Treatment Repurposing using Literature-Related Discovery.

by

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ABSTRACT

Treatment Repurposing is the application of a treatment to diseases or symptoms of interest other than the disease(s) or symptom(s) for which the treatment was developed (and used) initially. It includes, but goes well beyond, Drug Repurposing. The present monograph uses Literature-Related Discovery (LRD) to identify treatments that could be repurposed for diseases of interest.

The LRD methodology for identifying candidate repurposable treatments is presented in detail, and illustrative examples are provided from a recent monograph on prevention and treatment of Alzheimer's Disease [Kostoff et al, 2018]. The present monograph also contains an extensive Bibliography of the core Treatment Repurposing literature, as well as two novel taxonomies of this literature. One taxonomy uses text clustering to display the myriad categories (and their relationships) in this Treatment Repurposing literature, and the other taxonomy uses factor analysis to display the myriad categories/themes in the same literature.

Chapter 1 - Introduction and Background

1A. Overview

Literature-Related Discovery (LRD) is a systematic approach to bridging unconnected disciplines based on text mining procedures [Kostoff et al, 2008a; Kostoff et al, 2008b; Kostoff, 2012]. In the LRD context, discovery is linking two or more literature concepts that have heretofore not been linked (i.e., disjoint), in order to produce novel, interesting, plausible, and intelligible knowledge.

In the medical arena, LRD can be used for identifying potentially new treatments for a disease (aka Treatment Repurposing), identifying potentially new contributing factors for a disease, identifying new biomarkers for a disease, etc. By 'new', we mean previously non-existent in the core biomedical literature for the disease of interest.

The present monograph presents a detailed description of LRD-based Treatment Repurposing (which includes Drug Repurposing, but goes well beyond drugs to include any type of treatment). It contains **illustrative examples** of Treatment Repurposing from a recent study on preventing and reversing Alzheimer's Disease (AD) [Kostoff et al, 2018], as well as an algorithm for generating voluminous Treatment Repurposing (see Appendix 1).

1B. Structure of Treatment Repurposing Literature

Treatment Repurposing (hereafter abbreviated as TR) is the application of a treatment to diseases or symptoms of interest other than the disease(s) or symptom(s) for which the treatment was developed (and used) initially. A number of comprehensive reviews of one component of TR, drug repurposing/repositioning, have been published recently [Xue et al, 2018; March-Vila et al, 2017; Yella et al, 2018; Karaman and Sippl, 2018; Sahu and Kharkar, 2016]. As shown in these reviews, as well as many other more narrowly-focused documents, there are myriad possible categorizations for the TR literature.

For example, some TR papers are:

*disease-focused [Abbruzzese et al, 2017; Abbasi, 2016];

*drug focused [Albinana et al, 2017; Ahmad et al, 2018];

*biomarker-focused [Amar et al, 2015; Kim et al, 2018; Ohmichi et al, 2018];

*prediction methodology-focused, etc.

The prediction methodology category includes, but is not limited to, the following sub-categories:

*text-mining [Abrams et al, 2015; Kuusisto et al, 2017; Tari and Patel, 2014; Brown and Patel, 2017; Jang et al, 2017; Yang et al, 2017];

*machine learning [Ekins et al, 2015; Huang et al, 2016; Jamal et al, 2015; Nath, Kumari, and Chaube, 2018];

*network-based [Alaimo et al, 2015; Azmi et al, 2013; Berenstein et al, 2016; Bourdakou, Athanasiadis, and Spyrou, 2016; Carson and Lu, 2015; Cheng et al, 2018; Fukuoka, Takei, and Ogawa, 2013];

*semantics [Cheng at al, 2014; Cohen et al, 2012; Liang, Sun, and Tao, 2015; Mullen et al, 2016; Qu et al, 2009];

*ligand-binding/ligand-protein docking/binding-site focused [Wang et al, 2017; Huang et al, 2017; Dash et al, 2018; Di Muzio, Toti, and Polticelli, 2017]; Chartier, Adriansen, and Najmanovich, 2016; Di Domizio et al, 2014];

*protein targeting [Huang et al, 2018; Li et al, 2018];

*transcriptional signature-focused [Iorio et al, 2010; Iorio et al, 2015].

The LRD approach of TR is in the text mining sub-category of prediction methodology-focused approaches. LRD-TR identifies treatments from the biomedical literature that alter combinations of markers (mainly biomarkers) in directions required to reverse target diseases of interest (see Appendix 1 for details).

A less subjective perspective on the structure of the TR literature is offered by text clustering. Appendix 2 contains a hierarchical taxonomy of the TR literature obtained with the CLUTO text clustering software [CLUTO, 2018]. This unique taxonomy presents the higher-level and most detailed categories that constitute the core TR biomedical literature. Additionally, the actual display of the taxonomy links to the titles of papers in the most detailed categories, in order to present the full spectrum of sub-themes contained within each of these detailed categories. Chapter 4 contains a more extensive Bibliography of TR (mainly drug repurposing) papers, with complete references.

1C. Structure of Monograph

Chapter 1, the Introduction and Background, is followed by Chapter 2, Methodology, Results, and Conclusions. Chapter 3 contains the text References and Appendices:

*Appendix 1 is the TR query;

*Appendix 2 contains the CLUTO text mining-based core TR literature taxonomy;

*Appendix 3 contains the VP factor analysis-based core TR literature taxonomy;

*Appendix 4 contains markers from the AD study, and their directions of change as a result of treatments or contributing factors.

Chapter 4 contains the core TR literature (mainly drug repurposing) Bibliography, with full references.

Chapter 2 - Methodology, Results, and Conclusions

2A. Overview of LRD-TR Methodology

Treatments of disease or causes of disease (contributing factors to disease) result in changes to myriad markers in the body, including, but not limited to:

*general biomarkers (e.g., neuroinflammation, neurodegeneration, DNA damage, mitochondrial dysfunction, oxidative stress, neurotransmission dysfunction; olfactory dysfunction, glutamate uptake, glucose homeostasis, etc);

*specific biomarkers (e.g., ATP, B12, B6, BACE-1, Bax, Bcl-2, BDNF, c-AMP, caspase, folate, GLP-1, GSK-3, etc);

*symptoms (e.g., insomnia, ataxia, dysphagia, etc);

*performance (e.g., memory, learning, cognition, etc);

*behaviors (e.g., apathy, depression, anxiety, aggression, agitation, etc);

*others.

Appendix 4 contains extensive examples of myriad markers from the AD study, and the directions in which they changed in association with the presence/imposition of AD contributing factors or the provision of AD treatments.

The TR discovery approach of the present monograph consists of a two-stage process:

Stage 1: identify critical markers associated with a disease of interest, and identify how the values of those markers change 1) when contributing factors to disease are operable and 2) when treatments are operable.

Stage 2: search the non-disease-of-interest literature for potential treatments that will change the markers of interest in the desired direction.

2B. Specific Methodology Adapted from AD Study [Kostoff et al, 2018]

Stage 1

2B-1A. Identify critical markers and their directions of change associated with existing AD contributing factors

The first step in Stage 1 of the AD study (and in a subsequent chronic disease reversal study being performed presently) was to 1) identify existing contributing factors (causes) to AD and 2) identify markers (mainly biomarkers) whose changes from the norm were associated with the AD contributing factors. A number of approaches were used to identify these existing AD contributing factors and their associated markers, since no one approach was fully comprehensive.

2B-1A1. Visual Inspection

A **Visual Inspection** approach was used initially for the AD study. It started by generating a database of millions of abstract phrases parsed from ~100,000 records that constituted the total AD core Medline literature. Then, tens of thousands of the highest frequency phrases were inspected visually, and those that appeared to be contributing factors to AD were selected. During this process, and in the subsequent confirmatory process that validated the selection of AD contributing factors, a number of non-biomedical terms were identified that were closely associated with the existing AD contributing factors (shown in section 1A2). These non-biomedical terms could then be (and were) used as 'linking terms', to target lower frequency phrases (among the millions of abstract phrases) that had high probability of being/including existing AD contributing factors.

2B-1A2. Linking Term

A number of **linking term** approaches were used to target records or phrases with high probability of containing existing AD contributing factors. These included:

***MeSH Qualifiers** associated strongly with contributing factors (e.g., adverse effects, toxicity, pathogenicity, poisoning);

*Relatively unambiguous **MeSH Headings** associated strongly with contributing factors (e.g., "Drug-Related Side Effects AND Adverse Reactions"; Abnormalities, Drug Induced; Air Pollutants, Occupational; Amphetamine Related Disorders; Carcinogens; Chemical Warfare Agents; Chemically-Induced Disorders, etc);

***Text terms** associated strongly with contributing factors (e.g., -induced; caused by; induced by; -contaminated; exposure to; exposure(s) [at end of phrase]; exposed to; poisoning [at end]; -exposed [at end]; -related; -associated; -infected; abuse*; toxicity).

These linking terms were especially valuable for accessing low-frequency existing AD contributing factors not accessible from visual inspection of the high-frequency phrases.

2B-1A3. Dot Product

A **dot product** approach was used to identify phrases that had high probability of being existing AD contributing factors. External lists of toxic substances generated by Federal government organizations, state regulatory agencies, and other major organizations were aggregated. The final list of toxic substances was intersected with the full list of millions of abstract phrases in the core AD literature, to identify additional existing AD contributing factors.

The total number of existing AD contributing factors identified by the above approaches (from the premier biomedical literature and validated) numbered about 400-600, depending on how the existing AD contributing factors were aggregated. In all the approaches to identifying existing AD contributing factors shown above, the initial existing AD contributing factors selected were confirmed and validated by detailed reading of the relevant abstracts.

During the confirmation and validation process, one or (usually) more record abstracts containing the candidate existing AD contributing factor term was read, and other relevant data in the abstract were recorded. These data included biomarkers, symptoms, and behaviors impacted by the existing AD contributing factor(s), and the directions in which these markers were moved (increased, decreased, etc). In some/many of these records, one or more existing AD treatment(s) were also identified, as well as the myriad markers associated with the existing AD treatments and the directions of change these markers experienced as a result of the existing AD treatment(s). These treatment-related data were also recorded.

2B-1B. Identify critical markers and their directions of change associated with existing AD treatments

The second step in Stage 1 of the AD study (and in a subsequent chronic disease reversal study being performed presently) was to 1) identify existing AD treatments and 2) identify markers (mainly biomarkers) whose changes from the norm were associated with the existing AD treatments. A number of approaches were used to identify these existing AD treatments and their associated markers, since no one approach was fully comprehensive.

2B-1B1. Visual Inspection

A **Visual Inspection** approach (actually part of the visual inspection approach described in section 1A1) was used, which consisted of reading the thousands of high frequency abstract phrases in the core AD literature, and selecting those that appeared to be treatments for AD. During this process, and in the subsequent confirmatory process that validated the selection of existing AD treatments, a number of non-biomedical terms were identified that were closely associated with the existing AD treatments (shown in 1B2). These non-biomedical terms could then be (and were) used as 'linking terms', to target phrases (among the millions of abstract phrases) that had high probability of being/including existing AD treatments.

2B-1B2. Linking Term

A number of **linking term** approaches were used to target records with high probability of containing existing AD treatments. These included:

*MeSH Qualifiers** associated strongly with treatments (e.g., diet therapy, drug therapy, prevention & control, therapeutic use, therapy, etc);

*Relatively unambiguous **MeSH Headings** associated strongly with treatments (e.g., Treatment Outcome, Neuroprotective Agents, Nootropic Agents, Plant Extracts, Phytotherapy, Dietary Supplements, Drugs, Chinese Herbal, etc);

*Text terms** associated strongly with treatments (treat*, therap*, prevent*, protect*, improv*, reduc*, attenuat*, ameliorat*, enhanc*, revers*, promot*, alleviat*, inhibit*, remov*, suppress*, mitigat*, restor*, lower*, preserv*, regenerat*, rescu*, slow*).

These linking terms were especially valuable for accessing existing low-frequency AD treatments not accessible from visual inspection of the high-frequency phrases. Some of these linking terms had higher efficiencies of identifying the treatment consequences of interest than others. Terms like prevent*, protect*, improv*, restor*, alleviat*, ameliorat*, mitigat*, etc, almost always gave the desired AD

markers and the direction in which they changed as a result of treatment. Terms like decreas*and increas* (used initially, then abandoned), reduc*, slow*, etc, could go either way. The former group of terms had the 'sense' of *improvement*, while the latter group of terms reflected *change* (positive or negative), and may or may not have reflected improvement.

The total number of existing AD treatments identified by the above approaches (from the premier biomedical literature and validated) numbered about 600-700, depending on how the existing AD treatments were aggregated. In all the approaches to identifying existing AD treatments shown above, the initial existing AD treatments selected were confirmed and validated by detailed reading of the relevant abstracts.

During the confirmation and validation process, one or (usually) more record abstracts containing the candidate existing AD treatment term was read, and other relevant data in the abstract were recorded. These data included biomarkers, symptoms, and behaviors impacted by the treatment(s), and the directions in which these markers were moved (increased, decreased, etc) associated with the treatment. In some/many of these records, one or more existing AD contributing factor(s) were also identified, as well as the myriad markers associated with the existing AD contributing factor(s) and the directions of change these markers experienced associated with the existing AD contributing factor(s). These contributing factor-related data were also recorded.

2B-1C. Identify critical markers and their directions of change not identified in 2B-1A or 2B-1B

The third step in Stage 1 of the AD study (and in a subsequent chronic disease reversal study being performed presently) was to identify existing AD markers of interest.

2B-1C1. Visual Inspection

During the **Visual Inspection** process used to identify the higher-frequency existing AD contributing factors and treatments, the higher-frequency existing AD markers were also recorded. During this process, and in the subsequent confirmatory process that validated the selection of existing AD markers, a number of non-biomedical terms were identified that were closely associated with the existing AD markers. These non-biomedical terms could then be used as 'linking terms', to target phrases (among the millions of abstract phrases) that had high probability of being/including existing AD markers.

For the most part, these marker 'linking terms' were included in the combined list of linking terms used to identify existing low-frequency AD contributing factors and treatments (see sections 1A2 and 1B2 for the contributing factor linking terms and the treatment linking terms, respectively). The existing low-frequency AD markers had been identified as part of the AD low-frequency contributing factor and treatment identification process.

In reality, the existing AD contributing factors and existing AD treatments identified in 1A, 1B, 1C, 2A, 2B above served effectively as linking terms to the existing AD markers in their own right.

A total of about 250 major and semi-major existing AD biomarkers, symptoms, behaviors, etc, were identified, of which about 200 were specific existing AD biomarkers. This number of existing AD markers was deemed sufficient to meet the study objectives and constraints; no other methods were used

to identify additional existing AD markers. One of these constraints was to identify only those existing markers whose values were altered due to the effects of existing AD contributing factors or existing AD treatments. This was achieved by extracting only those markers related to existing AD contributing factors and existing AD treatments.

If any of the readers have applications where markers beyond those co-occurring with contributing factors or treatments would be required, then some of the techniques listed in sections 2B-1A and 2B-1B above could be used to generate these additional markers. One obvious example would be to use the relatively unambiguous MeSH Heading 'Biomarkers' as an effective linking term for identifying existing markers. The MeSH Heading 'Biomarkers' would contain biomarkers in myriad contexts, some of which may not be associated with contributing factors or treatments in the articles.

It should be noted that

*additional linking term approaches and text linking terms could have been identified;

*linking term patterns (combinations of linking terms) could have been identified for greater precision in predicting high probability existing AD biomarker phrases;

*not all linking terms identified were used;

*not all existing AD markers appeared in text in proximity to the identified linking terms, or to the identified contributing factors and treatments;

*software limitations on extracted phrase length excluded those existing AD markers not in very close proximity to the identified linking terms.

An expanded study could have easily overcome these limitations, and possibly doubled the number of existing AD biomarkers identified. The present ongoing new chronic disease study is exploiting these lessons from the AD study, and many more existing markers have been identified.

Stage 2: search the non-disease-of-interest literature for potential treatments that will change the markers of interest in the desired direction.

Text mining of the AD biomedical literature (especially records focused on treatments and contributing factors) identified the critical markers associated with AD, and identified the directions in which these critical markers needed to change for potential AD alleviation/reversal [Kostoff et al, 2018; also, see Appendix 4 of the present document]. For example, critical general biomarkers for AD and their desired directions of change included 'reduce oxidative stress', 'alleviate mitochondrial dysfunction', 'prevent apoptosis', etc. Critical specific biomarkers for AD and their desired directions of change included 'reduce BACE1', 'increase Bcl-2', 'enhance ADAM10', etc.

From these markers and their desired directions of change for effective treatment of AD, a query was developed to 1) identify potential AD treatments from 2) treatments used in the non-AD literature (see Appendix 1 for query details). The non-AD biomedical literature was then searched for records including one or more of these AD markers that moved in desired directions as a result of treatments (e.g.,

reduced Abeta; increased Bcl-2; reduced tau hyperphosphorylation; restricted NFKappaB signaling; reduced inflammation; reduced oxidative stress; enhanced Nrf2, etc).

Searching for records that had a threshold of including *at least one* of these desired marker alterations produced a voluminous retrieval. To keep the records retrieved at a manageable level, the requirement that a record in the non-AD literature must contain *at least two* AD markers (that moved in the appropriate direction in conjunction with a treatment) to be retrieved was imposed. Even then, the retrieval was voluminous, indicating the wealth of potential AD treatment repurposing possible from an expanded well-resourced study.

As a practical matter, combinations of the more fundamental and less AD-specific linking phrases were used for the treatment repurposing query. The general form of the query was 1) combinations of the markers and their desired directions of change followed by 2) negation of records that contained existing AD treatments. These existing AD treatments had been obtained in the first part of the AD study [Kostoff et al, 2018].

As an example of the query format:

((((increas* OR enhanc* OR restor*) NEAR/3 "norepinephrine") AND ((increas* OR enhanc* OR restor*) NEAR/3 "Nrf2"))

NOT

((alzheimer* OR dementia OR "mild cognitive impairment") OR {existing AD treatments}).

While terms such as 'reduce Abeta' or 'reduce tau phosphorylation' may be efficient for extracting *existing* AD treatments from the AD literature, they are very inefficient, either in isolation or especially in combination, for AD treatment *repurposing* from the non-AD literature. It is difficult to imagine people doing research in reducing Abeta or reducing tau hyperphosphorylation (much less doing research in both) not emphasizing the AD/dementia applications in their publications.

Finally, there are no restrictions on the numbers of treatments that could be repurposed for any disease of interest. For example, assume that a patient has been diagnosed with a specific disease, characterized by three abnormal biomarker values. The query could be applied to identify/discover 1) one treatment that would bring all three of the biomarkers back to normal, or 2) one treatment that would bring two of the biomarkers back to normal and one treatment that would bring the third biomarker back to normal, or 3) three treatments, each of which would bring one of the biomarkers back to normal. Obviously, the repurposed treatments in 2) and 3) would have to be compatible, but the technique offers a wide variety of options.

2C. Results

Appendix 1 contains the details of the actual query used to identify potential repurposed treatments for AD. Since the treatment repurposing described in the AD study was a proof-of-principle demonstration of the latest incarnation of our LRDI approach, only a few examples were provided for illustrative purposes. These examples were based on using *combinations of two biomarkers only* in the query, and are contained in the following table:

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Table 2C-1: Illustrative LRD-TR Results from AD Study

EXAMPLES OF POTENTIAL REPURPOSED AD TREATMENTS

- Fortunellin protects against high fructose-induced diabetic heart injury in mice by *suppressing inflammation* and *oxidative stress* via AMPK/*Nrf-2* pathway regulation []

- Protective effects of sarains on H2O2-induced mitochondrial dysfunction and oxidative stress; *improving mitochondrial function* and *decreasing reactive oxygen species* levels; ability to block the mPTP and to *enhance the Nrf2* pathway []

- Carboxyamidotriazole alleviates muscle atrophy in tumor-bearing mice by *inhibiting NF-kappaB* and *activating SIRT1*; CAI restricted the NF-kappaB signaling, *downregulated the level of TNF-alpha* in muscle and both *TNF-alpha and IL-6 levels* in serum, directly stimulated SIRT1 activity in vitro, and *increased SIRT1* content in muscle []

- Protective effects and mechanism of meretrix meretrix oligopeptides (MMO) against nonalcoholic fatty liver disease; MMO inhibited the activation of cell death-related pathways, based on *reduced p-JNK*, *Bax expression*, *tumor necrosis factor-alpha, caspase-9, and caspase-3* activity in the NAFLD model cells, and *Bcl-2 expression was enhanced* in the NAFLD model cells []

- Extract from Periostracum cicadae *inhibits oxidative stress* and *inflammation* induced by Ultraviolet B Irradiation; *decreased reactive oxygen species (ROS) production*. The extract *attenuates the expression of interleukin-6 (IL-6), matrix metalloproteinase-2 (MMP-2), and MMP-9* in UVB-treated HaCaT cells. Also, P. cicadae *abrogated* UVB-induced *activation of NF-kappaB, p53, and activator protein-1 (AP-1);* accumulation and *expression of NF-E2-related factor (Nrf2) were increased* []

Note that while the query was limited to combinations of two biomarkers only as selection criteria, the actual numbers of biomarkers in the retrieved records that moved in the desired directions for healing were typically greater (sometimes much greater) than two.

2D. Validation of TR Candidates

The final step involved in converting an existing treatment in the non-AD literature to a repurposed AD treatment is validation that the potential AD treatment has not been associated with AD application in the literature. Each candidate potential AD repurposed treatment retrieved using the query in Appendix 1 was subject to this validation before becoming a potential AD repurposed treatment. The candidate potential AD repurposed treatment was intersected with the core AD literature, and was validated only after this intersection showed orthogonality.

For example, the candidate potential AD repurposed treatment "fortunellin" was retrieved because it satisfied the desired query general biomarker combination of *reducing inflammation and oxidative stress*. Fortunellin also had the additional specific biomarkers-based benefits of *reducing the pro-inflammatory cytokines and the expression of p-IkappaB kinase alpha, p-IkappaBalpha, and p-nuclear factor-kappaB*, while significantly *enhancing superoxide dismutase, catalase, heme oxygenase-*

1and p-AMP-activated protein kinase. Fortunellin was intersected with the core AD biomedical literature retrieval terms (alzheimer* OR dementia OR "mild cognitive impairment"), and no records were retrieved, demonstrating that fortunellin could not be found in the core AD literature. Fortunellin was therefore validated as a potential AD repurposed treatment (LRD Discovery).

2E. Conclusions

The LRD-TR approach has evolved from its initial structure in 2008 [Kostoff et al, 2008a, 2008b] to the more advanced and targeted process described in the present monograph. It has the capability to generate voluminous TR results for any disease or symptom of interest; the only limitations are study resources.

The same generic process can be applied to identifying contributing factors to a symptom or disease of interest that have not been existent previously in the core biomedical literature of that disease or symptom of interest, but have been existent in the core biomedical literature of other diseases or symptoms. The same extrapolation process can be used for myriad markers as well.

Chapter 3 - References and Appendices

<u>3A. References</u>

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3B. Appendix 1 - Query for Identifying Potential AD Repurposed Treatments

The most general form of the TR query can incorporate any number of biomarkers and other markers of interest. For AD, a two biomarker query was deemed adequate for demonstration purposes. The generic form of the two biomarker AD treatment repurposing query is

(A and B) not (C or D), where

A is a biomarker and its associated desired direction of change

B is another biomarker and its associated direction of change

C is the query used to retrieve the AD core literature

D is a list of existing AD treatments identified in the initial part of the AD study

Thus, the combination (A and B) retrieves ALL records from the biomedical literature that contain potential AD treatments based on the two desired characteristics A and B, while (C or D) subtracts those records associated with the AD core literature. The remainder is non-AD records with substances that could be candidate repurposed AD treatments, based on the requirement that A and B must be present.

Twenty of the more than 200 biomarkers identified in the AD study (through text mining techniques) were selected for the query. The query was run in Thompson-Reuters-Medline, since its search engine allows for proximity searching (e.g., [direction] within three words of [biomarker], or [direction] near/3 [biomarker]). In modular form, each query term is shown as follows:

#1 - (reduc* OR decreas* OR prevent* OR attenuat* OR suppress* OR alleviat* OR ameliorat*) near/3 "oxidative stress"

#2 - (reduc* OR decreas* OR prevent* OR attenuat* OR suppress* OR alleviat* OR ameliorat*) near/3 "apoptosis"

#3 - ((protect* OR improv* OR enhanc* OR restor* OR preserv*) near/3 "mitochondrial function") OR ((reduc* OR decreas* OR prevent* OR attenuat* OR suppress* OR alleviat* OR ameliorat*) near/3 "mitochondrial dysfunction")

#4 - (inhibit* OR reduc* OR attenuat* OR decreas*) near/3 "BACE1"

#5 - (modulat* OR attenuat* OR reduc* OR inhibit* OR decreas*) near/3 "gamma-secretase"

#6 - (enhanc* OR increas* OR improv* OR protect*) near/3 "autophagy"

#7 - (attenuat* OR reduc* OR prevent* OR inhibit*) near/3 ("caspase* activ*" OR "caspase* express*")

#8 - (increas* OR restor* OR enhanc*) near/3 "Bcl-2"

#9 - (attenuat* OR reduc* OR inhibit* OR decreas* OR prevent*) near/3 "NF-kappaB"

#10 - (increas* OR enhanc* OR restor*) near/3 "ADAM10"

#11 - (increas* OR restor* OR enhanc*) near/3 "CREB"

#12 - (inhibit* OR decreas* OR reduc* OR attenuat*) near/3 "GSK-3"

#13 - (increas* OR enhanc* OR restor*) near/3 "GLP-1"

#14 - (increas* OR enhanc* OR restor*) near/3 "ABCA1"

#15 - (increas* OR enhanc* OR restor*) near/3 "norepinephrine"

#16 - (increas* OR enhanc* OR restor*) near/3 "Nrf2"

#17 - (increas* OR enhanc* OR restor*) near/3 "seladin-1"

#18 - (increas* OR enhanc* OR restor*) near/3 "LRP1"

#19 - (increas* OR enhanc* OR restor*) near/3 "SIRT1"

#20 - (attenuat* OR reduc* OR inhibit* OR decreas*) near/3 "beclin1"

NOT ((#21 - alzheimer* OR dementia OR "mild cognitive impairment") [Core AD Literature]

OR

Existing AD Treatments

#22 - ("donepezil" OR "memantine" OR "Rivastigmine" OR "galantamine" OR "Tacrine" OR "hormone replacement therapy" OR "vitamin E" OR "risperidone" OR "Curcumin" OR "melatonin" OR "docosahexaenoic" OR "olanzapine" OR "walking" OR "nicotine" OR "folate" OR "17 beta-estradiol" OR "physostigmine" OR "lithium" OR "vitamin B-12" OR "neurotrophin" OR "quetiapine" OR "omega-3 fatty acid" OR "Haloperidol" OR "huperzine" OR "psychotherapy" OR "music therapy" OR "occupational therapy" OR "acupuncture" OR "social interaction" OR "resveratrol" OR "polyunsaturated fatty acids" OR "neural stem cells" OR "transcranial magnetic stimulation" OR "vitamin D" OR "selegiline" OR "piracetam" OR "citalopram" OR "Testosterone" OR "folic acid" OR "vitamin C" OR "muscarinic agonist" OR "clioquinol" OR "ibuprofen" OR "Nimodipine" OR "simvastatin" OR "Carbamazepine" OR "electroconvulsive therapy" OR "rapamycin" OR "clozapine" OR "caffeine" OR "cannabinoid" OR "extract EGb 761" OR "tetrahydroaminoacridine" OR "alpha tocopherol" OR "ECT" OR "leisure activity" OR "Ginseng" OR "Mediterranean diet" OR "acetyl-L-carnitine" OR "metrifonate" OR "Aricept" OR "Bapineuzumab" OR "mesenchymal stem cells" OR "trazodone" OR "Cerebrolysin" OR "Epigallocatechin-3-gallate" OR "humanin" OR "reminiscence therapy" OR "B vitamin" OR "sertraline" OR "solanezumab" OR "Ginsenoside" OR "aerobic exercise" OR "pioglitazone" OR "Retinoic acid" OR "deep brain stimulation" OR "indomethacin" OR "leptin" OR "aromatherapy" OR "Cognitive Stimulation Therapy" OR "insulin therapy" OR "Intravenous immunoglobulin" OR "L-deprenyl" OR "turmeric" OR "galanin" OR "selenium" OR "treadmill" OR "coffee" OR "DHEA" OR "progesterone" OR "Atorvastatin" OR "massage" OR "electroacupuncture" OR "fluoxetine" OR "memory training" OR "phosphatidylserine" OR "rosiglitazone" OR "phosphatidylcholine" OR "semagacestat" OR

"Green tea" OR "nicotinamide" OR "physical therapy" OR "Aripiprazole" OR "rTMS" OR "bright light therapy" OR "quercetin" OR "fish oil" OR "phenserine" OR "S-adenosylmethionine" OR "saponin" OR "alpha lipoic acid" OR "amylin" OR "environmental enrichment" OR "Propentofylline" OR "social activity" OR "vitamin B-6" OR "cobalamin" OR "flurbiprofen" OR "methylene blue" OR "metformin" OR "rasagiline" OR "Group Therapy" OR "catechin" OR "coumarin" OR "lipoic acid" OR "lovastatin" OR "berberine" OR "ferulic acid" OR "small interfering RNA" OR "cognitive behavioral therapy" OR "DNA vaccine" OR "Reminyl" OR "velnacrine" OR "bexarotene" OR "carotenoid" OR "Citicoline" OR "desferrioxamine" OR "Huperzia serrata" OR "Liraglutide" OR "Thiamine" OR "morphine" OR "N-acetylcysteine" OR "amantadine" OR "ascorbic acid" OR "caloric restriction" OR "Dimebon" OR "erythropoietin" OR "genistein" OR "grape" OR "lamotrigine" OR "red wine" OR "behavioral therapy" OR "curcuminoid" OR "medroxyprogesterone" OR "methylphenidate" OR "pravastatin" OR "scyllo-inositol" OR "Xanomeline" OR "divalproex" OR "gabapentin" OR "lavender" OR "levetiracetam" OR "raloxifene" OR "transcranial direct current stimulation" OR "validation therapy" OR "ziprasidone" OR "arecoline" OR "idebenone" OR "ladostigil" OR "minocycline" OR "nicergoline" OR "PBT2" OR "perindopril" OR "soy" OR "Chondroitin sulfate" OR "etanercept" OR "hydergine" OR "piperidine" OR "sodium valproate" OR "sulfonamide" OR "animal-assisted therapy" OR "clonazepam" OR "Cognex" OR "deferoxamine" OR "multisensory stimulation" OR "allopregnanolone" OR "buspirone" OR "clonidine" OR "coenzyme Q10" OR "cyclophilin" OR "fluvoxamine" OR "garlic" OR "Imipramine" OR "tarenflurbil" OR "transcutaneous electrical nerve stimulation" OR "AF102B" OR "anthocyanin" OR "citrus" OR "embryonic stem cell" OR "escitalopram" OR "Higher education level" OR "Alpha2 macroglobulin" OR "Amaryllidaceae" OR "aminoguanidine" OR "art therapy" OR "benzothiazole" OR "Caffeic acid" OR "doxycycline" OR "Eptastigmine" OR "exendin-4" OR "gelsolin" OR "Icariin" OR "M30" OR "resistance training" OR "Tai Chi" OR "tanshinone" OR "Vinpocetine" OR "Yizhi" OR "Bacopa" OR "bisdemethoxycurcumin" OR "cocoa" OR "Colostrinin" OR "gantenerumab" OR "Geniposide" OR "hydrogen sulfide" OR "moxibustion" OR "oxiracetam" OR "Reality orientation therapy" OR "rifampicin" OR "strength training" OR "9-Amino-1,2,3,4-tetrahydroacridine" OR "apigenin" OR "cinnamon" OR "cognitive therapy" OR "D-cycloserine" OR "propargylamine" OR "rosmarinic acid" OR "telmisartan" OR "topiramate" OR "Tramiprosate" OR "blueberry" OR "Fortasyn" OR "hyperforin" OR "Kampo" OR "mirtazapine" OR "N-benzylpiperidine" OR "Panax notoginseng" OR "Salvia miltiorrhiza" OR "Taurine" OR "yoga" OR "aniracetam" OR "CHF5074" OR "colostrum" OR "dantrolene" OR "Ghrelin" OR "grape seed" OR "hyperbaric oxygen" OR "linopirdine" OR "oleic acid" OR "propranolol" OR "pyridostigmine" OR "retinoid*" OR "saffron" OR "trehalose" OR "AF150" OR "captopril" OR "Crocus sativus" OR "demethoxycurcumin" OR "H2S" OR "latrepirdine" OR "lycopene" OR "piperazine" OR "Polygala tenuifolia" OR "ramelteon" OR "Riluzole" OR "tiapride" OR "beer" OR "clomipramine" OR "dance therapy" OR "Doll therapy" OR "gold nanoparticles" OR "Huannao Yicong" OR "lentiviral vectors" OR "Luteolin" OR "memoquin" OR "Nefiracetam" OR "pitavastatin" OR "pomegranate" OR "Puerarin" OR "scFv antibody" OR "zolpidem" OR "acupressure" OR "AF267B" OR "anandamide" OR "apomorphine" OR "ASS234" OR "Curcuma longa" OR "dihydrotestosterone" OR "glatiramer acetate" OR "horticultural therapy" OR "ketogenic diet" OR "L-3-n-butylphthalide" OR "losartan" OR "rutin" OR "tea polyphenols" OR "Zingiber" OR "7,8-dihydroxyflavone" OR "Aducanumab" OR "aged garlic extract" OR "amiridin" OR "apocynin" OR "baicalein" OR "Centella asiatica" OR "Danshen" OR "edaravone" OR "focused ultrasound" OR "HP 029" OR "Huprine" OR "milieu therapy" OR "natural origin" OR "paeoniflorin" OR "R-flurbiprofen" OR "retinoic acid receptor" OR "Selenate" OR "single-chain antibody" OR "Withania somnifera" OR "Acori graminei" OR "akatinol"

OR "beta-asarone" OR "cotinine" OR "cryptotanshinone" OR "cyproterone" OR "dronabinol" OR "ganstigmine" OR "laser therapy" OR "Lavandula angustifolia" OR "naringenin" OR "Noopept" OR "oleocanthal" OR "pepper" OR "pet therapy" OR "ponezumab" OR "Pyritinol" OR "Rehmannia glutinosa" OR "Salidroside" OR "Salvianolic acid" OR "silymarin" OR "T0901317" OR "Tauroursodeoxycholic acid" OR "thalidomide" OR "triflusal" OR "Triptolide" OR "valsartan" OR "AMPK activation" OR "Colivelin" OR "fullerene*" OR "gastrodin" OR "hesperidin" OR "JWH-133" OR "Naftidrofuryl" OR "naringin" OR "neuroglobin" OR "nobiletin" OR "Oleuropein aglycone" OR "sodium butyrate" OR "talsaclidine" OR "Tannic acid" OR "Tetrahydrohyperforin" OR "Tiaoxin" OR "Uncaria rhynchophylla" OR "4-Phenylbutyrate" OR "asiatic acid" OR "benzylpiperidine" OR "Capsaicin" OR "Carnosic acid" OR "Catalpol" OR "D609" OR "Danggui-Shaoyao-San" OR "dihydroergotoxine" OR "ellagic acid" OR "fingolimod" OR "FLZ" OR "glycosaminoglycan polysulfate" OR "granulocyte colony-stimulating factor" OR "graphene" OR "IKKbeta" OR "mifepristone" OR "osthole" OR "protocatechuic acid" OR "Qingxin Kaiqiao" OR "rhynchophylline" OR "S14G-HN" OR "Selenomethionine" OR "Sodium selenate" OR "umbilical cord blood cells" OR "vagus nerve stimulation" OR "Wuzi Yanzong" OR "Xanthoceras" OR "xanthoceraside" OR "Xiusanzhen" OR "yi-gan" OR "Abeta12-28P" OR "carvedilol" OR "Choto-san" OR "cyclandelate" OR "cytidinediphosphocholine" OR "ebselen" OR "fucoidan" OR "H-89" OR "Hericium erinaceus mycelia" OR "JTP-4819" OR "L-theanine" OR "low molecular weight heparin" OR "Namaste Care" OR "Naoling" OR "neotrofin" OR "Noninvasive Brain Stimulation" OR "Oligonol" OR "red mold" OR "retinoid x receptor alpha" OR "S-allyl-l-cysteine" OR "Scutellaria baicalensis" OR "spatial training" OR "SuHeXiang" OR "Tolfenamic acid" OR "Tong Luo Jiu Nao" OR "touch intervention" OR "Valeriana amurensis" OR "15-deoxy-Delta(12,14)-PGJ(2)" OR "17-AAG" OR "4-O-methylhonokiol" OR "alpha-Mangostin" OR "Anatabine" OR "angiotensin-(1-7)" OR "Arundic acid" OR "bee venom" OR "betaine" OR "Cinnamomum" OR "coconut" OR "coptisine" OR "corticotropin-releasing factor receptor" OR "Cranberry" OR "diallyl disulfide" OR "Emblica officinalis" OR "Fucoxanthin" OR "Fuzhisan" OR "Gamma-hydroxybutyrate" OR "intermittent fasting" OR "isorhynchophylline" OR "Isradipine" OR "morin" OR "neural stem cell transplantation" OR "neuritin" OR "Nicotinamide mononucleotide" OR "pifithrin-alpha" OR "PQCA" OR "s-Ethyl cysteine" OR "s-propyl cysteine" OR "scFv-h3D6" OR "sulforaphane" OR "synj1" OR "tamibarotene" OR "targretin" OR "tenuifolin" OR "Tetrandrine" OR "Thymoquinone" OR "tropisetron" OR "vildagliptin" OR "3,6'-dithiothalidomide" OR "4% figs" OR "6-shogaol" OR "A-887755" OR "Activated protein C" OR "AF151" OR "Agmatine" OR "aminopyridazines" OR "apple juice concentrate" OR "arachidonic acid ARA" OR "AVP-786" OR "benfotiamine" OR "BMP9 administration" OR "BMS-299897" OR "compound-1" OR "CREB-binding protein CBP" OR "crocetin" OR "cyclophilin A." OR "Cystatin B deletion" OR "dasatinib" OR "delta-9-tetrahydrocannabinol" OR "derivative of benzothiazole aniline" OR "diazoxide" OR "Dl-PHPB" OR "Drp1 inhibitors" OR "Enoxaparin" OR "ergothioneine" OR "Fbx2" OR "glycyrrhizic acid" OR "Gossypium herbaceam" OR "Human amniotic epithelial cells" OR "hunger" OR "Hydroxysafflor yellow" OR "ICI 118,551" OR "IL-33" OR "ILEI" OR "indirubin-3'-monoxime" OR "iododiflunisal" OR "isoliquiritigenin" OR "L803-mts" OR "linagliptin" OR "Memogain" OR "Meserine" OR "mithramycin" OR "MMP9 gene" OR "Ophiopogon japonicus" OR "PEI-conjugated R8-Abeta(25-35)" OR "phloroglucinol" OR "PLD2 ablation" OR "protein-iPSCs" OR "rexinoid*" OR "RNS60" OR "Safflower yellow" OR "salubrinal" OR "saxagliptin" OR "Sendai virus" OR "single-walled carbon nanotubes" OR "Smart Soup" OR "sodium benzoate" OR "sulfomucopolysaccharide" OR "T-817MA" OR "tetrathiomolybdate" OR "WAY-100635" OR "WIN55212-2" OR "2-methyl-5-(3-{4-[(S)-

methylsulfinyl]phenyl}-1-benzofuran-5-yl" OR "2-phenylethynyl-butyltellurium" OR "2S -neoeriocitrin" OR "3,4-dihydroxyphenylethanol" OR "3-alpha-akebonoic acid" OR "40 Hz light-flickering regime" OR "AA3E2" OR "AAD-2004" OR "AAV-p75ECD" OR "Abeta-HBc VLPs" OR "ACAT1 gene ablation" OR "acetate extract of Centipedegrass" OR "Activase rt-PA" OR "activation-inhibitory Lactobacillus pentosus" OR "AD-35" OR "adipose-derived stem cell-conditioned medium" OR "allicin" OR "alpha-chymotrypcin" OR "alpha-tocopherol quinine" OR "alpha-Zearalanol" OR "Anhydroexfoliamycin" OR "anthoxanthin" OR "anti-dementia effects of s-limonene" OR "anti-TLR2 antibody" OR "arctigenin" OR "AS2030680" OR "AS2674723" OR "ASP5736" OR "AVP-923" OR "beta-caryophyllene" OR "Bis(9)-(-)-nor-meptazinol" OR "BMS-289948" OR "BMS-708,163" OR "BRET-Qdot-emitted NIR" OR "butyrolactone" OR "C-30-27" OR "Cardiotrophin-1" OR "Cassia obtusifolia" OR "catechin hydrate" OR "chitosan oligosaccharides" OR "chloroquine derivatives" OR "chronic intranasal treatment" OR "ciproxifan" OR "collagen VI" OR "Cudrania cochinchinensis" OR "cyclophilin B" OR "Cyperus rotundus" OR "cytosine-guanosine-containing DNA oligodeoxynucleotides" OR "DA-JC4" OR "Dalesconol B" OR "Daucosterol palmitate" OR "DcR3" OR "Dehydroevodiamine" OR "deleting Nogo" OR "Dendrobium Nobile Lindl" OR "deoxyschisandrin" OR "dexamethasone exposure during pregnancy" OR "Dietary niacin" OR "Dihydromyricetin" OR "dipotassium N-stearoyltyrosinate" OR "dynorphin A-(1-13)" OR "dZip1 inhibition" OR "ephrinB1/Fc" OR "Eugenia jambolana" OR "EUK1001" OR "exogenous Abeta fibrillar seeds" OR "fenugreek seed powder" OR "Fructus mume" OR "Fumanjian" OR "Gami-Chunghyuldan" OR "genetic deletion of 12/15LO" OR "Genetic deletion of eIF2alpha" OR "Gfa2-VIVIT" OR "GSM-2" OR "Harpagoside" OR "hemizygous deletion of Synj1" OR "high potassium intakes" OR "hunger-inducing drug" OR "HX630" OR "hypericin" OR "IL-1R blocking Ab" OR "illite" OR "Inhibition of GIVA-PLA(2)" OR "Interleukin-34" OR "iso-alpha-acids" OR "JC-124" OR "JM6" OR "Jujuboside" OR "K6Abeta1-30[E18E19]" OR "kallikrein 7" OR "Kamikihi-to" OR "kappacarrageenanderived pentasaccharide" OR "L-NNNBP" OR "laminin 1" OR "Lentiviral ABN" OR "low-intensity pulsed LIP ultrasound" OR "LX2343" OR "Magnesium sulfate treatment" OR "maltolyl p-coumarate" OR "Marapuama" OR "MER5101" OR "MOG45D" OR "MS-275" OR "murine pathogen-free" OR "MW01-2-069A-SRM" OR "MW01-2-151SRM" OR "N-butylidenephthalide" OR "NButGT" OR "Neuropep-1" OR "ninjin'yoeito" OR "NRG1" OR "P. frutescens extract" OR "P11-hEGF" OR "Paeng-Jo-Yeon-Nyeon-Baek-Ja-In-Hwan" OR "Pantethine" OR "pBri-peptide-based immunomodulation" OR "PD146176" OR "pentamidine" OR "peoniflorin" OR "pharmacological inducer of HO-1" OR "PHF13" OR "Pleurotus ostreatus" OR "PP-3copy-Abeta1-6-loop123" OR "pratensein" OR "proteolytic nanobodies" OR "Pterocarpus marsupium" OR "pulsed ultrasound" OR "Qifu-Yin" OR "recombinant brain-targeted neprilysin ASN12" OR "reduced InsP3R1 expression" OR "reduction in mTOR signaling" OR "Reduction of exosome secretion" OR "repeated cognitive enrichment" OR "replace the endogenous apoE" OR "Rhizophora mucronata" OR "RP-1" OR "S1 peptide" OR "Saengshik" OR "Salvia sahendica" OR "Satureja bachtiarica" OR "scanning ultrasound" OR "Schisantherin B" OR "selenofuranoside" OR "Shengmai" OR "shRNA in the dentate" OR "Sia hydroxamate" OR "skeletal analogues of gambierol" OR "ST09" OR "SUN11602" OR "TAK-070" OR "tangeretin" OR "TAT-BDNF peptide" OR "TAT-haFGF" OR "tenascin-C-deficient" OR "TG101209" OR "TNFSF10 neutralizing antibody" OR "Tongmai Yizhi Decoction" OR "Transplantation of neural progenitor" OR "tri-lithium pyrroloquinoline quinone" OR "tricyclodecan-9-xanthogenate" OR "unmethylated DNA CpG motif" OR "Wen-Dan-Tang" OR "Y-29794" OR "yonkenafil" OR "Zataria multiflora Boiss" OR "zinc/copper chelators"))

The final query actually entered into the search engine was:

(#1 AND (#2 OR #3 OR #4 OR #5 OR #6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#2 AND (#3 OR #4 OR #5 OR #6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#3 AND (#4 OR #5 OR #6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#4 AND (#5 OR #6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#5 AND (#6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#6 AND (#7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

#7 AND (#8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#8 AND (#9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#9 AND (#10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#10 AND (#11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#11 AND (#12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#12 AND (#13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#13 AND (#14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#14 AND (#15 OR #16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#15 AND (#16 OR #17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#16 AND (#17 OR #18 OR #19 OR #20)) NOT (#21 OR #22)

(#17 AND (#18 OR #19 OR #20)) NOT (#21 OR #22)

(#18 AND (#19 OR #20)) NOT (#21 OR #22)

(#19 AND (#20)) NOT (#21 OR #22)

3B. Appendix 2 - TR Literature Taxonomy based on Text Clustering

A2-1. Overview of TR text clustering literature taxonomy

The 2890 Medline records that constitute the core TR (mainly drug repurposing) literature were sub-divided into a 32 cluster hierarchical taxonomy using the CLUTO text clustering software [CLUTO, 2018]. Both the top-level aggregated clusters in the taxonomy (Table A2-1) and the 32 elemental clusters (the lowest and most detailed level of the taxonomy-Table A2-2) will be presented in the following sections.

The 32 elemental cluster presentation will include the titles of records assigned to each cluster by the algorithm. The version of CLUTO used for this analysis does not include fuzzy clustering, so each record is assigned to one cluster only. A number of the records contained multiple themes, and could have been assigned to more than one cluster. Nevertheless, the taxonomy does provide a unique and interesting perspective on the structure of the TR literature.

The themes of the clusters shown in Tables A2-1 and A2-2 are, of necessity, very broad. The titles are provided for each of the 32 elemental clusters shown in Table A2-2 to provide the full spectrum of sub-themes within each elemental cluster, and allow the interested reader to identify specific sub-themes of personal interest within the cluster. The full reference for each title is provided in Chapter 4, Bibliography, which will allow the reader to pursue the full text for further information.

Before the details of the 32 'leaf' (lowest level) clusters are presented, a high-level (top three levels) view of the TR text clustering taxonomy is shown in Table A2-1.

Table A2-1: TOP-LEVEL TR TEXT CLUSTERING TAXONOMY

(number of records in each cluster shown in parenthesis ())

SECOND LEVEL	THIRD LEVEL	FOURTH LEVEL
Cluster 58 (1096) Drug repurposing prediction	Cluster 51 (439) - Gene expression; protein interaction network	Cluster 35 (193) - Drug-disease associations; protein interaction networks
		Cluster 41 (246) - Gene expression; genome wide association
	Cluster 56 (657) - Drug-target interaction	Cluster 48 (276) - Drug-target interaction; protein-protein interaction
		Cluster 49 (381) - Computer-aided drug repositioning; drug discovery
Cluster 61 (1793) Disease treatment	Cluster 59 (569) - Drug-resistant tuberculosis; infectious diseases	Cluster 7 (114) - Drug-resistant tuberculosis
		Cluster 57 (455) - Viral/bacterial infections; parasites
	Cluster 60 (1224) - chronic disease treatments; cancer; neurodegenerative diseases	Cluster 52 (590) - Cancer treatment
		Cluster 55 (634) - Neurodegenerative disease treatment

The first bifurcated level of the hierarchical taxonomy shows two definite thrust areas: Methods for drug repurposing prediction (Cluster 58), and disease treatments that resulted from drug repositioning (Cluster 61). The next two levels of the hierarchy are self-explanatory.

Table A2-2 relates the eight fourth-level clusters shown above in Table A2-1 to the 32 elemental leaf clusters.

Table A2-2: LOWEST LEVEL TR TEXT CLUSTERING TAXONOMY

(number of records in each cluster shown in parenthesis (); this number is hyperlinked to the actual record titles)

FOURTH LEVEL	LOWEST LEVEL (LEAF CLUSTERS)
Cluster 35 (193) - Drug-disease associations; protein interaction networks	Cluster 4 (47) - drug-disease associations
	Cluster 18 (146) - network-based prediction, especially protein interaction networks
Cluster 41 (246) - Genome-wide associations; gene expression	Cluster 16 (65) - genome-wide associations
	Cluster 21 (181) - gene expression, especially gene expression signatures and gene expression profiles
Cluster 48 (276) - Drug-target interaction prediction; protein-protein interaction	Cluster 13 (100) - drug-target interaction prediction
	Cluster 22 (176) - ligand binding-sites, protein-ligand interactions, and protein-protein interactions
Cluster 49 (381) - Computer-aided drug repositioning; drug discovery	Cluster 9 (37) - rare diseases
	Cluster 20 (91) - computational drug repositioning
	Cluster 26 (86) - marketing aspects of drug repurposing
	Cluster 29 (167) - drug development and discovery
Cluster 7 (114) - Drug-resistant tuberculosis	Cluster 7 (114) - drug-resistant tuberculosis
Cluster 57 (455) - Viral/bacterial infections; parasites	Cluster 1 (41) - antiviral treatments for viral infections, especially Ebola virus
	Cluster 0 (21) - antiviral treatments for viral infections, especially Zika virus
	Cluster 15 (80) - antiviral treatments for other viral infections, especially dengue virus, hepatitis B virus, chikungunya virus, human immunodeficiency virus, japanese encephalitis virus, rift valley fever virus, human cytomegalovirus, respiratory syncytial virus, west nile virus
	Cluster 14 (62) - treatments for parasites, especially trypanosoma cruzi, african trypanosomiasi, trypanosoma brucei, leishmania amazonensi
	Cluster 19 (93) - treatments for parasites, especially plasmodium falciparum, schistosoma mansoni, toxoplasma gondii
	Cluster 6 (45) - antifungal treatments
	Cluster 17 (113) - antimicrobial and antibiotic treatments for infections

Cluster 52 (590) - Cancer treatment	Cluster 23 (93) - repurposing kinase inhibitors, especially for treatment of acute myeloid leukemia
	Cluster 12 (59) - ovarian cancer treatments, especially niclosamide
	Cluster 27 (160) - treatments that destroy cancer cells
	Cluster 25 (171) - anti-cancer treatments
	Cluster 5 (41) - treatments for pancreatic cancer, especially Metformin
	Cluster 11 (66) - breast cancer treatments
Cluster 55 (634) - Neurodegenerative disease treatment	Cluster 2 (48) - Alzheimer's Disease treatments
	Cluster 8 (30) - neurodegenerative disease treatments, especially Parkinson's Disease
	Cluster 24 (117) - treatments for brain disease, especially stroke
	Cluster 3 (33) - drug repurposing patent applications
	Cluster 10 (46) - glioblastoma treatments
	Cluster 31 (151) - anti-inflammatory treatments
	Cluster 28 (97) - treatments for addiction disorders (especially alcohol use) and chronic pain
	Cluster 30 (112) - cancer treatments, especially metronomic chemotherapy

The details of each of the leaf clusters in which the eight fourth level categories have been sub-divided (by the CLUTO text clustering algorithm) will now be presented in some detail. In the presentation structure, each fourth-level cluster (shown in both tables above) will be followed by its constituent leaf clusters. For each leaf cluster, there will be a summary of its biomedical thrust, followed by the titles of the records in the leaf cluster. These record titles in each cluster are hyperlinked to the corresponding cluster number shown in Table A2-2. To obtain the full reference for any title(s) of interest, the reader needs to search the Bibliography references in Chapter 4.

A2-2. Details of leaf clusters

The first time a leaf cluster is presented, its number will be followed by the number of records contained within the cluster, in parentheses. For example, in section A2-2a, 'Cluster 4 (47)' means the leaf Cluster #4 contains 47 records.

A2-2a. Leaf clusters under Cluster 35

There are two leaf clusters under Cluster 35: Cluster 4 (47) and Cluster 18 (146).

*Cluster 4 focuses on drug-disease associations;

*Cluster 18 focuses on network-based prediction, especially using protein interaction networks.

A2-2a1. Cluster 4 record titles

1. Predicting drug-disease associations and their therapeutic function based on the drug-disease association bipartite network.

2. Inferring drug-disease associations from integration of chemical, genomic and phenotype data using network propagation.

3. DR2DI: a powerful computational tool for predicting novel drug-disease associations.

4. Inferring drug-disease associations based on known protein complexes.

5. Prediction of new drug indications based on clinical data and network modularity.

6. Drug Repositioning by Integrating Known Disease-Gene and Drug-Target Associations in a Semi-supervised Learning Model.

7. Network-based inference methods for drug repositioning.

8. Computational drug repositioning using low-rank matrix approximation and randomized algorithms.

9. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data.

10. A miRNA-driven inference model to construct potential drug-disease associations for drug repositioning.

11. Drug repositioning based on comprehensive similarity measures and Bi-Random walk algorithm.

12. LRSSL: predict and interpret drug-disease associations based on data integration using sparse subspace learning.

13. Predicting drug-disease interactions by semi-supervised graph cut algorithm and three-layer data integration.

14. Towards drug repositioning: a unified computational framework for integrating multiple aspects of drug similarity and disease similarity.

15. Matrix Factorization-Based Prediction of Novel Drug Indications by Integrating Genomic Space.

16. Scoring multiple features to predict drug disease associations using information fusion and aggregation.

17. Drug-disease association and drug-repositioning predictions in complex diseases using causal inference-probabilistic matrix factorization.

18. Linking PharmGKB to phenotype studies and animal models of disease for drug repurposing.

19. Inferring disease association using clinical factors in a combinatorial manner and their use in drug repositioning.

20. The extraction of drug-disease correlations based on module distance in incomplete human interactome.

21. Inferring new indications for approved drugs via random walk on drug-disease heterogenous networks.

22. Predicting Potential Drugs for Breast Cancer based on miRNA and Tissue Specificity.

23. Compensating for literature annotation bias when predicting novel drug-disease relationships through Medical Subject Heading Over-representation Profile (MeSHOP) similarity.

24. Computational drug repurposing to predict approved and novel drug-disease associations.

25. An Integrated Data Driven Approach to Drug Repositioning Using Gene-Disease Associations.

26. Network-based in silico drug efficacy screening.

27. DrPOCS: Drug repositioning based on projection onto convex sets.

28. Prediction of Novel Drugs and Diseases for Hepatocellular Carcinoma Based on Multi-Source Simulated Annealing Based Random Walk.

29. Drug repositioning based on triangularly balanced structure for tissue-specific diseases in incomplete interactome.

30. Drug repositioning by kernel-based integration of molecular structure, molecular activity, and phenotype data.

31. Heter-LP: A heterogeneous label propagation algorithm and its application in drug repositioning.

32. Identification of associations between small molecule drugs and miRNAs based on functional similarity.

33. Prediction of Novel Drugs for Hepatocellular Carcinoma Based on Multi-Source Random Walk.

34. On the Integration of In Silico Drug Design Methods for Drug Repurposing.

35. Prediction of Non-coding RNAs as Drug Targets.

36. Large-scale extraction of accurate drug-disease treatment pairs from biomedical literature for drug repurposing.

37. ANTENNA, a Multi-Rank, Multi-Layered Recommender System for Inferring Reliable Drug-Gene-Disease Associations: Repurposing Diazoxide as a Targeted Anti-Cancer Therapy.

38. Inferring novel indications of approved drugs via a learning method with local and global consistency.

39. Identification association of drug-disease by using functional gene module for breast cancer.

40. miREFRWR: a novel disease-related microRNA-environmental factor interactions prediction method.

41. Network-based approach to prediction and population-based validation of in silico drug repurposing.

42. Construction of an miRNA-regulated drug-pathway network reveals drug repurposing candidates for myasthenia gravis.

43. Deciphering miRNA transcription factor feed-forward loops to identify drug repurposing candidates for cystic fibrosis.

44. Drug voyager: a computational platform for exploring unintended drug action.

45. Systematical analysis of lncRNA-mRNA competing endogenous RNA network in breast cancer subtypes.

46. Linking molecular feature space and disease terms for the immunosuppressive drug rapamycin.

47. Word-of-Mouth Innovation: Hypothesis Generation for Supplement Repurposing based on Consumer Reviews.

A2-2a2. Cluster 18 record titles

1. Building a drug-target network and its applications.

2. Prediction of novel drug indications using network driven biological data prioritization and integration.

3. Network-based prediction and knowledge mining of disease genes.

4. Human pathway-based disease network.

5. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies.

6. DrugNet: network-based drug-disease prioritization by integrating heterogeneous data.

7. Drug target prediction and repositioning using an integrated network-based approach.

8. Computational drug repositioning through heterogeneous network clustering.

9. Fusing literature and full network data improves disease similarity computation.

10. Network approaches to drug discovery.

11. Discovering gene re-ranking efficiency and conserved gene-gene relationships derived from gene co-expression network analysis on breast cancer data.

12. Network mirroring for drug repositioning.

13. A Systematic Framework for Drug Repositioning from Integrated Omics and Drug Phenotype Profiles Using Pathway-Drug Network.

14. Drug repositioning by integrating target information through a heterogeneous network model.

15. Drug repositioning using disease associated biological processes and network analysis of drug targets.

16. Ariadne's ChemEffect and Pathway Studio knowledge base.

17. Mining integrated semantic networks for drug repositioning opportunities.

18. GUILDify: a web server for phenotypic characterization of genes through biological data integration and network-based prioritization algorithms.

19. DNetDB: The human disease network database based on dysfunctional regulation mechanism.

20. Towards building a disease-phenotype knowledge base: extracting disease-manifestation relationship from literature.

21. Systematic integration of biomedical knowledge prioritizes drugs for repurposing.

22. Network-based machine learning and graph theory algorithms for precision oncology.

23. Drug Repositioning Through Network Pharmacology.

24. Prediction of drugs having opposite effects on disease genes in a directed network.

25. Human disease-drug network based on genomic expression profiles.

26. Construction of drug network based on side effects and its application for drug repositioning.

27. A comparative study of disease genes and drug targets in the human protein interactome.

28. A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer.

29. The human disease network in terms of dysfunctional regulatory mechanisms.

30. Learning disease relationships from clinical drug trials.

31. Computational drug repositioning with random walk on a heterogeneous network.

32. DiseaseConnect: a comprehensive web server for mechanism-based disease-disease connections.

33. Advanced systems biology methods in drug discovery and translational biomedicine.

34. A review of network-based approaches to drug repositioning.

35. dRiskKB: a large-scale disease-disease risk relationship knowledge base constructed from biomedical text.

36. Inferring novel disease indications for known drugs by semantically linking drug action and disease mechanism relationships.

37. Literature-based discovery of new candidates for drug repurposing.

38. Constructing Disease Similarity Networks Based on Disease Module Theory.

39. Rectifying cancer drug discovery through network pharmacology.

40. Network-based drug repositioning.

41. Informed walks: whispering hints to gene hunters inside networks' jungle.

42. DrugGenEx-Net: a novel computational platform for systems pharmacology and gene expression-based drug repurposing.

43. Unveiling the role of network and systems biology in drug discovery.

44. Generating Gene Ontology-Disease Inferences to Explore Mechanisms of Human Disease at the Comparative Toxicogenomics Database.

45. Rational drug repositioning guided by an integrated pharmacological network of protein, disease and drug.

46. Disease classification: from phenotypic similarity to integrative genomics and beyond.

47. Network-based drug ranking and repositioning with respect to DrugBank therapeutic categories.

48. ProphTools: general prioritization tools for heterogeneous biological networks.

49. A two-step drug repositioning method based on a protein-protein interaction network of genes shared by two diseases and the similarity of drugs.

50. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association.

51. Generation and application of drug indication inference models using typed network motif comparison analysis.

52. Identifying aberrant pathways through integrated analysis of knowledge in pharmacogenomics.

53. A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes.

54. Drug repositioning through incomplete bi-cliques in an integrated drug-target-disease network.

55. A disease similarity matrix based on the uniqueness of shared genes.

56. Cancer based pharmacogenomics network supported with scientific evidences: from the view of drug repurposing.

57. COMPUTING THERAPY FOR PRECISION MEDICINE: COLLABORATIVE FILTERING INTEGRATES AND PREDICTS MULTI-ENTITY INTERACTIONS.

58. Diffusion mapping of drug targets on disease signaling network elements reveals drug combination strategies.

59. Large-scale data-driven integrative framework for extracting essential targets and processes from disease-associated gene data sets.

60. Pathway-based drug repositioning using causal inference.

61. Data integration to prioritize drugs using genomics and curated data.

62. Pathway and network-based strategies to translate genetic discoveries into effective therapies.

63. Co-expression Network Approach Reveals Functional Similarities among Diseases Affecting Human Skeletal Muscle.

64. Proximal Pathway Enrichment Analysis for Targeting Comorbid Diseases via Network Endopharmacology.

65. A systems-level analysis of drug-target-disease associations for drug repositioning.

66. Biomolecular Network Controllability With Drug Binding Information.

67. Network insights into the genes regulated by hepatocyte nuclear factor 4 in response to drug induced perturbations: a review.

68. Network and matrix analysis of the respiratory disease interactome.

69. Network biology concepts in complex disease comorbidities.

70. Network-Based Drug Discovery: Coupling Network Pharmacology with Phenotypic Screening for Neuronal Excitability.

71. PISTON: Predicting drug indications and side effects using topic modeling and natural language processing.

72. Computational Drug Repurposing: Current Trends.

73. Toward creation of a cancer drug toxicity knowledge base: automatically extracting cancer drug-side effect relationships from the literature.

74. Systematic drug repositioning based on clinical side-effects.

75. Convergent downstream candidate mechanisms of independent intergenic polymorphisms between co-classified diseases implicate epistasis among noncoding elements.

76. Comparing a knowledge-driven approach to a supervised machine learning approach in large-scale extraction of drug-side effect relationships from free-text biomedical literature.

77. Large-scale automatic extraction of side effects associated with targeted anticancer drugs from full-text oncological articles.

78. Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computer-Aided Drug Repurposing.

79. Inferring new drug indications using the complementarity between clinical disease signatures and drug effects.

80. A two-tiered unsupervised clustering approach for drug repositioning through heterogeneous data integration.

81. Combined Analysis of Phenotypic and Target-Based Screening in Assay Networks.

82. RANKS: a flexible tool for node label ranking and classification in biological networks.

83. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing.

84. MTGO: PPI Network Analysis Via Topological and Functional Module Identification.

85. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge.

86. Community-driven roadmap for integrated disease maps.

87. Pharmacodynamics and Systems Pharmacology Approaches to Repurposing Drugs in the Wake of Global Health Burden.

88. Prediction of drug gene associations via ontological profile similarity with application to drug repositioning.

89. Network-based drug repositioning: A novel strategy for discovering potential antidepressants and their mode of action.

90. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing.

91. Drug repurposing by integrated literature mining and drug-gene-disease triangulation.

92. DeCoST: A New Approach in Drug Repurposing From Control System Theory.

93. Drug Repurposing Hypothesis Generation Using the "RE:fine Drugs" System.

94. Identifying Candidates for Breast Cancer Using Interactions of Chemicals and Proteins.

95. Complex-disease networks of trait-associated single-nucleotide polymorphisms (SNPs) unveiled by information theory.

96. Automatic construction of a large-scale and accurate drug-side-effect association knowledge base from biomedical literature.

97. A bidirectional drug repositioning approach for Parkinson's disease through network-based inference.

98. Discovering discovery patterns with Predication-based Semantic Indexing.

99. A systematic analysis of FDA-approved anticancer drugs.

100. Computational Study of Drugs by Integrating Omics Data with Kernel Methods.

101. Network medicine in disease analysis and therapeutics.

102. Combining automatic table classification and relationship extraction in extracting anticancer drug-side effect pairs from full-text articles.

103. Finding complex biological relationships in recent PubMed articles using Bio-LDA.

104. Literature-based prediction of novel drug indications considering relationships between entities.

105. The pain interactome: connecting pain-specific protein interactions.

106. DenguePredict: An Integrated Drug Repositioning Approach towards Drug Discovery for Dengue.

107. MeSHDD: Literature-based drug-drug similarity for drug repositioning.

108. DSviaDRM: an R package for estimating disease similarity via dysfunctional regulation mechanism.

109. Chemotext: A Publicly Available Web Server for Mining Drug-Target-Disease Relationships in PubMed.

110. Chemical-induced disease extraction via recurrent piecewise convolutional neural networks.

111. Integrative network modeling approaches to personalized cancer medicine.

112. Large-scale integration of heterogeneous pharmacogenomic data for identifying drug mechanism of action.

113. Integrative Cancer Pharmacogenomics to Infer Large-Scale Drug Taxonomy.

114. Uncovering novel repositioning opportunities using the Open Targets platform.

115. Changing Trends in Computational Drug Repositioning.

116. MediSyn: uncertainty-aware visualization of multiple biomedical datasets to support drug treatment selection.

117. Inflammatory pathway network-based drug repositioning and molecular phenomics.

118. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach.

119. Drug repurposing: a better approach for infectious disease drug discovery?

120. Computational methods and opportunities for phosphorylation network medicine.

121. DESM: portal for microbial knowledge exploration systems.

122. Exploring the pharmacogenomics knowledge base (PharmGKB) for repositioning breast cancer drugs by leveraging Web ontology language (OWL) and cheminformatics approaches.

123. Multi-aspect candidates for repositioning: data fusion methods using heterogeneous information sources.

124. Drug knowledge bases and their applications in biomedical informatics research.

125. Medical concept normalization in social media posts with recurrent neural networks.

126. Using predicate and provenance information from a knowledge graph for drug efficacy screening.

127. DrugMap Central: an on-line query and visualization tool to facilitate drug repositioning studies.

128. Automated QuantMap for rapid quantitative molecular network topology analysis.

129. Network-assisted prediction of potential drugs for addiction.

130. Neighbours of cancer-related proteins have key influence on pathogenesis and could increase the drug target space for anticancer therapies.

131. 'RE:fine drugs': an interactive dashboard to access drug repurposing opportunities.

132. Systems Pharmacology Links GPCRs with Retinal Degenerative Disorders.

133. A physarum-inspired prize-collecting steiner tree approach to identify subnetworks for drug repositioning.

134. Graph theory enables drug repurposing--how a mathematical model can drive the discovery of hidden mechanisms of action.

135. A phenome-guided drug repositioning through a latent variable model.

136. Drug repositioning for prostate cancer: using a data-driven approach to gain new insights.

137. Investigating drug repositioning opportunities in FDA drug labels through topic modeling.

138. Early repositioning through compound set enrichment analysis: a knowledge-recycling strategy.

139. A Simple Text Mining Approach for Ranking Pairwise Associations in Biomedical Applications.

140. Correction: A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer.

141. Linking biochemical pathways and networks to adverse drug reactions.

142. Big Data Mining and Adverse Event Pattern Analysis in Clinical Drug Trials.

143. A diseasome cluster-based drug repurposing of soluble guanylate cyclase activators from smooth muscle relaxation to direct neuroprotection.

144. Information exploration system for sickle cell disease and repurposing of hydroxyfasudil.

145. A systems pharmacology-oriented discovery of a new therapeutic use of the TCM formula Liuweiwuling for liver failure.

146. Neuroprotective Drug for Nerve Trauma Revealed Using Artificial Intelligence.

A2-2b. Leaf clusters under Cluster 41

There are two leaf clusters under Cluster 41: Cluster 16 (65) and Cluster 21 (181).

*Cluster 16 focuses on genome-wide associations;

*Cluster 21 focuses on gene expression, especially gene expression signatures and gene expression profiles.

A2-2b1. Cluster 16 record titles

1. Genome-wide association studies of cancer: current insights and future perspectives.

2. Use of genome-wide association studies for drug repositioning.

3. From the era of genome analysis to the era of genomic drug discovery: a pioneering example of rheumatoid arthritis.

4. Genetics of rheumatoid arthritis contributes to biology and drug discovery.

5. Analysis of genome-wide association data highlights candidates for drug repositioning in psychiatry.

6. [GWAS of Rheumatoid Arthritis and Drug Discovery].

7. GWAS and drug targets.

8. Drug enrichment and discovery from schizophrenia genome-wide association results: an analysis and visualisation approach.

9. Identification of novel therapeutics for complex diseases from genome-wide association data.

10. A meta-analysis of reflux genome-wide association studies in 6750 Northern Europeans from the general population.

11. Connecting genetics and gene expression data for target prioritisation and drug repositioning.

12. Use of genome-wide association studies for cancer research and drug repositioning.

13. Learning Opportunities for Drug Repositioning via GWAS and PheWAS Findings.

14. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases.

15. Gene-set analysis based on the pharmacological profiles of drugs to identify repurposing opportunities in schizophrenia.

16. Enhancing the Promise of Drug Repositioning through Genetics.

17. New pathogenic insights into rheumatoid arthritis.

18. Schizophrenia interactome with 504 novel protein-protein interactions.

19. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis.

20. Update on the genetic architecture of rheumatoid arthritis.

21. The druggable genome and support for target identification and validation in drug development.

22. Computational drug repositioning: from data to therapeutics.

23. Future Directions of Genomics Research in Rheumatic Diseases.

24. Approaches for establishing the function of regulatory genetic variants involved in disease.

25. Targeting the schizophrenia genome: a fast track strategy from GWAS to clinic.

26. Phenome-wide association studies: a new method for functional genomics in humans.

27. Novel therapeutics for coronary artery disease from genome-wide association study data.

28. Genome-wide association analyses for lung function and chronic obstructive pulmonary disease identify new loci and potential druggable targets.

29. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis.

30. Molecular mechanisms underlying variations in lung function: a systems genetics analysis.

31. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia.

32. Identification of ST3AGL4, MFHAS1, CSNK2A2 and CD226 as loci associated with systemic lupus erythematosus (SLE) and evaluation of SLE genetics in drug repositioning.

33. Shared genetic origin of asthma, hay fever and eczema elucidates allergic disease biology.

34. The emergence of genome-based drug repositioning.

35. Mood, stress and longevity: convergence on ANK3.

36. Genetic and molecular aspects of hypertension.

37. Functional genomics of pain in analgesic drug development and therapy.

38. Human CCL3L1 copy number variation, gene expression, and the role of the CCL3L1-CCR5 axis in lung function.

39. Systems Pharmacology-Based Approach of Connecting Disease Genes in Genome-Wide Association Studies with Traditional Chinese Medicine.

40. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients.

41. Opportunities for drug repositioning from phenome-wide association studies.

42. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants.

43. Drug repositioning for diabetes based on 'omics' data mining.

44. Computational functional genomics-based approaches in analgesic drug discovery and repurposing.

45. Explore Small Molecule-induced Genome-wide Transcriptional Profiles for Novel Inflammatory Bowel Disease Drug.

46. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets.

47. A perspective on genomic-guided anthelmintic discovery and repurposing using Haemonchus contortus.

48. Drug Repositioning in Inflammatory Bowel Disease Based on Genetic Information.

49. A phenome-wide association study of a lipoprotein-associated phospholipase A2 loss-of-function variant in 90 000 Chinese adults.

50. Bioinformatics analysis reveals transcriptome and microRNA signatures and drug repositioning targets for IBD and other autoimmune diseases.

51. Repositioning of drugs using open-access data portal DTome: A test case with probenecid (Review).

52. A machine-learned computational functional genomics-based approach to drug classification.

53. Precision medicine for suicidality: from universality to subtypes and personalization.

54. Omics studies: their use in diagnosis and reclassification of SLE and other systemic autoimmune diseases.

55. Calcium channel blockers as drug repurposing candidates for gestational diabetes: Mining large scale genomic and electronic health records data to repurpose medications.

56. ZikaVR: An Integrated Zika Virus Resource for Genomics, Proteomics, Phylogenetic and Therapeutic Analysis.

57. Towards precision medicine-based therapies for glioblastoma: interrogating human disease genomics and mouse phenotypes.

58. Drug repurposing for glioblastoma based on molecular subtypes.

59. Personalized Proteomics for Precision Health: Identifying Biomarkers of Vitreoretinal Disease.

60. Drug repositioning in SLE: crowd-sourcing, literature-mining and Big Data analysis.

61. Repurpose terbutaline sulfate for amyotrophic lateral sclerosis using electronic medical records.

62. Opportunities for Web-based Drug Repositioning: Searching for Potential Antihypertensive Agents with Hypotension Adverse Events.

63. Systems pharmacology of adverse event mitigation by drug combinations.

64. Simvastatin offers new prospects for the treatment of Duchenne muscular dystrophy.

65. A second look: Efforts to repurpose old drugs against Zika cast a wide net.

A2-2b2. Cluster 21 record titles

1. Connectivity mapping using a combined gene signature from multiple colorectal cancer datasets identified candidate drugs including existing chemotherapies.

2. Drug similarity search based on combined signatures in gene expression profiles.

3. Finding the targets of a drug by integration of gene expression data with a protein interaction network.

4. Discovery of the neuroprotective effects of alvespimycin by computational prioritization of potential anti-Parkinson agents.

5. Harnessing the biological complexity of Big Data from LINCS gene expression signatures.

6. New drug candidates for treatment of atypical meningiomas: An integrated approach using gene expression signatures for drug repurposing.

7. Gene-Set Local Hierarchical Clustering (GSLHC)--A Gene Set-Based Approach for Characterizing Bioactive Compounds in Terms of Biological Functional Groups.

8. ADEPTUS: a discovery tool for disease prediction, enrichment and network analysis based on profiles from many diseases.

9. Statistically controlled identification of differentially expressed genes in one-to-one cell line comparisons of the CMAP database for drug repositioning.

10. A novel computational approach for drug repurposing using systems biology.

11. Cogena, a novel tool for co-expressed gene-set enrichment analysis, applied to drug repositioning and drug mode of action discovery.

12. MD-Miner: a network-based approach for personalized drug repositioning.

13. Utilizing Cancer - Functional Gene Set - Compound Networks to Identify Putative Drugs for Breast Cancer.

14. Revisiting Connectivity Map from a gene co-expression network analysis.

15. DeSigN: connecting gene expression with therapeutics for drug repurposing and development.

16. Drug repositioning for orphan genetic diseases through Conserved Anticoexpressed Gene Clusters (CAGCs).

17. Drug repositioning: a machine-learning approach through data integration.

18. A Computational Systems Biology Approach for Identifying Candidate Drugs for Repositioning for Cardiovascular Disease.

19. Network-based analysis of transcriptional profiles from chemical perturbations experiments.

20. DIGEP-Pred: web service for in silico prediction of drug-induced gene expression profiles based on structural formula.

21. Multi-target drug repositioning by bipartite block-wise sparse multi-task learning.

22. Integrating Clinical Phenotype and Gene Expression Data to Prioritize Novel Drug Uses.

23. DrugSig: A resource for computational drug repositioning utilizing gene expression signatures.

24. From gene networks to drugs: systems pharmacology approaches for AUD.

25. Master Regulators Connectivity Map: A Transcription Factors-Centered Approach to Drug Repositioning.

26. Repositioning drugs by targeting network modules: a Parkinson's disease case study.

27. Transcriptional data: a new gateway to drug repositioning?

28. Drug Intervention Response Predictions with PARADIGM (DIRPP) identifies drug resistant cancer cell lines and pathway mechanisms of resistance.

29. A computational method for drug repositioning using publicly available gene expression data.

30. Identifying prognostic features by bottom-up approach and correlating to drug repositioning.

31. Functional Module Connectivity Map (FMCM): a framework for searching repurposed drug compounds for systems treatment of cancer and an application to colorectal adenocarcinoma.

32. GeneExpressionSignature: an R package for discovering functional connections using gene expression signatures.

33. Drug Selection in the Genomic Age: Application of the Coexpression Extrapolation Principle for Drug Repositioning in Cancer Therapy.

34. Gene Vector Analysis (Geneva): a unified method to detect differentially-regulated gene sets and similar microarray experiments.

35. Personalised drug repositioning for Clear Cell Renal Cell Carcinoma using gene expression.

36. Pathway-based Bayesian inference of drug-disease interactions.

37. DvD: An R/Cytoscape pipeline for drug repurposing using public repositories of gene expression data.

38. Improved anticancer drug response prediction in cell lines using matrix factorization with similarity regularization.

39. Drug-Path: a database for drug-induced pathways.

40. Drug Repurposing Using Deep Embeddings of Gene Expression Profiles.

41. Prioritizing therapeutics for lung cancer: an integrative meta-analysis of cancer gene signatures and chemogenomic data.

42. A cross-species analysis method to analyze animal models' similarity to human's disease state.

43. GDA, a web-based tool for Genomics and Drugs integrated analysis.

44. cudaMap: a GPU accelerated program for gene expression connectivity mapping.

45. Integrating systems biology sources illuminates drug action.

46. Identification of small molecules enhancing autophagic function from drug network analysis.

47. DSigDB: drug signatures database for gene set analysis.

48. Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis.

49. Drug Repositioning through Systematic Mining of Gene Coexpression Networks in Cancer.

50. Linking drug target and pathway activation for effective therapy using multi-task learning.

51. Systematic Identification and Assessment of Therapeutic Targets for Breast Cancer Based on Genome-Wide RNA Interference Transcriptomes.

52. Discovery of drug mode of action and drug repositioning from transcriptional responses.

53. Cell-specific prediction and application of drug-induced gene expression profiles.

54. Connection Map for Compounds (CMC): A Server for Combinatorial Drug Toxicity and Efficacy Analysis.

55. Integrated analysis of numerous heterogeneous gene expression profiles for detecting robust disease-specific biomarkers and proposing drug targets.

56. Synergistic drug combinations from electronic health records and gene expression.

57. Transcriptomic-Guided Drug Repositioning Supported by a New Bioinformatics Search Tool: geneXpharma.

58. Drug repositioning framework by incorporating functional information.

59. Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference.

60. BRCA-Monet: a breast cancer specific drug treatment mode-of-action network for treatment effective prediction using large scale microarray database.

61. The use of a gene expression signature and connectivity map to repurpose drugs for bipolar disorder.

62. Drug-repurposing identified the combination of Trolox C and Cytisine for the treatment of type 2 diabetes.

63. An integrated network platform for contextual prioritization of drugs and pathways.

64. Discovery and preclinical validation of drug indications using compendia of public gene expression data.

65. Using gene expression signatures to identify novel treatment strategies in gulf war illness.

66. Probabilistic drug connectivity mapping.

67. An integrative approach using real-world data to identify alternative therapeutic uses of existing drugs.

68. Network analysis of immunotherapy-induced regressing tumours identifies novel synergistic drug combinations.

69. DMAP: a connectivity map database to enable identification of novel drug repositioning candidates.

70. PREDICT: a method for inferring novel drug indications with application to personalized medicine.

71. A network based approach to drug repositioning identifies plausible candidates for breast cancer and prostate cancer.

72. ksRepo: a generalized platform for computational drug repositioning.

73. Systematic drug safety evaluation based on public genomic expression (Connectivity Map) data: myocardial and infectious adverse reactions as application cases.

74. Transcriptomic Analysis of the Host Response and Innate Resilience to Enterotoxigenic Escherichia coli Infection in Humans.

75. Identification of common biological pathways and drug targets across multiple respiratory viruses based on human host gene expression analysis.

76. Elucidating the modes of action for bioactive compounds in a cell-specific manner by large-scale chemically-induced transcriptomics.

77. A Semi-Supervised Approach for Refining Transcriptional Signatures of Drug Response and Repositioning Predictions.

78. CellFateScout - a bioinformatics tool for elucidating small molecule signaling pathways that drive cells in a specific direction.

79. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning.

80. Using functional signatures to identify repositioned drugs for breast, myelogenous leukemia and prostate cancer.

81. Exploring the molecular mechanisms of Traditional Chinese Medicine components using gene expression signatures and connectivity map.

82. Introduction: Cancer Gene Networks.

83. Bioinformatics methods in drug repurposing for Alzheimer's disease.

84. Gene expression-based drug repurposing to target aging.

85. Application of Atlas of Cancer Signalling Network in preclinical studies.

86. gene2drug: a computational tool for pathway-based rational drug repositioning.

87. Using Big Data to Discover Diagnostics and Therapeutics forGastrointestinal and Liver Diseases.

88. NetwoRx: connecting drugs to networks and phenotypes in Saccharomyces cerevisiae.

89. Gene expression-based chemical genomics identifies potential therapeutic drugs in hepatocellular carcinoma.

90. Drug Repositioning for Cancer Therapy Based on Large-Scale Drug-Induced Transcriptional Signatures.

91. PATIENT-SPECIFIC DATA FUSION FOR CANCER STRATIFICATION AND PERSONALISED TREATMENT.

92. Classifying cancer genome aberrations by their mutually exclusive effects on transcription.

93. Comparing structural and transcriptional drug networks reveals signatures of drug activity and toxicity in transcriptional responses.

94. Drugs that reverse disease transcriptomic signatures are more effective in a mouse model of dyslipidemia.

95. Objective assessment of cancer genes for drug discovery.

96. EMUDRA: Ensemble of Multiple Drug Repositioning Approaches to improve prediction accuracy.

97. Mantra 2.0: an online collaborative resource for drug mode of action and repurposing by network analysis.

98. Drug Targeting and Biomarkers in Head and Neck Cancers: Insights from Systems Biology Analyses.

99. Prediction of anti-cancer drug response by kernelized multi-task learning.

100. High-throughput screening for the identification of new therapeutic options for metastatic pheochromocytoma and paraganglioma.

101. Computational identification of multi-omic correlates of anticancer therapeutic response.

102. Signatures for drug repositioning.

103. [Identification of key pathways and drug repurposing for anaplastic thyroid carcinoma by integrated bioinformatics analysis].

104. A Biologically-Based Computational Approach to Drug Repurposing for Anthrax Infection.

105. A cellular genetics approach identifies gene-drug interactions and pinpoints drug toxicity pathway nodes.

106. Machine learning prediction of cancer cell sensitivity to drugs based on genomic and chemical properties.

107. Identify potential drugs for cardiovascular diseases caused by stress-induced genes in vascular smooth muscle cells.

108. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases.

109. Cancer Drug Response Profile scan (CDRscan): A Deep Learning Model That Predicts Drug Effectiveness from Cancer Genomic Signature.

110. A subpathway-based method of drug reposition for polycystic ovary syndrome.

111. Mining the transcriptome for rare disease therapies: a comparison of the efficiencies of two data mining approaches and a targeted cell-based drug screen.

112. EHFPI: a database and analysis resource of essential host factors for pathogenic infection.

113. In search for geroprotectors: in silico screening and in vitro validation of signalome-level mimetics of young healthy state.

114. Drug repositioning discovery for early- and late-stage non-small-cell lung cancer.

115. Exploration of the Anti-Inflammatory Drug Space Through Network Pharmacology: Applications for Drug Repurposing.

116. Pathway analysis for drug repositioning based on public database mining.

117. Rational drug repurposing using sscMap analysis in a HOX-TALE model of leukemia.

118. Predicting High-Impact Pharmacological Targets by Integrating Transcriptome and Text-Mining Features.

119. Integrative bioinformatic analyses of an oncogenomic profile reveal the biology of endometrial cancer and guide drug discovery.

120. Computational approaches for drug repositioning and combination therapy design.

121. Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis.

122. Drug discovery in the age of systems biology: the rise of computational approaches for data integration.

123. Text Mining and Data Modeling of Karyotypes to aid in Drug Repurposing Efforts.

124. Bioinformatics: Novel Insights from Genomic Information.

125. Nucleosome Repositioning: A Novel Mechanism for Nicotine- and Cocaine-Induced Epigenetic Changes.

126. Drug repositioning for schizophrenia and depression/anxiety disorders: A machine learning approach leveraging expression data.

127. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification.

128. Context-specific functional module based drug efficacy prediction.

129. Antiviral effects of inhibiting host gene expression.

130. The functional therapeutic chemical classification system.

131. Drug repurposing in idiopathic pulmonary fibrosis filtered by a bioinformatics-derived composite score.

132. Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data.

133. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine.

134. A computational method for clinically relevant cancer stratification and driver mutation module discovery using personal genomics profiles.

135. Integrative omics analyses broaden treatment targets in human cancer.

136. Computational repositioning and preclinical validation of mifepristone for human vestibular schwannoma.

137. NMR spectroscopy-based metabolic profiling of drug-induced changes in vitro can discriminate between pharmacological classes.

138. Significance and suppression of redundant IL17 responses in acute allograft rejection by bioinformatics based drug repositioning of fenofibrate.

139. Drug repositioning for non-small cell lung cancer by using machine learning algorithms and topological graph theory.

140. Mining Exosomal Genes for Pancreatic Cancer Targets.

141. Drug repurposing and therapeutic anti-microRNA predictions for inhibition of oxidized low-density lipoprotein-induced vascular smooth muscle cell-associated diseases.

142. A chemical-genetic interaction map of small molecules using high-throughput imaging in cancer cells.

143. Molecular property diagnostic suite for diabetes mellitus (MPDSDM): An integrated web portal for drug discovery and drug repurposing.

144. Discovery of novel therapeutic properties of drugs from transcriptional responses based on multi-label classification.

145. Radiation protective effects of baclofen predicted by a computational drug repurposing strategy.

146. Bioinformatic and biological avenues for understanding alcohol use disorder.

147. Genomic perturbations reveal distinct regulatory networks in intrahepatic cholangiocarcinoma.

148. A Computational Workflow Translates a 58-Gene Signature to a Formalin-Fixed, Paraffin-Embedded Sample-Based Companion Diagnostic for Personalized Treatment of the BRAF-Mutation-Like Subtype of Colorectal Cancers.

149. Clobetasol and Halcinonide Act as Smoothened Agonists to Promote Myelin Gene Expression and RxRgamma Receptor Activation.

150. Gaining insight into off-target mediated effects of drug candidates with a comprehensive systems chemical biology analysis.

151. Exploration and analysis of drug modes of action through feature integration.

152. Predicting and characterizing selective multiple drug treatments for metabolic diseases and cancer.

153. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning.

154. Neuroblastoma, a Paradigm for Big Data Science in Pediatric Oncology.

155. siRNA Genome Screening Approaches to Therapeutic Drug Repositioning.

156. Integrated Computational Analysis of Genes Associated with Human Hereditary Insensitivity to Pain. A Drug Repurposing Perspective.

157. Myotonic dystrophy: candidate small molecule therapeutics.

158. Drug-target based cross-sectional analysis of olfactory drug effects.

159. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes.

160. Advances in epilepsy gene discovery and implications for epilepsy diagnosis and treatment.

161. IMPACT web portal: oncology database integrating molecular profiles with actionable therapeutics.

162. Combined analysis of gene expression and genome binding profiles identified potential therapeutic targets of ciclopirox in Ewing sarcoma.

163. RDF SKETCH MAPS - KNOWLEDGE COMPLEXITY REDUCTION FOR PRECISION MEDICINE ANALYTICS.

164. From the Viewpoint of Drug Metabolism Research.

165. A structure- and chemical genomics-based approach for repositioning of drugs against VCP/p97 ATPase.

166. Personalizing Chinese medicine by integrating molecular features of diseases and herb ingredient information: application to acute myeloid leukemia.

167. Drug repurposing for aging research using model organisms.

168. A profound computational study to prioritize the disease-causing mutations in PRPS1 gene.

169. High-Throughput Flow Cytometry Drug Combination Discovery with Novel Synergy Analysis Software, SynScreen.

170. A Computational Drug Repositioning Approach for Targeting Oncogenic Transcription Factors.

171. Integrative clinical transcriptomics analyses for new therapeutic intervention strategies: a psoriasis case study.

172. Identification of Atorvastatin for Moderate toSevere Hidradenitis through Drug Repositioning Using Public Gene ExpressionDatasets.

173. Drug Synergy Slows Aging and Improves Healthspan through IGF and SREBP Lipid Signaling.

174. Olfactory drug effects approached from human-derived data.

175. The prescribable drugs with efficacy in experimental epilepsies (PDE3) database for drug repurposing research in epilepsy.

176. A network pharmacology approach reveals new candidate caloric restriction mimetics in C. elegans.

177. A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors.

178. Registered report: Discovery and preclinical validation of drug indications using compendia of public gene expression data.

179. Mining mouse behavior for patterns predicting psychiatric drug classification.

180. Identification of Alpha-Adrenergic Agonists asPotential Therapeutic Agents for Dermatomyositis through Drug-Repurposing Using Public Expression Datasets.

181. Mixed outcomes for computational predictions.

A2-2c. Leaf clusters under Cluster 48

There are two leaf clusters under Cluster 48: Cluster 13 (100) and Cluster 22 (176).

*Cluster 13 focuses on drug-target interaction prediction;

*Cluster 22 focuses on ligand binding-sites, protein-ligand interactions, and protein-protein interactions.

A2-2c1. Cluster 13 record titles

1. Drug-Target Interactions: Prediction Methods and Applications.

2. Some Remarks on Prediction of Drug-Target Interaction with Network Models.

3. Recent advances in the machine learning-based drug-target interaction prediction.

4. Prediction of drug-target interaction by label propagation with mutual interaction information derived from heterogeneous network.

5. Toward more realistic drug-target interaction predictions.

6. Deep-Learning-Based Drug-Target Interaction Prediction.

7. Link prediction in drug-target interactions network using similarity indices.

8. Predicting Drug-Target Interactions With Multi-Information Fusion.

9. Computational Prediction of Drug?Target Interactions Using Chemical, Biological, and Network Features.

10. Computational Discovery of Putative Leads for Drug Repositioning through Drug-Target Interaction Prediction.

11. Prediction of Human Drug Targets and Their Interactions Using Machine Learning Methods: Current and Future Perspectives.

12. A network integration approach for drug-target interaction prediction and computational drug repositioning from heterogeneous information.

13. Predicting drug-target interactions using restricted Boltzmann machines.

14. Mining significant substructure pairs for interpreting polypharmacology in drug-target network.

15. Predicting Drug-Target Interactions via Within-Score and Between-Score.

16. Drug-target interaction prediction by integrating multiview network data.

17. SELF-BLM: Prediction of drug-target interactions via self-training SVM.

18. A computational approach to finding novel targets for existing drugs.

19. Prediction of drug-target interactions for drug repositioning only based on genomic expression similarity.

20. Drug-target interaction prediction: A Bayesian ranking approach.

21. Drug-target interaction prediction by integrating chemical, genomic, functional and pharmacological data.

22. Drug target prediction using adverse event report systems: a pharmacogenomic approach.

23. Predicting drug-target interaction for new drugs using enhanced similarity measures and super-target clustering.

24. Global optimization-based inference of chemogenomic features from drug-target interactions.

25. Recommendation Techniques for Drug-Target Interaction Prediction and Drug Repositioning.

26. SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drug-target interactions and drug repositioning.

27. Large-Scale Prediction of Drug-Target Interaction: a Data-Centric Review.

28. Screening drug-target interactions with positive-unlabeled learning.

29. MPGraph: multi-view penalised graph clustering for predicting drug-target interactions.

30. Prediction of drug-target interactions and drug repositioning via network-based inference.

31. Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors.

32. RepTB: a gene ontology based drug repurposing approach for tuberculosis.

33. Drug-Target Networks.

34. Polypharmacological Drug-target Inference for Chemogenomics.

35. An improved approach for predicting drug-target interaction: proteochemometrics to molecular docking.

36. Prediction of polypharmacological profiles of drugs by the integration of chemical, side effect, and therapeutic space.

37. DT-Web: a web-based application for drug-target interaction and drug combination prediction through domain-tuned network-based inference.

38. Predicting drug-target interactions using probabilistic matrix factorization.

39. Open-source chemogenomic data-driven algorithms for predicting drug-target interactions.

40. Improved prediction of drug-target interactions using regularized least squares integrating with kernel fusion technique.

41. Large-Scale Off-Target Identification Using Fast and Accurate Dual Regularized One-Class Collaborative Filtering and Its Application to Drug Repurposing.

42. Updates on drug-target network; facilitating polypharmacology and data integration by growth of DrugBank database.

43. A simple mathematical approach to the analysis of polypharmacology and polyspecificity data.

44. Identification of drug candidates and repurposing opportunities through compound-target interaction networks.

45. Design of a tripartite network for the prediction of drug targets.

46. BalestraWeb: efficient online evaluation of drug-target interactions.

47. Computational Drug Target Screening through Protein Interaction Profiles.

48. Clustering drug-drug interaction networks with energy model layouts: community analysis and drug repurposing.

49. Drug Target Commons 2.0: a community platform for systematic analysis of drug-target interaction profiles.

50. Analysis of A Drug Target-based Classification System using Molecular Descriptors.

51. Predicting new indications for approved drugs using a proteochemometric method.

52. Leveraging 3D chemical similarity, target and phenotypic data in the identification of drug-protein and drug-adverse effect associations.

53. A New Method for Computational Drug Repositioning Using Drug Pairwise Similarity.

54. Target-Based Drug Repositioning Using Large-Scale Chemical-Protein Interactome Data.

55. The role of drug profiles as similarity metrics: applications to repurposing, adverse effects detection and drug-drug interactions.

56. Network predicting drug's anatomical therapeutic chemical code.

57. Drug Target Commons: A Community Effort to Build a Consensus Knowledge Base for Drug-Target Interactions.

58. Drug repositioning by applying 'expression profiles' generated by integrating chemical structure similarity and gene semantic similarity.

59. Drug repurposing based on drug-drug interaction.

60. A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case.

61. Mouse model phenotypes provide information about human drug targets.

62. A Multilayer Network Approach for Guiding Drug Repositioning in Neglected Diseases.

63. Similarity-based prediction for Anatomical Therapeutic Chemical classification of drugs by integrating multiple data sources.

64. Prediction of chemical-protein interactions network with weighted network-based inference method.

65. C-SPADE: a web-tool for interactive analysis and visualization of drug screening experiments through compound-specific bioactivity dendrograms.

66. In silico prediction of chemical mechanism of action via an improved network-based inference method.

67. Large-scale Direct Targeting for Drug Repositioning and Discovery.

68. Drug target central.

69. Many approved drugs have bioactive analogs with different target annotations.

70. Drug target prediction by multi-view low rank embedding.

71. Prediction of drug indications based on chemical interactions and chemical similarities.

72. Prediction of drug's Anatomical Therapeutic Chemical (ATC) code by integrating drug-domain network.

73. REPRODUCIBLE DRUG REPURPOSING: WHEN SIMILARITY DOES NOT SUFFICE.

74. A hybrid method for prediction and repositioning of drug Anatomical Therapeutic Chemical classes.

75. Experimental confirmation of new drug-target interactions predicted by Drug Profile Matching.

76. Logical comparison over RDF resources in bio-informatics.

77. Drug Repositioning Strategies for the Identification of Novel Therapies for Rheumatic Autoimmune Inflammatory Diseases.

78. Predicting anatomic therapeutic chemical classification codes using tiered learning.

79. Extracting drug-enzyme relation from literature as evidence for drug drug interaction.

80. Relating anatomical therapeutic indications by the ensemble similarity of drug sets.

81. In silico repositioning-chemogenomics strategy identifies new drugs with potential activity against multiple life stages of Schistosoma mansoni.

82. Realizing drug repositioning by adapting a recommendation system to handle the process.

83. Concept-based semi-automatic classification of drugs.

84. Exploring drug-target interaction networks of illicit drugs.

85. Large-Scale Prediction of Beneficial Drug Combinations Using Drug Efficacy and Target Profiles.

86. Drug Repurposing by Simulating Flow Through Protein-Protein Interaction Networks.

87. Drug repositioning using in silico compound profiling.

88. Target-similarity search using Plasmodium falciparum proteome identifies approved drugs with anti-malarial activity and their possible targets.

89. IDMap: facilitating the detection of potential leads with therapeutic targets.

90. Clustering based drug-drug interaction networks for possible repositioning of drugs against EGFR mutations: Clustering based DDI networks for EGFR mutations.

91. DrugBank 5.0: a major update to the DrugBank database for 2018.

92. From malaria to cancer: Computational drug repositioning of amodiaquine using PLIP interaction patterns.

93. Defining the Schistosoma haematobium kinome enables the prediction of essential kinases as anti-schistosome drug targets.

94. Genetic screens for the control of influenza virus replication: from meta-analysis to drug discovery.

95. Protein localization vector propagation: a method for improving the accuracy of drug repositioning.

96. Computational drug repositioning for peripheral arterial disease: prediction of anti-inflammatory and pro-angiogenic therapeutics.

97. Predict drug permeability to blood-brain-barrier from clinical phenotypes: drug side effects and drug indications.

98. Interaction and localization diversities of global and local hubs in human protein-protein interaction networks.

99. Correction: Large-Scale Off-Target Identification Using Fast and Accurate Dual Regularized One-Class Collaborative Filtering and Its Application to Drug Repurposing.

100. US science: The Obama experiment.

A2-2c2. Cluster 22 record titles

1. eModel-BDB: a database of comparative structure models of drug-target interactions from the Binding Database.

2. Polypharmacology rescored: protein-ligand interaction profiles for remote binding site similarity assessment.

3. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison.

4. eMatchSite: sequence order-independent structure alignments of ligand binding pockets in protein models.

5. Virtual target screening: validation using kinase inhibitors.

6. ProBiS-ligands: a web server for prediction of ligands by examination of protein binding sites.

7. Characterizing the pocketome of Mycobacterium tuberculosis and application in rationalizing polypharmacological target selection.

8. Drug Promiscuity in PDB: Protein Binding Site Similarity Is Key.

9. Protein-ligand-based pharmacophores: generation and utility assessment in computational ligand profiling.

10. Binding site matching in rational drug design: algorithms and applications.

11. Identify drug repurposing candidates by mining the protein data bank.

12. Reverse Screening Methods to Search for the Protein Targets of Chemopreventive Compounds.

13. Large-scale detection of drug off-targets: hypotheses for drug repurposing and understanding side-effects.

14. Assessing protein kinase target similarity: Comparing sequence, structure, and cheminformatics approaches.

15. Comparative assessment of strategies to identify similar ligand-binding pockets in proteins.

16. BioGPS: The Music for the Chemo- and Bioinformatics Walzer.

17. High-Throughput parallel blind Virtual Screening using BINDSURF.

18. SPILLO-PBSS: detecting hidden binding sites within protein 3D-structures through a flexible structure-based approach.

19. In Silico target fishing: addressing a "Big Data" problem by ligand-based similarity rankings with data fusion.

20. BioGPS: navigating biological space to predict polypharmacology, off-targeting, and selectivity.

21. Predicting targeted polypharmacology for drug repositioning and multi- target drug discovery.

22. An integrated structure- and system-based framework to identify new targets of metabolites and known drugs.

23. Detection of Binding Site Molecular Interaction Field Similarities.

24. TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database.

25. Structure Investigation, Enrichment Analysis and Structure-based Repurposing of FDA-approved Drugs as Inhibitors of BET-BRD4.

26. Local Alignment of Ligand Binding Sites in Proteins for Polypharmacology and Drug Repositioning.

27. Chemical-protein interactome and its application in off-target identification.

28. Homopharma: a new concept for exploring the molecular binding mechanisms and drug repurposing.

29. Computational profiling of bioactive compounds using a target-dependent composite workflow.

30. A large-scale computational approach to drug repositioning.

31. Docking-based inverse virtual screening: methods, applications, and challenges.

32. From laptop to benchtop to bedside: structure-based drug design on protein targets.

33. TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds.

34. RepurposeVS: A Drug Repurposing-Focused Computational Method for Accurate Drug-Target Signature Predictions.

35. Exploring polypharmacology using a ROCS-based target fishing approach.

36. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites.

37. What is the potential of structure-based target prediction methods?

38. Proteome-scale docking: myth and reality.

39. Exploring Polypharmacology in Drug Discovery and Repurposing Using the CANDO Platform.

40. Old friends in new guise: repositioning of known drugs with structural bioinformatics.

41. PDID: database of molecular-level putative protein-drug interactions in the structural human proteome.

42. ChemMapper: a versatile web server for exploring pharmacology and chemical structure association based on molecular 3D similarity method.

43. Bioinformatics and Drug Discovery.

44. Comparing Drug Images and Repurposing Drugs with BioGPS and FLAPdock: The Thymidylate Synthase Case.

45. Drugs Polypharmacology by In Silico Methods: New Opportunities in Drug Discovery.

46. The CARLSBAD database: a confederated database of chemical bioactivities.

47. SPIDR: small-molecule peptide-influenced drug repurposing.

48. PROMISCUOUS: a database for network-based drug-repositioning.

49. Implications of the small number of distinct ligand binding pockets in proteins for drug discovery, evolution and biochemical function.

50. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies.

51. Uncovering Drug Mechanism of Action by Proteome Wide- Identification of Drug-Binding Proteins.

52. Characterizing protein domain associations by Small-molecule ligand binding.

53. A machine learning-based method to improve docking scoring functions and its application to drug repurposing.

54. Docking of a novel DNA methyltransferase inhibitor identified from high-throughput screening: insights to unveil inhibitors in chemical databases.

55. Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach.

56. Prediction of off-target drug effects through data fusion.

57. MOST: most-similar ligand based approach to target prediction.

58. Detecting drug promiscuity using Gaussian ensemble screening.

59. Reverse docking: a powerful tool for drug repositioning and drug rescue.

60. A combined systems and structural modeling approach repositions antibiotics for Mycoplasma genitalium.

61. Incorporating Protein Dynamics Through Ensemble Docking in Machine Learning Models to Predict Drug Binding.

62. Review and comparative assessment of similarity-based methods for prediction of drug-protein interactions in the druggable human proteome.

63. A drug target slim: using gene ontology and gene ontology annotations to navigate protein-ligand target space in ChEMBL.

64. Comprehensive prediction of drug-protein interactions and side effects for the human proteome.

65. Methods to Profile the Macromolecular Targets of Small Compounds.

66. A novel multi-modal drug repurposing approach for identification of potent ACK1 inhibitors.

67. GES polypharmacology fingerprints: a novel approach for drug repositioning.

68. A review of MED-SuMo applications.

69. Orphan receptor ligand discovery by pickpocketing pharmacological neighbors.

70. Explicit Drug Re-positioning: Predicting Novel Drug-Target Interactions of the Shelved Molecules with QM/MM Based Approaches.

71. The purchasable chemical space: a detailed picture.

72. Tools for in silico target fishing.

73. Enhancing the Enrichment of Pharmacophore-Based Target Prediction for the Polypharmacological Profiles of Drugs.

74. Advances in the Development of Shape Similarity Methods and Their Application in Drug Discovery.

75. Polypharmacology in Drug Discovery: A Review from Systems Pharmacology Perspective.

76. Using reverse docking for target identification and its applications for drug discovery.

77. Finding off-targets, biological pathways, and target diseases for chymase inhibitors via structure-based systems biology approach.

78. CANDO and the infinite drug discovery frontier.

79. Exploring the anti-proliferative activity of Pelargonium sidoides DC with in silico target identification and network pharmacology.

80. Molecular Connectivity Predefines Polypharmacology: Aliphatic Rings, Chirality, and sp3 Centers Enhance Target Selectivity.

81. Checking the STEP-Associated Trafficking and Internalization of Glutamate Receptors for Reduced Cognitive Deficits: A Machine Learning Approach-Based Cheminformatics Study and Its Application for Drug Repurposing.

82. Discovery of Novel Liver-Stage Antimalarials through Quantum Similarity.

83. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach.

84. Data Sets Representative of the Structures and Experimental Properties of FDA-Approved Drugs.

85. DPDR-CPI, a server that predicts Drug Positioning and Drug Repositioning via Chemical-Protein Interactome.

86. Exploring the associations between drug side-effects and therapeutic indications.

87. Human enterovirus 71 protein interaction network prompts antiviral drug repositioning.

88. Network measures for chemical library design.

89. Development of a Sigma-2 Receptor affinity filter through a Monte Carlo based QSAR analysis.

90. Target Fishing by Cross-Docking to Explain Polypharmacological Effects.

91. Discovery of Surface Target Proteins Linking Drugs, Molecular Markers, Gene Regulation, Protein Networks, and Disease by Using a Web-Based Platform Targets-search.

92. Assessing relative bioactivity of chemical substances using quantitative molecular network topology analysis.

93. Reactions of model proteins with aurothiomalate, a clinically established gold(I) drug: The comparison with auranofin.

94. Exploring the relationship between drug side-effects and therapeutic indications.

95. FDA approved drugs complexed to their targets: evaluating pose prediction accuracy of docking protocols.

96. The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing.

97. Identifying the macromolecular targets of de novo-designed chemical entities through self-organizing map consensus.

98. Cyclotides as Tools in Chemical Biology.

99. Drug design targeting protein-protein interactions (PPIs) using multiple ligand simultaneous docking (MLSD) and drug repositioning: discovery of raloxifene and bazedoxifene as novel inhibitors of IL-6/GP130 interface.

100. Polypharmacology: challenges and opportunities in drug discovery.

101. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology.

102. IsoMIF Finder: online detection of binding site molecular interaction field similarities.

103. Recognizing drug targets using evolutionary information: implications for repurposing FDA-approved drugs against Mycobacterium tuberculosis H37Rv.

104. High-throughput identification of off-targets for the mechanistic study of severe adverse drug reactions induced by analgesics.

105. Can sodium/hydrogen exchange inhibitors be repositioned for treating attention deficit hyperactivity disorder? An in silico approach.

106. Exploiting large-scale drug-protein interaction information for computational drug repurposing.

107. Visual Analysis of Biological Activity Data with Scaffold Hunter.

108. The bitter pill: clinical drugs that activate the human bitter taste receptor TAS2R14.

109. A potential target of Tanshinone IIA for acute promyelocytic leukemia revealed by inverse docking and drug repurposing.

110. [Research advance in the drug target prediction based on chemoinformatics].

111. DockingApp: a user friendly interface for facilitated docking simulations with AutoDock Vina.

112. Targeting the off-targets: a computational bioinformatics approach to understanding the polypharmacology of nelfinavir.

113. DRAR-CPI: a server for identifying drug repositioning potential and adverse drug reactions via the chemical-protein interactome.

114. Identification of cisapride as new inhibitor of putrescine uptake in Trypanosoma cruzi by combined ligand- and structure-based virtual screening.

115. Mapping Protein Targets of Bioactive Small Molecules Using Lipid-Based Chemical Proteomics.

116. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation.

117. Computational tools for polypharmacology and repurposing.

118. Beyond Channel Activity: Protein-Protein Interactions Involving Viroporins.

119. Pharmacological use of a novel scaffold, anomeric N,N-diarylamino tetrahydropyran: molecular similarity search, chemocentric target profiling, and experimental evidence.

120. Prediction of chemical-protein interactions: multitarget-QSAR versus computational chemogenomic methods.

121. Multiscale modelling of relationships between protein classes and drug behavior across all diseases using the CANDO platform.

122. In Silico Receptorome Screening of Antipsychotic Drugs.

123. Benchmarking human protein complexes to investigate drug-related systems and evaluate predicted protein complexes.

124. Insights from pharmacological similarity of epigenetic targets in epipolypharmacology.

125. Accidental interaction between PDZ domains and diclofenac revealed by NMR-assisted virtual screening.

126. Compound promiscuity: what can we learn from current data?

127. SWEETLEAD: an in silico database of approved drugs, regulated chemicals, and herbal isolates for computer-aided drug discovery.

128. Steroids-specific target library for steroids target prediction.

129. DeCAF-Discrimination, Comparison, Alignment Tool for 2D PHarmacophores.

130. POAP: A GNU parallel based multithreaded pipeline of open babel and AutoDock suite for boosted high throughput virtual screening.

131. Cascade Ligand- and Structure-Based Virtual Screening to Identify New Trypanocidal Compounds Inhibiting Putrescine Uptake.

132. Multivariate analysis in the identification of biological targets for designed molecular structures: the BIOTA protocol.

133. How Reliable Are Ligand-Centric Methods for Target Fishing?

134. Catecholamine receptors: prototypes for GPCR-based drug discovery.

135. New opportunities for kinase drug repurposing and target discovery.

136. Activity-Based Protein Profiling for the Study of Parasite Biology.

137. Heme Oxygenase Database (HemeOxDB) and QSAR Analysis of Isoform?1 Inhibitors.

138. Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing.

139. Macromolecular target prediction by self-organizing feature maps.

140. A quality alert and call for improved curation of public chemistry databases.

141. [Adverse Effect Predictions Based on Computational Toxicology Techniques and Large-scale Databases].

142. Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding.

143. Microbial protein targets: towards understanding and intervention.

144. Hit Recycling: Discovery of a Potent Carbonic Anhydrase Inhibitor by in Silico Target Fishing.

145. Pharmacophore-based screening and drug repurposing exemplified on glycogen synthase kinase-3 inhibitors.

146. A rapid and affordable screening platform for membrane protein trafficking.

147. How good are publicly available web services that predict bioactivity profiles for drug repurposing?

148. A chemo-centric view of human health and disease.

149. Drug repurposing: mining protozoan proteomes for targets of known bioactive compounds.

150. Identification of FDA-approved drugs that computationally bind to MDM2.

151. Identification of Potential Therapeutics to Conquer Drug Resistance in Salmonella typhimurium: Drug Repurposing Strategy.

152. Correction to "Machine learning-based method to improve docking scoring functions and its application to drug repurposing".

153. Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity.

154. Many drugs contain unique scaffolds with varying structural relationships to scaffolds of currently available bioactive compounds.

155. Fragment-based drug design and drug repositioning using multiple ligand simultaneous docking (MLSD): identifying celecoxib and template compounds as novel inhibitors of signal transducer and activator of transcription 3 (STAT3).

156. A tool to utilize adverse effect profiles to identify brain-active medications for repurposing.

157. Structural analysis of dihydrofolate reductases enables rationalization of antifolate binding affinities and suggests repurposing possibilities.

158. Molecular Topology and other Promiscuity Determinants as Predictors of Therapeutic Class- A Theoretical Framework to guide Drug Repositioning?

159. Repurposing of Potent Drug Candidates for Multiparasite Targeting.

160. Virtual screening and repositioning of inconclusive molecules of beta-lactamase Bioassays-A data mining approach.

161. HEDD: the human epigenetic drug database.

162. G Protein-Coupled Receptors as Targets for Approved Drugs: How Many Targets and How Many Drugs?

163. Substrate-driven mapping of the degradome by comparison of sequence logos.

164. DRABAL: novel method to mine large high-throughput screening assays using Bayesian active learning.

165. Repurposed FDA-approved drugs targeting genes influencing aging can extend lifespan and healthspan in rotifers.

166. Quantification of quaternary structure stability in aggregation-prone proteins under physiological conditions: the transthyretin case.

167. Design of efficient computational workflows for in silico drug repurposing.

168. Repurposing FDA-approved drugs for anti-aging therapies.

169. Computational Drug Repositioning by Target Hopping: A Use Case in Chagas Disease.

170. Repositioning organohalogen drugs: a case study for identification of potent B-Raf V600E inhibitors via docking and bioassay.

171. Database of Optimized Proteomic Quantitative Methods for Human Drug Disposition-Related Proteins for Applications in Physiologically Based Pharmacokinetic Modeling.

172. Drug repositioning for enzyme modulator based on human metabolite-likeness.

173. Understanding organellar protein folding capacities and assessing their pharmacological modulation by small molecules.

174. MSBIS: A Multi-Step Biomedical Informatics Screening Approach for Identifying Medications that Mitigate the Risks of Metoclopramide-Induced Tardive Dyskinesia.

175. Anticonvulsant activity of artificial sweeteners: a structural link between sweet-taste receptor T1R3 and brain glutamate receptors.

176. Predicting unintended effects of drugs based on off-target tissue effects.

A2-2d. Leaf clusters under Cluster 49

There are four leaf clusters under Cluster 49: Cluster 9 (37), Cluster 20 (91), Cluster 26 (86), and Cluster 29 (167).

*Cluster 9 focuses on rare diseases;

*Cluster 20 focuses on computational drug repositioning;

*Cluster 26 focuses on marketing aspects of drug repurposing;

*Cluster 29 focuses on drug development and discovery.

A2-2d1. Cluster 9 record titles

1. Database identifies FDA-approved drugs with potential to be repurposed for treatment of orphan diseases.

2. Computational drug repositioning for rare diseases in the era of precision medicine.

3. Rare Diseases: Drug Discovery and Informatics Resource.

4. Trends of Clinical Trials for Drug Development in Rare Diseases.

5. Large-scale computational drug repositioning to find treatments for rare diseases.

6. Collaboration for rare disease drug discovery research.

7. Drug discovery and development for rare genetic disorders.

8. Repositioning 'old' drugs to treat rare diseases: arguing from the mechanism of action.

9. Potential Reuse of Oncology Drugs in the Treatment of Rare Diseases.

10. High-content drug screening for rare diseases.

11. In silico repositioning of approved drugs for rare and neglected diseases.

12. eRepo-ORP: Exploring the Opportunity Space to Combat Orphan Diseases with Existing Drugs.

13. The TREAT-NMD advisory committee for therapeutics (TACT): an innovative de-risking model to foster orphan drug development.

14. Finding promiscuous old drugs for new uses.

15. Pharmacology and drug development in rare diseases: the attractiveness and expertise of the French medical pharmacology.

16. Drug repositioning for orphan diseases.

17. Repositioning Drugs for Rare Immune Diseases: Hopes and Challenges for a Precision Medicine.

18. A generalizable pre-clinical research approach for orphan disease therapy.

19. [Possible framework and best practices in the future for prescriptions outside market authorization indications for rare diseases?].

20. Incentives to Repurpose Existing Drugs for Orphan Indications.

21. Transcriptomic RNAseq drug screen in cerebrocortical cultures: toward novel neurogenetic disease therapies.

22. Personalized drug discovery: HCA approach optimized for rare diseases at Tel Aviv University.

23. The roles of academia, rare diseases, and repurposing in the development of the most transformative drugs.

24. Affordable orphan drugs: a role for not-for-profit organizations.

25. Shining a light in the black box of orphan drug pricing.

26. Drug repositioning can accelerate discovery of pharmacological chaperones.

27. Concept Modeling-based Drug Repositioning.

28. NFFinder: an online bioinformatics tool for searching similar transcriptomics experiments in the context of drug repositioning.

29. The Power of Rare: An Opportunity to Repurpose an Old Drug for Mitochondrial Cardiomyopathy.

30. New Therapeutic Uses for Existing Drugs.

31. Drug repositioning in sarcomas and other rare tumors.

32. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs.

33. Infectious diseases. Drug developers finally take aim at a neglected disease.

34. [What's new in dermatology?].

35. [Baclofen: Innovative treatment or French controversy?].

36. Biomedicine. NIH's secondhand shop for tried-and-tested drugs.

37. NIH gambles on recycled drugs.

A2-2d2. Cluster 20 record titles

1. Drug repositioning: identifying and developing new uses for existing drugs.

2. Computational and experimental advances in drug repositioning for accelerated therapeutic stratification.

3. Computational drug repositioning for cancer therapeutics.

4. Exploiting drug-disease relationships for computational drug repositioning.

5. Drug repositioning from the combined evaluation of phenotypic and target-based screening.

6. A Review of Computational Drug Repositioning Approaches.

7. Computational Drug Repositioning: A Lateral Approach to Traditional Drug Discovery?

8. A survey of current trends in computational drug repositioning.

9. Challenges and opportunities of drug repositioning.

10. Review of Drug Repositioning Approaches and Resources.

11. High-throughput drug repositioning for the discovery of new treatments for Chagas disease.

12. Drug repositioning: re-investigating existing drugs for new therapeutic indications.

13. A review of validation strategies for computational drug repositioning.

14. Toward better drug repositioning: prioritizing and integrating existing methods into efficient pipelines.

15. Recent advances in drug repositioning for the discovery of new anticancer drugs.

16. In vitro screening for drug repositioning.

17. In silico drug repositioning: what we need to know.

18. The value of drug repositioning in the current pharmaceutical market.

19. Serological biochemical markers of surrogate efficacy and safety as a novel approach to drug repositioning.

20. Mining drug-disease relationships as a complement to medical genetics-based drug repositioning: Where a recommendation system meets genome-wide association studies.

21. Drug repositioning approaches to parasitic diseases: a medicinal chemistry perspective.

22. Back to the future - Is the drug repositioning concept applicable to vaccines?

23. Computational and Practical Aspects of Drug Repositioning.

24. Drug repositioning, a new alternative in infectious diseases.

25. Novel insight into drug repositioning: Methylthiouracil as a case in point.

26. In Silico Chemogenomics Drug Repositioning Strategies for Neglected Tropical Diseases.

27. Drug repositioning summit: finding new routes to success.

28. Drug repositioning for personalized medicine.

29. Systematic analyses of drugs and disease indications in RepurposeDB reveal pharmacological, biological and epidemiological factors influencing drug repositioning.

30. An integrated dataset for in silico drug discovery.

31. In vivo phenotypic screening: clinical proof of concept for a drug repositioning approach.

32. Drug combination therapy increases successful drug repositioning.

33. Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets.

34. A standard database for drug repositioning.

35. Drug repositioning by structure-based virtual screening.

36. Antiprotozoal Activity Profiling of Approved Drugs: A Starting Point toward Drug Repositioning.

37. Repositioning of Drugs in Cardiometabolic Disorders: Importance and Current Scenario.

38. Leveraging Population-Based Clinical Quantitative Phenotyping for Drug Repositioning.

39. Identification of anti-melanogenic natural compounds from Galega officinalis and further drug repositioning.

40. Neglected Tropical Protozoan Diseases: Drug Repositioning as a Rational Option.

41. Reply to Rational drug repositioning by medical genetics.

42. Rational drug repositioning by medical genetics.

43. Drug repositioning: playing dirty to kill pain.

44. Computer-guided drug repurposing: identification of trypanocidal activity of clofazimine, benidipine and saquinavir.

45. DRUGSURV: a resource for repositioning of approved and experimental drugs in oncology based on patient survival information.

46. Pharmacological approach for drug repositioning against cardiorenal diseases.

47. Drug repositioning for treatment of movement disorders: from serendipity to rational discovery strategies.

48. Laying in silico pipelines for drug repositioning: a paradigm in ensemble analysis for neurodegenerative diseases.

49. [Drug Repositioning Research Utilizing a Large-scale Medical Claims Database to Improve Survival Rates after Cardiopulmonary Arrest].

50. Nonprofit disease groups earmark grants for drug repositioning.

51. Drug repositioning and repurposing: terminology and definitions in literature.

52. A Network-Biology Informed Computational Drug Repositioning Strategy to Target Disease Risk Trajectories and Comorbidities of Peripheral Artery Disease.

53. Drug-repositioning opportunities for cancer therapy: novel molecular targets for known compounds.

54. Editorial: Drug Repositioning: Current Advances and Future Perspectives.

55. Baseline Regularization for Computational Drug Repositioning with Longitudinal Observational Data.

56. The Importance of Bioactivation in Computer-Guided Drug Repositioning. Why the Parent Drug is Not Always Enough.

57. Drug Repositioning and Off-Label Use-Finding the Balance and Understanding the Differences: Interview with David Cavalla, MA, PhD, Founder, Numedicus.

58. Computational Drug Repositioning Using Continuous Self-Controlled Case Series.

59. Systematic evaluation of drug-disease relationships to identify leads for novel drug uses.

60. Systematic drug repositioning through mining adverse event data in ClinicalTrials.gov.

61. Opportunities in systems biology to discover mechanisms and repurpose drugs for CNS diseases.

62. Challenges in secondary analysis of high throughput screening data.

63. Drug screening: Drug repositioning needs a rethink.

64. Drug Signature-based Finding of Additional Clinical Use of LC28-0126 for Neutrophilic Bronchial Asthma.

65. A Practical Guide for Exploring Opportunities of Repurposing Drugs for CNS Diseases in Systems Biology.

66. Genomics-enabled drug repositioning and repurposing: insights from an IOM Roundtable activity.

67. Pioneering government-sponsored drug repositioning collaborations: progress and learning.

68. Correction to: Realizing drug repositioning by adapting a recommendation system to handle the process.

69. The CTSA Pharmaceutical Assets Portal - a public-private partnership model for drug repositioning.

70. PhenoPredict: A disease phenome-wide drug repositioning approach towards schizophrenia drug discovery.

71. Applications and implications of heparin and protamine in tissue engineering and regenerative medicine.

72. Application of drug repositioning strategy to TOFISOPAM.

73. Therapeutic drug repositioning using personalized proteomics of liquid biopsies.

74. Recycling side-effects into clinical markers for drug repositioning.

75. Phenytoin repositioned in wound healing: clinical experience spanning 60 years.

76. New therapeutic bearings for repositioned drugs.

77. Mefloquine neurotoxicity and gap junction blockade: critical insights in drug repositioning.

78. [Drug repositioning in neuro-oncology-targeting GSK3beta for glioblastoma].

79. Computational repositioning and experimental validation of approved drugs for HIF-prolyl hydroxylase inhibition.

80. Overcoming Obstacles to Drug Repositioning in Japan.

81. Medical genetic inspirations for anticancer drug repurposing.

82. Exploiting drug repositioning and the brain microenvironment to treat brain metastases.

83. [Discovering L-type calcium channels inhibitors of antihypertensive drugs based on drug repositioning].

84. The Immunogenetics of Psoriasis and Implications for Drug Repositioning.

85. Measuring cognitive effects: cognition in drug development and repositioning.

86. Interview with Farid Khan, PhD.

87. Interview with Raul Insa, MD, PhD.

88. Encouraging New Uses for Old Drugs.

89. Correction: In Silico Repositioning-Chemogenomics Strategy Identifies New Drugs with Potential Activity against Multiple Life Stages of Schistosoma mansoni.

90. Current Progress in Bioinformatics 2016.

91. Make better, safer biomaterials.

A2-2d3. Cluster 26 record titles

1. The year's new drugs and biologics--2006.

2. The year's new drugs and biologics--2007.

3. Editorial: Old Drugs Learn New Tricks: Advances and Applications for Drug Repurposing.

4. The Year's New Drugs & Biologics - 2009.

5. The year's new drugs & biologics - 2008.

6. Scientific advice - is drug repurposing missing a trick?

7. Filling the gap in CNS drug development: evaluation of the role of drug repurposing.

8. Repurposing medicinal compounds for blood cancer treatment.

9. Challenges and Benefits of Repurposing Products for Use during a Radiation Public Health Emergency: Lessons Learned from Biological Threats and other Disease Treatments.

10. Drug repurposing from the perspective of pharmaceutical companies.

11. Drug reformulations and repositioning in the pharmaceutical industry and their impact on market access: regulatory implications.

12. Editorial: computational methods for drug repurposing.

13. Drug reformulations and repositioning in pharmaceutical industry and its impact on market access: reassessment of nomenclature.

14. The promise of genomics-based drug repurposing.

15. Regulatory pitfalls and opportunities when repurposing for inhalation therapy.

16. Drug Repurposing as An Efficient Strategy In Drug Development - Example Of Cns Area.

17. Purposeful learning with drug repurposing.

18. Challenges and Benefits of Repurposing Licensed/Approved/Cleared Products for a Radiation Indication.

19. Drug repurposing in pharmaceutical industry and its impact on market access: market access implications.

20. Overcoming Drug Development Bottlenecks With Repurposing: Old drugs learn new tricks.

21. [Development of new indications for old products: difficulties and search for solutions].

22. Lost interest for existing compounds: New boosts.

23. Teaching old drugs new tricks.

24. Can you teach old drugs new tricks?

25. Extensions of indication throughout the drug product lifecycle: a quantitative analysis.

26. Industrial perspective of gastroretentive drug delivery systems: physicochemical, biopharmaceutical, technological and regulatory consideration.

27. Drug repurposing and adverse event prediction using high-throughput literature analysis.

28. Drug repurposing in oncology--patient and health systems opportunities.

29. Systematic drug repurposing through text mining.

30. Drug repurposing in pediatrics and pediatric hematology oncology.

31. Overcoming the legal and regulatory barriers to drug repurposing.

32. Expanding the scope of drug repurposing in pediatrics: the Children's Pharmacy Collaborative.

33. Wish-fulfilling jewel pills: Tibetan medicines from exclusivity to ubiquity.

34. Teaching Old Drugs New Tricks: Repositioning Pharmaceuticals for Bench to Bedside Success.

35. Using Social Media Data to Identify Potential Candidates for Drug Repurposing: A Feasibility Study.

36. Biocomputing drug repurposing toward targeted therapies.

37. Drug Repurposing for the Development of Novel Analgesics.

38. Retrospective clinical analysis for drug rescue: for new indications or stratified patient groups.

39. Medication Repurposing in Pediatric Patients: Teaching Old Drugs New Tricks.

40. Regulatory exclusivities for medicinal products for human use in the EU.

41. Molecular Docking for Identification of Potential Targets for Drug Repurposing.

42. Repurposing old drugs in oncology: Opportunities with clinical and regulatory challenges ahead.

43. Drug repurposing and the medicinal chemist.

44. How Much Nonclinical Safety Data Are Required for a Clinical Study in Ophthalmology?

45. The Rescue and Repurposing of Pharmaceuticals: Augmenting the Drug Development Paradigm.

46. A Special Focus on Drug Repurposing, Rescue, and Repositioning.

47. Innovating by developing new uses of already-approved drugs: trends in the marketing approval of supplemental indications.

48. The promise and challenges of drug repurposing in psychiatry.

49. Hangover free! The social and material trajectories of PartySmart.

50. Drug repurposing programmes get lift off.

51. [Dutch Medicines Act also applicable to repurposing].

52. Drug repurposing: identify, develop and commercialize new uses for existing or abandoned drugs. Part I.

53. [New indications for existing drugs; repurposing in psychiatry and addiction medicine].

54. APT drug R&D: the right active ingredient in the right presentation for the right therapeutic use.

55. Changes on the Horizon for Drug Repurposing, Rescue, and Repositioning at ASSAY.

56. Drug repurposing: identify, develop and commercialize new uses for existing or abandoned drugs. Part II.

57. Creating a unique, multi-stakeholder Paediatric Oncology Platform to improve drug development for children and adolescents with cancer.

58. Why Do Promising Therapies Stall in Development and How Can We Move Them Forward?

59. Drug repurposing a reality: from computers to the clinic.

60. Editorial (Thematic Issue: Drug Reprofiling: An Alternative Path to Drug Discovery).

61. A bibliometric review of drug repurposing.

62. Mendelian randomization: a novel approach for the prediction of adverse drug events and drug repurposing opportunities.

63. EDITORIAL: Repurposing Niacin as Antiplatelet Drug?

64. Formalizing drug indications on the road to therapeutic intent.

65. Pimping up Drugs Recovered, Superannuated and Under Exploited Drugs - An Introduction to the Basics of Drug Reprofiling.

66. NCATS launches drug repurposing program.

67. Inventing new therapies without reinventing the wheel: the power of drug repurposing.

68. Editorial: Computational and Experimental Approaches in Multi-target Pharmacology.

69. Creating New Economic Incentives for Repurposing Generic Drugs for Unsolved Diseases Using Social Finance.

70. Hard Drug Repurposing for Precision Oncology: The Missing Link?

71. Recent European legal developments on second medical uses and dosage regimes.

72. Drug repurposing and beyond: the fundamental role of pharmacology.

73. Supplementary protection certificates on reformulations and new uses after Neurim: where do we go from here?

74. Second act: Drug repurposing gets a boost as academic researchers join the search for novel uses of existing drugs.

75. Psychedelic drugs should be legally reclassified so that researchers can investigate their therapeutic potential.

76. Busting the billion-dollar myth: how to slash the cost of drug development.

77. Drug Repurposing and Artificial Intelligence: From Liaison to Marriage.

78. Finding Hsp90 inhibitors by drug repurposing: the power of chemical genetics.

79. Drug repurposing to target proteostasis and prevent neurodegeneration: accelerating translational efforts.

80. New Formulations of Old Analgesics and Repurposing of Old Drugs as "New" Analgesics.

81. The Drug Repurposing Hub: a next-generation drug library and information resource.

82. New Indications and a Sense of (Re)purpose.

83. Integrative cancer pharmacogenomics to establish drug mechanism of action: drug repurposing.

84. [Exception drugs status: specific characteristics and the role in the proper use of drugs].

85. Could repurposing existing drugs be an efficient protective method against microbial biologic threats?

86. Advocating for mutually beneficial access to shelved compounds.

A2-2d4. Cluster 29 record titles

1. A Perspective on Implementing a Quantitative Systems Pharmacology Platform for Drug Discovery and the Advancement of Personalized Medicine.

2. [Identification of a molecular mechanism for actions of existing medicines and its application for drug development].

3. Drug discovery in a multidimensional world: systems, patterns, and networks.

4. Drug discovery and development focusing on existing medicines: drug re-profiling strategy.

5. Contributions from emerging transcriptomics technologies and computational strategies for drug discovery.

6. Drug repurposing: translational pharmacology, chemistry, computers and the clinic.

7. Quality by design (QbD) approach of pharmacogenomics in drug designing and formulation development for optimization of drug delivery systems.

8. High-field MRS in clinical drug development.

9. An Insight into Drug Repositioning for the Development of Novel Anti-Cancer Drugs.

10. Bioinformatics in translational drug discovery.

11. Use of big data in drug development for precision medicine.

12. The University of New Mexico Center for Molecular Discovery.

13. Harnessing Polypharmacology with Computer-Aided Drug Design and Systems Biology.

14. Drug discovery in academia.

15. Systems chemical biology and the Semantic Web: what they mean for the future of drug discovery research.

16. In silico methods to address polypharmacology: current status, applications and future perspectives.

17. Renovation as innovation: is repurposing the future of drug discovery research?

18. Computational polypharmacology: a new paradigm for drug discovery.

19. Applications of chemogenomic library screening in drug discovery.

20. Improving the efficacy-safety balance of polypharmacology in multi-target drug discovery.

21. Target repurposing for neglected diseases.

22. Advancing cancer drug discovery towards more agile development of targeted combination therapies.

23. Expediting the Design, Discovery and Development of Anticancer Drugs using Computational Approaches.

24. Reverse pharmacognosy: another way to harness the generosity of nature.

25. Integrative methods for analyzing big data in precision medicine.

26. The Influence of Big (Clinical) Data and Genomics on Precision Medicine and Drug Development.

27. Genomic medicine: a decade of successes, challenges, and opportunities.

28. The opportunities of mining historical and collective data in drug discovery.

29. The prince and the pauper. A tale of anticancer targeted agents.

30. Drug discovery for neglected tropical diseases at the Sandler Center.

31. Computational approaches for innovative antiepileptic drug discovery.

32. Chemical & RNAi screening at MSKCC: a collaborative platform to discover & repurpose drugs to fight disease.

33. Recent trends and future prospects in computational GPCR drug discovery: from virtual screening to polypharmacology.

34. Systems biology-embedded target validation: improving efficacy in drug discovery.

35. Revisiting Repurposing.

36. Multitasking models for quantitative structure-biological effect relationships: current status and future perspectives to speed up drug discovery.

37. New sources of drugs for hematologic malignancies.

38. Small-Molecule Screens: A Gateway to Cancer Therapeutic Agents with Case Studies of Food and Drug Administration-Approved Drugs.

39. Structure based drug discovery for designing leads for the non-toxic metabolic targets in multi drug resistant Mycobacterium tuberculosis.

40. The polypharmacology of natural products.

41. Chromone as a Privileged Scaffold in Drug Discovery: Recent Advances.

42. Biocomputational resources useful for drug discovery against compartmentalized targets.

43. Mining small-molecule screens to repurpose drugs.

44. Web-based drug repurposing tools: a survey.

45. Shifting from the single to the multitarget paradigm in drug discovery.

46. Systems medicine: evolution of systems biology from bench to bedside.

47. In silico methods for drug repurposing and pharmacology.

48. Genomes, structural biology and drug discovery: combating the impacts of mutations in genetic disease and antibiotic resistance.

49. Repurposing High-Throughput Image Assays Enables Biological Activity Prediction for Drug Discovery.

50. Back to the Roots: Prediction of Biologically Active Natural Products from Ayurveda Traditional Medicine.

51. Individualized network-based drug repositioning infrastructure for precision oncology in the panomics era.

52. Pharmacology and Clinical Drug Candidates in Redox Medicine.

53. Drug repurposing in chemical genomics: can we learn from the past to improve the future?

54. The ReFRAME library as a comprehensive drug repurposing library and its application to the treatment of cryptosporidiosis.

55. Polypharmacology in Precision Oncology: Current Applications and Future Prospects.

56. Open-source approaches for the repurposing of existing or failed candidate drugs: learning from and applying the lessons across diseases.

57. Pharmacogenomics to Revive Drug Development in Cardiovascular Disease.

58. New horizons for old drugs and drug leads.

59. The Repurposing of Old Drugs or Unsuccessful Lead Compounds by in Silico Approaches: New Advances and Perspectives.

60. Accelerating Precision Drug Development and Drug Repurposing by Leveraging Human Genetics.

61. Modern Approaches for the Discovery of Anti-Infectious Drugs for the Treatment of Neglected Diseases.

62. Connections in pharmacology: innovation serving translational medicine.

63. Process Pharmacology: A Pharmacological Data Science Approach to Drug Development and Therapy.

64. Phosphoproteomics in drug discovery.

65. Recent Advances and Emerging Applications in Text and Data Mining for Biomedical Discovery.

66. An integrated drug development approach applying topological descriptors.

67. Predicting new indications of compounds with a network pharmacology approach: Liuwei Dihuang Wan as a case study.

68. Cheaper faster drug development validated by the repositioning of drugs against neglected tropical diseases.

69. Rational application of drug promiscuity in medicinal chemistry.

70. Polypharmacology - foe or friend?

71. Scaffold Repurposing of Old Drugs Towards New Cancer Drug Discovery.

72. Transplantomics: Toward Precision Medicine in Transplantation Research.

73. PubChem applications in drug discovery: a bibliometric analysis.

74. Third-generation sequencing techniques and applications to drug discovery.

75. Polypharmacology in Drug Development: A Minireview of Current Technologies.

76. Getting the most out of PubChem for virtual screening.

77. Clinical Trials and Therapeutic Rationale for Drug Repurposing in Schizophrenia.

78. Drug repurposing: far beyond new targets for old drugs.

79. Drug Repurposing from an Academic Perspective.

80. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective.

81. Surveying Recent Themes in Translational Bioinformatics: Big Data in EHRs, Omics for Drugs, and Personal Genomics.

82. The use of transcriptomic biomarkers for personalized medicine.

83. Phenotypic screening of the Prestwick library for treatment of Parkinson's tremor symptoms using a humanized quantitative systems pharmacology platform.

84. Complementary new approaches enable repositioning of failed drug candidates.

85. IBM Watson: How Cognitive Computing Can Be Applied to Big Data Challenges in Life Sciences Research.

86. Discovery and development of DNA methyltransferase inhibitors using in silico approaches.

87. Use of Computational Functional Genomics in Drug Discovery and Repurposing for Analgesic Indications.

88. Insights into respiratory disease through bioinformatics.

89. Drug discovery and repurposing at Memorial Sloan Kettering Cancer Center: chemical biology drives translational medicine.

90. Repurposing Drugs to Target the Diabetes Epidemic.

91. Chapter 7: Pharmacogenomics.

92. Pharmacogenomic approaches to lipid-regulating trials.

93. CancerHSP: anticancer herbs database of systems pharmacology.

94. Drug Repurposing Is a New Opportunity for Developing Drugs against Neuropsychiatric Disorders.

95. Exploring the epigenetic drug discovery landscape.

96. Turning omics data into therapeutic insights.

97. e-Drug3D: 3D structure collections dedicated to drug repurposing and fragment-based drug design.

98. Identifying Novel Cancer Therapies Using Chemical Genetics and Zebrafish.

99. Literature mining, ontologies and information visualization for drug repurposing.

100. Multi-target pharmacology: possibilities and limitations of the "skeleton key approach" from a medicinal chemist perspective.

101. Assessment of berberine as a multi-target antimicrobial: a multi-omics study for drug discovery and repositioning.

102. Schistosomiasis: from drug deployment to drug development.

103. PregOMICS-Leveraging systems biology and bioinformatics for drug repurposing in maternal-child health.

104. Nuclear matrix, nuclear envelope and premature aging syndromes in a translational research perspective.

105. beta3-Adrenoceptor agonists for overactive bladder syndrome: Role of translational pharmacology in a repositioning clinical drug development project.

106. In silico frameworks for systematic pre-clinical screening of potential anti-leukemia therapeutics.

107. High-throughput analysis of behavior for drug discovery.

108. Systems Medicine Approaches to Improving Understanding, Treatment, and Clinical Management of Neuroendocrine Prostate Cancer.

109. Clinical Trial Designs in Amyotrophic Lateral Sclerosis: Does One Design Fit All?

110. Repurposing strategies for tropical disease drug discovery.

111. Drug target identification in protozoan parasites.

112. Repurposing drugs to treat l-DOPA-induced dyskinesia in Parkinson's disease.

113. Genetics and pharmacology of longevity: the road to therapeutics for healthy aging.

114. Beyond new chemical entities: advancing drug development based on functional versatility of antibodies.

115. The thiol-polyamine metabolism of Trypanosoma cruzi: molecular targets and drug repurposing strategies.

116. Reprint of: Highthroughtput analysis of behavior for drug discovery.

117. Opportunities and challenges provided by cloud repositories for bioinformatics-enabled drug discovery.

118. Pathogenesis of thrombosis: cellular and pharmacogenetic contributions.

119. Predicting New Target Conditions for Drug Retesting Using Temporal Patterns in Clinical Trials: A Proof of Concept.

120. KCa 3.1-a microglial target ready for drug repurposing?

121. New approach to generating insights for aging research based on literature mining and knowledge integration.

122. Discovery of New Potential Anti-Infective Compounds Based on Carbonic Anhydrase Inhibitors by Rational Target-Focused Repurposing Approaches.

123. Toward a Reasoned Classification of Diseases Using Physico-Chemical Based Phenotypes.

124. Recent advances in technologies for developing drugs against Chlamydia pneumoniae.

125. Repurposing metformin: an old drug with new tricks in its binding pockets.

126. Novel Phenotypic Outcomes Identified for a Public Collection of Approved Drugs from a Publicly Accessible Panel of Assays.

127. Therapeutic Approaches to Prion Diseases.

128. Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates.

129. The NCGC pharmaceutical collection: a comprehensive resource of clinically approved drugs enabling repurposing and chemical genomics.

130. fMRI in analgesic drug discovery.

131. Is it time for a paradigm shift in drug research and development in endometriosis/adenomyosis?

132. Literature Based Discovery: Models, methods, and trends.

133. Drugs in clinical development for the treatment of amyotrophic lateral sclerosis.

134. Using genetics to inform new therapeutics for diabetes.

135. Computational Multitarget Drug Design.

136. Managing Bardet-Biedl Syndrome-Now and in the Future.

137. Therapeutic Manipulation of Ageing: Repurposing Old Dogs and Discovering New Tricks.

138. Repurposing as a strategy for the discovery of new anti-leishmanials: the-state-of-the-art.

139. Clinical neuroscience of addiction: similarities and differences between alcohol and other drugs.

140. The Repurposing Drugs in Oncology (ReDO) Project.

141. Epigenetic drugs: from chemistry via biology to medicine and back.

142. Repurposing available drugs for neurodevelopmental disorders: The fragile X experience.

143. When Enough Is Enough: Decision Criteria for Moving a Known Drug into Clinical Testing for a New Indication in the Absence of Preclinical Efficacy Data.

144. Beyond multiple mechanisms and a unique drug: Defective autophagy as pivotal player in cerebral cavernous malformation pathogenesis and implications for targeted therapies.

145. Drug discovery. Repurposing with a difference.

146. Drug discovery for the treatment of substance use disorders: novel targets, repurposing, and the need for new paradigms.

147. Designer Drugs 2.0.

148. Mendelian randomisation in cardiovascular research: an introduction for clinicians.

149. Repositioning the substrate activity screening (SAS) approach as a fragment-based method for identification of weak binders.

150. Discontinued anxiolytic drugs (2009 - 2014).

151. Antifungal drug discovery: something old and something new.

152. Identifying new antiepileptic drugs through genomics-based drug repurposing.

153. Looking Back, Looking Forward at Halogen Bonding in Drug Discovery.

154. Help luck along to find psychiatric medicines.

155. Computer-Aided Identification of Anticonvulsant Effect of Natural Nonnutritive Sweeteners Stevioside and Rebaudioside A.

156. Old friends in new guise: exploiting privileged structures for scaffold re-evolution/refining.

157. How will insights from genetics translate to clinical practice in inflammatory bowel disease?

158. Is there a relationship between sweet taste and seizures? Anticonvulsant and proconvulsant effects of non-nutritive sweeteners.

159. Exploring old drugs for the treatment of hematological malignancies.

160. Lithium Pharmacogenetics: Where Do We Stand?

161. The genome of Onchocerca volvulus, agent of river blindness.

162. Psilocybin: Good Trip or Bad Trip.

163. The Second Insubria Autumn School on Neuroimmune Pharmacology: Repurposing Established Drugs for Novel Indications.

164. Pharmacologic Treatment of Polycystic Ovary Syndrome: Alternate and Future Paths.

165. The rise of translational bioinformatics.

166. Use of venlafaxine in psychiatric disorders and climacteric syndrome: is a therapeutic bridge?

167. Mental health: depression needs large human-genetics studies.

A2-2e. Leaf clusters under Cluster 7

*Cluster 7 (114) is a leaf cluster, and focuses on treatments for drug-resistant tuberculosis.

A2-2e1. Cluster 7 record titles

1. Tuberculosis clinical trial update and the current anti-tuberculosis drug portfolio.

2. Clinical management of adults and children with multidrug-resistant and extensively drug-resistant tuberculosis.

3. Repurposing and Revival of the Drugs: A New Approach to Combat the Drug Resistant Tuberculosis.

4. The potential role of trimethoprim-sulfamethoxazole in the treatment of drug-resistant tuberculosis.

5. Drug-resistant tuberculosis: An update on disease burden, diagnosis and treatment.

6. Host Directed Therapies for Tuberculosis: Futures Strategies for an Ancient Disease.

7. Pipeline of drugs for related diseases: tuberculosis.

8. null

9. New anti-tuberculosis drugs and regimens: 2015 update.

10. Tuberculosis: From an incurable scourge to a curable disease - journey over a millennium.

11. Recent controversies about MDR and XDR-TB: Global implementation of the WHO shorter MDR-TB regimen and bedaquiline for all with MDR-TB?

12. Discovery of antitubercular 2,4-diphenyl-1H-imidazoles from chemical library repositioning and rational design.

13. The challenge of new drug discovery for tuberculosis.

14. New drugs and perspectives for new anti-tuberculosis regimens.

15. Repurposing-a ray of hope in tackling extensively drug resistance in tuberculosis.

16. New Antituberculosis Drugs: From Clinical Trial to Programmatic Use.

17. Evolution of drug resistance in Mycobacterium tuberculosis: a review on the molecular determinants of resistance and implications for personalized care.

18. Host-Directed Therapies for Tackling Multi-Drug Resistant Tuberculosis: Learning From the Pasteur-Bechamp Debates.

19. An optimized background regimen for treatment of active tuberculosis with the next-generation benzothiazinone Macozinone (PBTZ169).

20. Meropenem-clavulanate for drug-resistant tuberculosis: a follow-up of relapse-free cases.

21. New and repurposed drugs to treat multidrug- and extensively drug-resistant tuberculosis.

22. New Approaches to the Treatment of Tuberculosis.

23. Is repositioning of drugs a viable alternative in the treatment of tuberculosis?

24. Management of drug-resistant tuberculosis in special sub-populations including those with HIV co-infection, pregnancy, diabetes, organ-specific dysfunction, and in the critically ill.

25. Rising to the challenge: new therapies for tuberculosis.

26. Totally drug-resistant tuberculosis and adjunct therapies.

27. Advances in the development of new tuberculosis drugs and treatment regimens.

28. The epidemiology, pathogenesis, transmission, diagnosis, and management of multidrug-resistant, extensively drug-resistant, and incurable tuberculosis.

29. Tuberculosis: progress and advances in development of new drugs, treatment regimens, and host-directed therapies.

30. Recent developments in genomics, bioinformatics and drug discovery to combat emerging drug-resistant tuberculosis.

31. New and Repurposed Drugs for Pediatric Multidrug-Resistant Tuberculosis. Practice-based Recommendations.

32. Management of drug-resistant TB in patients with HIV co-infection.

33. Mechanisms of drug resistance in Mycobacterium tuberculosis: update 2015.

34. Turning the tide against tuberculosis.

35. Tuberculosis--advances in development of new drugs, treatment regimens, host-directed therapies, and biomarkers.

36. Current therapies for the treatment of multidrug-resistant tuberculosis in children in India.

37. New drugs and regimens for tuberculosis.

38. Neuroleptic drugs in the treatment of tuberculosis: Minimal inhibitory concentrations of different phenothiazines against Mycobacterium tuberculosis.

39. New drugs for the treatment of Mycobacterium tuberculosis infection.

40. Bis-biguanide dihydrochloride inhibits intracellular replication of M. tuberculosis and controls infection in mice.

41. Methodological considerations in clinical trials for new MDR-TB treatment regimens.

42. Current status of pharmacokinetic and safety studies of multidrug-resistant tuberculosis treatment in children.

43. In Vitro Activity and MIC of Sitafloxacin against Multidrug-Resistant and Extensively Drug-Resistant Mycobacterium tuberculosis Isolated in Thailand.

44. Drug repositioning in the treatment of malaria and TB.

45. Pros and cons of the tuberculosis drugome approach--an empirical analysis.

46. Treatment of drug-resistant tuberculosis among people living with HIV.

47. Successful shortening of tuberculosis treatment using adjuvant host-directed therapy with FDA-approved phosphodiesterase inhibitors in the mouse model.

48. Interplay of DDP4 and IP-10 as a Potential Mechanism for Cell Recruitment to Tuberculosis Lesions.

49. Aerosolized gentamicin reduces the burden of tuberculosis in a murine model.

50. Mycobacterium tuberculosis... Can we beat it? Report from a Euroscicon conference 2013.

51. Exploring the potential of adjunct therapy in tuberculosis.

52. Mode of Action of Clofazimine and Combination Therapy with Benzothiazinones against Mycobacterium tuberculosis.

53. Docking-based virtual screening of known drugs against murE of Mycobacterium tuberculosis towards repurposing for TB.

54. Mefloquine and its oxazolidine derivative compound are active against drug-resistant Mycobacterium tuberculosis strains and in a murine model of tuberculosis infection.

55. Recent therapeutic approaches for the management of tuberculosis: Challenges and opportunities.

56. Clofazimine in the treatment of extensively drug-resistant tuberculosis with HIV coinfection in South Africa: a retrospective cohort study.

57. The role of moxifloxacin in tuberculosis therapy.

58. Emerging strategies for the treatment of pulmonary tuberculosis: promise and limitations?

59. Tackling tuberculosis: Insights from an international TB Summit in London.

60. Challenges of using new and repurposed drugs for the treatment of multidrug-resistant tuberculosis in children.

61. Recent Developments and Future Opportunities in the Treatment of Tuberculosis in Children.

62. Translating the Tuberculosis Research Agenda: Much Accomplished, but Much More to Be Done.

63. Tuberculosis: An Inorganic Medicinal Chemistry Perspective.

64. Perspectives on Advances in Tuberculosis Diagnostics, Drugs, and Vaccines.

65. Advancing host-directed therapy for tuberculosis.

66. Repurposing drugs for treatment of tuberculosis: a role for non-steroidal anti-inflammatory drugs.

67. The DprE1 enzyme, one of the most vulnerable targets of Mycobacterium tuberculosis.

68. Antitubercular activity of disulfiram, an antialcoholism drug, against multidrug- and extensively drug-resistant Mycobacterium tuberculosis isolates.

69. Bioinformatics approach to prioritize known drugs towards repurposing for tuberculosis.

70. Host-directed therapy targeting the Mycobacterium tuberculosis granuloma: a review.

71. Newer patents in antimycobacterial therapy.

72. Performance of the GenoType MTBDRsl assay for the detection second-line anti-tuberculosis drug resistance.

73. Reduced emergence of isoniazid resistance with concurrent use of thioridazine against acute murine tuberculosis.

74. [New drugs against multidrug-resistant tuberculosis].

75. Drug discovery using chemical systems biology: repositioning the safe medicine Comtan to treat multi-drug and extensively drug resistant tuberculosis.

76. Priming the tuberculosis drug pipeline: new antimycobacterial targets and agents.

77. Evaluation of the efficacy of valproic acid and suberoylanilide hydroxamic acid (vorinostat) in enhancing the effects of first-line tuberculosis drugs against intracellular Mycobacterium tuberculosis.

78. Inhibiting Mycobacterium tuberculosis within and without.

79. Safety and availability of clofazimine in the treatment of multidrug and extensively drug-resistant tuberculosis: analysis of published guidance and meta-analysis of cohort studies.

80. Meta-analysis of human gene expression in response to Mycobacterium tuberculosis infection reveals potential therapeutic targets.

81. Statistical considerations for pediatric multidrug-resistant tuberculosis efficacy trials.

82. Bedaquiline and Repurposed Drugs for Fluoroquinolone-Resistant MDR-TB: How Much Better Are They?

83. New antituberculosis drugs, regimens, and adjunct therapies: needs, advances, and future prospects.

84. Estimated generic prices for novel treatments for drug-resistant tuberculosis.

85. Simvastatin increases the in vivo activity of the first-line tuberculosis regimen.

86. Sharpening nature's tools for efficient tuberculosis control: A review of the potential role and development of host-directed therapies and strategies for targeted respiratory delivery.

87. Design and synthesis of novel anti-tuberculosis agents from the celecoxib pharmacophore.

88. Old Drugs and New Targets as an Outlook for the Treatment of Tuberculosis.

89. Targeting intracellular p-aminobenzoic acid production potentiates the anti-tubercular action of antifolates.

90. Bactericidal activity of pyrazinamide and clofazimine alone and in combinations with pretomanid and bedaquiline.

91. Pharmacologically active metabolites, combination screening and target identification-driven drug repositioning in antituberculosis drug discovery.

92. An allosteric inhibitor of Mycobacterium tuberculosis ArgJ: Implications to a novel combinatorial therapy.

93. Functional drug screening reveals anticonvulsants as enhancers of mTOR-independent autophagic killing of Mycobacterium tuberculosis through inositol depletion.

94. Novel Pharmacological Activity of Artesunate and Artemisinin: Their Potential as Anti-Tubercular Agents.

95. Interaction of Mycobacterium tuberculosis Virulence Factor RipA with Chaperone MoxR1 Is Required for Transport through the TAT Secretion System.

96. Identifying and Tackling Emergent Vulnerability in Drug-Resistant Mycobacteria.

97. Loperamide Restricts Intracellular Growth of Mycobacterium tuberculosis in Lung Macrophages.

98. Zafirlukast inhibits complexation of Lsr2 with DNA and growth of Mycobacterium tuberculosis.

99. Impact of Clofazimine Dosing on Treatment Shortening of the First-Line Regimen in a Mouse Model of Tuberculosis.

100. Combined chemical genetics and data-driven bioinformatics approach identifies receptor tyrosine kinase inhibitors as host-directed antimicrobials.

101. Synthetic lethality reveals mechanisms of Mycobacterium tuberculosis resistance to beta-lactams.

102. Evaluation of anti-tubercular activity of linolenic acid and conjugated-linoleic acid as effective inhibitors against Mycobacterium tuberculosis.

103. Thioridazine pharmacokinetic-pharmacodynamic parameters "Wobble" during treatment of tuberculosis: a theoretical basis for shorter-duration curative monotherapy with congeners.

104. Three-dimensional models of Mycobacterium tuberculosis proteins Rv1555, Rv1554 and their docking analyses with sildenafil, tadalafil, vardenafil drugs, suggest interference with quinol binding likely to affect protein's function.

105. The EU approved antimalarial pyronaridine shows antitubercular activity and synergy with rifampicin, targeting RNA polymerase.

106. Resistance to Thiacetazone Derivatives Active against Mycobacterium abscessus Involves Mutations in the MmpL5 Transcriptional Repressor MAB_4384.

107. The trials and tribulations of repurposing metformin and other generic drugs for tuberculosis.

108. Synthesis and SAR evaluation of novel thioridazine derivatives active against drug-resistant tuberculosis.

109. Repurposing of a drug scaffold: Identification of novel sila analogues of rimonabant as potent antitubercular agents.

110. The anti-tubercular drug delamanid as a potential oral treatment for visceral leishmaniasis.

111. High-throughput screening for daunorubicin-mediated drug resistance identifies mometasone furoate as a novel ABCB1-reversal agent.

112. Synthesis and in vitro investigation of halogenated 1,3-bis(4-nitrophenyl)triazenide salts as antitubercular compounds.

113. We need a global system to help identify new uses for existing drugs.

114. New cures sought from old drugs.

A2-2f. Leaf clusters under Cluster 57

There are seven leaf clusters under Cluster 57: Cluster 1 (41), Cluster 0 (21), Cluster 15 (80), Cluster 14 (62), Cluster 19 (93), Cluster 6 (45), and Cluster 17 (113).

*Cluster 1 focuses on antiviral treatments for viral infections, especially Ebola virus;

*Cluster 0 focuses on antiviral treatments for viral infections, especially Zika virus;

*Cluster 15 focuses on antiviral treatments for other viral infections, especially dengue virus, hepatitis B virus, chikungunya virus, human immunodeficiency virus, japanese encephalitis virus, rift valley fever virus, human cytomegalovirus, respiratory syncytial virus, west nile virus.

*Cluster 14 focuses on treatments for parasites, especially trypanosoma cruzi, african trypanosomiasi, trypanosoma brucei, leishmania amazonensi.

*Cluster 19 focuses on treatments for parasites, especially plasmodium falciparum, schistosoma mansoni, toxoplasma gondii.

*Cluster 6 focuses on antifungal treatments

*Cluster 17 focuses on antimicrobial and antibiotic treatments for infections.

A2-2f1. Cluster 1 record titles

1. Ebola virus: A gap in drug design and discovery - experimental and computational perspective.

2. Teicoplanin inhibits Ebola pseudovirus infection in cell culture.

3. Identification of 53 compounds that block Ebola virus-like particle entry via a repurposing screen of approved drugs.

4. Ebola therapy: Developing new drugs or repurposing old ones?

5. Ibuprofen as a template molecule for drug design against Ebola virus.

6. Repurposed therapeutic agents targeting the Ebola virus: a protocol for a systematic review.

7. A Systematic Review of Computational Drug Discovery, Development, and Repurposing for Ebola Virus Disease Treatment.

8. Advances in Designing and Developing Vaccines, Drugs, and Therapies to Counter Ebola Virus.

9. Virtual screen for repurposing approved and experimental drugs for candidate inhibitors of EBOLA virus infection.

10. Improving attrition rates in Ebola virus drug discovery.

11. Will There Be a Cure for Ebola?

12. In Vitro and In Vivo Activity of Amiodarone Against Ebola Virus.

13. Combating Ebola with Repurposed Therapeutics Using the CANDO Platform.

14. Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology.

15. Hyperimmune serum from healthy vaccinated individuals for Ebola virus disease?

16. FDA approved drugs as potential Ebola treatments.

17. A response adaptive randomization platform trial for efficient evaluation of Ebola virus treatments: A model for pandemic response.

18. A screen of approved drugs and molecular probes identifies therapeutics with anti-Ebola virus activity.

19. Antiviral Screening of Multiple Compounds against Ebola Virus.

20. FDA-approved selective estrogen receptor modulators inhibit Ebola virus infection.

21. Against the clock towards new Ebola virus therapies.

22. Did Ebola survivors use plant medicines, and if so, which ones?

23. High-throughput drug screening using the Ebola virus transcription- and replication-competent virus-like particle system.

24. Repurposed Therapeutic Agents Targeting the Ebola Virus: A Systematic Review.

25. Screening of FDA-Approved Drugs for Treatment of Emerging Pathogens.

26. Drug repurposing for Ebola virus disease: principles of consideration and the Animal Rule.

27. [Integrating clinical research into epidemic response: the field perspective in the Ebola experience].

28. Synergistic drug combination effectively blocks Ebola virus infection.

29. Rethinking the development of Ebola treatments.

30. Infectious diseases. Debate erupts on 'repurposed' drugs for Ebola.

31. Machine learning models identify molecules active against the Ebola virus in vitro.

32. Evaluation of Ebola Virus Inhibitors for Drug Repurposing.

33. Repurposing of clinically developed drugs for treatment of Middle East respiratory syndrome coronavirus infection.

34. Current treatment options and the role of peptides as potential therapeutic components for Middle East Respiratory Syndrome (MERS): A review.

35. A systematic screen of FDA-approved drugs for inhibitors of biological threat agents.

36. Abelson Kinase Inhibitors Are Potent Inhibitors of Severe Acute Respiratory Syndrome Coronavirus and Middle East Respiratory Syndrome Coronavirus Fusion.

37. Alternative screening approaches for discovery of Middle East respiratory syndrome coronavirus inhibitors.

38. Middle East Respiratory Syndrome and Severe Acute Respiratory Syndrome: Current Therapeutic Options and Potential Targets for Novel Therapies.

39. Treatment With Lopinavir/Ritonavir or Interferon-beta1b Improves Outcome of MERS-CoV Infection in a Nonhumand Primate Model of Common Marmoset.

40. Quantitative structure-activity relationship and molecular docking revealed a potency of anti-hepatitis C virus drugs against human corona viruses.

41. Repurposing potential of 1st generation H1-specific antihistamines as anti-filovirus therapeutics.

A2-2f2. Cluster 0 record titles

1. A Screen of FDA-Approved Drugs for Inhibitors of Zika Virus Infection.

2. Drug Repurposing: New Treatments for Zika Virus Infection?

3. Chloroquine, a FDA-approved Drug, Prevents Zika Virus Infection and its Associated Congenital Microcephaly in Mice.

4. Pediatric Drug Nitazoxanide: A Potential Choice for Control of Zika.

5. The A-Z of Zika drug discovery.

6. The antimalarial drug amodiaquine possesses anti-ZIKA virus activities.

7. Advances in Developing Therapies to Combat Zika Virus: Current Knowledge and Future Perspectives.

8. Repurposing of the anti-malaria drug chloroquine for Zika Virus treatment and prophylaxis.

9. Host-Directed Antivirals: A Realistic Alternative to Fight Zika Virus.

10. Recent trends in ZikV research: A step away from cure.

11. Repurposing drugs for use against Zika virus infection.

12. Identification of small-molecule inhibitors of Zika virus infection and induced neural cell death via a drug repurposing screen.

13. Novel antiviral activity and mechanism of bromocriptine as a Zika virus NS2B-NS3 protease inhibitor.

14. 2,8-bis(trifluoromethyl)quinoline analogs show improved anti-Zika virus activity, compared to mefloquine.

15. Cell-line dependent antiviral activity of sofosbuvir against Zika virus.

16. Heparin prevents Zika virus induced-cytopathic effects in human neural progenitor cells.

17. Can an FDA-Approved Alzheimer's Drug Be Repurposed for Alleviating Neuronal Symptoms of Zika Virus?

18. Stem Cell Hydrogel, Jump-Starting Zika Drug Discovery, and Engineering RNA Recognition.

19. Repurposing Drugs to Treat Zika.

20. Novel strategies for discovering inhibitors of Dengue and Zika fever.

21. Cases of babies in Brazil born with thalidomide defects.

A2-2f3. Cluster 15 record titles

1. N-Desmethylclozapine, Fluoxetine, and Salmeterol Inhibit Postentry Stages of the Dengue Virus Life Cycle.

2. Drug repurposing approaches to fight Dengue virus infection and related diseases.

3. Nitazoxanide: a first-in-class broad-spectrum antiviral agent.

4. Past, Current, and Future Developments of Therapeutic Agents for Treatment of Chronic Hepatitis B Virus Infection.

5. Repurposing Kinase Inhibitors as Antiviral Agents to Control Influenza A Virus Replication.

6. Drug repurposing of quinine as antiviral against dengue virus infection.

7. Meeting report: 28th International Conference on Antiviral Research in Rome, Italy.

8. Repurposing of prochlorperazine for use against dengue virus infection.

9. Drug repurposing of minocycline against dengue virus infection.

10. Repurposed FDA-Approved drug sorafenib reduces replication of Venezuelan equine encephalitis virus and other alphaviruses.

11. Drug Repurposing for Viral Infectious Diseases: How Far Are We?

12. Clinically Approved Ion Channel Inhibitors Close Gates for Hepatitis C Virus and Open Doors for Drug Repurposing in Infectious Viral Diseases.

13. A perspective on targeting non-structural proteins to combat neglected tropical diseases: Dengue, West Nile and Chikungunya viruses.

14. Screening of FDA-Approved Drugs for Inhibitors of Japanese Encephalitis Virus Infection.

15. Natural Products as Promising Therapeutics for Treatment of Influenza Disease.

16. Use of attenuated paramyxoviruses for cancer therapy.

17. H7N9 and other pathogenic avian influenza viruses elicit a three-pronged transcriptomic signature that is reminiscent of 1918 influenza virus and is associated with lethal outcome in mice.

18. Targeting organic anion transporter 3 with probenecid as a novel anti-influenza a virus strategy.

19. Molecular Basis for the Selective Inhibition of Respiratory Syncytial Virus RNA Polymerase by 2'-Fluoro-4'-Chloromethyl-Cytidine Triphosphate.

20. Screening and Identification of Lassa Virus Entry Inhibitors from an FDA-Approved Drug Library.

21. High-content assay to identify inhibitors of dengue virus infection.

22. Development of Direct-acting Antiviral and Host-targeting Agents for Treatment of HBV Infection.

23. The HIV integrase inhibitor raltegravir inhibits felid alphaherpesvirus 1 (FeHV-1) replication by targeting both DNA replication and late gene expression.

24. Drug Repurposing Approach Identifies Inhibitors of the Prototypic Viral Transcription Factor IE2 that Block Human Cytomegalovirus Replication.

25. Direct-acting antivirals and host-targeting strategies to combat enterovirus infections.

26. Dengue Antiviral Development: A Continuing Journey.

27. Current Strategies for Inhibition of Chikungunya Infection.

28. Hyphenated 3D-QSAR statistical model-drug repurposing analysis for the identification of potent neuraminidase inhibitor.

29. Use of minocycline in viral infections.

30. Identification of FDA-approved drugs that target hepatitis B virus transcription.

31. Kinome Profiling Identifies Druggable Targets for Novel Human Cytomegalovirus (HCMV) Antivirals.

32. Repurposing the clinically approved calcium antagonist manidipine dihydrochloride as a new early inhibitor of human cytomegalovirus targeting the Immediate-Early 2 (IE2) protein.

33. West Nile virus drug discovery.

34. A dual drug regimen synergistically blocks human parainfluenza virus infection.

35. Antiviral activity of cationic amphiphilic drugs.

36. Irbesartan, an FDA approved drug for hypertension and diabetic nephropathy, is a potent inhibitor for hepatitis B virus entry by disturbing Na(+)-dependent taurocholate cotransporting polypeptide activity.

37. Identification of Retinoic Acid Receptor Agonists as Potent Hepatitis B Virus Inhibitors via a Drug Repurposing Screen.

38. Antiviral activity of doxycycline against vesicular stomatitis virus in vitro.

39. Repurposing of the antihistamine chlorcyclizine and related compounds for treatment of hepatitis C virus infection.

40. Identification of resveratrol analogs as potent anti-dengue agents using a cell-based assay.

41. Metformin inhibits hepatitis B virus protein production and replication in human hepatoma cells.

42. The combination effects of licl and the active leflunomide metabolite, A771726, on viral-induced interleukin 6 production and EV-A71 replication.

43. Phosphorylation of Single Stranded RNA Virus Proteins and Potential for Novel Therapeutic Strategies.

44. Identification of KX2-391 as an inhibitor of HBV transcription by a recombinant HBV-based screening assay.

45. Structure-based discovery of the novel antiviral properties of naproxen against the nucleoprotein of influenza A virus.

46. Antiviral activity of micafungin against enterovirus 71.

47. Feasibility and biological rationale of repurposing sunitinib and erlotinib for dengue treatment.

48. Transcriptomic characterization of the novel avian-origin influenza A (H7N9) virus: specific host response and responses intermediate between avian (H5N1 and H7N7) and human (H3N2) viruses and implications for treatment options.

49. Repurposing FDA-approved drugs as therapeutics to treat Rift Valley fever virus infection.

50. Management and Treatment of Dengue and Chikungunya - Natural Products to the Rescue.

51. Enterovirus replication: go with the (counter)flow.

52. Computer-Aided Structure Based Drug Design Approaches for the Discovery of New Anti-CHIKV Agents.

53. Antiviral activity of gemcitabine against human rhinovirus invitro and invivo.

54. Inhibition of Rift Valley fever virus replication and perturbation of nucleocapsid-RNA interactions by suramin.

55. Repurposing of Kinase Inhibitors as Broad-Spectrum Antiviral Drugs.

56. Treating Influenza Infection, From Now and Into the Future.

57. Drug Repurposing Identifies Inhibitors of Oseltamivir-Resistant Influenza Viruses.

58. New developments in flavivirus drug discovery.

59. Inhibitors for the hepatitis C virus RNA polymerase explored by SAR with advanced machine learning methods.

60. [Open Sesame: regulation of hepatitis C virus entry into hepatocytes].

61. Hydroxyurea inhibits parvovirus B19 replication in erythroid progenitor cells.

62. Developing a dengue vaccine: progress and future challenges.

63. Exploiting drug repositioning for discovery of a novel HIV combination therapy.

64. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway.

65. Evaluation of Crimean-Congo hemorrhagic fever virus in vitro inhibition by chloroquine and chlorpromazine, two FDA approved molecules.

66. Identification of potential anti-hepatitis C virus agents targeting non structural protein 5B using computational techniques.

67. Investigational drugs in early development for treating dengue infection.

68. Using HIV drugs to target human papilloma virus.

69. [L-Lysine-alpha-Oxidase in vitro Activity in Experiments on Models of Viruses Sindbis, Forest-Spring Encephalitis, Western Nile, Tyaginya and Dhori].

70. LEDGIN-mediated Inhibition of Integrase-LEDGF/p75 Interaction Reduces Reactivation of Residual Latent HIV.

71. Rhinovirus - From bench to bedside.

72. Artemisinin analogues as potent inhibitors of in vitro hepatitis C virus replication.

73. Fighting viruses with antibiotics: an overlooked path.

74. Pentosan Polysulfate: a Novel Glycosaminoglycan-Like Molecule for Effective Treatment of Alphavirus-Induced Cartilage Destruction and Inflammatory Disease.

75. Repurposing of HDAC inhibitors toward anti-hepatitis C virus drug discovery: teaching an old dog new tricks.

76. Pharmacophore anchor models of flaviviral NS3 proteases lead to drug repurposing for DENV infection.

77. Repurposing of rutin for the inhibition of norovirus replication.

78. Drug Repurposing: Tolfenamic Acid Inactivates PrbP, a Transcriptional Accessory Protein in Liberibacter asiaticus.

79. Analysis and assay of oseltamivir-resistant mutants of influenza neuraminidase via direct observation of drug unbinding and rebinding in simulation.

80. Old and new uses of surfactant.

A2-2f4. Cluster 14 record titles

1. Synergy testing of FDA-approved drugs identifies potent drug combinations against Trypanosoma cruzi.

2. Targeting calcium homeostasis as the therapy of Chagas' disease and leishmaniasis - a review.

3. In vitro and in vivo studies of the antiparasitic activity of sterol 14alpha-demethylase (CYP51) inhibitor VNI against drug-resistant strains of Trypanosoma cruzi.

4. In vitro activity of the antifungal azoles itraconazole and posaconazole against Leishmania amazonensis.

5. Optimization of Physicochemical Properties for 4-Anilinoquinoline Inhibitors of Plasmodium falciparum Proliferation.

6. Novel cruzipain inhibitors for the chemotherapy of chronic Chagas disease.

7. Discovery of novel polyamine analogs with anti-protozoal activity by computer guided drug repositioning.

8. Stairway to Heaven or Hell? Perspectives and Limitations of Chagas Disease Chemotherapy.

9. Pyrazinoates as antiparasitic agents against Trypanosoma cruzi.

10. Kinase scaffold repurposing for neglected disease drug discovery: discovery of an efficacious, lapatinib-derived lead compound for trypanosomiasis.

11. Identification of Trypanocidal Activity for Known Clinical Compounds Using a New Trypanosoma cruzi Hit-Discovery Screening Cascade.

12. The human Aurora kinase inhibitor danusertib is a lead compound for anti-trypanosomal drug discovery via target repurposing.

13. Discovery of a Carbazole-Derived Lead Drug for Human African Trypanosomiasis.

14. Benznidazole/Itraconazole Combination Treatment Enhances Anti-Trypanosoma cruzi Activity in Experimental Chagas Disease.

15. The susceptibility of trypanosomatid pathogens to PI3/mTOR kinase inhibitors affords a new opportunity for drug repurposing.

16. Repurposing of the Open Access Malaria Box for Kinetoplastid Diseases Identifies Novel Active Scaffolds against Trypanosomatids.

17. Drug repurposing strategy against Trypanosoma cruzi infection: In vitro and in vivo assessment of the activity of metronidazole in mono- and combined therapy.

18. Repositioning FDA Drugs as Potential Cruzain Inhibitors from Trypanosoma cruzi: Virtual Screening, In Vitro and In Vivo Studies.

19. Therapeutical approaches under investigation for treatment of Chagas disease.

20. The Oral Antimalarial Drug Tafenoquine Shows Activity against Trypanosoma brucei.

21. Repurposing Strategy of Atorvastatin against Trypanosoma cruzi: In Vitro Monotherapy and Combined Therapy with Benznidazole Exhibit Synergistic Trypanocidal Activity.

22. Repurposing of Human Kinase Inhibitors in Neglected Protozoan Diseases.

23. New chemical scaffolds for human african trypanosomiasis lead discovery from a screen of tyrosine kinase inhibitor drugs.

24. Trypanocidal Effect of Isotretinoin through the Inhibition of Polyamine and Amino Acid Transporters in Trypanosoma cruzi.

25. Activity of anti-cancer protein kinase inhibitors against Leishmania spp.

26. Cruzain inhibitors: efforts made, current leads and a structural outlook of new hits.

27. Novel lead compounds in pre-clinical development against African sleeping sickness.

28. Repurposing human PDE4 inhibitors for neglected tropical diseases: design, synthesis and evaluation of cilomilast analogues as Trypanosoma brucei PDEB1 inhibitors.

29. Polypharmacology in the treatment of Chagas disease.

30. Recent developments in rationally designed multitarget antiprotozoan agents.

31. Synthesis and in vitro evaluation of Ca2+ channel blockers 1,4-dihydropyridines analogues against Trypanosoma cruzi and Leishmania amazonensis: SAR analysis.

32. Ketanserin, an antidepressant, exerts its antileishmanial action via inhibition of 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGR) enzyme of Leishmania donovani.

33. Imidazolium salts as innovative agents against Leishmania amazonensis.

34. Ibandronate metal complexes: solution behavior and antiparasitic activity.

35. The antifungal compound butenafine eliminates promastigote and amastigote forms of Leishmania (Leishmania) amazonensis and Leishmania (Viannia) braziliensis.

36. 2-acylamino-5-nitro-1,3-thiazoles: preparation and in vitro bioevaluation against four neglected protozoan parasites.

37. Antileishmanial Activity of Ezetimibe: Inhibition of Sterol Biosynthesis, In Vitro Synergy with Azoles, and Efficacy in Experimental Cutaneous Leishmaniasis.

38. Identification of levothyroxine antichagasic activity through computer-aided drug repurposing.

39. Application of computer-aided drug repurposing in the search of new cruzipain inhibitors: discovery of amiodarone and bromocriptine inhibitory effects.

40. Repurposing human PDE4 inhibitors for neglected tropical diseases. Evaluation of analogs of the human PDE4 inhibitor GSK-256066 as inhibitors of PDEB1 of Trypanosoma brucei.

41. Dose-dependent effect and pharmacokinetics of fexinidazole and its metabolites in a mouse model of human African trypanosomiasis.

42. Activity of imidazole compounds on Leishmania (L.) infantum chagasi: reactive oxygen species induced by econazole.

43. Nanoliposomal Buparvaquone Immunomodulates Leishmania infantum-Infected Macrophages and Is Highly Effective in a Murine Model.

44. Leishmaniasis treatment: update of possibilities for drug repurposing.

45. In vitro additive interaction between ketoconazole and antimony against intramacrophage Leishmania (Leishmania) amazonensis amastigotes.

46. In vitro leishmanicidal effects of the anti-fungal drug natamycin are mediated through disruption of calcium homeostasis and mitochondrial dysfunction.

47. An invitro and invivo evaluation of new potential trans-sialidase inhibitors of Trypanosoma cruzi predicted by a computational drug repositioning method.

48. Nelfinavir and lopinavir impair Trypanosoma cruzi trypomastigote infection in mammalian host cells and show anti-amastigote activity.

49. Engineering Synergistically Active and Bioavailable Cost-effective Medicines for Neglected Tropical Diseases; The Role of Excipients.

50. Drug repurposing for Leishmania. Molecular basis of the leishmanicidal activity of the antidepressant sertraline.

51. In silico drug re-purposing against African sleeping sickness using GlcNAc-PI de-N-acetylase as an experimental target.

52. Development of a semi-automated image-based high-throughput drug screening system.

53. CYP51 as drug targets for fungi and protozoan parasites: past, present and future.

54. Histamine H1-receptor antagonists against Leishmania (L.) infantum: an in vitro and in vivo evaluation using phosphatidylserine-liposomes.

55. Repositioning Antitubercular 6-Nitro-2,3-dihydroimidazo[2,1-b][1,3]oxazoles for Neglected Tropical Diseases: Structure-Activity Studies on a Preclinical Candidate for Visceral Leishmaniasis.

56. Development of anti-fungal pesticides from protein kinase inhibitor-based anticancer agents.

57. CYP51 is an essential drug target for the treatment of primary amoebic meningoencephalitis (PAM).

58. Repurposing N,N'-bis-(arylamidino)-1,4-piperazinedicarboxamidines: An unexpected class of potent inhibitors of cholinesterases.

59. Treatment of Disseminated Leishmaniasis With Liposomal Amphotericin B.

60. Is the pharmaceutical industry's preoccupation with the monotherapy drug model stifling the development of effective new drug therapies?

61. Repurposing an old anti-fungal drug as a Hedgehog inhibitor.

62. Low-Income Countries And Repurposed Drugs.

A2-2f5. Cluster 19 record titles

1. A class of tricyclic compounds blocking malaria parasite oocyst development and transmission.

2. Antimalarial activity of novel 4-cyano-3-methylisoquinoline inhibitors against Plasmodium falciparum: design, synthesis and biological evaluation.

3. Efficacy of Synriam, a new antimalarial combination of OZ277 and piperaquine, against different developmental stages of Schistosoma mansoni.

4. Expanding the Antimalarial Drug Arsenal-Now, But How?

5. Repurposing drugs to target the malaria parasite unfolding protein response.

6. Antimalarials in the treatment of schistosomiasis.

7. Chemical signatures and new drug targets for gametocytocidal drug development.

8. Activity Profile of an FDA-Approved Compound Library against Schistosoma mansoni.

9. Screening a repurposing library, the Medicines for Malaria Venture Stasis Box, against Schistosoma mansoni.

10. Small molecule inhibition of apicomplexan FtsH1 disrupts plastid biogenesis in human pathogens.

11. Drug repurposing and human parasitic protozoan diseases.

12. Repurposing of anticancer drugs: in vitro and in vivo activities against Schistosoma mansoni.

13. Controlling schistosomiasis with praziquantel: How much longer without a viable alternative?

14. New leads for drug repurposing against malaria.

15. In vitro and in vivo antischistosomal activity of ferroquine derivatives.

16. Repositioning: the fast track to new anti-malarial medicines?

17. Approved oncology drugs lack in vivo activity against Trichuris muris despite in vitro activity.

18. Miltefosine Lipid Nanocapsules for Single Dose Oral Treatment of Schistosomiasis Mansoni: A Preclinical Study.

19. Exploring anti-malarial potential of FDA approved drugs: an in silico approach.

20. Auranofin is highly efficacious against Toxoplasma gondii in vitro and in an in vivo experimental model of acute toxoplasmosis.

21. Drug Repurposing Screening Identifies Novel Compounds That Effectively Inhibit Toxoplasma gondii Growth.

22. Treatment of Schistosoma mansoni with miltefosine in vitro enhances serological recognition of defined worm surface antigens.

23. Lysine Deacetylase Inhibitors in Parasites: Past, Present, and Future Perspectives.

24. Drug Repurposing for Schistosomiasis: Combinations of Drugs or Biomolecules.

25. High-throughput screen of drug repurposing library identifies inhibitors of Sarcocystis neurona growth.

26. Drug discovery for schistosomiasis: hit and lead compounds identified in a library of known drugs by medium-throughput phenotypic screening.

27. Screening of chemical compound libraries identified new anti-Toxoplasma gondii agents.

28. High-Throughput Screening of Entamoeba Identifies Compounds Which Target Both Life Cycle Stages and Which Are Effective Against Metronidazole Resistant Parasites.

29. Review of Experimental Compounds Demonstrating Anti-Toxoplasma Activity.

30. The Glucose Transporter PfHT1 Is an Antimalarial Target of the HIV Protease Inhibitor Lopinavir.

31. Miltefosine lipid nanocapsules: Intersection of drug repurposing and nanotechnology for single dose oral treatment of pre-patent schistosomiasis mansoni.

32. Repositioning of chlorambucil as a potential anti-schistosomal agent.

33. Distinct effects of HIV protease inhibitors and ERAD inhibitors on zygote to ookinete transition of the malaria parasite.

34. Ion channels and drug transporters as targets for anthelmintics.

35. Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine.

36. Activity of mefloquine and mefloquine derivatives against Echinococcus multilocularis.

37. Identification of Cryptosporidium parvum active chemical series by Repurposing the open access malaria box.

38. A systematic and prospectively validated approach for identifying synergistic drug combinations against malaria.

39. Viability Screen of LOPAC1280 Reveals Phosphorylation Inhibitor Auranofin as a Potent Inhibitor of Blastocystis Subtype 1, 4, and 7 Isolates.

40. Repurposing auranofin as a lead candidate for treatment of lymphatic filariasis and onchocerciasis.

41. Repurposing of antiparasitic drugs: the hydroxy-naphthoquinone buparvaquone inhibits vertical transmission in the pregnant neosporosis mouse model.

42. Sertraline, Paroxetine, and Chlorpromazine Are Rapidly Acting Anthelmintic Drugs Capable of Clinical Repurposing.

43. Antischistosomal agents: state of art and perspectives.

44. Re-positioning protein-kinase inhibitors against schistosomiasis.

45. Investigating antimalarial drug interactions of emetine dihydrochloride hydrate using CalcuSyn-based interactivity calculations.

46. Repurposing pharma assets: an accelerated mechanism for strengthening the schistosomiasis drug development pipeline.

47. Evaluation of methylene blue, pyrimethamine and its combination on an in vitro Neospora caninum model.

48. Clinically Available Medicines Demonstrating Anti-Toxoplasma Activity.

49. Toward organometallic antischistosomal drug candidates.

50. Drug repositioning as a route to anti-malarial drug discovery: preliminary investigation of the in vitro anti-malarial efficacy of emetine dihydrochloride hydrate.

51. The potential of quinoline derivatives for the treatment of Toxoplasma gondii infection.

52. Repurposing drugs for the treatment and control of helminth infections.

53. Road towards new antimalarials - overview of the strategies and their chemical progress.

54. Anthelmintics - from discovery to resistance.

55. Phase I Clinical Trial Results of Auranofin, a Novel Antiparasitic Agent.

56. A reprofiled drug, auranofin, is effective against metronidazole-resistant Giardia lamblia.

57. In vitro activity of immunosuppressive drugs against Plasmodium falciparum.

58. A repurposing strategy for Hsp90 inhibitors demonstrates their potency against filarial nematodes.

59. Auranofin inactivates Trichomonas vaginalis thioredoxin reductase and is effective against trichomonads in vitro and in vivo.

60. Screening of the Open Source Malaria Box Reveals an Early Lead Compound for the Treatment of Alveolar Echinococcosis.

61. Adverse neuropsychiatric effects of antimalarial drugs.

62. Synergic in vitro combinations of artemisinin, pyrimethamine and methylene blue against Neospora caninum.

63. Arylpyrrole and fipronil analogues that inhibit the motility and/or development of Haemonchus contortus in vitro.

64. A high-throughput phenotypic screen identifies clofazimine as a potential treatment for cryptosporidiosis.

65. Nanotechnology as a potential therapeutic alternative for schistosomiasis.

66. In vitro effects of new artemisinin derivatives in Neospora caninum-infected human fibroblasts.

67. Methylene blue inhibits lumefantrine-resistant Plasmodium berghei.

68. Gefitinib inhibits the growth of Toxoplasma gondii in HeLa cells.

69. Drug repurposing screen reveals FDA-approved inhibitors of human HMG-CoA reductase and isoprenoid synthesis that block Cryptosporidium parvum growth.

70. Drug repositioning for novel antitrichomonas from known antiprotozoan drugs using hierarchical screening.

71. Oral treatments of Echinococcus multilocularis-infected mice with the antimalarial drug mefloquine that potentially interacts with parasite ferritin and cystatin.

72. Repositioning of an existing drug for the neglected tropical disease Onchocerciasis.

73. Chloroquine and beyond: exploring anti-rheumatic drugs to reduce immune hyperactivation in HIV/AIDS.

74. Artemisinin derivatives: a patent review (2006 - present).

75. Drug repositioning and pharmacophore identification in the discovery of hookworm MIF inhibitors.

76. Repurposing of approved drugs from the human pharmacopoeia to target Wolbachia endosymbionts of onchocerciasis and lymphatic filariasis.

77. Chloroquine analogues in drug discovery: new directions of uses, mechanisms of actions and toxic manifestations from malaria to multifarious diseases.

78. Treatment of Cryptosporidium: What We Know, Gaps, and the Way Forward.

79. Chloroquine: An Old Drug with New Perspective Against Giardiasis.

80. Repositioning of DHFR Inhibitors.

81. Modeling of Plasmodium falciparum Telomerase Reverse Transcriptase Ternary Complex: Repurposing of Nucleoside Analog Inhibitors.

82. Repurposing isoxazoline veterinary drugs for control of vector-borne human diseases.

83. Preclinical drug evaluation system in the Plasmodium knowlesi baboon model of malaria: the methotrexate study.

84. Structural basis for inactivation of Giardia lamblia carbamate kinase by disulfiram.

85. Short communication: Nitazoxanide inhibits HIV viral replication in monocyte-derived macrophages.

86. A novel cell-based high-throughput screen for inhibitors of HIV-1 gene expression and budding identifies the cardiac glycosides.

87. Ivermectin: repurposing an old drug to complement malaria vector control.

88. Microplate fluorescence protease assays test the inhibition of select North American snake venoms' activities with an anti-proteinase library.

89. Drug repurposing: An approach to tackle drug resistance in S. typhimurium.

90. Laboratory testing of clinically approved drugs against Balamuthia mandrillaris.

91. Preclinical activity of the repurposed drug auranofin in classical Hodgkin lymphoma.

92. Prospects for Moxidectin as a New Oral Treatment for Human Scabies.

93. Considerations in the repurposing of mefloquine for prevention and treatment of osteoporosis.

A2-2f6. Cluster 6 record titles

1. Novel Antifungal Compounds Discovered in Medicines for Malaria Venture's Malaria Box.

2. High-throughput screening of a collection of known pharmacologically active small compounds for identification of Candida albicans biofilm inhibitors.

3. Strategies in the discovery of novel antifungal scaffolds.

4. Antifungals.

5. Synergistic combinations of antifungals and anti-virulence agents to fight against Candida albicans.

6. Antifungal application of nonantifungal drugs.

7. Antifungal adjuvants: Preserving and extending the antifungal arsenal.

8. Screening a Repurposing Library for Inhibitors of Multidrug-Resistant Candida auris Identifies Ebselen as a Repositionable Candidate for Antifungal Drug Development.

9. Repurposing auranofin as an antifungal: In vitro activity against a variety of medically important fungi.

10. Virtual screening and drug repositioning as strategies for the discovery of new antifungal inhibitors of oxidosqualene cyclase.

11. Repurposing antipsychotic drugs into antifungal agents: Synergistic combinations of azoles and bromperidol derivatives in the treatment of various fungal infections.

12. Repurposing Approach Identifies Auranofin with Broad Spectrum Antifungal Activity That Targets Mia40-Erv1 Pathway.

13. The triphenylethylenes, a novel class of antifungals.

14. Reversal of Azole Resistance in Candida albicans by Sulfa Antibacterial Drugs.

15. Candidiasis and the impact of flow cytometry on antifungal drug discovery.

16. Quinacrine inhibits Candida albicans growth and filamentation at neutral pH.

17. Repurposing as a means to increase the activity of amphotericin B and caspofungin against Candida albicans biofilms.

18. Antifungal Phenothiazines: Optimization, Characterization of Mechanism, and Modulation of Neuroreceptor Activity.

19. In vitro analysis of finasteride activity against Candida albicans urinary biofilm formation and filamentation.

20. Anticancer Drugs as Antibiofilm Agents in Candida albicans: Potential Targets.

21. Antifungal amphiphilic kanamycins: new life for an old drug.

22. The anti-Aspergillus drug pipeline: Is the glass half full or empty?

23. Repurposing FDA approved drugs against the human fungal pathogen, Candida albicans.

24. Antifungal properties of the anti-hypertensive drug: aliskiren.

25. Cancer drugs inhibit morphogenesis in the human fungal pathogen, Candida albicans.

26. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation.

27. Newer patents in antimycotic therapy.

28. Cross-species discovery of syncretic drug combinations that potentiate the antifungal fluconazole.

29. The Anti-helminthic Compound Mebendazole Has Multiple Antifungal Effects against Cryptococcus neoformans.

30. How promising are combinatorial drug strategies in combating Candida albicans biofilms?

31. Rapid identification of antifungal compounds against Exserohilum rostratum using high throughput drug repurposing screens.

32. Artemisinins, new miconazole potentiators resulting in increased activity against Candida albicans biofilms.

33. Repurposing drugs to fast-track therapeutic agents for the treatment of cryptococcosis.

34. A repurposing approach identifies off-patent drugs with fungicidal cryptococcal activity, a common structural chemotype, and pharmacological properties relevant to the treatment of cryptococcosis.

35. Drugs currently under investigation for the treatment of invasive candidiasis.

36. Estrogen receptor antagonists are anti-cryptococcal agents that directly bind EF hand proteins and synergize with fluconazole in vivo.

37. Repositioning of Endonuclear Receptors Binders as Potential Antibacterial and Antifungal Agents. Eptyloxim: A Potential and Novel Gyrase B and Cytochrome Cyp51 Inhibitor.

38. Can repurposing of existing drugs provide more effective therapies for invasive fungal infections?

39. Topical delivery of ebselen encapsulated in biopolymeric nanocapsules: drug repurposing enhanced antifungal activity.

40. Antiviral, antifungal, and antiparasitic activities of fluoroquinolones optimized for treatment of bacterial infections: a puzzling paradox or a logical consequence of their mode of action?

41. Toward improved anti-cryptococcal drugs: Novel molecules and repurposed drugs.

42. New applications for known drugs: Human glycogen synthase kinase 3 inhibitors as modulators of Aspergillus fumigatus growth.

43. Atorvastatin as a promising anticryptococcal agent.

44. Fluoxetine and thioridazine inhibit efflux and attenuate crystalline biofilm formation by Proteus mirabilis.

45. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs.

A2-2f7. Cluster 17 record titles

1. Repurposing Non-Antimicrobial Drugs and Clinical Molecules to Treat Bacterial Infections.

2. Drug repurposing as an alternative for the treatment of recalcitrant bacterial infections.

3. Repurposing auranofin for the treatment of cutaneous staphylococcal infections.

4. Repurposing of Anticancer Drugs for the Treatment of Bacterial Infections.

5. Innovative approaches to treat Staphylococcus aureus biofilm-related infections.

6. Repurposing the antihistamine terfenadine for antimicrobial activity against Staphylococcus aureus.

7. Repurposing salicylanilide anthelmintic drugs to combat drug resistant Staphylococcus aureus.

8. Drug repurposing for the treatment of staphylococcal infections.

9. Repurposing Ivacaftor for treatment of Staphylococcus aureus infections.

10. In vitro antibacterial effects of statins against bacterial pathogens causing skin infections.

11. Repurposing Clinical Molecule Ebselen to Combat Drug Resistant Pathogens.

12. Screening a Commercial Library of Pharmacologically Active Small Molecules against Staphylococcus aureus Biofilms.

13. Repurposing celecoxib as a topical antimicrobial agent.

14. Exploring simvastatin, an antihyperlipidemic drug, as a potential topical antibacterial agent.

15. Antibacterial activity and mechanism of action of auranofin against multi-drug resistant bacterial pathogens.

16. Antibiotic resistance breakers: can repurposed drugs fill the antibiotic discovery void?

17. In Vitro Screening of an FDA-Approved Library Against ESKAPE Pathogens.

18. Repurposing of nucleoside- and nucleobase-derivative drugs as antibiotics and biofilm inhibitors.

19. In vitro antimicrobial activity of monensin against common clinical isolates associated with canine otitis externa.

20. Repurposing FDA-approved drugs to combat drug-resistant Acinetobacter baumannii.

21. Drug repositioning: auranofin as a prospective antimicrobial agent for the treatment of severe staphylococcal infections.

22. Repurposing the anticancer drug mitomycin C for the treatment of persistent Acinetobacter baumannii infections.

23. Drug repurposing: a new front in the war against Staphylococcus aureus.

24. Statins and Antimicrobial Effects: Simvastatin as a Potential Drug against Staphylococcus aureus Biofilm.

25. Novel Polymyxin Combination With Antineoplastic Mitotane Improved the Bacterial Killing Against Polymyxin-Resistant Multidrug-Resistant Gram-Negative Pathogens.

26. The Immunomodulatory Drug Glatiramer Acetate is Also an Effective Antimicrobial Agent that Kills Gram-negative Bacteria.

27. Recent Drug-Repurposing-Driven Advances in the Discovery of Novel Antibiotics.

28. Screening a repurposing library for potentiators of antibiotics against Staphylococcus aureus biofilms.

29. New Role for FDA-Approved Drugs in Combating Antibiotic-Resistant Bacteria.

30. Inhibition of Fosfomycin Resistance Protein FosA by Phosphonoformate (Foscarnet) in Multidrug-Resistant Gram-Negative Pathogens.

31. Pathogenicity phenomena in three model systems: from network mining to emerging system-level properties.

32. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae.

33. Triclosan Is an Aminoglycoside Adjuvant for Eradication of Pseudomonas aeruginosa Biofilms.

34. Repurposing niclosamide as a versatile antimicrobial surface coating against device-associated, hospital-acquired bacterial infections.

35. Non-anti-infective effects of antimicrobials and their clinical applications: a review.

36. Host-directed antimicrobial drugs with broad-spectrum efficacy against intracellular bacterial pathogens.

37. Repurposing screens identify rifamycins as potential broad-spectrum therapy for multidrug-resistant Acinetobacter baumannii and select agent microorganisms.

38. Combination therapy: the propitious rationale for drug development.

39. Host response to respiratory bacterial pathogens as identified by integrated analysis of human gene expression data.

40. An FDA-Drug Library Screen for Compounds with Bioactivities against Meticillin-Resistant Staphylococcus aureus (MRSA).

41. New frontiers for anti-biofilm drug development.

42. Identification of Agents Active against Methicillin-Resistant Staphylococcus aureus USA300 from a Clinical Compound Library.

43. Repurposing ebselen for treatment of multidrug-resistant staphylococcal infections.

44. Repurposing of gallium-based drugs for antibacterial therapy.

45. Resistance-resistant antibiotics.

46. From Breast Cancer to Antimicrobial: Combating Extremely Resistant Gram-Negative "Superbugs" Using Novel Combinations of Polymyxin B with Selective Estrogen Receptor Modulators.

47. Statins: antimicrobial resistance breakers or makers?

48. Repurposing the antimycotic drug flucytosine for suppression of Pseudomonas aeruginosa pathogenicity.

49. Is There Potential for Repurposing Statins as Novel Antimicrobials?

50. Antimicrobial Activity of Gallium Compounds on ESKAPE Pathogens.

51. Extensive impact of non-antibiotic drugs on human gut bacteria.

52. Repurposing Zidovudine in combination with Tigecycline for treating carbapenem-resistant Enterobacteriaceae infections.

53. Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence.

54. Strategies to overcome the action of aminoglycoside-modifying enzymes for treating resistant bacterial infections.

55. Tedizolid Activity Against Clinical Mycobacterium abscessus Complex Isolates-An in vitro Characterization Study.

56. In-house chemical library repurposing: A case example for Pseudomonas aeruginosa antibiofilm activity and quorum sensing inhibition.

57. Identification and Validation of an Antivirulence Agent Targeting HlyU-Regulated Virulence in Vibrio vulnificus.

58. Repurposing Toremifene for Treatment of Oral Bacterial Infections.

59. Auranofin and its Analogues Show Potent Antimicrobial Activity Covering Multiresistant Pathogens: Structure-Activity Relationships.

60. Anthelmintic closantel enhances bacterial killing of polymyxin B against multidrug-resistant Acinetobacter baumannii.

61. Identification of antimicrobial activity among FDA-approved drugs for combating Mycobacterium abscessus and Mycobacterium chelonae.

62. Evaluating New Compounds to Treat Burkholderia pseudomallei Infections.

63. In vitro activity of the antiasthmatic drug zafirlukast against the oral pathogens Porphyromonas gingivalis and Streptococcus mutans.

64. Repurposing the Nonsteroidal Anti-inflammatory Drug Diflunisal as an Osteoprotective, Antivirulence Therapy for Staphylococcus aureus Osteomyelitis.

65. Comparative analysis of methicillin-sensitive and resistant Staphylococcus aureus exposed to emodin based on proteomic profiling.

66. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox.

67. New Antimicrobial Approaches: Reuse of Old Drugs.

68. Identification of novel drug targets in bovine respiratory disease: an essential step in applying biotechnologic techniques to develop more effective therapeutic treatments.

69. Alternative clinical indications for novel antibiotics licensed for skin and soft tissue infection?

70. Real-Time High-Throughput Drug and Synergy Testing for Multidrug-Resistant Bacterial Infection: A Case Report.

71. Prospects for Anti-Biofilm Pharmaceuticals.

72. Combating Multidrug-Resistant Pathogens with Host-Directed Nonantibiotic Therapeutics.

73. Ribavirin suppresses bacterial virulence by targeting LysR-type transcriptional regulators.

74. Drug Repositioning to Alleviate Systemic Inflammatory Response Syndrome Caused by Gram-Negative Bacterial Outer Membrane Vesicles.

75. Repurposing of Existing Statin drugs for treatment of Microbial Infections: How much Promising?

76. Combating Intracellular Pathogens with Repurposed Host-Targeted Drugs.

77. Skin and Soft Tissue Infections Due to Nontuberculous Mycobacteria.

78. Repositioning of Memantine as a Potential Novel Therapeutic Agent against Meningitic E. coli-Induced Pathogenicities through Disease-Associated Alpha7 Cholinergic Pathway and RNA Sequencing-Based Transcriptome Analysis of Host Inflammatory Responses.

79. Drug repurposing screens and synergistic drug-combinations for infectious diseases.

80. A Drug Repositioning Approach Reveals that Streptococcus mutans Is Susceptible to a Diverse Range of Established Antimicrobials and Nonantibiotics.

81. Editorial: Alternative Therapeutics against MDR Bacteria - "Fighting the Epidemic of Antibiotic Resistance".

82. Antibacterial effects of antiretrovirals, potential implications for microbiome studies in HIV.

83. A drug-repositioning screening identifies pentetic acid as a potential therapeutic agent for suppressing the elastase-mediated virulence of Pseudomonas aeruginosa.

84. Mode of action and resistance studies unveil new roles for tropodithietic acid as an anticancer agent and the gamma-glutamyl cycle as a proton sink.

85. Lytic activity of the staphylolytic Twort phage endolysin CHAP domain is enhanced by the SH3b cell wall binding domain.

86. [Reinstating cloxacilin for empiric antibiotic in late-onset sepsis].

87. Characterization of a Francisella tularensis-Caenorhabditis elegans Pathosystem for the Evaluation of Therapeutic Compounds.

88. Bedaquiline Inhibits the ATP Synthase in Mycobacterium abscessus and Is Effective in Infected Zebrafish.

89. Inhibition of adenovirus infection by mifepristone.

90. Target mechanism-based whole-cell screening identifies bortezomib as an inhibitor of caseinolytic protease in mycobacteria.

91. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens.

92. Protein kinase C-delta inhibitor, Rottlerin inhibits growth and survival of mycobacteria exclusively through Shikimate kinase.

93. New antibacterial, non-genotoxic materials, derived from the functionalization of the anti-thyroid drug methimazole with silver ions.

94. Repurposing the anthelmintic drug niclosamide to combat Helicobacter pylori.

95. Antidepressants, antimicrobials or both? Gut microbiota dysbiosis in depression and possible implications of the antimicrobial effects of antidepressant drugs for antidepressant effectiveness.

96. L-Captopril and its derivatives as potential inhibitors of microbial enzyme DapE: A combined approach of drug repurposing and similarity screening.

97. Toward Repositioning Niclosamide for Antivirulence Therapy of Pseudomonas aeruginosa Lung Infections: Development of Inhalable Formulations through Nanosuspension Technology.

98. Screening of a Drug Library Identifies Inhibitors of Cell Intoxication by CNF1.

99. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides.

100. Development of inhalable hyaluronan/mannitol composite dry powders for flucytosine repositioning in local therapy of lung infections.

101. [Nonantibiotic properties of macrolides and their role in modulation of the inflammatory reaction].

102. Mutational patterns in the HIV genome and cross-resistance following nucleoside and nucleotide analogue drug exposure.

103. Pharmacophore-Based Repositioning of Approved Drugs as Novel Staphylococcus aureus NorA Efflux Pump Inhibitors.

104. Potential repurposing of known drugs as potent bacterial beta-glucuronidase inhibitors.

105. Structural Basis of Metallo-beta-Lactamase Inhibition by Captopril Stereoisomers.

106. HIV reverse transcriptase: structural interpretation of drug resistant genetic variants from India.

107. Antibiotic shortages: effective alternatives in the face of a growing problem.

108. Exposure Matching of Pediatric Anti-infective Drugs: Review of Drugs Submitted to the Food and Drug Administration for Pediatric Approval.

109. In Vitro and Intracellular Activity of Imipenem Combined with Rifabutin and Avibactam against Mycobacterium abscessus.

110. Repurposing an old drug: aztreonam as a new treatment strategy for gonorrhoea.

111. Structural basis for the resilience of efavirenz (DMP-266) to drug resistance mutations in HIV-1 reverse transcriptase.

112. L-Lysine-alpha-Oxidase: Acidovorax citrulli Bacterium Inhibitor.

113. Rapid Recovery of Clofazimine-Loaded Nanoparticles with Long-Term Storage Stability as Anti-Cryptosporidium Therapy.

A2-2g. Leaf clusters under Cluster 52

There are six leaf clusters under Cluster 52: Cluster 23 (93), Cluster 12 (59), Cluster 27 (160), Cluster 25 (171), Cluster 5 (41), Cluster 11 (66).

*Cluster 23 focuses on repurposing kinase inhibitors, especially for treatment of acute myeloid leukemia

*Cluster 12 focuses on ovarian cancer treatments, especially niclosamide

*Cluster 27 focuses on treatments that destroy cancer cells

*Cluster 25 focuses on anti-cancer treatments

*Cluster 5 focuses on treatments for pancreatic cancer, especially Metformin

*Cluster 11 focuses on breast cancer treatments

A2-2g1. Cluster 23 record titles

1. The potent Cdc7-Dbf4 (DDK) kinase inhibitor XL413 has limited activity in many cancer cell lines and discovery of potential new DDK inhibitor scaffolds.

2. K-Map: connecting kinases with therapeutics for drug repurposing and development.

3. Competitive Kinase Enrichment Proteomics Reveals that Abemaciclib Inhibits GSK3beta and Activates WNT Signaling.

4. Covalent inhibitors of EGFR family protein kinases induce degradation of human Tribbles 2 (TRIB2) pseudokinase in cancer cells.

5. Inhibitor repurposing reveals ALK, LTK, FGFR, RET and TRK kinases as the targets of AZD1480.

6. Kinase Inhibitor Screening in Myeloid Malignancies.

7. Identification of Novel Cdc7 Kinase Inhibitors as Anti-Cancer Agents that Target the Interaction with Dbf4 by the Fragment Complementation and Drug Repositioning Approach.

8. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia.

9. Bioinformatics-driven discovery of rational combination for overcoming EGFR-mutant lung cancer resistance to EGFR therapy.

10. One reporter for in-cell activity profiling of majority of protein kinase oncogenes.

11. Drug combination approach to overcome resistance to EGFR tyrosine kinase inhibitors in lung cancer.

12. Fluvastatin inhibits FLT3 glycosylation in human and murine cells and prolongs survival of mice with FLT3/ITD leukemia.

13. Re-purposing clinical kinase inhibitors to enhance chemosensitivity by overriding checkpoints.

14. Individualized systems medicine strategy to tailor treatments for patients with chemorefractory acute myeloid leukemia.

15. Multi-pathway cellular analysis of compound selectivity.

16. Axitinib effectively inhibits BCR-ABL1(T315I) with a distinct binding conformation.

17. Monocyte-macrophage differentiation of acute myeloid leukemia cell lines by small molecules identified through interrogation of the Connectivity Map database.

18. High-Throughput Flow Cytometry Identifies Small-Molecule Inhibitors for Drug Repurposing in T-ALL.

19. Repositioning of bromocriptine for treatment of acute myeloid leukemia.

20. Redox modulation of adjacent thiols in VLA-4 by AS101 converts myeloid leukemia cells from a drug-resistant to drug-sensitive state.

21. In silico drug repurposing of FDA-approved drugs to predict new inhibitors for drug resistant T315I mutant and wild-type BCR-ABL1: A virtual screening and molecular dynamics study.

22. Drug screen in patient cells suggests quinacrine to be repositioned for treatment of acute myeloid leukemia.

23. Drug repurposing for chronic myeloid leukemia: in silico and in vitro investigation of DrugBank database for allosteric Bcr-Abl inhibitors.

24. Genome-wide CRISPR-Cas9 Screen Identifies Leukemia-Specific Dependence on a Pre-mRNA Metabolic Pathway Regulated by DCPS.

25. Dual MET and SMO Negative Modulators Overcome Resistance to EGFR Inhibitors in Human Nonsmall Cell Lung Cancer.

26. In silico identification of potent small molecule inhibitors targeting epidermal growth factor receptor 1.

27. Chemogenomic Landscape of RUNX1-mutated AML Reveals Importance of RUNX1 Allele Dosage in Genetics and Glucocorticoid Sensitivity.

28. Structural insight into selectivity and resistance profiles of ROS1 tyrosine kinase inhibitors.

29. Ex vivo drug response profiling detects recurrent sensitivity patterns in drug-resistant acute lymphoblastic leukemia.

30. A Receptor Tyrosine Kinase Inhibitor, Dovitinib (TKI-258), Enhances BMP-2-Induced Osteoblast Differentiation In Vitro.

31. Structure based discovery of clomifene as a potent inhibitor of cancer-associated mutant IDH1.

32. Hydroxyurea synergizes with valproic acid in wild-type p53 acute myeloid leukaemia.

33. Valproic acid in the complex therapy of malignant tumors.

34. Towards repositioning of quinacrine for treatment of acute myeloid leukemia - Promising synergies and in vivo effects.

35. In silico identification of novel kinase inhibitors targeting wild-type and T315I mutant ABL1 from FDA-approved drugs.

36. Beyond standard therapy: drugs under investigation for the treatment of gastrointestinal stromal tumor.

37. The protein kinase 2 inhibitor CX-4945 regulates osteoclast and osteoblast differentiation in vitro.

38. Coming full circle: 70 years of chronic lymphocytic leukemia cell redistribution, from glucocorticoids to inhibitors of B-cell receptor signaling.

39. PPARgamma agonists sensitize PTEN-deficient resistant lung cancer cells to EGFR tyrosine kinase inhibitors by inducing autophagy.

40. A screen for Fli-1 transcriptional modulators identifies PKC agonists that induce erythroid to megakaryocytic differentiation and suppress leukemogenesis.

41. Repurposing anticancer drugs for targeting necroptosis.

42. Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors.

43. Bisphosphonates inactivate human EGFRs to exert antitumor actions.

44. Upgrading gemcitabine with recycled kinase inhibitors.

45. Inhibition of EGFR Signaling Protects from Mucormycosis.

46. The photosensitizer verteporfin has light-independent anti-leukemic activity for Ph-positive acute lymphoblastic leukemia and synergistically works with dasatinib.

47. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer.

48. Cyclic AMP efflux inhibitors as potential therapeutic agents for leukemia.

49. Drug-Repositioning Screens Identify Triamterene as a Selective Drug for the Treatment of DNA Mismatch Repair Deficient Cells.

50. Structure-based repurposing of FDA-approved drugs as inhibitors of NEDD8-activating enzyme.

51. Drug repurposing for gastrointestinal stromal tumor.

52. Discovery of Novel SPAK Inhibitors That Block WNK Kinase Signaling to Cation Chloride Transporters.

53. Combined inhibition of atypical PKC and histone deacetylase 1 is cooperative in basal cell carcinoma treatment.

54. Inhibiting Drivers of Non-mutational Drug Tolerance Is a Salvage Strategy for Targeted Melanoma Therapy.

55. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage.

56. Propofol enhances BCR-ABL TKIs' inhibitory effects in chronic myeloid leukemia through Akt/mTOR suppression.

57. FDA-approved drugs selected using virtual screening bind specifically to G-quadruplex DNA.

58. Targeted therapy for Epstein-Barr virus-associated gastric carcinoma using low-dose gemcitabine-induced lytic activation.

59. Fluvastatin activates sirtuin 6 to regulate sterol regulatory element-binding proteins and AMP-activated protein kinase in HepG2 cells.

60. Meclozine facilitates proliferation and differentiation of chondrocytes by attenuating abnormally activated FGFR3 signaling in achondroplasia.

61. Copper is required for oncogenic BRAF signalling and tumorigenesis.

62. Molecular therapeutic strategies for FGFR3 gene-related skeletal dysplasia.

63. 5-azacytidine inhibits nonsense-mediated decay in a MYC-dependent fashion.

64. Drug repurposing identifies a synergistic combination therapy with imatinib mesylate for gastrointestinal stromal tumor.

65. A protein folding molecular imaging biosensor monitors the effects of drugs that restore mutant p53 structure and its downstream function in glioblastoma cells.

66. Comparison of Quantitative Mass Spectrometry Platforms for Monitoring Kinase ATP Probe Uptake in Lung Cancer.

67. Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues.

68. Repurposing existing drugs for new AMPK activators as a strategy to extend lifespan: a computer-aided drug discovery study.

69. A High-Content Screening of Anticancer Compounds Suggests the Multiple Tyrosine Kinase Inhibitor Ponatinib for Repurposing in Neuroblastoma Therapy.

70. In silico and in vitro drug screening identifies new therapeutic approaches for Ewing sarcoma.

71. Molecular docking studies on thirteen fluoroquinolines with human topoisomerase II a and b.

72. Discovery of alkyl bis(oxy)dibenzimidamide derivatives as novel protein arginine methyltransferase 1 (PRMT1) inhibitors.

73. Repurposing the antihelmintic mebendazole as a hedgehog inhibitor.

74. A comprehensive approach to identifying repurposed drugs to treat SCN8A epilepsy.

75. Could the FDA-approved anti-HIV PR inhibitors be promising anticancer agents? An answer from enhanced docking approach and molecular dynamics analyses.

76. A Dual Readout Assay Based on Fluorescence Polarization and Time-Resolved Fluorescence Resonance Energy Transfer to Screen for RSK1 Inhibitors.

77. Identification of FDA-approved drugs as novel allosteric inhibitors of human executioner caspases.

78. Identification of toxin inhibitors using a magnetic nanosensor-based assay.

79. Auranofin induces lethal oxidative and endoplasmic reticulum stress and exerts potent preclinical activity against chronic lymphocytic leukemia.

80. A small molecule screen identifies an inhibitor of DNA repair inducing the degradation of TFIIH and the chemosensitization of tumor cells to platinum.

81. Identification of novel small-molecule inhibitors targeting menin-MLL interaction, repurposing the antidiarrheal loperamide.

82. Unveiling anticancer potential of glibenclamide: Its synergistic cytotoxicity with doxorubicin on cancer cells.

83. Response to hydralazine-valproate in a patient with mycosis fungoides.

84. Cooperative recognition of T:T mismatch by echinomycin causes structural distortions in DNA duplex.

85. Repurposing the Clinically Efficacious Antifungal Agent Itraconazole as an Anticancer Chemotherapeutic.

86. Toward drug repurposing in epigenetics: olsalazine as a hypomethylating compound active in a cellular context.

87. Selected drugs with reported secondary cell-differentiating capacity prime latent HIV-1 infection for reactivation.

88. Thermal profiling reveals phenylalanine hydroxylase as an off-target of panobinostat.

89. Inhibition of Peroxidase Activity of Cytochrome c: De Novo Compound Discovery and Validation.

90. Drug repurposing identifies therapeutic agents for gastrointestinal stromal tumors.

91. Butamben derivatives enhance BMP-2-stimulated commitment of C2C12 cells into osteoblasts with induction of voltage-gated potassium channel expression.

92. PP2A Controls Genome Integrity by Integrating Nutrient-Sensing and Metabolic Pathways with the DNA Damage Response.

93. Cell reprogramming for skeletal dysplasia drug repositioning.

A2-2g2. Cluster 12 record titles

1. A Blockade of IGF Signaling Sensitizes Human Ovarian Cancer Cells to the Anthelmintic Niclosamide-Induced Anti-Proliferative and Anticancer Activities.

2. Niclosamide and its analogs are potent inhibitors of Wnt/beta-catenin, mTOR and STAT3 signaling in ovarian cancer.

3. Evaluation of Effects of Metformin in Primary Ovarian Cancer Cells.

4. Bithionol inhibits ovarian cancer cell growth in vitro - studies on mechanism(s) of action.

5. Metformin and epithelial ovarian cancer therapeutics.

6. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo.

7. Ormeloxifene efficiently inhibits ovarian cancer growth.

8. A new niclosamide derivatives-B17 can inhibit urological cancers growth through apoptosis-related pathway.

9. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition.

10. Assessment of the antitumor potential of Bithionol in vivo using a xenograft model of ovarian cancer.

11. Mevalonate Pathway Antagonist Suppresses Formation of Serous Tubal Intraepithelial Carcinoma and Ovarian Carcinoma in Mouse Models.

12. Using a novel computational drug-repositioning approach (DrugPredict) to rapidly identify potent drug candidates for cancer treatment.

13. A Small-molecule Kinase Inhibitor, CEP-1347, Inhibits Survivin Expression and Sensitizes Ovarian Cancer Stem Cells to Paclitaxel.

14. Ritonavir blocks AKT signaling, activates apoptosis and inhibits migration and invasion in ovarian cancer cells.

15. Licofelone Enhances the Efficacy of Paclitaxel in Ovarian Cancer by Reversing Drug Resistance and Tumor Stem-like Properties.

16. Drug Repurposing of the Anthelmintic Niclosamide to Treat Multidrug-Resistant Leukemia.

17. Discovering drugs to overcome chemoresistance in ovarian cancers based on the cancer genome atlas tumor transcriptome profile.

18. The anthelmintic niclosamide inhibits colorectal cancer cell lines via modulation of the canonical and noncanonical Wnt signaling pathway.

19. The Anthelmintic Drug Niclosamide Inhibits the Proliferative Activity of Human Osteosarcoma Cells by Targeting Multiple Signal Pathways.

20. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer.

21. Niclosamide enhances ROS-mediated cell death through c-Jun activation.

22. Niclosamide, a Drug with Many (Re)purposes.

23. Niclosamide Exhibits Potent Anticancer Activity and Synergizes with Sorafenib in Human Renal Cell Cancer Cells.

24. Niclosamide Induces Epiboly Delay During Early Zebrafish Embryogenesis.

25. Drug repositioning of mevalonate pathway inhibitors as antitumor agents for ovarian cancer.

26. Valproic Acid Promotes Apoptosis and Cisplatin Sensitivity Through Downregulation of H19 Noncoding RNA in Ovarian A2780 Cells.

27. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling.

28. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling.

29. Disulfiram/copper causes redox-related proteotoxicity and concomitant heat shock response in ovarian cancer cells that is augmented by auranofin-mediated thioredoxin inhibition.

30. Antihelminthic drug niclosamide inhibits CIP2A and reactivates tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells.

31. Antibiotic drug rifabutin is effective against lung cancer cells by targeting the eIF4E-beta-catenin axis.

32. Pyrvinium Sensitizes Clear Cell Renal Cell Carcinoma Response to Chemotherapy Via Casein Kinase 1alpha-Dependent Inhibition of Wnt/beta-Catenin.

33. beta-catenin and PI3Kdelta inhibition expands precursor Th17 cells with heightened stemness and antitumor activity.

34. Identification of Niclosamide as a Novel Anticancer Agent for Adrenocortical Carcinoma.

35. Albumin nanoparticles increase the anticancer efficacy of albendazole in ovarian cancer xenograft model.

36. In vivo loss-of-function screens identify KPNB1 as a new druggable oncogene in epithelial ovarian cancer.

37. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis.

38. A convenient synthesis of lubeluzole and its enantiomer: evaluation as chemosensitizing agents on human ovarian adenocarcinoma and lung carcinoma cells.

39. Doxycycline inhibits proliferation and induces apoptosis of both human papillomavirus positive and negative cervical cancer cell lines.

40. Antimalarial drug mefloquine inhibits nuclear factor kappa B signaling and induces apoptosis in colorectal cancer cells.

41. Inhibition of mTOR/eIF4E by anti-viral drug ribavirin effectively enhances the effects of paclitaxel in oral tongue squamous cell carcinoma.

42. Identification of Chemical Inhibitors of beta-Catenin-Driven Liver Tumorigenesis in Zebrafish.

43. Repositioning of anti-viral drugs as therapy for cervical cancer.

44. Identification of known drugs that act as inhibitors of NF-kappaB signaling and their mechanism of action.

45. A Novel High Content Imaging-Based Screen Identifies the Anti-Helminthic Niclosamide as an Inhibitor of Lysosome Anterograde Trafficking and Prostate Cancer Cell Invasion.

46. Drug-dependent functionalization of wild-type and mutant p53 in cisplatin-resistant human ovarian tumor cells.

47. Doxycycline is an NF-kappaB inhibitor that induces apoptotic cell death in malignant T-cells.

48. Repurposing the anti-malarial drug dihydroartemisinin suppresses metastasis of non-small-cell lung cancer via inhibiting NF-kappaB/GLUT1 axis.

49. Evaluating class III antiarrhythmic agents as novel MYC targeting drugs in ovarian cancer.

50. Bioinformatics and in vitro experimental analyses identify the selective therapeutic potential of interferon gamma and apigenin against cervical squamous cell carcinoma and adenocarcinoma.

51. Effects of digitoxin on cell migration in ovarian cancer inflammatory microenvironment.

52. Mechanism-informed Repurposing of Minocycline Overcomes Resistance to Topoisomerase Inhibition for Peritoneal Carcinomatosis.

53. Ribavirin as a tri-targeted antitumor repositioned drug.

54. Computational drugs repositioning identifies inhibitors of oncogenic PI3K/AKT/P70S6K-dependent pathways among FDA-approved compounds.

55. Repurposing disulfiram for cancer therapy via targeted nanotechnology through enhanced tumor mass penetration and disassembly.

56. Chemoprevention of head and neck squamous cell carcinoma through inhibition of NF-kappaB signaling.

57. Oncogenic targets Mmp7, S100a9, Nppb and Aldh1a3 from transcriptome profiling of FAP and Pirc adenomas are downregulated in response to tumor suppression by Clotam.

58. Repurposing the FDA-approved pinworm drug pyrvinium as a novel chemotherapeutic agent for intestinal polyposis.

59. Repurposing cationic amphiphilic drugs as adjuvants to induce lysosomal siRNA escape in nanogel transfected cells.

A2-2g3. Cluster 27 record titles

1. Delineation of biological and molecular mechanisms underlying the diverse anticancer activities of mycophenolic acid.

2. Transcriptomic changes induced by mycophenolic acid in gastric cancer cells.

3. Therapeutic Effect of Quinacrine, an Antiprotozoan Drug, by Selective Suppression of p-CHK1/2 in p53-Negative Malignant Cancers.

4. A novel anti-cancer role of beta-apopicropodophyllin against non-small cell lung cancer cells.

5. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment.

6. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin.

7. Drug Repurposing Screening Identifies Tioconazole as an ATG4 Inhibitor that Suppresses Autophagy and Sensitizes Cancer Cells to Chemotherapy.

8. New insight for pharmacogenomics studies from the transcriptional analysis of two large-scale cancer cell line panels.

9. New derivatives of the antimalarial drug Pyrimethamine in the control of melanoma tumor growth: an in vitro and in vivo study.

10. The combination astemizole-gefitinib as a potential therapy for human lung cancer.

11. The antiparasitic drug, potassium antimony tartrate, inhibits tumor angiogenesis and tumor growth in nonsmall-cell lung cancer.

12. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo.

13. Proton pump inhibitor ilaprazole suppresses cancer growth by targeting T-cell-originated protein kinase.

14. Repurposing of phentolamine as a potential anticancer agent against human castration-resistant prostate cancer: A central role on microtubule stabilization and mitochondrial apoptosis pathway.

15. The anti-fibrotic agent pirfenidone synergizes with cisplatin in killing tumor cells and cancer-associated fibroblasts.

16. Screening of a composite library of clinically used drugs and well-characterized pharmacological compounds for cystathionine beta-synthase inhibition identifies benserazide as a drug potentially suitable for repurposing for the experimental therapy of colon cancer.

17. Nelfinavir, a new anti-cancer drug with pleiotropic effects and many paths to autophagy.

18. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells.

19. Eritoran Suppresses Colon Cancer by Altering a Functional Balance in Toll-like Receptors That Bind Lipopolysaccharide.

20. Auranofin-mediated inhibition of PI3K/AKT/mTOR axis and anticancer activity in non-small cell lung cancer cells.

21. Benserazide, a dopadecarboxylase inhibitor, suppresses tumor growth by targeting hexokinase 2.

22. Repurposing the anti-malarial drug artesunate as a novel therapeutic agent for metastatic renal cell carcinoma due to its attenuation of tumor growth, metastasis, and angiogenesis.

23. Identification of repurposed small molecule drugs for chordoma therapy.

24. Computational Cell Cycle Profiling of Cancer Cells for Prioritizing FDA-Approved Drugs with Repurposing Potential.

25. Down-regulating IL-6/GP130 targets improved the anti-tumor effects of 5-fluorouracil in colon cancer.

26. Nrf2 inhibition reverses the resistance of cisplatin-resistant head and neck cancer cells to artesunate-induced ferroptosis.

27. Effects of repurposed drug candidates nitroxoline and nelfinavir as single agents or in combination with erlotinib in pancreatic cancer cells.

28. Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing.

29. CLC-Pred: A freely available web-service for in silico prediction of human cell line cytotoxicity for drug-like compounds.

30. Repositioning of amprenavir as a novel extracellular signal-regulated kinase-2 inhibitor and apoptosis inducer in MCF-7 human breast cancer.

31. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage.

32. Glutamate release inhibitor, Riluzole, inhibited proliferation of human hepatocellular carcinoma cells by elevated ROS production.

33. Parainfluenza Virus Infection Sensitizes Cancer Cells to DNA-Damaging Agents: Implications for Oncolytic Virus Therapy.

34. p73 as a pharmaceutical target for cancer therapy.

35. Quantitative high-throuput drug screening identifies novel classes of drugs with anticancer activity in thyroid cancer cells: opportunities for repurposing.

36. Verteporfin inhibits gastric cancer cell growth by suppressing adhesion molecule FAT1.

37. Gene-expression data integration to squamous cell lung cancer subtypes reveals drug sensitivity.

38. Repositioning of difluorinated propanediones as inhibitors of histone methyltransferases and their biological evaluation in human leukemic cell lines.

39. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function.

40. The Antiarrhythmic Drug, Amiodarone, Decreases AKT Activity and Sensitizes Human Acute Myeloid Leukemia Cells to Apoptosis by ABT-263.

41. Autophagy Induced by Naftopidil Inhibits Apoptosis of Human Gastric Cancer Cells.

42. Lymphoma and myeloma cells are highly sensitive to growth arrest and apoptosis induced by artesunate.

43. Repositioning of the anthelmintic drug mebendazole for the treatment for colon cancer.

44. Drug Repurposing Approach Identifies a Synergistic Drug Combination of an Antifungal Agent and an Experimental Organometallic Drug for Melanoma Treatment.

45. Pharmacological targeting of p38 MAP-Kinase 6 (MAP2K6) inhibits the growth of esophageal adenocarcinoma.

46. Identification of thiazolo[5,4-d]pyrimidine derivatives as potent antiproliferative agents through the drug repurposing strategy.

47. Autophagy in HIV-induced T cell death.

48. SIS3, a specific inhibitor of Smad3 reverses ABCB1- and ABCG2-mediated multidrug resistance in cancer cell lines.

49. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways.

50. Four clinically utilized drugs were identified and validated for treatment of adrenocortical cancer using quantitative high-throughput screening.

51. In Silico Identification and In Vitro and In Vivo Validation of Anti-Psychotic Drug Fluspirilene as a Potential CDK2 Inhibitor and a Candidate Anti-Cancer Drug.

52. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs.

53. Repurposing itraconazole to the benefit of skin cancer treatment: A combined azole-DDAB nanoencapsulation strategy.

54. Targeting Phosphatidylinositol 4-Kinase IIIalpha for Radiosensitization: A Potential Model of Drug Repositioning Using an Anti-Hepatitis C Viral Agent.

55. Anticancer Properties of Fenofibrate: A Repurposing Use.

56. Structure-based identification of a NEDD8-activating enzyme inhibitor via drug repurposing.

57. A tumor deconstruction platform identifies definitive end points in the evaluation of drug responses.

58. Repositioning "old" drugs for new causes: identifying new inhibitors of prostate cancer cell migration and invasion.

59. Anthelmintic mebendazole enhances cisplatin's effect on suppressing cell proliferation and promotes differentiation of head and neck squamous cell carcinoma (HNSCC).

60. Identification of endoplasmic reticulum stress-inducing agents by antagonizing autophagy: a new potential strategy for identification of anti-cancer therapeutics in B-cell malignancies.

61. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress.

62. P-gp Inhibition by the Anti-psychotic Drug Pimozide Increases Apoptosis, as well as Expression of pRb and pH2AX in Highly Drug-resistant KBV20C Cells.

63. Luteolin Impacts on the DNA Damage Pathway in Oral Squamous Cell Carcinoma.

64. Synergistic combination of flavopiridol and carfilzomib targets commonly dysregulated pathways in adrenocortical carcinoma and has biomarkers of response.

65. Three-Dimensional Cell Culture-Based Screening Identifies the Anthelmintic Drug Nitazoxanide as a Candidate for Treatment of Colorectal Cancer.

66. Growth-suppressive activity of raloxifene on liver cancer cells by targeting IL-6/GP130 signaling.

67. Multiple effects of digoxin on subsets of cancer-associated genes through the alternative splicing pathway.

68. High-throughput drug library screening identifies colchicine as a thyroid cancer inhibitor.

69. Emerging roles of Myc in stem cell biology and novel tumor therapies.

70. Induction of DNA damage and apoptosis in human leukemia cells by efavirenz.

71. From ancient herb to modern drug: Artemisia annua and artemisinin for cancer therapy.

72. Identifying candidate agents for lung adenocarcinoma by walking the human interactome.

73. Angiotensin II type 1 receptor blocker telmisartan induces apoptosis and autophagy in adult T-cell leukemia cells.

74. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors.

75. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent.

76. In silico prediction and in vitro and in vivo validation of acaricide fluazuron as a potential inhibitor of FGFR3 and a candidate anticancer drug for bladder carcinoma.

77. Ex vivo drug sensitivity testing as a means for drug repurposing in esophageal adenocarcinoma.

78. Artemisinin and Its Derivatives as a Repurposing Anticancer Agent: What Else Do We Need to Do?

79. Therapeutic Effect of Repurposed Temsirolimus in Lung Adenocarcinoma Model.

80. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death.

81. Repositioning of anti-cancer drug candidate, AZD7762, to an anti-allergic drug suppressing IgE-mediated mast cells and allergic responses via the inhibition of Lyn and Fyn.

82. Tumor deconstruction as a tool for advanced drug screening and repositioning.

83. Carfilzomib is an effective anticancer agent in anaplastic thyroid cancer.

84. Expression Profiling Identifies Bezafibrate as Potential Therapeutic Drug for Lung Adenocarcinoma.

85. N-bromotaurine surrogates for loss of antiproliferative response and enhances cisplatin efficacy in cancer cells with impaired glucocorticoid receptor.

86. In vitro and in vivo study of hydralazine, a potential anti-angiogenic agent.

87. Identification of Existing Drugs That Effectively Target NTRK1 and ROS1 Rearrangements in Lung Cancer.

88. Increasing procaspase 8 expression using repurposed drugs to induce HIV infected cell death in ex vivo patient cells.

89. Revisiting old drugs as novel agents for retinoblastoma: in vitro and in vivo antitumor activity of cardenolides.

90. Therapeutic synergy between tigecycline and venetoclax in a preclinical model of MYC/BCL2 double-hit B cell lymphoma.

91. Pharmacological exploitation of the phenothiazine antipsychotics to develop novel antitumor agents-A drug repurposing strategy.

92. Biotin-targeted Pluronic() P123/F127 mixed micelles delivering niclosamide: A repositioning strategy to treat drug-resistant lung cancer cells.

93. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma.

94. PPARgamma agonists promote differentiation of cancer stem cells by restraining YAP transcriptional activity.

95. Preclinical Evaluation of Vemurafenib as Therapy for BRAFV600E Mutated Sarcomas.

96. Concise Review: Cell Surface N-Linked Glycoproteins as Potential Stem Cell Markers and Drug Targets.

97. Mebendazole stimulates CD14+ myeloid cells to enhance T-cell activation and tumour cell killing.

98. Immunomodulatory effects of cyclophosphamide and implementations for vaccine design.

99. Combination of cationic dexamethasone derivative and STAT3 inhibitor (WP1066) for aggressive melanoma: a strategy for repurposing a phase I clinical trial drug.

100. Repositioning antipsychotic chlorpromazine for treating colorectal cancer by inhibiting sirtuin 1.

101. Repurposed drug screen identifies cardiac glycosides as inhibitors of TGF-beta-induced cancer-associated fibroblast differentiation.

102. Concise Review: Cell Surface N-Linked Glycoproteins as Potential Stem Cell Markers and Drug Targets.

103. Repositioning FDA-Approved Drugs in Combination with Epigenetic Drugs to Reprogram Colon Cancer Epigenome.

104. Possible targets on carcinoma for bMAb retargeting of lymphocyte or drug cytotoxicity.

105. Repositioning proton pump inhibitors as anticancer drugs by targeting the thioesterase domain of human fatty acid synthase.

106. Repurposing of nitroxoline as a potential anticancer agent against human prostate cancer: a crucial role on AMPK/mTOR signaling pathway and the interplay with Chk2 activation.

107. Piperazine-based Alpha-1 AR Blocker, Naftopidil, Selectively Suppresses Malignant Human Bladder Cells via Induction of Apoptosis.

108. Vitamin K and hepatocellular carcinoma: The basic and clinic.

109. Identification of a new pharmacological activity of the phenylpiperazine derivative naftopidil: tubulin-binding drug.

110. Auranofin induces apoptosis by ROS-mediated ER stress and mitochondrial dysfunction and displayed synergistic lethality with piperlongumine in gastric cancer.

111. High-throughput screening identified selective inhibitors of exosome biogenesis and secretion: A drug repurposing strategy for advanced cancer.

112. Albendazole as a promising molecule for tumor control.

113. Drug repurposing screening identifies bortezomib and panobinostat as drugs targeting cancer associated fibroblasts (CAFs) by synergistic induction of apoptosis.

114. Drug Repositioning of Proton Pump Inhibitors for Enhanced Efficacy and Safety of Cancer Chemotherapy.

115. Repurposing the anti-epileptic drug sodium valproate as an adjuvant treatment for diffuse intrinsic pontine glioma.

116. HMG-CoA Reductase Inhibition Delays DNA Repair and Promotes Senescence After Tumor Irradiation.

117. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma.

118. Aging-related Repositioned Drugs, Donepezil and Sildenafil Citrate, Increase Apoptosis of Anti-mitotic Drug-resistant KBV20C Cells Through Different Molecular Mechanisms.

119. Highly Halaven-resistant KBV20C Cancer Cells Can Be Sensitized by Co-treatment with Fluphenazine.

120. The human immunodeficiency virus protease inhibitor ritonavir is potentially active against urological malignancies.

121. FTY720 inhibits mesothelioma growth in vitro and in a syngeneic mouse model.

122. Synthesis and biological evaluation of thiabendazole derivatives as anti-angiogenesis and vascular disrupting agents.

123. Phenotypic identification of the redox dye methylene blue as an antagonist of heat shock response gene expression in metastatic melanoma cells.

124. Combination treatment with naftopidil increases the efficacy of radiotherapy in PC-3 human prostate cancer cells.

125. Fenofibrate Suppresses Oral Tumorigenesis via Reprogramming Metabolic Processes: Potential Drug Repurposing for Oral Cancer.

126. Computational repositioning and preclinical validation of pentamidine for renal cell cancer.

127. The repurposed anthelmintic mebendazole in combination with trametinib suppresses refractory NRASQ61K melanoma.

128. Prevention of skin carcinogenesis by the beta-blocker carvedilol.

129. Ferroquine, the next generation antimalarial drug, has antitumor activity.

130. Comparative oncology approach to drug repurposing in osteosarcoma.

131. The EYA tyrosine phosphatase activity is pro-angiogenic and is inhibited by benzbromarone.

132. Quinacrine in endometrial cancer: Repurposing an old antimalarial drug.

133. Reprofiling using a zebrafish melanoma model reveals drugs cooperating with targeted therapeutics.

134. Three-Dimensional in Vitro Cell Culture Models in Drug Discovery and Drug Repositioning.

135. New HSP27 inhibitors efficiently suppress drug resistance development in cancer cells.

136. Regorafenib overcomes chemotherapeutic multidrug resistance mediated by ABCB1 transporter in colorectal cancer: Invitro and invivo study.

137. A statin-regulated microRNA represses human c-Myc expression and function.

138. Repurposing tofacitinib as an anti-myeloma therapeutic to reverse growth-promoting effects of the bone marrow microenvironment.

139. Replication Study: Discovery and preclinical validation of drug indications using compendia of public gene expression data.

140. Stromal microenvironment in type VII collagen-deficient skin: The ground for squamous cell carcinoma development.

141. Auranofin: repurposing an old drug for a golden new age.

142. Repurposing cephalosporin antibiotics as pro-senescent radiosensitizers.

143. Discovery of rafoxanide as a dual CDK4/6 inhibitor for the treatment of skin cancer.

144. The Hippo pathway in normal development and cancer.

145. Activation of PP2A by perphenazine induces apoptosis in T-ALL.

146. Antitumor effects of a drug combination targeting glycolysis, glutaminolysis and de novo synthesis of fatty acids.

147. Mevalonate pathway blockage enhances the efficacy of mTOR inhibitors with the activation of retinoblastoma protein in renal cell carcinoma.

148. Repurposing of Drugs Targeting YAP-TEAD Functions.

149. Homology modelling and molecular docking of MDR1 with chemotherapeutic agents in non-small cell lung cancer.

150. Clomipramine kills Trypanosoma brucei by apoptosis.

151. Autophagy Modulation in Disease Therapy: Where Do We Stand?

152. Hydralazine-valproate: a repositioned drug combination for the epigenetic therapy of cancer.

153. Novel spirobicyclic artemisinin analogues (artemalogues): Synthesis and antitumor activities.

154. Ibrutinib repurposing: from B-cell malignancies to solid tumors.

155. Drug repurposing using high-throughput screening identifies a promising drug combination to treat adrenocortical carcinoma.

156. Repurposing Vitamin D as an Anticancer Drug.

157. Molecular mimicry-based repositioning of nutlin-3 to anti-apoptotic Bcl-2 family proteins.

158. Selective inhibition of host cell signaling for rotavirus antivirals: PI3K/Akt/mTOR-mediated rotavirus pathogenesis.

159. [Role of bioinformatics in research and development of antipsychotic agents].

160. Chlorambucil in indolent mantle cell lymphoma--just another old drug for a new disease?

A2-2g4. Cluster 25 record titles

1. Repurposing Tecfidera for cancer.

2. Drug repurposing in cancer.

3. Biomarker-guided repurposing of chemotherapeutic drugs for cancer therapy: a novel strategy in drug development.

4. Revisiting Non-Cancer Drugs for Cancer Therapy.

5. Cancer Prevention and Interception: A New Era for Chemopreventive Approaches.

6. A novel method of transcriptional response analysis to facilitate drug repositioning for cancer therapy.

7. The potential to treat lung cancer via inhalation of repurposed drugs.

8. Drug Repurposing in the Development of Anticancer Agents.

9. Phospholipase PLA2G7, associated with aggressive prostate cancer, promotes prostate cancer cell migration and invasion and is inhibited by statins.

10. Drug Repositioning for Effective Prostate Cancer Treatment.

11. Drug Repurposing for Cancer Therapy.

12. Systematic repurposing screening in xenograft models identifies approved drugs with novel anti-cancer activity.

13. Targeting ADAM17 Sheddase Activity in Cancer.

14. Repurposing Drugs in Oncology (ReDO)-nitroglycerin as an anti-cancer agent.

15. Molecular pathways: trafficking of metabolic resources in the tumor microenvironment.

16. Potential anti-cancer drugs commonly used for other indications.

17. Repositioning of drugs for intervention in tumor progression and metastasis: Old drugs for new targets.

18. Drug Repurposing in Anticancer Reagent Development.

19. Leucovorin Enhances the Anti-cancer Effect of Bortezomib in Colorectal Cancer Cells.

20. Repurposing Drugs in Oncology (ReDO)-mebendazole as an anti-cancer agent.

21. Cancer drug discovery by repurposing: teaching new tricks to old dogs.

22. Colorectal Cancer Consensus Molecular Subtypes Translated to Preclinical Models Uncover Potentially Targetable Cancer Cell Dependencies.

23. [Chemoprevention of colorectal cancer for broad clinical use in the future].

24. Glipizide suppresses prostate cancer progression in the TRAMP model by inhibiting angiogenesis.

25. The impact of transcription on metabolism in prostate and breast cancers.

26. Cell line modeling for systems medicine in cancers (review).

27. Repositioning approved drugs for the treatment of problematic cancers using a screening approach.

28. Repurposing Drugs in Oncology (ReDO)-itraconazole as an anti-cancer agent.

29. Repurposing Drugs for Cancer Prevention.

30. A novel two-stage, transdisciplinary study identifies digoxin as a possible drug for prostate cancer treatment.

31. CONCORD biomarker prediction for novel drug introduction to different cancer types.

32. Transforming Cancer Prevention through Precision Medicine and Immune-oncology.

33. Metabolic reprogramming: the emerging concept and associated therapeutic strategies.

34. Repositioning of proton pump inhibitors in cancer therapy.

35. Combining genomic and network characteristics for extended capability in predicting synergistic drugs for cancer.

36. Misfolded proteins: from little villains to little helpers in the fight against cancer.

37. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors.

38. Repurposing Drugs in Oncology (ReDO)-Propranolol as an anti-cancer agent.

39. Identification of driver copy number alterations in diverse cancer types and application in drug repositioning.

40. [Metabolic Competition in Tumor Microenvironment].

41. Patient derived organoids to model rare prostate cancer phenotypes.

42. Tumor progression: the neuronal input.

43. Memantine induces apoptosis and inhibits cell cycle progression in LNCaP prostate cancer cells.

44. Irreversible LSD1 Inhibitors: Application of Tranylcypromine and Its Derivatives in Cancer Treatment.

45. Novel drug candidates for the treatment of metastatic colorectal cancer through global inverse gene-expression profiling.

46. Unexploited Antineoplastic Effects of Commercially Available Anti-Diabetic Drugs.

47. Barriers to preventive therapy for breast and other major cancers and strategies to improve uptake.

48. Metformin for Prevention and Treatment of Colon Cancer: A Reappraisal of Experimental and Clinical Data.

49. From drug response profiling to target addiction scoring in cancer cell models.

50. Repurposing Metformin as Therapy for Prostate Cancer within the STAMPEDE Trial Platform.

51. Repurposing of FDA-approved drugs against cancer - focus on metastasis.

52. In silico prescription of anticancer drugs to cohorts of 28 tumor types reveals targeting opportunities.

53. Repurposing drugs in oncology (ReDO)-cimetidine as an anti-cancer agent.

54. The positive inotropic agent DPI-201106 selectively reverses ABCB1-mediated multidrug resistance in cancer cell lines.

55. Identification of an old antibiotic clofoctol as a novel activator of unfolded protein response pathways and an inhibitor of prostate cancer.

56. Loss of BRCA1 in the Cells of Origin of Ovarian Cancer Induces Glycolysis: A Window of Opportunity for Ovarian Cancer Chemoprevention.

57. Statin and rottlerin small-molecule inhibitors restrict colon cancer progression and metastasis via MACC1.

58. Alcohol-abuse drug disulfiram targets cancer via p97 segregase adaptor NPL4.

59. Patient-Customized Drug Combination Prediction and Testing for T-cell Prolymphocytic Leukemia Patients.

60. Anti-cancer potential of a novel SERM ormeloxifene.

61. The mortality reducing effect of aspirin in colorectal cancer patients: Interpreting the evidence.

62. Repurposing Drugs in Oncology (ReDO)-diclofenac as an anti-cancer agent.

63. Repurposing itraconazole as an anticancer agent.

64. The Emerging Facets of Non-Cancerous Warburg Effect.

65. Therapeutic Effects of Repurposed Therapies in Non-Small Cell Lung Cancer: What Is Old Is New Again.

66. Personalization of cancer treatment using predictive simulation.

67. Repurposing Drugs in Oncology: Next Steps.

68. Identification of Small-Molecule Inhibitors of Human Golgi Mannosidase via a Drug Repositioning Screen.

69. Discovery and validation of the antimetastatic activity of citalopram in colorectal cancer.

70. The fatty acid synthase inhibitor triclosan: repurposing an anti-microbial agent for targeting prostate cancer.

71. The Concept of Hormesis in Cancer Therapy - Is Less More?

72. Possibility as an anti-cancer drug of astemizole: Evaluation of arrhythmogenicity by the chronic atrioventricular block canine model.

73. Repurposing psychiatric drugs as anti-cancer agents.

74. Targeting ion channels for cancer therapy by repurposing the approved drugs.

75. Pharmacotherapeutic Targeting of G Protein-Coupled Receptors in Oncology: Examples of Approved Therapies and Emerging Concepts.

76. Rho-associated kinase signalling and the cancer microenvironment: novel biological implications and therapeutic opportunities.

77. Designing novel therapies against sarcomas in the era of personalized medicine and economic crisis.

78. Role of ion channels in natural killer cell function towards cancer.

79. Anakoinosis: Communicative Reprogramming of Tumor Systems - for Rescuing from Chemorefractory Neoplasia.

80. Discovery and development of Seliciclib. How systems biology approaches can lead to better drug performance.

81. In Silico-Based Repositioning of Phosphinothricin as a Novel Technetium-99m Imaging Probe with Potential Anti-Cancer Activity.

82. Challenges and perspective of drug repurposing strategies in early phase clinical trials.

83. Repurposing and Rescuing of Mibefradil, an Antihypertensive, for Cancer: A Case Study.

84. Could cancer drugs be repurposed for use in Parkinson's and Alzheimer's?

85. Old-School Chemotherapy in Immunotherapeutic Combination in Cancer, A Low-cost Drug Repurposed.

86. The Architecture and Function of Monoclonal Antibody-Functionalized Mesoporous Silica Nanoparticles Loaded with Mifepristone: Repurposing Abortifacient for Cancer Metastatic Chemoprevention.

87. A chemical genomics approach to drug reprofiling in oncology: Antipsychotic drug risperidone as a potential adenocarcinoma treatment.

88. The Amide Local Anesthetic Lidocaine in Cancer Surgery-Potential Antimetastatic Effects and Preservation of Immune Cell Function? A Narrative Review.

89. A combinatorial screen of the CLOUD uncovers a synergy targeting the androgen receptor.

90. Repositioning therapy for thyroid cancer: new insights on established medications.

91. Immune Cell Metabolism in Tumor Microenvironment.

92. A Second WNT for Old Drugs: Drug Repositioning against WNT-Dependent Cancers.

93. Repurposing drugs in oncology (ReDO)-selective PDE5 inhibitors as anti-cancer agents.

94. Targeting the ubiquitin-proteasome system for cancer treatment: discovering novel inhibitors from nature and drug repurposing.

95. Cancer Drug Development Using Drosophila as an in vivo Tool: From Bedside to Bench and Back.

96. Seek and destroy: relating cancer drivers to therapies.

97. S100A4 in Cancer Metastasis: Wnt Signaling-Driven Interventions for Metastasis Restriction.

98. The wisdom of crowds and the repurposing of artesunate as an anticancer drug.

99. Drug repositioning for gynecologic tumors: a new therapeutic strategy for cancer.

100. An overview of angiogenesis inhibitors in Phase II studies for non-small-cell lung cancer.

101. Orlistat as a FASN inhibitor and multitargeted agent for cancer therapy.

102. Targeting Mevalonate Pathway in Cancer Treatment: Repurposing of Statins.

103. Mouse hospital and co-clinical trial project--from bench to bedside.

104. Insights into the Link Between Obesity and Cancer.

105. Drug Repurposing for Terminal-Stage Cancer Patients.

106. Reprofiling of Troglitazone Towards More Active and Less Toxic Derivatives: A New Hope for Cancer Treatment?

107. Pharmacological targeting of ion channels for cancer therapy: In vivo evidences.

108. Inhibition of LSD1 by Pargyline inhibited process of EMT and delayed progression of prostate cancer invivo.

109. The multitargeted drug ivermectin: from an antiparasitic agent to a repositioned cancer drug.

110. Some leopards can change their spots: potential repositioning of stem cell reprogramming compounds as anti-cancer agents.

111. Molecular-targeted nanotherapies in cancer: enabling treatment specificity.

112. Repurposing drugs in your medicine cabinet: untapped opportunities for cancer therapy?

113. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types.

114. CaV channels and cancer: canonical functions indicate benefits of repurposed drugs as cancer therapeutics.

115. The antineoplastic properties of FTY720: evidence for the repurposing of fingolimod.

116. Repurposing Drugs in Oncology (ReDO)-clarithromycin as an anti-cancer agent.

117. Anti-malarials are anti-cancers and vice versa - one arrow two sparrows.

118. Poly lactic-co-glycolic acid controlled delivery of disulfiram to target liver cancer stem-like cells.

119. Discovering proteasomal deubiquitinating enzyme inhibitors for cancer therapy: lessons from rational design, nature and old drug reposition.

120. Idiopathic pulmonary fibrosis and cancer: do they really look similar?

121. Drug repurposing for the treatment of glioblastoma multiforme.

122. Feedback Activation of STAT3 as a Cancer Drug-Resistance Mechanism.

123. Novel therapeutic strategy for cancer and autoimmune conditions: Modulating cell metabolism and redox capacity.

124. Repurposing itraconazole for the treatment of cancer.

125. SRSF6-regulated alternative splicing that promotes tumour progression offers a therapy target for colorectal cancer.

126. Role of TGFbeta in regulation of the tumor microenvironment and drug delivery (review).

127. Roles of the RANKL-RANK axis in antitumour immunity - implications for therapy.

128. [Paradigms, doses and controversies in cancer therapy].

129. Copper Complexes in Cancer Therapy.

130. Cancer: fundamentals behind pH targeting and the double-edged approach.

131. Anticancer and Immunogenic Properties of Cardiac Glycosides.

132. Aldo-Keto Reductase (AKR) 1C3 inhibitors: a patent review.

133. Drug Repurposing of Metabolic Agents in Malignant Glioma.

134. New use for old drugs? Prospective targets of chloroquines in cancer therapy.

135. Chemoprevention agents for melanoma: a path forward into phase 3 clinical trials.

136. Development and Characterization of Bladder Cancer Patient-Derived Xenografts for Molecularly Guided Targeted Therapy.

137. Study finds possible role for aspirin as treatment for colon cancer.

138. Low-dose salinomycin induces anti-leukemic responses in AML and MLL.

139. Repurposing apoptosis-inducing cancer drugs to treat schistosomiasis.

140. Metabolic reprogramming in clear cell renal cell carcinoma.

141. Drug Repositioning Meets Precision in Glioblastoma.

142. Teaching an old dog new tricks: drug repositioning in small cell lung cancer.

143. Overcoming Drug Development Bottlenecks With Repurposing: Repurposing biguanides to target energy metabolism for cancer treatment.

144. Repurposing Cationic Amphiphilic Antihistamines for Cancer Treatment.

145. Revisiting nomenclature for the description of prostate cancer androgen-responsiveness.

146. Perioperative therapies - Enhancing the impact of cancer surgery with repurposed drugs.

147. Trimodal Therapy: Combining Hyperthermia with Repurposed Bexarotene and Ultrasound for Treating Liver Cancer.

148. Radiation-Drug Combinations to Improve Clinical Outcomes and Reduce Normal Tissue Toxicities: Current Challenges and New Approaches: Report of the Symposium Held at the 63rd Annual Meeting of the Radiation Research Society, 15-18 October 2017; Cancun, Mexico.

149. A screening cascade to identify ERbeta ligands.

150. Hyaluronan-Derived Swelling of Solid Tumors, the Contribution of Collagen and Cancer Cells, and Implications for Cancer Therapy.

151. Repositioning compounds from cancer drug discovery to IPF: PI3K inhibition.

152. Case Report: Propranolol increases the therapeutic response to temozolomide in a patient with metastatic paraganglioma.

153. Appraisal of mechanisms of radioprotection and therapeutic approaches of radiation countermeasures.

154. Mitochondrial dysfunction and potential anticancer therapy.

155. Deploying ibrutinib to lung cancer: another step in the quest towards drug repurposing.

156. Nanomedicine for prostate cancer using nanoemulsion: A review.

157. The repositioning of the anti-fungal agent ciclopirox olamine as a novel therapeutic agent for the treatment of haematologic malignancy.

158. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases.

159. Summary of the 45th annual meeting on women's cancers.

160. Drug repositioning from bench to bedside: tumour remission by the antihelmintic drug mebendazole in refractory metastatic colon cancer.

161. Targeting Hypoxia-Inducible Factors for Antiangiogenic Cancer Therapy.

162. Repurposing cancer drugs to treat neurological diseases - Src inhibitors as examples.

163. Chloroquine-containing compounds: a patent review (2010 - 2014).

164. Marketed drugs used for the management of hypercholesterolemia as anticancer armament.

165. Cell Metabolism Clinical and Translational Reports.

166. The spatial organization of intra-tumour heterogeneity and evolutionary trajectories of metastases in hepatocellular carcinoma.

167. Cancer immunotherapy without frontiers: 2nd Annual Immuno-Oncology Meeting of the Centro de Investigacion de Cancer en Sonora (CICS), Ciudad Obregon, Sonora Mexico, Dec 2-4, 2016.

168. Does the oncology community have a rejection bias when it comes to repurposed drugs?

169. Nonprofit drugs as the salvation of the world's healthcare systems: the case of Antabuse (disulfiram).

170. Repurposing approved and abandoned drugs for the treatment and prevention of cancer through public-private partnership.

171. Clarithromycin as a "repurposing drug" against MALT lymphoma.

A2-2g5. Cluster 5 record titles

1. Modified Metformin as a More Potent Anticancer Drug: Mitochondrial Inhibition, Redox Signaling, Antiproliferative Effects and Future EPR Studies.

2. No association between metformin use and survival in patients with pancreatic cancer: An observational cohort study.

3. Metformin in patients with advanced pancreatic cancer: a double-blind, randomised, placebo-controlled phase 2 trial.

4. Mitochondria-targeted metformins: anti-tumour and redox signalling mechanisms.

5. Model-based unsupervised learning informs metformin-induced cell-migration inhibition through an AMPK-independent mechanism in breast cancer.

6. Repurposing of metformin and aspirin by targeting AMPK-mTOR and inflammation for pancreatic cancer prevention and treatment.

7. Old drug, new trick: repurposing metformin for gynecologic cancers?

8. Repositioning metformin in cancer: genetics, drug targets, and new ways of delivery.

9. Metformin directly acts on mitochondria to alter cellular bioenergetics.

10. Repurposing metformin for the prevention of cancer and cancer recurrence.

11. Metformin as a geroprotector: experimental and clinical evidence.

12. Metformin: its emerging role in oncology.

13. MATE2 Expression Is Associated with Cancer Cell Response to Metformin.

14. [New perspectives for metformin in cancer therapy].

15. Metformin use and gynecological cancers: A novel treatment option emerging from drug repositioning.

16. Metformin for non-small cell lung cancer patients: Opportunities and pitfalls.

17. Mitochondria-Targeted Analogues of Metformin Exhibit Enhanced Antiproliferative and Radiosensitizing Effects in Pancreatic Cancer Cells.

18. Metformin Use in Relation With Survival Outcomes of Patients With Renal Cell Carcinoma.

19. Metformin repositioning as antitumoral agent: selective antiproliferative effects in human glioblastoma stem cells, via inhibition of CLIC1-mediated ion current.

20. Prediction of Candidate Drugs for Treating Pancreatic Cancer by Using a Combined Approach.

21. The Role of Common Pharmaceutical Agents on the Prevention and Treatment of Pancreatic Cancer.

22. One-carbon metabolism: an aging-cancer crossroad for the gerosuppressant metformin.

23. Validating drug repurposing signals using electronic health records: a case study of metformin associated with reduced cancer mortality.

24. Expression of DRD2 Is Increased in Human Pancreatic Ductal Adenocarcinoma and Inhibitors Slow Tumor Growth in Mice.

25. Use of metformin and survival of patients with high-grade glioma.

26. Metformin as a repurposed therapy in advanced non-small cell lung cancer (NSCLC): results of a phase II trial.

27. Repurposing old drugs to chemoprevention: the case of metformin.

28. A drug-repositioning screen for primary pancreatic ductal adenocarcinoma cells identifies 6-thioguanine as an effective therapeutic agent for TPMT-low cancer cells.

29. A selective mitochondrial-targeted chlorambucil with remarkable cytotoxicity in breast and pancreatic cancers.

30. A novel chemoradiation targeting stem and nonstem pancreatic cancer cells by repurposing disulfiram.

31. Blocking IL-6/GP130 signaling inhibits cell viability/proliferation, glycolysis, and colony forming activity in human pancreatic cancer cells.

32. Warfarin Blocks Gas6-Mediated Axl Activation Required for Pancreatic Cancer Epithelial Plasticity and Metastasis.

33. Bazedoxifene as a Novel GP130 Inhibitor for Pancreatic Cancer Therapy.

34. Challenges and future directions in therapeutics for pancreatic ductal adenocarcinoma.

35. Repurposing Established Compounds to Target Pancreatic Cancer Stem Cells (CSCs).

36. Study protocol of a phase IB/II clinical trial of metformin and chloroquine in patients with IDH1-mutated or IDH2-mutated solid tumours.

37. Potentiating the effects of radiotherapy in rectal cancer: the role of aspirin, statins and metformin as adjuncts to therapy.

38. Pancreas Cancer Precision Treatment Using Avatar Mice from a Bioinformatics Perspective.

39. A therapy for FXS?

40. Metastasis and chemoresistance in CD133 expressing pancreatic cancer cells are dependent on their lipid raft integrity.

41. High-throughput screening of FDA-approved drugs using oxygen biosensor plates reveals secondary mitofunctional effects.

A2-2g6. Cluster 11 record titles

1. Doxycycline inhibits the cancer stem cell phenotype and epithelial-to-mesenchymal transition in breast cancer.

2. PAF-Wnt signaling-induced cell plasticity is required for maintenance of breast cancer cell stemness.

3. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy.

4. Identification of FDA-approved drugs targeting breast cancer stem cells along with biomarkers of sensitivity.

5. Drug repurposing screen identifies lestaurtinib amplifies the ability of the poly (ADP-ribose) polymerase 1 inhibitor AG14361 to kill breast cancer associated gene-1 mutant and wild type breast cancer cells.

6. Tumor selective cytotoxic action of a thiomorpholin hydroxamate inhibitor (TMI-1) in breast cancer.

7. Buformin inhibits the stemness of erbB-2-overexpressing breast cancer cells and premalignant mammary tissues of MMTV-erbB-2 transgenic mice.

8. FoxO3a Mediates the Inhibitory Effects of the Antiepileptic Drug Lamotrigine on Breast Cancer Growth.

9. Pathway-Based Drug Repositioning for Breast Cancer Molecular Subtypes.

10. Existing drugs and their application in drug discovery targeting cancer stem cells.

11. Pre-clinical effects of metformin and aspirin on the cell lines of different breast cancer subtypes.

12. Inhibitors of Cancer Stem Cells.

13. The CARMA3-Bcl10-MALT1 Signalosome Drives NFkappaB Activation and Promotes Aggressiveness in Angiotensin II Receptor-Positive Breast Cancer.

14. The novel JNK inhibitor AS602801 inhibits cancer stem cells in vitro and in vivo.

15. Metformin and propranolol combination prevents cancer progression and metastasis in different breast cancer models.

16. Breast cancer cells condition lymphatic endothelial cells within pre-metastatic niches to promote metastasis.

17. Novel modeling of cancer cell signaling pathways enables systematic drug repositioning for distinct breast cancer metastases.

18. Cytogenomic profiling of breast cancer brain metastases reveals potential for repurposing targeted therapeutics.

19. Repositioning of antibiotic levofloxacin as a mitochondrial biogenesis inhibitor to target breast cancer.

20. Anti-protozoal and anti-bacterial antibiotics that inhibit protein synthesis kill cancer subtypes enriched for stem cell-like properties.

21. [Cancer stem cells as the therapeutic target of tomorrow].

22. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer.

23. Integration of a prognostic gene module with a drug sensitivity module to identify drugs that could be repurposed for breast cancer therapy.

24. Propranolol and breast cancer-a work in progress.

25. Emerging nanotherapeutic strategies in breast cancer.

26. Aripiprazole, an Antipsychotic and Partial Dopamine Agonist, Inhibits Cancer Stem Cells and Reverses Chemoresistance.

27. Drug-repositioning screening identified piperlongumine as a direct STAT3 inhibitor with potent activity against breast cancer.

28. Cadherin-11 in poor prognosis malignancies and rheumatoid arthritis: common target, common therapies.

29. New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate.

30. An Integrative Drug Repurposing Pipeline: Switching Viral Drugs to Breast Cancer.

31. Hiding in plain view: the potential for commonly used drugs to reduce breast cancer mortality.

32. Mucuna pruriens (L.) DC chemo sensitize human breast cancer cells via downregulation of prolactin-mediated JAK2/STAT5A signaling.

33. Doxycycline and therapeutic targeting of the DNA damage response in cancer cells: old drug, new purpose.

34. Imidazole Antifungal Drugs Inhibit the Cell Proliferation and Invasion of Human Breast Cancer Cells.

35. Repositioning chloroquine and metformin to eliminate cancer stem cell traits in pre-malignant lesions.

36. Simultaneous blockade of IL-6 and CCL5 signaling for synergistic inhibition of triple-negative breast cancer growth and metastasis.

37. The heterogeneity of cancer stem-like cells at the invasive front.

38. Cancer stem cell (CSC) inhibitors: a review of recent patents (2012-2015).

39. The Tissue-Reconstructing Ability of Colon CSCs Is Enhanced by FK506 and Suppressed by GSK3 Inhibition.

40. The sodium channel-blocking antiepileptic drug phenytoin inhibits breast tumour growth and metastasis.

41. Targeting cancer stem cells with dietary phytochemical - Repositioned drug combinations.

42. PEGylated chitosan nanoparticles potentiate repurposing of ormeloxifene in breast cancer therapy.

43. Repurposing atovaquone: targeting mitochondrial complex III and OXPHOS to eradicate cancer stem cells.

44. Use of monoclonal antibody-IRDye800CW bioconjugates in the resection of breast cancer.

45. Chk1 as a new therapeutic target in triple-negative breast cancer.

46. Mitochondrial biogenesis is required for the anchorage-independent survival and propagation of stem-like cancer cells.

47. Targeting of embryonic annexin A2 expressed on ovarian and breast cancer by the novel monoclonal antibody 2448.

48. Inhibition of PI4K IIIalpha radiosensitizes in human tumor xenograft and immune-competent syngeneic murine tumor model.

49. Carglumic acid promotes apoptosis and suppresses cancer cell proliferation in vitro and in vivo.

50. Therapeutic potential for phenytoin: targeting Na(v)1.5 sodium channels to reduce migration and invasion in metastatic breast cancer.

51. Repositioning of Anti-parasitic Drugs in Cyclodextrin Inclusion Complexes for Treatment of Triple-Negative Breast Cancer.

52. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs).

53. Repurposing of bisphosphonates for the prevention and therapy of nonsmall cell lung and breast cancer.

54. Inhibition of Wnt signalling and breast tumour growth by the multi-purpose drug suramin through suppression of heterotrimeric G proteins and Wnt endocytosis.

55. Targeting epithelial-mesenchymal plasticity in cancer: clinical and preclinical advances in therapy and monitoring.

56. Virtual screening-driven repositioning of etoposide as CD44 antagonist in breast cancer cells.

57. Reactivation of cAMP Pathway by PDE4D Inhibition Represents a Novel Druggable Axis for Overcoming Tamoxifen Resistance in ER-positive Breast Cancer.

58. Folate Receptor-Targeted Polymeric Micellar Nanocarriers for Delivery of Orlistat as a Repurposed Drug against Triple-Negative Breast Cancer.

59. Voltage-gated sodium channels and metastatic disease.

60. [Novel strategies of ovarian cancer treatment].

61. Repurposing Registered Drugs as Antagonists for Protease-Activated Receptor

62. Optimized acriflavine-loaded lipid nanocapsules as a safe and effective delivery system to treat breast cancer.

63. Olanzapine, an Atypical Antipsychotic, Inhibits Survivin Expression and Sensitizes Cancer Cells to Chemotherapeutic Agents.

64. Angiotensin inhibition enhances drug delivery and potentiates chemotherapy by decompressing tumour blood vessels.

65. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen.

66. Voltage-gated sodium channel as a target for metastatic risk reduction with re-purposed drugs.

A2-2h. Leaf clusters under Cluster 55

There are eight leaf clusters under Cluster 55: Cluster 2 (48), Cluster 8 (30), Cluster 24 (117), Cluster 3 (33), Cluster 10 (46), Cluster 31 (151), Cluster 28 (97), Cluster 30 (112).

*Cluster 2 focuses on Alzheimer's Disease treatments

*Cluster 8 focuses on neurodegenerative disease treatments, especially Parkinson's Disease

*Cluster 24 focuses on treatments for brain disease, especially stroke

*Cluster 3 focuses on drug repurposing patent applications

*Cluster 10 focuses on glioblastoma treatments

*Cluster 31 focuses on anti-inflammatory treatments

*Cluster 28 focuses on treatments for addiction disorders (especially alcohol use) and chronic pain

*Cluster 30 focuses on cancer treatments, especially metronomic chemotherapy

A2-2h1. Cluster 2 record titles

1. Emerging amyloid and tau targeting treatments for Alzheimer's disease.

2. Alzheimer's Disease (AD) therapeutics - 1: Repeated clinical failures continue to question the amyloid hypothesis of AD and the current understanding of AD causality.

3. Drug repositioning: an opportunity to develop novel treatments for Alzheimer's disease.

4. Discovering new treatments for Alzheimer's disease by repurposing approved medications.

5. [A review of drugs for treatment of Alzheimer's disease in clinical trials: main trends].

6. Emerging treatments for Alzheimer's disease for non-amyloid and non-tau targets.

7. Drug repositioning approaches for the discovery of new therapeutics for Alzheimer's disease.

8. A review: treatment of Alzheimer's disease discovered in repurposed agents.

9. Approved drugs are to be studied for use in Alzheimer's disease.

10. Cyclin dependent kinase 5: A novel avenue for Alzheimer's disease.

11. Potential repurposing of oncology drugs for the treatment of Alzheimer's disease.

12. Challenges for Alzheimer's Disease Therapy: Insights from Novel Mechanisms Beyond Memory Defects.

13. Progresses in treating agitation: a major clinical challenge in Alzheimer's disease.

14. Drug Repositioning for Alzheimer's Disease Based on Systematic 'omics' Data Mining.

15. Medical genetics-based drug repurposing for Alzheimer's disease.

16. Repurposed Drugs as Potential Therapeutic Candidates for the Management of Alzheimer's Disease.

17. Drugs in Clinical Trials for Alzheimer's Disease: The Major Trends.

18. Clozapine Improves Memory Impairment and Reduces Abeta Level in the Tg-APPswe/PS1dE9 Mouse Model of Alzheimer's Disease.

19. Metabolic Dysfunction in Alzheimer's Disease: From Basic Neurobiology to Clinical Approaches.

20. The Coming of Age of the Angiotensin Hypothesis in Alzheimer's Disease: Progress Toward Disease Prevention and Treatment?

21. Recent progress in repositioning Alzheimer's disease drugs based on a multitarget strategy.

22. Latest treatment options for Alzheimer's disease, Parkinson's disease dementia and dementia with Lewy bodies.

23. Repurposing diabetes drugs for brain insulin resistance in Alzheimer disease.

24. Microglial KCa3.1 Channels as a Potential Therapeutic Target for Alzheimer's Disease.

25. Molecular investigations of protriptyline as a multi-target directed ligand in Alzheimer's disease.

26. Do Cancer Drugs Counteract Neurodegeneration? Repurposing forAlzheimer's Disease.

27. Is a potential Alzheimer's therapy already in use for other conditions? Can medications for hypertension, diabetes and acne help with the symptoms?

28. Drug repositioning for Alzheimer's disease.

29. T3D-959: A Multi-Faceted Disease Remedial Drug Candidate for the Treatment of Alzheimer's Disease.

30. [Alzheimer disease: the temptation coming from off-label use].

31. Combining in vitro and in silico Approaches to Find New Candidate Drugs Targeting the Pathological Proteins Related to the Alzheimer's Disease.

32. Insights into the Drug Repositioning Applied to the Alzheimer's Disease Treatment and Future Perspectives.

33. Research and development of anti-Alzheimer's disease drugs: an update from the perspective of technology flows.

34. Advanced Assay Monitoring APP-Carboxyl-Terminal Fragments as Markers of APP Processing in Alzheimer Disease Mouse Models.

35. In silico repurposing of antipsychotic drugs for Alzheimer's disease.

36. iPSC-Based Compound Screening and InVitro Trials Identify a Synergistic Anti-amyloid beta Combination for Alzheimer's Disease.

37. Exploring the nexus of Alzheimer's disease and related dementias with cancer and cancer therapies: A convening of the Alzheimer's Association & Alzheimer's Drug Discovery Foundation.

38. Drug repositioning in Alzheimer's disease.

39. AlzhCPI: A knowledge base for predicting chemical-protein interactions towards Alzheimer's disease.

40. Design, Synthesis, and Biological Evaluation of Orally Available First-Generation Dual-Target Selective Inhibitors of Acetylcholinesterase (AChE) and Phosphodiesterase 5 (PDE5) for the Treatment of Alzheimer's Disease.

41. One for All? Hitting Multiple Alzheimer's Disease Targets with One Drug.

42. Mild cognitive impairment due to Alzheimer disease: Contemporary approaches to diagnostics and pharmacological intervention.

43. Alzheimer's disease master regulators analysis: search for potential molecular targets and drug repositioning candidates.

44. Epigenetic Drug Repositioning for Alzheimer's Disease Based on Epigenetic Targets in Human Interactome.

45. Tacrine-deferiprone hybrids as multi-target-directed metal chelators against Alzheimer's disease: a two-in-one drug.

46. Value added medicines: what value repurposed medicines might bring to society?

47. Application of molecular framework-based data-mining method in the search for beta-secretase 1 inhibitors through drug repurposing.

48. The case of galantamine: repurposing and late blooming of a cholinergic drug.

A2-2h2. Cluster 8 record titles

1. Drug Repurposing in Parkinson's Disease.

2. Repurposed drugs for use in Parkinson's disease.

3. Advances in drug development for Parkinson's disease: present status.

4. Recent Advances in Drug Repurposing for Parkinson's Disease.

5. Cell specificity dictates similarities in gene expression in multiple sclerosis, Parkinson's disease, and Alzheimer's disease.

6. Linked clinical trials--the development of new clinical learning studies in Parkinson's disease using screening of multiple prospective new treatments.

7. Combining Human Disease Genetics and Mouse Model Phenotypes towards Drug Repositioning for Parkinson's disease.

8. Old wines in new bottles: Repurposing opportunities for Parkinson's disease.

9. Validating the Predicted Effect of Astemizole and Ketoconazole Using a Drosophila Model of Parkinson's Disease.

10. Repurposing sex steroids and related drugs as potential treatment for Parkinson's disease.

11. Biomarker repurposing: Therapeutic drug monitoring of serum theophylline offers a potential diagnostic biomarker of Parkinson's disease.

12. Old Drugs as New Treatments for Neurodegenerative Diseases.

13. The Linked Clinical Trials Initiative (LCT) for Parkinson's disease.

14. In silico drug screening by using genome-wide association study data repurposed dabrafenib, an anti-melanoma drug, for Parkinson's disease.

15. Exenatide and the treatment of patients with Parkinson's disease.

16. Clinical utility of neuroprotective agents in neurodegenerative diseases: current status of drug development for Alzheimer's, Parkinson's and Huntington's diseases, and amyotrophic lateral sclerosis.

17. CNS repurposing - Potential new uses for old drugs: Examples of screens for Alzheimer's disease, Parkinson's disease and spasticity.

18. Repurposing of Copper(II)-chelating Drugs for the Treatment of Neurodegenerative Diseases.

19. Using Drugs as Molecular Probes: AComputational Chemical Biology Approach in Neurodegenerative Diseases.

20. Overcoming obstacles to repurposing for neurodegenerative disease.

21. From stroke to neurodegenerative diseases: The multi-target neuroprotective effects of 3-n-butylphthalide and its derivatives.

22. Neurodegenerative disease: Halting neurodegeneration - are repurposed drugs the answer?

23. Exploiting the therapeutic potential of ready-to-use drugs: Repurposing antibiotics against amyloid aggregation in neurodegenerative diseases.

24. Neurotrophin strategies for neuroprotection: are they sufficient?

25. Can commonly prescribed drugs be repurposed for the prevention or treatment of Alzheimer's and other neurodegenerative diseases? Protocol for an observational cohort study in the UK Clinical Practice Research Datalink.

26. Six psychotropics for pre-symptomatic & early Alzheimer's (MCI), Parkinson's, and Huntington's disease modification.

27. Intelligent and effective informatic deconvolution of "Big Data" and its future impact on the quantitative nature of neurodegenerative disease therapy.

28. Approaches for discovering anti-prion compounds: lessons learned and challenges ahead.

29. Repackaging FDA-approved drugs for degenerative diseases: promises and challenges.

30. Drugs in search of diseases.

A2-2h3. Cluster 24 record titles

1. Advanced neuroprotection for brain ischemia: an alternative approach to minimize stroke damage.

2. Minocycline repurposing in critical illness: focus on stroke.

3. Drug repurposing for vascular protection after acute ischemic stroke.

4. Drug repurposing for immune modulation in acute ischemic stroke.

5. Poly(ADP-ribose) polymerase is not involved in the neuroprotection exerted by azithromycin against ischemic stroke in mice.

6. Mmp-9 inhibition: a therapeutic strategy in ischemic stroke.

7. Drug repurposing for drug development in stroke.

8. A Combination of Three Repurposed Drugs Administered at Reperfusion as a Promising Therapy for Postischemic Brain Injury.

9. Azithromycin protects mice against ischemic stroke injury by promoting macrophage transition towards M2 phenotype.

10. Stroke is one of the most common and undertreated diseases in the world, and ischemic stroke makes up more than 85% of all strokes. Introduction.

11. Clinical validation of blood/brain glutamate grabbing in acute ischemic stroke.

12. Activation of RXR/PPARgamma underlies neuroprotection by bexarotene in ischemic stroke.

13. Dexpramipexole improves bioenergetics and outcome in experimental stroke.

14. Pharmacological treatment and prevention of cerebral small vessel disease: a review of potential interventions.

15. Development of a stretch-induced neurotrauma model for medium-throughput screening in vitro: identification of rifampicin as a neuroprotectant.

16. Senicapoc: Repurposing a Drug to Target Microglia KCa3.1 in Stroke.

17. Re-engineering a neuroprotective, clinical drug as a procognitive agent with high in vivo potency and with GABAA potentiating activity for use in dementia.

18. Repurposing an old drug to improve the use and safety of tissue plasminogen activator for acute ischemic stroke: minocycline.

19. Parkinson's Disease, Diabetes and Cognitive Impairment.

20. Combination of acamprosate and baclofen as a promising therapeutic approach for Parkinson's disease.

21. Post-ischemic treatment with azithromycin protects ganglion cells against retinal ischemia/reperfusion injury in the rat.

22. Repurposing an old drug to improve the use and safety of tissue plasminogen activator for acute ischemic stroke: minocycline.

23. Exendin-4 ameliorates traumatic brain injury-induced cognitive impairment in rats.

24. Fast, non-competitive and reversible inhibition of NMDA-activated currents by 2-BFI confers neuroprotection.

25. alpha-Methyl-alpha-phenylsuccinimide ameliorates neurodegeneration in a C. elegans model of TDP-43 proteinopathy.

26. Combining two repurposed drugs as a promising approach for Alzheimer's disease therapy.

27. Repurposed drugs targeting eIF2?-P-mediated translational repression prevent neurodegeneration in mice.

28. Doxycycline counteracts neuroinflammation restoring memory in Alzheimer's disease mouse models.

29. Modulation of GLP-1 signaling as a novel therapeutic approach in the treatment of Alzheimer's disease pathology.

30. Potential repositioning of exemestane as a neuroprotective agent for Parkinson's disease.

31. Repurposing and repositioning neurosteroids in the treatment of traumatic brain injury: A report from the trenches.

32. Sulforaphane Prevents Neuronal Apoptosis and Memory Impairment in Diabetic Rats.

33. Hippocampal Neurophysiologic Changes after Mild Traumatic Brain Injury and Potential Neuromodulation Treatment Approaches.

34. Drug repurposing for drug development in stroke.

35. Metformin treatment ameliorates diabetes-associated decline in hippocampal neurogenesis and memory via phosphorylation of insulin receptor substrate 1.

36. Utility of Induced Pluripotent Stem Cells for the Study and Treatment of Genetic Diseases: Focus on Childhood Neurological Disorders.

37. High-Throughput Screening forIdentification of Blood-Brain Barrier Integrity Enhancers: A Drug Repurposing Opportunity to Rectify Vascular Amyloid Toxicity.

38. A staged screening of registered drugs highlights remyelinating drug candidates for clinical trials.

39. Acetaminophen attenuates dopamine neuron degeneration in animal models of Parkinson's disease.

40. Modeling Niemann Pick type C1 using human embryonic and induced pluripotent stem cells.

41. Human Pluripotent Stem Cell-derived Cortical Neurons for High Throughput Medication Screening in Autism: A Proof of Concept Study in SHANK3 Haploinsufficiency Syndrome.

42. Neuroprotective and immunomodulatory effects of raloxifene in the myenteric plexus of a mouse model of Parkinson's disease.

43. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease.

44. A phase Ib multiple ascending dose study of the safety, tolerability, and central nervous system availability of AZD0530 (saracatinib) in Alzheimer's disease.

45. Platelet Hyperreactivity in Diabetes: Focus on GPVI Signaling-Are Useful Drugs Already Available?

46. Polytherapy with a combination of three repurposed drugs (PXT3003) down-regulates Pmp22 over-expression and improves myelination, axonal and functional parameters in models of CMT1A neuropathy.

47. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease.

48. Strategy for identifying repurposed drugs for the treatment of cerebral cavernous malformation.

49. The proton-pump inhibitor lansoprazole enhances amyloid beta production.

50. Ursocholanic acid rescues mitochondrial function in common forms of familial Parkinson's disease.

51. Identification of new EphA4 inhibitors by virtual screening of FDA-approved drugs.

52. Folic Acid Exerts Post-Ischemic Neuroprotection In Vitro Through HIF-1alpha Stabilization.

53. Preclinical Evidence Supporting Early Initiation of Citalopram Treatment in Machado-Joseph Disease.

54. CK2 inhibition confers functional protection to young and aging axons against ischemia by differentially regulating the CDK5 and AKT signaling pathways.

55. Opportunities for the repurposing of PARP inhibitors for the therapy of non-oncological diseases.

56. Repositioning drugs for traumatic brain injury - N-acetyl cysteine and Phenserine.

57. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist.

58. Cell-based screening identifies paroxetine as an inhibitor of diabetic endothelial dysfunction.

59. Myelination induction by a histamine H3 receptor antagonist in a mouse model of preterm white matter injury.

60. Rationale for an experimental treatment of retinitis pigmentosa: 140-month test of hypothesis with one patient.

61. Novel Tadalafil Derivatives Ameliorates Scopolamine-Induced Cognitive Impairment in Mice via Inhibition of Acetylcholinesterase (AChE) and Phosphodiesterase 5 (PDE5).

62. The Src/c-Abl pathway is a potential therapeutic target in amyotrophic lateral sclerosis.

63. Isogenic FUS-eGFP iPSC Reporter Lines Enable Quantification of FUS Stress Granule Pathology that Is Rescued by Drugs Inducing Autophagy.

64. Systemic hemin therapy attenuates blood-brain barrier disruption after intracerebral hemorrhage.

65. DPP-4 inhibitors promote proliferation and migration of rat brain microvascular endothelial cells under hypoxic/high-glucose conditions, potentially through the SIRT1/HIF-1/VEGF pathway.

66. Stem cells in pediatric cardiology.

67. Candesartan stimulates reparative angiogenesis in ischemic retinopathy model: role of hemeoxygenase-1 (HO-1).

68. Quantitative high-throughput screening identifies cytoprotective molecules that enhance SUMO conjugation via the inhibition of SUMO-specific protease (SENP)2.

69. Repositioning of Omarigliptin as a once-weekly intranasal Anti-parkinsonian Agent.

70. Liraglutide attenuates the depressive- and anxiety-like behaviour in the corticosterone induced depression model via improving hippocampal neural plasticity.

71. Modeling cerebrovascular pathophysiology in amyloid-beta metabolism using neural-crest-derived smooth muscle cells.

72. Spironolactone is an antagonist of NRG1-ERBB4 signaling and schizophrenia-relevant endophenotypes in mice.

73. Inhibition of ACE Retards Tau Hyperphosphorylation and Signs of Neuronal Degeneration in Aged Rats Subjected to Chronic Mild Stress.

74. Protein Kinases and Parkinson's Disease.

75. Neuron-specific regulation of class I PI3K catalytic subunits and their dysfunction in brain disorders.

76. The dual targeting of EGFR and ErbB2 with the inhibitor Lapatinib corrects high glucose-induced apoptosis and vascular dysfunction by opposing multiple diabetes-induced signaling changes.

77. Repurposing HAMI3379 to Block GPR17 and Promote Rodent and Human Oligodendrocyte Differentiation.

78. Effects of Benzothiazolamines on Voltage-Gated Sodium Channels.

79. Combination of valproic acid and morpholino splice-switching oligonucleotide produces improved outcomes in spinal muscular atrophy patient-derived fibroblasts.

80. Reduction of amyloid-beta deposition and attenuation of memory deficits by tolfenamic acid.

81. Citalopram Reduces Aggregation of ATXN3 in a YAC Transgenic Mouse Model of Machado-Joseph Disease.

82. Minocycline attenuates mechanical allodynia and expression of spinal NMDA receptor 1 subunit in rat neuropathic pain model.

83. Nitrosylation of GAPDH augments pathological tau acetylation upon exposure to amyloid-beta.

84. Development of Molecular Therapies for Venous Malformations.

85. SUMOylation in brain ischemia: Patterns, targets, and translational implications.

86. Stress-Activated Kinase Mitogen-Activated Kinase Kinase-7 Governs Epigenetics of Cardiac Repolarization for Arrhythmia Prevention.

87. Fine-tuning PERK signaling for neuroprotection.

88. Small Molecules in Development for the Treatment of Spinal Muscular Atrophy.

89. Paroxetine-mediated GRK2 inhibition reverses cardiac dysfunction and remodeling after myocardial infarction.

90. Tamoxifen Provides Structural and Functional Rescue in Murine Models of Photoreceptor Degeneration.

91. Nutrients, neurogenesis and brain ageing: From disease mechanisms to therapeutic opportunities.

92. Drug Repurposing for Duchenne Muscular Dystrophy: The Monoamine Oxidase B Inhibitor Safinamide Ameliorates the Pathological Phenotype in mdx Mice and in Myogenic Cultures From DMD Patients.

93. Clobetasol promotes remyelination in a mouse model of neuromyelitis optica.

94. Neutrophil Infiltration and Matrix Metalloproteinase-9 in Lacunar Infarction.

95. Rescue of cell death and inflammation of a mouse model of complex 1-mediated vision loss by repurposed drug molecules.

96. Interferons in Traumatic Brain and Spinal Cord Injury: Current Evidence for Translational Application.

97. Ebselen inhibits the activity of acetylcholinesterase globular isoform G4 in vitro and attenuates scopolamine-induced amnesia in mice.

98. Treating the dysfunctional placenta.

99. Amino acid conjugated chitosan nanoparticles for the brain targeting of a model dipeptidyl peptidase-4 inhibitor.

100. Repositioning tolcapone as a potent inhibitor of transthyretin amyloidogenesis and associated cellular toxicity.

101. Prevention of Epilepsy: Issues and Innovations.

102. Screening and personalizing nootropic drugs and cognitive modulator regimens in silico.

103. ERK and ROCK functionally interact in a signaling network that is compensationally upregulated in Spinal Muscular Atrophy.

104. The FDA-approved natural product dihydroergocristine reduces the production of the Alzheimer's disease amyloid-beta peptides.

105. Targeting phosphodiesterase 5 as a therapeutic option against myocardial ischaemia/reperfusion injury and for treating heart failure.

106. Mechanistic insights into epigenetic modulation of ethanol consumption.

107. A Drug Screen using Human iPSC-Derived Hepatocyte-like Cells Reveals Cardiac Glycosides as a Potential Treatment for Hypercholesterolemia.

108. alpha2-Adrenergic blockade rescues hypoglossal motor defense against obstructive sleep apnea.

109. Interactions of Selective Serotonin Reuptake Inhibitors with beta-Amyloid.

110. A review of contemporary options for medical management of hemangiomas, other vascular tumors, and vascular malformations.

111. Oral administration of erythromycin decreases RNA toxicity in myotonic dystrophy.

112. Mitochondrial protein sorting as a therapeutic target for ATP synthase disorders.

113. Pharmacokinetic and protein binding profile of peptidomimetic DPP-4 inhibitor - Teneligliptin in rats using liquid chromatography-tandem mass spectrometry.

114. Repurposing the Selective Oestrogen Receptor Modulator Tamoxifen for the Treatment of Duchenne Muscular Dystrophy.

115. Disease Modifying Potential of Glatiramer Acetate in Huntington's Disease.

116. Do traditional anti-seizure drugs have a future? A review of potential anti-seizure drugs in clinical development.

117. Diabetes Drug Receives New Indication.

A2-2h4. Cluster 3 record titles

1. Drug Repurposing Patent Applications July-September 2015.

2. Drug Repurposing Patent Applications April-June 2015.

3. Drug Repurposing Patent Applications April-June 2016.

4. Drug Repurposing Patent Applications July-September 2016.

5. Drug Repurposing Patent Applications January-March 2017.

6. Drug Repurposing Patent Applications October-December 2016.

7. Drug Repurposing Patent Applications January-March 2018.

8. Drug Repurposing Patent Applications October-December 2017.

9. Second medical use in Turkey.

10. Drug repurposing and the prior art patents of competitors.

11. Sources and Targets for Drug Repurposing: Landscaping Transitions in Therapeutic Space.

12. Use patents can be useful: the case of rescued drugs.

13. Patent review.

14. Patent review.

15. Computational Approaches for Translational Oncology: Concepts and Patents.

16. A perspective on second medical indication patents in Brazil.

17. What are the risks of second medical use and dosing regimens in pharmaceutical patenting?

18. Therapeutic compositions and uses of alpha1-antitrypsin: a patent review (2012 - 2015).

19. The problem with repurposing: Is there really an alternative to Big Pharma for developing new drugs for multiple sclerosis?

20. Tecfidera(): an approach for repurposing.

21. Computational biology: future challenges for the patenting of repurposed drugs.

22. New drugs or alternative therapy to blurring the symptoms of fibromyalgia-a patent review.

23. Predictive methods in drug repurposing: gold mine or just a bigger haystack?

24. Drug Repositioning in the Mirror of Patenting: Surveying and Mining Uncharted Territory.

25. Patent cliff mitigation strategies: giving new life to blockbusters.

26. Future perspectives for cryptococcosis treatment.

27. Finding new uses for existing medications.

28. Second medical use claims and 'skinny' labels: clear guidance at last?

29. Enforceability of second medical use claims in the UK.

30. Repurposing of drugs for dermatologic applications: five key medications.

31. [Modern disease-modifying antirheumatic drugs].

32. Drug repurposing for neuroregeneration in multiple sclerosis.

33. [Supervised off-label prescribing of topiramate for binge eating disorder within the system CAMTEA].

A2-2h5. Cluster 10 record titles

1. Disulfiram, a drug widely used to control alcoholism, suppresses the self-renewal of glioblastoma and over-rides resistance to temozolomide.

2. Evidence for the efficacy of disulfiram and copper combination in glioblastoma multiforme - A propos of a case.

3. Drug Repositioning in Glioblastoma: A Pathway Perspective.

4. Targeting Gliomas: Can a New Alkylating Hybrid Compound Make a Difference?

5. Concise review: bullseye: targeting cancer stem cells to improve the treatment of gliomas by repurposing disulfiram.

6. Inhibition of Radiation and Temozolomide-Induced Invadopodia Activity in Glioma Cells Using FDA-Approved Drugs.

7. Recycling drug screen repurposes hydroxyurea as a sensitizer of glioblastomas to temozolomide targeting de novo DNA synthesis, irrespective of molecular subtype.

8. Identification of thioridazine, an antipsychotic drug, as an antiglioblastoma and anticancer stem cell agent using public gene expression data.

9. Identification of antipsychotic drug fluspirilene as a potential anti-glioma stem cell drug.

10. Bacoside A Induces Tumor Cell Death in Human Glioblastoma Cell Lines through Catastrophic Macropinocytosis.

11. Case-specific potentiation of glioblastoma drugs by pterostilbene.

12. Identification of repaglinide as a therapeutic drug for glioblastoma multiforme.

13. Biological basis and clinical study of glycogen synthase kinase- 3beta-targeted therapy by drug repositioning for glioblastoma.

14. Proscillaridin A exerts anti-tumor effects through GSK3beta activation and alteration of microtubule dynamics in glioblastoma.

15. Fluvoxamine, an anti-depressant, inhibits human glioblastoma invasion by disrupting actin polymerization.

16. Thioridazine inhibits autophagy and sensitizes glioblastoma cells to temozolomide.

17. Identification of Mitoxantrone as a TRAIL-sensitizing agent for Glioblastoma Multiforme.

18. Repurposing drugs for glioblastoma: From bench to bedside.

19. Disulfiram is a direct and potent inhibitor of human O6-methylguanine-DNA methyltransferase (MGMT) in brain tumor cells and mouse brain and markedly increases the alkylating DNA damage.

20. Promoting oligodendroglial-oriented differentiation of glioma stem cell: a repurposing of quetiapine for the treatment of malignant glioma.

21. Use of an anti-viral drug, Ribavirin, as an anti-glioblastoma therapeutic.

22. Drug repurposing: sulfasalazine sensitizes gliomas to gamma knife radiosurgery by blocking cystine uptake through system Xc-, leading to glutathione depletion.

23. Repurposing phenformin for the targeting of glioma stem cells and the treatment of glioblastoma.

24. The anti-hypertensive drug prazosin inhibits glioblastoma growth via the PKCdelta-dependent inhibition of the AKT pathway.

25. Repurposing some older drugs that cross the blood-brain barrier and have potential anticancer activity to provide new treatment options for glioblastoma.

26. Repositioning of the antipsychotic trifluoperazine: Synthesis, biological evaluation and in silico study of trifluoperazine analogs as anti-glioblastoma agents.

27. A conceptually new treatment approach for relapsed glioblastoma: coordinated undermining of survival paths with nine repurposed drugs (CUSP9) by the International Initiative for Accelerated Improvement of Glioblastoma Care.

28. Repositioning chlorpromazine for treating chemoresistant glioma through the inhibition of cytochrome c oxidase bearing the COX4-1 regulatory subunit.

29. A Repurposed Drug for Brain Cancer: Enhanced Atovaquone Amorphous Solid Dispersion by Combining a Spontaneously Emulsifying Component with a Polymer Carrier.

30. Disulfiram's Anticancer Activity: Evidence and Mechanisms.

31. Do statins, ACE inhibitors or sartans improve outcome in primary glioblastoma?

32. Adaptive mitochondrial reprogramming and resistance to PI3K therapy.

33. Disulfiram with or without metformin inhibits oesophageal squamous cell carcinoma invivo.

34. Dual Targeting of the Autophagic Regulatory Circuitry in Gliomas with Repurposed Drugs Elicits Cell-Lethal Autophagy and Therapeutic Benefit.

35. Improving contrast enhancement in magnetic resonance imaging using 5-aminolevulinic acid-induced protoporphyrin IX for high-grade gliomas.

36. Development and optimization of an injectable formulation of copper diethyldithiocarbamate, an active anticancer agent.

37. Modulating the metabolism by trimetazidine enhances myoblast differentiation and promotes myogenesis in cachectic tumor-bearing c26 mice.

38. Diethyldithiocarbamate complex with copper: the mechanism of action in cancer cells.

39. Posttranslational Regulation of O(6)-Methylguanine-DNA Methyltransferase (MGMT) and New Opportunities for Treatment of Brain Cancers.

40. Recent Advances in Antabuse (Disulfiram): The Importance of its Metal-binding Ability to its Anticancer Activity.

41. Establishing a Preclinical Multidisciplinary Board for Brain Tumors.

42. Nanoscale Reaction Vessels Designed for Synthesis of Copper-Drug Complexes Suitable for Preclinical Development.

43. Glioma: Repurposed drugs combined to amplify autophagy.

44. Elesclomol restores mitochondrial function in genetic models of copper deficiency.

45. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin.

46. Disulfiram as a novel inactivator of Giardia lamblia triosephosphate isomerase with antigiardial potential.

A2-2h6. Cluster 31 record titles

1. Ameliorative effect of methylthiouracil on TGFBIp-induced septic responses.

2. Anti-inflammatory effects of methylthiouracil in vitro and in vivo.

3. Repurposing an orally available drug for the treatment of geographic atrophy.

4. Suppressive effects of methylthiouracil on polyphosphate-mediated vascular inflammatory responses.

5. Anti-inflammatory effects of dabrafenib in vitro and in vivo.

6. Repositioning drugs for inflammatory disease - fishing for new anti-inflammatory agents.

7. Antiseptic effects of dabrafenib on TGFBIp-induced septic responses.

8. beta-Caryophyllene protects against alcoholic steatohepatitis by attenuating inflammation and metabolic dysregulation in mice.

9. Anti-inflammatory effects of dabrafenib on polyphosphate-mediated vascular disruption.

10. Repositioning of 2,4-dichlorophenoxy acetic acid as a potential anti-inflammatory agent: in silico and pharmaceutical formulation study.

11. Antifibrotic effect of pirfenidone in a mouse model of human nonalcoholic steatohepatitis.

12. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer.

13. Methylthiouracil, a new treatment option for sepsis.

14. Fibrosis in systemic sclerosis: common and unique pathobiology.

15. A Zebrafish Drug-Repurposing Screen Reveals sGC-Dependent and sGC-Independent Pro-Inflammatory Activities of Nitric Oxide.

16. Fibrosis in systemic sclerosis: emerging concepts and implications for targeted therapy.

17. Understanding fibrosis in systemic sclerosis: shifting paradigms, emerging opportunities.

18. Toll-Like Receptor-4 Signaling Drives Persistent Fibroblast Activation and Prevents Fibrosis Resolution in Scleroderma.

19. ACTH: The forgotten therapy.

20. Immunomodulatory tetracyclines shape the intestinal inflammatory response inducing mucosal healing and resolution.

21. 3, 5, 3'-Triiodothyroacetic acid (TRIAC) is an anti-inflammatory drug that targets toll-like receptor 2.

22. Propofol post-conditioning alleviates hepatic ischaemia reperfusion injury via BRG1-mediated Nrf2/HO-1 transcriptional activation in human and mice.

23. Adrenergic regulation of innate immunity: a review.

24. Fishing Anti-Inflammatories from Known Drugs: In Silico Repurposing, Design, Synthesis and Biological Evaluation of Bisacodyl Analogues.

25. Identification and validation of uterine stimulant methylergometrine as a potential inhibitor of caspase-1 activation.

26. Identification of Iguratimod as an Inhibitor of Macrophage Migration Inhibitory Factor (MIF) with Steroid-sparing Potential.

27. Suppressive effects of dabrafenibon endothelial protein C receptor shedding.

28. Connectivity mapping (ssCMap) to predict A20-inducing drugs and their antiinflammatory action in cystic fibrosis.

29. Glybenclamide: an antidiabetic with in vivo antithrombotic activity.

30. The possible repositioning of an oral anti-arthritic drug, auranofin, for Nrf2-activating therapy: The demonstration of Nrf2-dependent anti-oxidative action using a zebrafish model.

31. Lansoprazole Upregulates Polyubiquitination of the TNF Receptor-Associated Factor 6 and Facilitates Runx2-mediated Osteoblastogenesis.

32. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent.

33. Functional genetics-directed identification of novel pharmacological inhibitors of FAS- and TNF-dependent apoptosis that protect mice from acute liver failure.

34. Interleukin-6, A Cytokine Critical to Mediation of Inflammation, Autoimmunity and Allograft Rejection: Therapeutic Implications of IL-6 Receptor Blockade.

35. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease.

36. Ibuprofen and diclofenac treatments reduce proliferation of pancreatic acinar cells upon inflammatory injury and mitogenic stimulation.

37. A signalome screening approach in the autoinflammatory disease TNF receptor associated periodic syndrome (TRAPS) highlights the anti-inflammatory properties of drugs for repurposing.

38. Drug-Repositioning Screening for Keap1-Nrf2 Binding Inhibitors using Fluorescence Correlation Spectroscopy.

39. Repurposing Treprostinil for Enhancing Hematopoietic Progenitor Cell Transplantation.

40. Characterization of drug-induced transcriptional modules: towards drug repositioning and functional understanding.

41. Repurposing ospemifene for potentiating an antigen-specific immune response.

42. Activation of MyD88-dependent TLR1/2 signaling by misfolded alpha-synuclein, a protein linked to neurodegenerative disorders.

43. Bromide supplementation exacerbated the renal dysfunction, injury and fibrosis in a mouse model of Alport syndrome.

44. Fenofibrate Attenuates Neutrophilic Inflammation in Airway Epithelia: Potential Drug Repurposing for Cystic Fibrosis.

45. Olaparib protects cardiomyocytes against oxidative stress and improves graft contractility during the early phase after heart transplantation in rats.

46. Osteoprotegerin and Denosumab Stimulate Human Beta Cell Proliferation through Inhibition of the Receptor Activator of NF-kappaB Ligand Pathway.

47. Repositioning of molsidomine for its efficacy in diabetes induced erectile dysfunction in rats: In silico, in vitro and in vivo approach.

48. Repositioning of Tak-475 In Mevalonate Kinase Disease: Translating Theory Into Practice.

49. Repurposing a novel parathyroid hormone analogue to treat hypoparathyroidism.

50. Dopaminergic Regulation of Innate Immunity: a Review.

51. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis.

52. An in vitro test system for compounds that modulate human inflammatory macrophage polarization.

53. Glycogen phosphorylase inhibition improves beta cell function.

54. Histamine-2 receptor antagonist famotidine modulates cardiac stem cell characteristics in hypertensive heart disease.

55. Inhibition of effector antigen-specific T cells by intradermal administration of heme oxygenase-1 inducers.

56. The clinically used PARP inhibitor olaparib improves organ function, suppresses inflammatory responses and accelerates wound healing in a murine model of third-degree burn injury.

57. The antidepressant 5-HT2A receptor antagonists pizotifen and cyproheptadine inhibit serotonin-enhanced platelet function.

58. Old drugs with new skills: fenoprofen as an allosteric enhancer at melanocortin receptor 3.

59. Modulating Innate and Adaptive Immunity by (R)-Roscovitine: Potential Therapeutic Opportunity in Cystic Fibrosis.

60. Repurposing an Osteoporosis Drug for beta Cell Regeneration in Diabetic Patients.

61. Treatment of experimental autoimmune uveoretinitis with peroxisome proliferator-activated receptor alpha agonist fenofibrate.

62. Rebamipide, an Amino Acid Analog of 2(1H)-Quinolinone, Inhibits the Formation of Human Osteoclasts.

63. Colonic delivery of celecoxib is a potential pharmaceutical strategy for repositioning the selective COX-2 inhibitor as an anti-colitic agent.

64. Oxidative stress during acetaminophen hepatotoxicity: Sources, pathophysiological role and therapeutic potential.

65. Pharmacological targeting of GSK-3 and NRF2 provides neuroprotection in a preclinical model of tauopathy.

66. Repurposing Lesogaberan to Promote Human Islet Cell Survival and beta-Cell Replication.

67. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs.

68. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain.

69. Tegaserod mimics the neurostimulatory glycan polysialic acid and promotes nervous system repair.

70. Molecular Characterization of GABA-A Receptor Subunit Diversity within Major Peripheral Organs and Their Plasticity in Response to Early Life Psychosocial Stress.

71. Repurposing an old drug for a new use: glybenclamide exerts antiplatelet activity by interacting with the thromboxane A(2) receptor.

72. Therapeutic modulators of peroxisome proliferator-activated receptors (PPAR): a patent review (2008-present).

73. Targeting Abl kinases to regulate vascular leak during sepsis and acute respiratory distress syndrome.

74. Inhibition of the insulin-like growth factor system is a potential therapy for rheumatoid arthritis.

75. Repositioning Potential of PAK4 to Osteoclastic Bone Resorption.

76. Exploring novel pharmacotherapeutic applications and repurposing potential of sodium glucose CoTransporter 2 inhibitors.

77. Repurposing matrine for the treatment of hepatosteatosis and associated disorders in glucose homeostasis in mice.

78. Mitigation of carbon tetrachloride-induced hepatic injury by methylene blue, a repurposed drug, is mediated by dual inhibition of GSK3beta downstream of PKA.

79. Evaluation of a systems biology approach to identify pharmacological correctors of the mutant CFTR chloride channel.

80. Identification of Febuxostat as a New Strong ABCG2 Inhibitor: Potential Applications and Risks in Clinical Situations.

81. Fragmin/protamine microparticle carriers as a drug repositioning strategy for cell transplantation.

82. Repurposing of Aspirin and Ibuprofen as Candidate Anti-Cryptococcus Drugs.

83. Drug Repositioning for Preeclampsia Therapeutics by In Vitro Screening: Phosphodiesterase-5 Inhibitor Vardenafil Restores Endothelial Dysfunction via Induction of Placental Growth Factor.

84. Novel Therapeutics Identification for Fibrosis in Renal Allograft Using Integrative Informatics Approach.

85. High-throughput screening for modulators of ACVR1 transcription: discovery of potential therapeutics for fibrodysplasia ossificans progressiva.

86. Repurposing the anti-malarial drug, quinacrine: new anti-colitis properties.

87. A glucagon-like peptide-1 receptor agonist reduces intracranial pressure in a rat model of hydrocephalus.

88. Fenoprofen -- an old drug rediscovered as a biased allosteric enhancer for melanocortin receptors.

89. Inflammation-dependent cerebrospinal fluid hypersecretion by the choroid plexus epithelium in posthemorrhagic hydrocephalus.

90. Hemin activation of innate cellular response blocks human immunodeficiency virus type-1-induced osteoclastogenesis.

91. Thiopurine Drugs Repositioned as Tyrosinase Inhibitors.

92. Repositioning Clofazimine as a Macrophage-Targeting Photoacoustic Contrast Agent.

93. Repurposing doxycycline for synucleinopathies: remodelling of alpha-synuclein oligomers towards non-toxic parallel beta-sheet structured species.

94. The Horizon of a Therapy for Rare Genetic Diseases: A "Druggable" Future for Fibrodysplasia Ossificans Progressiva.

95. Therapeutic Approaches to Type I Interferonopathies.

96. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma.

97. The chaperone activity of 4PBA ameliorates the skeletal phenotype of Chihuahua, a zebrafish model for dominant osteogenesis imperfecta.

98. Anti-obesogenic and hypolipidemic effects of a glucagon-like peptide-1 receptor agonist derived from the saliva of the Gila monster.

99. Investigating Drug Repositioning Approach to Design Novel Prodrugs for Colon-specific Release of Fexofenadine for Ulcerative Colitis.

100. Alendronate inhalation ameliorates elastase-induced pulmonary emphysema in mice by induction of apoptosis of alveolar macrophages.

101. Carbamazepine alone and in combination with doxycycline attenuates isoproterenol-induced cardiac hypertrophy.

102. Repositioning of Thiourea-Containing Drugs as Tyrosinase Inhibitors.

103. Prilocaine hydrochloride protects zebrafish from lethal effects of ionizing radiation: role of hematopoietic cell expansion.

104. Personalized Proteomics in Proliferative Vitreoretinopathy Implicate Hematopoietic Cell Recruitment and mTOR as a Therapeutic Target.

105. Structure-based repurposing of FDA-approved drugs as TNF-alpha inhibitors.

106. New culture medium concepts for cell transplantation.

107. Captopril mitigates splenomegaly and myelofibrosis in the Gata1low murine model of myelofibrosis.

108. Newly Identified Targets of Aspirin and Its Primary Metabolite, Salicylic Acid.

109. Drug-Mediated Regulation of Glycosaminoglycan Biosynthesis.

110. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C.

111. Calcineurin-NFAT signalling in myeloid leucocytes: new prospects and pitfalls in immunosuppressive therapy.

112. [Doxycycline or how to create new with the old?].

113. GDC-0879, a BRAFV600E Inhibitor, Protects Kidney Podocytes from Death.

114. Tezosentan inhibits uptake of proinflammatory endothelin-1 in stenotic aortic valves.

115. Chloroquine upregulates TRAIL/TRAILR2 expression and potentiates doxorubicin anti-tumor activity in thioacetamide-induced hepatocellular carcinoma model.

116. Pluripotent Stem Cell Platforms for Drug Discovery.

117. A common rejection module (CRM) for acute rejection across multiple organs identifies novel therapeutics for organ transplantation.

118. Tyrosinase inhibitors: a patent review (2011-2015).

119. Alternative molecular formats and therapeutic applications for bispecific antibodies.

120. Liraglutide modulates gut microbiota and reduces NAFLD in obese mice.

121. Promethazine Hydrochloride Inhibits Ectopic Fat Cell Formation in Skeletal Muscle.

122. Metabolic switch during adipogenesis: From branched chain amino acid catabolism to lipid synthesis.

123. Discovery of antiandrogen activity of nonsteroidal scaffolds of marketed drugs.

124. Clinical dosage of meclozine promotes longitudinal bone growth, bone volume, and trabecular bone quality in transgenic mice with achondroplasia.

125. Repurposing of Proton Pump Inhibitors as first identified small molecule inhibitors of endo-beta-N-acetylglucosaminidase (ENGase) for the treatment of NGLY1 deficiency, a rare genetic disease.

126. Lethal action of the nitrothiazolyl-salicylamide derivative nitazoxanide via induction of oxidative stress in Leishmania (L.) infantum.

127. Valproic acid mediates miR-124 to down-regulate a novel protein target, GNAI1.

128. IL-4 as a Repurposed Biological Drug for Myocardial Infarction through Augmentation of Reparative Cardiac Macrophages: Proof-of-Concept Data in Mice.

129. YAP/TAZ Are Mechanoregulators of TGF-beta-Smad Signaling and Renal Fibrogenesis.

130. Targeting transcriptional control of soluble guanylyl cyclase via NOTCH for prevention of cardiovascular disease.

131. A Topical Zinc Ionophore Blocks Tumorigenic Progression in UV-exposed SKH-1 High-risk Mouse Skin.

132. Nucleoside reverse transcriptase inhibitors possess intrinsic anti-inflammatory activity.

133. Neural Crossroads in the Hematopoietic Stem Cell Niche.

134. Developmental toxicity of auranofin in zebrafish embryos.

135. Sympathoadrenergic modulation of hematopoiesis: a review of available evidence and of therapeutic perspectives.

136. In silico model of the human ClC-Kb chloride channel: pore mapping, biostructural pathology and drug screening.

137. Identification of the antiarrhythmic drugs amiodarone and lorcainide as potent H3 histamine receptor inverse agonists.

138. Tetracycline hydrochloride: A potential clinical drug for radioprotection.

139. SIRT1 activation by methylene blue, a repurposed drug, leads to AMPK-mediated inhibition of steatosis and steatohepatitis.

140. In vitro biological evaluation of glyburide as potential inhibitor of collagenases.

141. Drug repurposing: In-vitro anti-glycation properties of 18 common drugs.

142. Structural Basis of Antisickling Effects of Selected FDA Approved Drugs: A Drug Repurposing Study.

143. Diclofenac Identified as a Kynurenine 3-Monooxygenase Binder and Inhibitor by Molecular Similarity Techniques.

144. Identification of raloxifene as a novel CB2 inverse agonist.

145. Repurposing an established drug: an emerging role for methylene blue in L-DOPA-induced dyskinesia.

146. Repurposing miltefosine for the treatment of immune-mediated disease?

147. Drug repurposing: Ibrutinib exhibits immunosuppressive potential in organ transplantation.

148. Mining Retrospective Data for Virtual Prospective Drug Repurposing: L-DOPA and Age-related Macular Degeneration.

149. Structural basis for the hepatoprotective effects of antihypertensive 1,4-dihydropyridine drugs.

150. In silico prediction of new inhibitors for the nucleotide pool sanitizing enzyme, MTH1, using drug repurposing.

151. Deal watch: IL-2 focus switches to stimulating Tregs.

A2-2h7. Cluster 28 record titles

1. More Treatments on Deck for Alcohol Use Disorder.

2. Medications for alcohol use disorders: An overview.

3. New pharmacological treatment strategies for relapse prevention.

4. New steps for treating alcohol use disorder.

5. Therapeutic Strategies for the Treatment of Alcoholic Hepatitis.

6. Delivering drugs to the lungs: The history of repurposing in the treatment of respiratory diseases.

7. Medication discovery for addiction: translating the dopamine D3 receptor hypothesis.

8. Buspirone Counteracts MK-801-Induced Schizophrenia-Like Phenotypes through Dopamine D3 Receptor Blockade.

9. Neuropathic Pain Creates an Enduring Prefrontal Cortex Dysfunction Corrected by the Type II Diabetic Drug Metformin But Not by Gabapentin.

10. Capsaicin: Current Understanding of Its Mechanisms and Therapy of Pain and Other Pre-Clinical and Clinical Uses.

11. Oral delivery of ivermectin using a fast dissolving oral film: Implications for repurposing ivermectin as a pharmacotherapy for alcohol use disorder.

12. Investigational drug therapies in phase I and phase II clinical trials for alcohol use disorders.

13. EMA401: an old antagonist of the AT2R for a new indication in neuropathic pain.

14. The neuroimmune transcriptome and alcohol dependence: potential for targeted therapies.

15. Microglial role in the development of chronic pain.

16. Ketamine for treatment-resistant unipolar depression: current evidence.

17. Repurposed drugs for the treatment of schizophrenia and bipolar disorders.

18. Fibrogenic Disorders in Human Diseases: From Inflammation to Organ Dysfunction.

19. Effects of the nicotinic agonist varenicline on the performance of tasks of cognition in aged and middle-aged rhesus and pigtail monkeys.

20. Antifibrotic Therapies: Where Are We Now?

21. Drug repurposing and emerging adjunctive treatments for schizophrenia.

22. Adjunct treatments for schizophrenia and bipolar disorder: what to try when you are out of ideas.

23. The effects of buspirone on occupancy of dopamine receptors and the rat gambling task.

24. Drug repurposing to treat asthma and allergic disorders: Progress and prospects.

25. Current and upcoming pharmacotherapy for non-alcoholic fatty liver disease.

26. Targeting CYP2J to reduce paclitaxel-induced peripheral neuropathic pain.

27. What We Know About the Pathogenesis of Idiopathic Pulmonary Fibrosis.

28. Repurposing drugs as inhaled therapies in asthma.

29. Topical phenytoin for the treatment of neuropathic pain.

30. Identification of Nitazoxanide as a Group I Metabotropic Glutamate Receptor Negative Modulator for the Treatment of Neuropathic Pain: An In Silico Drug Repositioning Study.

31. Effects of lorcaserin and buspirone, administered alone and as a mixture, on cocaine self-administration in male and female rhesus monkeys.

32. Ketamine: repurposing and redefining a multifaceted drug.

33. Preclinical development of moxidectin as a novel therapeutic for alcohol use disorder.

34. Drug repurposing may generate novel approaches to treating depression.

35. Inhalation of repurposed drugs to treat pulmonary hypertension.

36. Inhaled mannitol in patients with cystic fibrosis: A randomised open-label dose response trial.

37. Symptomatic thinking: the current state of Phase III and IV clinical trials for cognition in schizophrenia.

38. Low Dose Loxapine: Neuromotor Side Effects and Tolerability in Autism Spectrum Disorders.

39. Repurposing Pentoxifylline for the Treatment of Fibrosis: An Overview.

40. The Significance of Hypothiocyanite Production via the Pendrin/DUOX/Peroxidase Pathway in the Pathogenesis of Asthma.

41. Benign Paroxysmal Positional Vertigo Following Sinus Floor Elevation in Patient with Antecedents of Vertigo.

42. Where do we stand in the field of anti-abuse drug discovery?

43. Sphingolipids as targets for inhalation treatment of cystic fibrosis.

44. Efficacy of SRM-IV Vestibular Function Diagnosis and Treatment System in Treating Benign Paroxysmal Positional Vertigo.

45. Larval zebrafish model for FDA-approved drug repositioning for tobacco dependence treatment.

46. Pharmacological targeting of dopamine D3 receptors: Possible clinical applications of selective drugs.

47. Repurposing Drugs for Cognition in Schizophrenia.

48. New drug candidates for depression - a nationwide population-based study.

49. How to study sex differences in addiction using animal models.

50. [Comparison of simple canalith repositioning treatment and medication therapeutic alliance in the management of canalithiasis associated with benign paroxysmal positional vertigo of the horizontal semicircular canal].

51. The proteasome inhibitor bortezomib attenuates renal fibrosis in mice via the suppression of TGF-beta1.

52. Repurposing steroidogenesis inhibitors for the therapy of neuropsychiatric disorders: Promises and caveats.

53. Genetic Mechanisms of Asthma and the Implications for Drug Repositioning.

54. Pediatric psychopharmacology: too much or too little?

55. Subanaesthetic dose of ketamine in intractable asthma.

56. Treatments: In the waiting room.

57. Pharmacologic treatments for pulmonary hypertension: exploring pharmacogenomics.

58. Neuropathy: A name for their pain.

59. Fragile Histidine Triad (FHIT), a Novel Modifier Gene in Pulmonary Arterial Hypertension.

60. [Experience of Vasonat usage in treatment of patients with chronic toxic hepatitis].

61. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research.

62. N-acetylcysteine prevents stress-induced anxiety behavior in zebrafish.

63. Loxapine add-on for adolescents and adults with autism spectrum disorders and irritability.

64. The promise and pitfalls of intranasally administering psychopharmacological agents for the treatment of psychiatric disorders.

65. Drug Repurposing of Histone Deacetylase Inhibitors That Alleviate Neutrophilic Inflammation in Acute Lung Injury and Idiopathic Pulmonary Fibrosis via Inhibiting Leukotriene A4 Hydrolase and Blocking LTB4 Biosynthesis.

66. Evaluation of safety and efficacy of brain targeted chitosan nanoparticles of minocycline.

67. For peace and pain: the medical legitimisation of Afghanistan's poppy crop.

68. [The assessment of sequential treatment for subjective and objective benign paroxysmal positional vertigo].

69. Dopamine antagonists for treatment resistance in autism spectrum disorders: review and focus on BDNF stimulators loxapine and amitriptyline.

70. Repurposing buspirone for drug addiction treatment.

71. Orally inhaled migraine therapy: Where are we now?

72. Metformin in Idiopathic Pulmonary Fibrosis "Seeking the Holy-Grail through Drug-Repositioning".

73. Cystic fibrosis transmembrane conductance regulator modulators in cystic fibrosis: current perspectives.

74. Exploration of alpha1-antitrypsin treatment protocol for islet transplantation: dosing plan and route of administration.

75. Repurposed drugs in metabolic disorders.

76. Advances in intravesical therapy for urinary tract disorders.

77. Repositioning Microtubule Stabilizing Drugs for Brain Disorders.

78. The behavioural profile of gamma-hydroxybutyrate, gamma-butyrolactone and 1,4-butanediol in humans.

79. [Effects of canalith repositioning procedures with anti-vertigo drugs on benign paroxysmal positional vertigo].

80. A Critical Review of Repurposing Apomorphine for Smoking Cessation.

81. Repurposing Resveratrol and Fluconazole To Modulate Human Cytochrome P450-Mediated Arachidonic Acid Metabolism.

82. Repurposing an old drug: A low-cost allergy medication provides new hope for hepatitis C patients.

83. Drug delivery for the treatment of endometriosis and uterine fibroids.

84. Metabolome analysis of effect of aspirin on Drosophila lifespan extension.

85. Microsomal cytochrome P450 as a target for drug discovery and repurposing.

86. Can anti-obesity drugs be repurposed to treat cocaine addiction?

87. [LIRAGUTIDE AT A DOSE OF 3.0 MG (SAXENDA): NEW INDICATION FOR THE TREATMENT OF OBESITY].

88. Continuous Suprascapular Nerve Block With a Perineural Catheter for Reverse Shoulder Arthroplasty Rescue Analgesia in a Patient With Severe Chronic Obstructive Pulmonary Disease.

89. JAK Inhibitors for Treatment of AlopeciaAreata.

90. [Utilization of veno-venous bypass in orthotopic liver transplantation].

91. Old and new applications of non-anticoagulant heparin.

92. Examining the potential preventative effects of minocycline prescribed for acne on the incidence of severe mental illnesses: A historical cohort study.

93. Identification of circadian clock modulators from existing drugs.

94. Repositioning of dexamethasone intravitreal implant (Ozurdex) migrated into the anterior chamber.

95. The potential for repositioning antithyroid agents as antiasthma drugs.

96. [To dare trying a diuretic in autism treatment].

97. [T stands for testosterone: do you have enough of it?].

A2-2h8. Cluster 30 record titles

1. Lessons from the Fourth Metronomic and Anti-angiogenic Therapy Meeting, 24-25 June 2014, Milan.

2. Effective Management of Advanced Angiosarcoma by the Synergistic Combination of Propranolol and Vinblastine-based Metronomic Chemotherapy: A Bench to Bedside Study.

3. Next generation metronomic chemotherapy-report from the Fifth Biennial International Metronomic and Anti-angiogenic Therapy Meeting, 6-8 May 2016, Mumbai.

4. Highlights from the 1st Latin American meeting on metronomic chemotherapy and drug repositioning in oncology, 27-28 May, 2016, Rosario, Argentina.

5. Targeted therapy with propranolol and metronomic chemotherapy combination: sustained complete response of a relapsing metastatic angiosarcoma.

6. Preliminary evaluation of children treated with metronomic chemotherapy and valproic acid in a low-income country: Metro-Mali-02.

7. The poor design of clinical trials of statins in oncology may explain their failure - Lessons for drug repurposing.

8. Statins in conditions other than hypocholesterolemic effects for chronic subdural hematoma therapy, old drug, new tricks?

9. Has the time come for metronomics in low-income and middle-income countries?

10. Metronomics: towards personalized chemotherapy?

11. Niacin as a drug repositioning candidate for hyperphosphatemia management in dialysis patients.

12. Sustained Complete Response to Metronomic Chemotherapy in a Child with Refractory Atypical Teratoid Rhabdoid Tumor: A Case Report.

13. The role of statins in inflammatory vasculitides.

14. Emerging drugs for primary progressive multiple sclerosis.

15. Repurposing of statins via inhalation to treat lung inflammatory conditions.

16. Therapeutic Advances and Future Prospects in Progressive Forms of Multiple Sclerosis.

17. Repurposing propranolol as a drug for the treatment of retinal haemangioblastomas in von Hippel-Lindau disease.

18. Multiple Sclerosis-Secondary Progressive Multi-Arm Randomisation Trial (MS-SMART): a multiarm phase IIb randomised, double-blind, placebo-controlled clinical trial comparing the efficacy of three neuroprotective drugs in secondary progressive multiple sclerosis.

19. Innovations in asthma therapy: is there a role for inhaled statins?

20. Propranolol for Off-label Treatment of Patients With Melanoma: Results From a Cohort Study.

21. Development of therapies for autoimmune disease at Stanford: a tale of multiple shots and one goal.

22. Repurposing existing medications as cancer therapy: design and feasibility of a randomized pilot investigating propranolol administration in patients receiving hematopoietic cell transplantation.

23. Are biologic treatments a potential approach to wear- and corrosion-related problems?

24. Simvastatin Therapy for Drug Repositioning to Reduce the Risk of Prostate Cancer Mortality in Patients With Hyperlipidemia.

25. A meta-analysis of randomized double-blind clinical trials in CMT1A to assess the change from baseline in CMTNS and ONLS scales after one year of treatment.

26. Hydroquinidine Prevents Life-Threatening Arrhythmic Events in Patients With ShortQTSyndrome.

27. Statin: new life for an old drug.

28. Drug Repurposing Screen Identifies Foxo1-Dependent Angiopoietin-2 Regulation in Sepsis.

29. Evaluation of multiday analgesia with etoricoxib in a double-blind, randomized controlled trial using the postoperative third-molar extraction dental pain model.

30. METFORMIN: NONGLYCEMIC EFFECTS AND POTENTIAL NOVEL INDICATIONS.

31. Insights from Second-Line Treatments for Idiopathic Dilated Cardiomyopathy.

32. Current and future immunotherapy targets in autoimmune neurology.

33. High-dose methotrexate with leucovorin rescue: For monumentally severe CNS inflammatory syndromes.

34. Erythropoietin, a novel repurposed drug: an innovative treatment for wound healing in patients with diabetes mellitus.

35. Repurposing Medications for Hospice/Palliative Care Symptom Control Is No Longer Sufficient: A Manifesto for Change.

36. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC).

37. Drug repurposing in kidney disease.

38. Metronomics: Intrinsic Anakoinosis Modulator?

39. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5.

40. Novel Therapeutic Approaches to Allosensitization and Antibody-Medicated Rejection.

41. Old drugs, new uses.

42. Drug repurposing in malignant pleural mesothelioma: a breath of fresh air?

43. Histone Deacetylase Inhibitors and Diabetic Kidney Disease.

44. Emerging therapeutic targets currently under investigation for the treatment of systemic amyloidosis.

45. Drug repurposing: a systematic approach to evaluate candidate oral neuroprotective interventions for secondary progressive multiple sclerosis.

46. Medical treatment in neurofibromatosis type 2. Review of the literature and presentation of clinical reports.

47. Paradoxical strategy for treating chronic diseases where the therapeutic effect is derived from compensatory response rather than drug effect.

48. [Fumaric acid as therapeutic agent for multiple sclerosis].

49. Systemic amyloidosis: novel therapies and role of biomarkers.

50. Current issues concerning drug development for pediatric hematologic malignancies.

51. Designing drugs that combat kidney damage.

52. Novel therapeutic approaches for chronic kidney disease due to glomerular disorders.

53. Repurposing of approved cardiovascular drugs.

54. Antidepressants in the Treatment of Functional Dyspepsia: A Systematic Review and Meta-Analysis.

55. Current and Future Use of Chloroquine and Hydroxychloroquine in Infectious, Immune, Neoplastic, and Neurological Diseases: A Mini-Review.

56. Metformin - The Drug for the Treatment of Autoimmune Diseases; A New Use of a Known Anti-Diabetic Drug.

57. Understanding and Treating Glioblastoma.

58. Topical isopropyl unoprostone for retinitis pigmentosa: microperimetric results of the phase 2 clinical study.

59. Evaluating a novel treatment for coronary artery inflammation in acute Kawasaki disease: A Phase I/IIa trial of atorvastatin.

60. beta2-Adrenoceptor agonists as novel, safe and potentially effective therapies for Amyotrophic lateral sclerosis (ALS).

61. Nutraceuticals and "repurposed" drugs of phytochemical origin in prevention and interception of chronic degenerative disease and cancer.

62. Advances in the therapeutic use of mammalian target of rapamycin (mTOR) inhibitors in dermatology.

63. Non-diabetic clinical applications of insulin.

64. [Possibilities and limits of topical hydrocortisone therapy. Experiences in general practice].

65. [Possibilities of the use of parenteral form of alpha- and beta-adrenoblocker for the treatment of hypertensive crises at prehospital stage].

66. Oleanolic acid derivatives for pharmaceutical use: a patent review.

67. Therapeutic compounds for Cushing's syndrome: a patent review (2012-2016).

68. Repurposing Valproate, Enteral Clonidine, and Phenobarbital for Comfort in Adult ICU Patients: A Literature Review with Practical Considerations.

69. Nilotinib - Differentiating the Hope fromtheHype.

70. Repurposing of sodium channel antagonists as potential new anti-myotonic drugs.

71. A multicenter, randomized, placebo-controlled trial for cilostazol in patients with mild cognitive impairment: The COMCID study protocol.

72. Pathology assessment is necessary to validate translational endpoints in preclinical aging studies.

73. Long-term safety and efficacy of twice-daily aclidinium bromide in patients with COPD.

74. New developments in the management of neurogenic orthostatic hypotension.

75. Balance and circumstance: The renin angiotensin system in wound healing and fibrosis.

76. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis.

77. Chloroquine and hydroxychloroquine are associated with reduced cardiovascular risk: a systematic review and meta-analysis.

78. Symptomatic therapy in multiple sclerosis: Big pharma should do more - NO.

79. Hydralazine and magnesium valproate as epigenetic treatment for myelodysplastic syndrome. Preliminary results of a phase-II trial.

80. Perhexiline maleate in the treatment of fibrodysplasia ossificans progressiva: an open-labeled clinical trial.

81. Molecular therapies for inherited epidermolysis bullosa.

82. Serendipity: How the search for meaning of serum uric acid might lead to the repurposing of an old drug in patients with cardiovascular disease.

83. [Pulmonary amniotic fluid embolism syndrome: case report and literature review].

84. Multiple sclerosis: Repurposing dopaminergic drugs for MS--the evidence mounts.

85. Multicentric study of monitoring alarms in the adult intensive care unit (ICU): a descriptive analysis.

86. Repurposing an Old Drug for a New Epidemic: Ursodeoxycholic Acid to Prevent Recurrent Clostridioides difficile Infection.

87. Repositioning Bevacizumab: A Promising Therapeutic Strategy for Cartilage Regeneration.

88. Vinblastine as a second rescue for the treatment of canine multicentric lymphoma in 39 cases (2005 to 2014).

89. [Effects of nutrition intervention for pressure ulcer patients--healing rate and speed of wound size and nutrition--].

90. ATTIRE: Albumin To prevenT Infection in chronic liveR failurE: study protocol for a single-arm feasibility trial.

91. Vinorelbine rescue therapy for dogs with primary urinary bladder carcinoma.

92. Current Care and Investigational Therapies in Achondroplasia.

93. Quantitative determination of sulfisoxazole and its three N-acetylated metabolites using HPLC-MS/MS, and the saturable pharmacokinetics of sulfisoxazole in mice.

94. Application of Pharmacokinetics and Pharmacodynamics in Product Life Cycle Management. A Case Study with a Carbidopa-Levodopa Extended-Release Formulation.

95. Comparing treatments for age-related macular degeneration: safety, effectiveness and cost.

96. [The Management of the Vertiginous Patient].

97. Diuretics with carbonic anhydrase inhibitory action: a patent and literature review (2005 - 2013).

98. Medical marijuana in the workplace: challenges and management options for occupational physicians.

99. Oral Paracetamol for Patent Ductus Arteriosus Rescue Closure.

100. Molecular determinants of high-affinity drug binding to HERG channels.

101. Non-contraceptive health benefits of intrauterine hormonal systems.

102. Sickle cell disease: a malady beyond a hemoglobin defect in cerebrovascular disease.

103. Drug rediscovery to prevent off-label prescription reduces health care costs: the case of tioguanine in the Netherlands.

104. Nanocarrier for poorly water-soluble anticancer drugs--barriers of translation and solutions.

105. Use of dilutional ultrasound monitoring to detect changes in recirculation during venovenous extracorporeal membrane oxygenation in swine.

106. Repurposing drugs to treat neurological diseases.

107. [Anti-VEGF: one drug for different conditions?].

108. Practice variation in the management of intrapartum fetal distress in The Netherlands and the Western world.

109. Inhibition of Cholesterol Esterification in the Adrenal Gland by ATR101/PD132301-2, A Promising Case of Drug Repurposing.

110. Deserves a hearing? A case report of remitting tinnitus with N-acetyl cysteine.

111. Reporting unexpected benefit through the yellow card system.

112. Eco-pharma of approved drug focused on mitochondria fission.

3B. Appendix 3 - TR Literature Taxonomy based on Factor Analysis

A3-1. Overview of TR literature taxonomy based on Factor Analysis

The previous appendix provided one perspective (text clustering) on the taxonomic structure of the TR literature. The CLUTO text clustering software incorporates all phrases (minus stop-words), and uses one selected algorithm to generate a hierarchical taxonomy. Another approach our group has used in the past to generate literature taxonomies is Factor Analysis. Here, only pre-selected phrases are used.

The present appendix contains the results of a 37 factor study. A factor matrix that identifies the main theme of each factor (and shows the key phrases that determine each theme) is presented. Additionally, the titles of the records associated with each of the key phrases in the 37 themes is presented as well (similar to what was done in Appendix 2 for each factor).

A3-2. Results of Factor Analysis

Figure A3-1 (in a companion file on this site) shows the factor matrix containing the 37 factors. Column B contains the factor themes and the key phrases that determined the theme of each factor. The line containing the number of each factor and its theme is highlighted in orange. Thus, this line for Factor 1 is: "**1. IN VITRO EXPERIMENTS OF REPURPOSED DRUG CANDIDATES ON CANCER CELL LINES**".

The key phrases that determine the main theme of each factor are listed under the orange line. Thus, for Factor 1, the key phrases include "cancer, cancer cells, cancer cell lines, cell lines, apoptosis, anticancer, tumor, cancers, cancer treatment, cell line, cancer cell line".

How is the order of these phrases determined; what makes them key phrases? The answer lies in the numbers contained in the appropriate column to the right of Column B. The heading for each column to the right of Column B is the factor number. The cells in each column are the factor loadings, weightings that determine the importance of each phrase to the central factor theme. The weightings are ordered by decreasing absolute value.

Thus, for Factor 1, the theme is determined mainly by the top phrases colored in medium green, with some input from the next group of phrases colored light green. Any remaining non-colored phrases provide confirmatory examples.

The weightings for any factor range from positive in value to negative. Typically, one 'tail' of this spectrum is large (at least one weighting has absval>0.3) and the other is small (absval<0.2). The 'tail' containing the large absval weighting determines the theme of the factor. In a few cases, both 'tails' will have at least one weighting absval>0.3. In these cases, the factor is split into two themes. In the present case, Factors 5, 8, and 11 have A and B components.

While many broad thematic categories were possible, four appeared to be dominant. These included: Repurposing Prediction Methodologies (PRED), Diseases (DISEASE), Biomarker Targets (BIOTARG), and Drug Types (DRUG). Figure A3-2 lists all the 37 factor themes, and Figure A3-3 shows the factor numbers under each major category. Note that some factors have been assigned to multiple categories in Figure A3-3.

Figure A3-2: FACTOR THEMES

(each factor hyperlinked to associated record titles)

1. In Vitro Experiments of Repurposed Drug Candidates on Cancer Cell Lines
2. Gene Expression Signatures for Predicting Repurposed Drugs
3. Antiviral Protease Inhibitors for Cancer Therapy
4. Neurodegenerative Diseases Biomarkers for Repurposing Targets
5a. Antifungal Applications of Non-Antifungal Drugs
5b. Network-Based Approaches to Drug Repositioning
6. Antimicrobial Applications of Repurposed Drugs
7. Repurposed Drugs or Antifungal Applications
8a. Use of Cellular Signatures Library to Provide Gene Expression Profiles for Drug Repurposing Prediction
8b. Ligand-Based Target Inference
9. Binding Site Analysis for Drug Repurposing
10. Antiinflammatory Applications for Repurposed Drugs
11a. Biomarkers for Repurposed Drug-Enhanced Apoptosis of Cancer Cells
11b. Repurposed Drugs for Oxidative Stress Reduction
12. Repurposed Drugs that Increase or Decrease ROS for Different Applications
13. Similarity Searching of Ligand-Target Sets for Drug Repurposing
14. AMPK Activation for Cancer Treatment, Emphasizing Anti-Diabetic Drug Metformin
15. Repurposing of Cholesterol-Lowering Drugs for Chronic and Infectious Diseases
16. Similarity-Based Methods for Drug Repurposing
17. Machine Learning-Based Drug Repurposing Prediction
18. Tyrosine Kinase Inhibitors Repurposed for Cancer Treatment
19. Chemical Structure Similarity for Repurposing Prediction
20. Network-Based Inference for Predicting Drug-Target Interaction
21. Drug Repurposing for Viral Diseases
22. Drug Repurposing for Anti-Parasitic Applications
23. Phosphodiesterase Inhibitors Repurposed from Predicitions of Drug Response Signatures
24. Inhibiting NF-KappaB Signaling for Cancer and Inflammation Treatment
25. Repurposing Based on Comprehensive Multi-Metric Similarity Measures
26. Genome-Wide Association-Based Networks for Repurposing
27. Drug Repurposing for Brain Cancer
28. Repurposing Anthelmintic Drugs for Cancer Treatment
29. Drug Repurposing for Neurodegenerative Diseases
30. Repurposed Drugs Targeting Glutamate Receptors
31. Repurposing Drugs that Target Oxidative and Inflammation Biomarkers VEGF, HO-1, iNOS, Nrf2
32. Computational Drug Repositioning Based on Similarity Networks
33. Repurposing Antipsychotic Drugs
34. Multiple Ligand Simultaneous Docking and Drug Repositioning for Cancer Therapy

Figure A3-3: MAIN TAXONOMY CATEGORIES FROM FACTOR ANALYSIS

CATEGORY	PRED	DISEASE	BIOTARG	DRUG
FACTOR #	2, 5B, 8A, 8B, 9, 13, 16, 17, 19, 20, 23, 25, 26, 32, 34	*CANCER* 1, 3, 11A, 14, 18, 24, 27, 28 *NEURODEGEN* 4, 29 *INFECTIOUS* 5A, 6, 7, 15, 21, 22	4, 10, 11A, 11B, 12, 14, 15, 18, 23, 24, 30, 31	3, 14, 18, 23, 33

A3-3. Factor Theme Summary

Figures A3-2 and A3-3 show the following broad characteristics of the TR literature. The main diseases studied are cancer (by far), neurodegenerative, and infectious. The main biomarker targets studied focus on oxidative stress and inflammatory metrics. While drugs of many ifferent classes have been researched for repurposing, the main drug classes as emphasized in Figure A3-2 are Inhibitors of myriad signaling pathways.

Finally, the main repurposing prediction methodologies studied focus on networks, similarity, machine learning, gene expression signatures, genome-wide associations, ligand-target interactions, and binding site analyses.

A3-4. Factor Theme Record Titles

In Figure A3-1, key phrases are listed under each factor. The remainder of the present section contains the titles for each record associated with those phrases listed in Figure A3-1. This listing allows the reader to examine the full spectrum of concepts that underlie each factor, and to retrieve the full record (from the full references provided in Chapter 4) for more detail. The presentation format is factor number/factor theme followed by the record title. Each factor listing of record titles below is hyperlinked to the appropriate factor number and theme in Figure A3-2. Thus, clicking on the hyperlinked "**1. In Vitro Experiments of Repurposed Drug Candidates on Cancer Cell Lines**" in Figure A3-2 will link to the beginning of the list of record titles in Factor 1.

FACTOR 1. In Vitro Experiments of Repurposed Drug Candidates on Cancer Cell Lines

1. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

2. 5-azacytidine inhibits nonsense-mediated decay in a MYC-dependent fashion

3. A Blockade of IGF Signaling Sensitizes Human Ovarian Cancer Cells to the Anthelmintic Niclosamide-Induced Anti-Proliferative and Anticancer Activities

4. A cellular genetics approach identifies gene-drug interactions and pinpoints drug toxicity pathway nodes

5. A chemical genomics approach to drug reprofiling in oncology: Antipsychotic drug risperidone as a potential adenocarcinoma treatment

6. A chemical-genetic interaction map of small molecules using high-throughput imaging in cancer cells

7. A Combination of Three Repurposed Drugs Administered at Reperfusion as a Promising Therapy for Postischemic Brain Injury

8. A combinatorial screen of the CLOUD uncovers a synergy targeting the androgen receptor

9. A comparative study of disease genes and drug targets in the human protein interactome

10. A comprehensive approach to identifying repurposed drugs to treat SCN8A epilepsy

11. A Computational Drug Repositioning Approach for Targeting Oncogenic Transcription Factors

12. A computational method for clinically relevant cancer stratification and driver mutation module discovery using personal genomics profiles

13. A computational method for drug repositioning using publicly available gene expression data

14. A Computational Systems Biology Approach for Identifying Candidate Drugs for Repositioning for Cardiovascular Disease

15. A Computational Workflow Translates a 58-Gene Signature to a Formalin-Fixed, Paraffin-Embedded Sample-Based Companion Diagnostic for Personalized Treatment of the BRAF-Mutation-Like Subtype of Colorectal Cancers

16. A conceptually new treatment approach for relapsed glioblastoma: coordinated undermining of survival paths with nine repurposed drugs (CUSP9) by the International Initiative for Accelerated Improvement of Glioblastoma Care

17. A convenient synthesis of lubeluzole and its enantiomer: evaluation as chemosensitizing agents on human ovarian adenocarcinoma and lung carcinoma cells

18. A cross-species analysis method to analyze animal models' similarity to human's disease state

19. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

20. A disease similarity matrix based on the uniqueness of shared genes

21. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

22. A drug-repositioning screen for primary pancreatic ductal adenocarcinoma cells identifies 6-thioguanine as an effective therapeutic agent for TPMT-low cancer cells

23. A High-Content Screening of Anticancer Compounds Suggests the Multiple Tyrosine Kinase Inhibitor Ponatinib for Repurposing in Neuroblastoma Therapy

24. A high-throughput phenotypic screen identifies clofazimine as a potential treatment for cryptosporidiosis

25. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research

26. A network based approach to drug repositioning identifies plausible candidates for breast cancer and prostate cancer

27. A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer

28. A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes

29. A new niclosamide derivatives-B17 can inhibit urological cancers growth through apoptosis-related pathway

30. A novel anti-cancer role of beta-apopicropodophyllin against non-small cell lung cancer cells

31. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia

32. A novel chemoradiation targeting stem and nonstem pancreatic cancer cells by repurposing disulfiram

33. A novel computational approach for drug repurposing using systems biology

34. A Novel High Content Imaging-Based Screen Identifies the Anti-Helminthic Niclosamide as an Inhibitor of Lysosome Anterograde Trafficking and Prostate Cancer Cell Invasion

35. A novel method of transcriptional response analysis to facilitate drug repositioning for cancer therapy

36. A novel multi-modal drug repurposing approach for identification of potent ACK1 inhibitors

37. A novel two-stage, transdisciplinary study identifies digoxin as a possible drug for prostate cancer treatment

38. A profound computational study to prioritize the disease-causing mutations in PRPS1 gene

39. A protein folding molecular imaging biosensor monitors the effects of drugs that restore mutant p53 structure and its downstream function in glioblastoma cells

40. A Receptor Tyrosine Kinase Inhibitor, Dovitinib (TKI-258), Enhances BMP-2-Induced Osteoblast Differentiation In Vitro

41. A Repurposed Drug for Brain Cancer: Enhanced Atovaquone Amorphous Solid Dispersion by Combining a Spontaneously Emulsifying Component with a Polymer Carrier

42. A repurposing strategy for Hsp90 inhibitors demonstrates their potency against filarial nematodes

43. A review of contemporary options for medical management of hemangiomas, other vascular tumors, and vascular malformations

44. A screen for Fli-1 transcriptional modulators identifies PKC agonists that induce erythroid to megakaryocytic differentiation and suppress leukemogenesis

45. A Screen of FDA-Approved Drugs for Inhibitors of Zika Virus Infection

46. A screening cascade to identify ERbeta ligands

47. A Second WNT for Old Drugs: Drug Repositioning against WNT-Dependent Cancers

48. A selective mitochondrial-targeted chlorambucil with remarkable cytotoxicity in breast and pancreatic cancers

49. A Semi-Supervised Approach for Refining Transcriptional Signatures of Drug Response and Repositioning Predictions

50. A signalome screening approach in the autoinflammatory disease TNF receptor associated periodic syndrome (TRAPS) highlights the anti-inflammatory properties of drugs for repurposing

51. A small molecule screen identifies an inhibitor of DNA repair inducing the degradation of TFIIH and the chemosensitization of tumor cells to platinum

52. A Small-molecule Kinase Inhibitor, CEP-1347, Inhibits Survivin Expression and Sensitizes Ovarian Cancer Stem Cells to Paclitaxel

53. A statin-regulated microRNA represses human c-Myc expression and function

54. A structure- and chemical genomics-based approach for repositioning of drugs against VCP/p97 ATPase

55. A survey of current trends in computational drug repositioning

56. A systematic analysis of FDA-approved anticancer drugs

57. A Systematic Framework for Drug Repositioning from Integrated Omics and Drug Phenotype Profiles Using Pathway-Drug Network

58. A systems pharmacology-oriented discovery of a new therapeutic use of the TCM formula Liuweiwuling for liver failure

59. A systems-level analysis of drug-target-disease associations for drug repositioning

60. A Topical Zinc Ionophore Blocks Tumorigenic Progression in UV-exposed SKH-1 High-risk Mouse Skin

61. A tumor deconstruction platform identifies definitive end points in the evaluation of drug responses

62. Abelson Kinase Inhibitors Are Potent Inhibitors of Severe Acute Respiratory Syndrome Coronavirus and Middle East Respiratory Syndrome Coronavirus Fusion

63. Activity of anti-cancer protein kinase inhibitors against Leishmania spp

64. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

65. Adaptive mitochondrial reprogramming and resistance to PI3K therapy

66. ADEPTUS: a discovery tool for disease prediction, enrichment and network analysis based on profiles from many diseases

67. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

68. Advancing cancer drug discovery towards more agile development of targeted combination therapies

69. Aging-related Repositioned Drugs, Donepezil and Sildenafil Citrate, Increase Apoptosis of Anti-mitotic Drug-resistant KBV20C Cells Through Different Molecular Mechanisms

70. Albendazole as a promising molecule for tumor control

71. Albumin nanoparticles increase the anticancer efficacy of albendazole in ovarian cancer xenograft model

72. Alcohol-abuse drug disulfiram targets cancer via p97 segregase adaptor NPL4

73. Aldo-Keto Reductase (AKR) 1C3 inhibitors: a patent review

74. Alendronate inhalation ameliorates elastase-induced pulmonary emphysema in mice by induction of apoptosis of alveolar macrophages

75. Alternative molecular formats and therapeutic applications for bispecific antibodies

76. Alternative screening approaches for discovery of Middle East respiratory syndrome coronavirus inhibitors

77. An improved approach for predicting drug-target interaction: proteochemometrics to molecular docking

78. An in vitro test system for compounds that modulate human inflammatory macrophage polarization

79. An Insight into Drug Repositioning for the Development of Novel Anti-Cancer Drugs

80. An integrated network platform for contextual prioritization of drugs and pathways

81. An Integrative Drug Repurposing Pipeline: Switching Viral Drugs to Breast Cancer

82. An overview of angiogenesis inhibitors in Phase II studies for non-small-cell lung cancer

83. Anakoinosis: Communicative Reprogramming of Tumor Systems - for Rescuing from Chemorefractory Neoplasia

84. Angiotensin II type 1 receptor blocker telmisartan induces apoptosis and autophagy in adult T-cell leukemia cells

85. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin

86. Angiotensin inhibition enhances drug delivery and potentiates chemotherapy by decompressing tumour blood vessels

87. ANTENNA, a Multi-Rank, Multi-Layered Recommender System for Inferring Reliable Drug-Gene-Disease Associations: Repurposing Diazoxide as a Targeted Anti-Cancer Therapy

88. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

89. Anthelmintic mebendazole enhances cisplatin's effect on suppressing cell proliferation and promotes differentiation of head and neck squamous cell carcinoma (HNSCC

90. Anti-cancer potential of a novel SERM ormeloxifene

91. Anti-inflammatory effects of dabrafenib in vitro and in vivo

92. Anti-inflammatory effects of dabrafenib on polyphosphate-mediated vascular disruption

93. Anti-inflammatory effects of methylthiouracil in vitro and in vivo

94. Anti-malarials are anti-cancers and vice versa - one arrow two sparrows

95. Anti-protozoal and anti-bacterial antibiotics that inhibit protein synthesis kill cancer subtypes enriched for stem cell-like properties

96. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

97. Antibiotic drug rifabutin is effective against lung cancer cells by targeting the eIF4E-beta-catenin axis

98. Anticancer and Immunogenic Properties of Cardiac Glycosides

99. Anticancer Drugs as Antibiofilm Agents in Candida albicans: Potential Targets

100. Anticancer Properties of Fenofibrate: A Repurposing Use

101. Antifibrotic effect of pirfenidone in a mouse model of human nonalcoholic steatohepatitis

102. Antifungal application of nonantifungal drugs

103. Antihelminthic drug niclosamide inhibits CIP2A and reactivates tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells

104. Antimalarial activity of novel 4-cyano-3-methylisoquinoline inhibitors against Plasmodium falciparum: design, synthesis and biological evaluation

105. Antimalarial drug mefloquine inhibits nuclear factor kappa B signaling and induces apoptosis in colorectal cancer cells

106. Antischistosomal agents: state of art and perspectives

107. Antitumor effects of a drug combination targeting glycolysis, glutaminolysis and de novo synthesis of fatty acids

108. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis

109. Application of Atlas of Cancer Signalling Network in preclinical studies

110. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

111. Appraisal of mechanisms of radioprotection and therapeutic approaches of radiation countermeasures

112. Approved oncology drugs lack in vivo activity against Trichuris muris despite in vitro activity

113. Aripiprazole, an Antipsychotic and Partial Dopamine Agonist, Inhibits Cancer Stem Cells and Reverses Chemoresistance

114. Artemisinin and Its Derivatives as a Repurposing Anticancer Agent: What Else Do We Need to Do

115. Assessment of the antitumor potential of Bithionol in vivo using a xenograft model of ovarian cancer

116. Atorvastatin as a promising anticryptococcal agent

117. Auranofin inactivates Trichomonas vaginalis thioredoxin reductase and is effective against trichomonads in vitro and in vivo

118. Auranofin induces apoptosis by ROS-mediated ER stress and mitochondrial dysfunction and displayed synergistic lethality with piperlongumine in gastric cancer

119. Auranofin induces lethal oxidative and endoplasmic reticulum stress and exerts potent preclinical activity against chronic lymphocytic leukemia

120. Auranofin-mediated inhibition of PI3K/AKT/mTOR axis and anticancer activity in non-small cell lung cancer cells

121. Auranofin: repurposing an old drug for a golden new age

122. Autophagy in HIV-induced T cell death

123. Autophagy Induced by Naftopidil Inhibits Apoptosis of Human Gastric Cancer Cells

124. Autophagy Modulation in Disease Therapy: Where Do We Stand

125. Axitinib effectively inhibits BCR-ABL1(T315I) with a distinct binding conformation

126. Bacoside A Induces Tumor Cell Death in Human Glioblastoma Cell Lines through Catastrophic Macropinocytosis

127. Barriers to preventive therapy for breast and other major cancers and strategies to improve uptake

128. Bazedoxifene as a Novel GP130 Inhibitor for Pancreatic Cancer Therapy

129. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

130. Benserazide, a dopadecarboxylase inhibitor, suppresses tumor growth by targeting hexokinase 2

131. beta-catenin and PI3Kdelta inhibition expands precursor Th17 cells with heightened stemness and antitumor activity

132. Beyond standard therapy: drugs under investigation for the treatment of gastrointestinal stromal tumor

133. Bioinformatics analysis reveals transcriptome and microRNA signatures and drug repositioning targets for IBD and other autoimmune diseases

134. Bioinformatics and in vitro experimental analyses identify the selective therapeutic potential of interferon gamma and apigenin against cervical squamous cell carcinoma and adenocarcinoma

135. Bioinformatics-driven discovery of rational combination for overcoming EGFR-mutant lung cancer resistance to EGFR therapy

136. Biological basis and clinical study of glycogen synthase kinase- 3beta-targeted therapy by drug repositioning for glioblastoma

137. Biomarker-guided repurposing of chemotherapeutic drugs for cancer therapy: a novel strategy in drug development

138. Biotin-targeted Pluronic() P123/F127 mixed micelles delivering niclosamide: A repositioning strategy to treat drug-resistant lung cancer cells

139. Bis-biguanide dihydrochloride inhibits intracellular replication of M. tuberculosis and controls infection in mice

140. Bisphosphonates inactivate human EGFRs to exert antitumor actions

141. Bithionol inhibits ovarian cancer cell growth in vitro - studies on mechanism(s) of action

142. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

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171. Chemoprevention agents for melanoma: a path forward into phase 3 clinical trials

172. Chemoprevention of colorectal cancer for broad clinical use in the future

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197. Computational Approaches for Translational Oncology: Concepts and Patents

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199. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

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201. Computational drugs repositioning identifies inhibitors of oncogenic PI3K/AKT/P70S6K-dependent pathways among FDA-approved compounds

202. Computational identification of multi-omic correlates of anticancer therapeutic response

203. Computational methods and opportunities for phosphorylation network medicine

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216. Could the FDA-approved anti-HIV PR inhibitors be promising anticancer agents? An answer from enhanced docking approach and molecular dynamics analyses

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221. Current and Future Use of Chloroquine and Hydroxychloroquine in Infectious, Immune, Neoplastic, and Neurological Diseases: A Mini-Review

222. Current issues concerning drug development for pediatric hematologic malignancies

223. Cyclic AMP efflux inhibitors as potential therapeutic agents for leukemia

224. CYP51 as drug targets for fungi and protozoan parasites: past, present and future

225. Cytogenomic profiling of breast cancer brain metastases reveals potential for repurposing targeted therapeutics

226. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer

227. Data integration to prioritize drugs using genomics and curated data

228. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

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230. Deep Learning Applications for Predicting Pharmacological Properties of Drugs and Drug Repurposing Using Transcriptomic Data

231. Delineation of biological and molecular mechanisms underlying the diverse anticancer activities of mycophenolic acid

232. DeSigN: connecting gene expression with therapeutics for drug repurposing and development

233. Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference

234. Designing novel therapies against sarcomas in the era of personalized medicine and economic crisis

235. Development and Characterization of Bladder Cancer Patient-Derived Xenografts for Molecularly Guided Targeted Therapy

236. Development and optimization of an injectable formulation of copper diethyldithiocarbamate, an active anticancer agent

237. Development of a stretch-induced neurotrauma model for medium-throughput screening in vitro: identification of rifampicin as a neuroprotectant

238. Development of Molecular Therapies for Venous Malformations

239. Developmental toxicity of auranofin in zebrafish embryos

240. Diethyldithiocarbamate complex with copper: the mechanism of action in cancer cells

241. Diffusion mapping of drug targets on disease signaling network elements reveals drug combination strategies

242. Discovering drugs to overcome chemoresistance in ovarian cancers based on the cancer genome atlas tumor transcriptome profile

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244. Discovering proteasomal deubiquitinating enzyme inhibitors for cancer therapy: lessons from rational design, nature and old drug reposition

245. Discovery and development of Seliciclib. How systems biology approaches can lead to better drug performance

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248. Discovery of drug mode of action and drug repositioning from transcriptional responses

249. Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues

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262. Identification of FDA-approved drugs targeting breast cancer stem cells along with biomarkers of sensitivity

263. Identification of key pathways and drug repurposing for anaplastic thyroid carcinoma by integrated bioinformatics analysis

264. Identification of Mitoxantrone as a TRAIL-sensitizing agent for Glioblastoma Multiforme

265. Identification of Niclosamide as a Novel Anticancer Agent for Adrenocortical Carcinoma

266. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs

267. Identification of novel therapeutics for complex diseases from genome-wide association data

268. Identification of potential anti-hepatitis C virus agents targeting non structural protein 5B using computational techniques

269. Identification of Potential Therapeutics to Conquer Drug Resistance in Salmonella typhimurium: Drug Repurposing Strategy

270. Identification of repaglinide as a therapeutic drug for glioblastoma multiforme

271. Identification of Retinoic Acid Receptor Agonists as Potent Hepatitis B Virus Inhibitors via a Drug Repurposing Screen

272. Identification of small molecules enhancing autophagic function from drug network analysis

273. Identification of ST3AGL4, MFHAS1, CSNK2A2 and CD226 as loci associated with systemic lupus erythematosus (SLE) and evaluation of SLE genetics in drug repositioning

274. Identification of thioridazine, an antipsychotic drug, as an antiglioblastoma and anticancer stem cell agent using public gene expression data

275. Identify potential drugs for cardiovascular diseases caused by stress-induced genes in vascular smooth muscle cells

276. Identifying aberrant pathways through integrated analysis of knowledge in pharmacogenomics

277. Identifying candidate agents for lung adenocarcinoma by walking the human interactome

278. Identifying Candidates for Breast Cancer Using Interactions of Chemicals and Proteins

279. Identifying new antiepileptic drugs through genomics-based drug repurposing

280. Identifying Novel Cancer Therapies Using Chemical Genetics and Zebrafish

281. Identifying prognostic features by bottom-up approach and correlating to drug repositioning

282. IL-4 as a Repurposed Biological Drug for Myocardial Infarction through Augmentation of Reparative Cardiac Macrophages: Proof-of-Concept Data in Mice

283. IMPACT web portal: oncology database integrating molecular profiles with actionable therapeutics

284. Improved anticancer drug response prediction in cell lines using matrix factorization with similarity regularization

285. In search for geroprotectors: in silico screening and in vitro validation of signalome-level mimetics of young healthy state

286. In Silico Identification and In Vitro and In Vivo Validation of Anti-Psychotic Drug Fluspirilene as a Potential CDK2 Inhibitor and a Candidate Anti-Cancer Drug

287. In silico methods for drug repurposing and pharmacology

288. In silico prediction and in vitro and in vivo validation of acaricide fluazuron as a potential inhibitor of FGFR3 and a candidate anticancer drug for bladder carcinoma

289. In silico prescription of anticancer drugs to cohorts of 28 tumor types reveals targeting opportunities

290. In vitro and in vivo study of hydralazine, a potential anti-angiogenic agent

291. In vivo loss-of-function screens identify KPNB1 as a new druggable oncogene in epithelial ovarian cancer

292. Inferring drug-disease associations based on known protein complexes

293. Inferring new drug indications using the complementarity between clinical disease signatures and drug effects

294. Inferring novel disease indications for known drugs by semantically linking drug action and disease mechanism relationships

295. Informed walks: whispering hints to gene hunters inside networks' jungle

296. Inhibition of ACE Retards Tau Hyperphosphorylation and Signs of Neuronal Degeneration in Aged Rats Subjected to Chronic Mild Stress

297. Inhibition of EGFR Signaling Protects from Mucormycosis

298. Inhibition of LSD1 by Pargyline inhibited process of EMT and delayed progression of prostate cancer invivo

299. Inhibition of mTOR/eIF4E by anti-viral drug ribavirin effectively enhances the effects of paclitaxel in oral tongue squamous cell carcinoma

300. Insights into respiratory disease through bioinformatics

301. Integrated Computational Analysis of Genes Associated with Human Hereditary Insensitivity to Pain. A Drug Repurposing Perspective

302. Integrating Clinical Phenotype and Gene Expression Data to Prioritize Novel Drug Uses

303. Integrating systems biology sources illuminates drug action

304. Integrative bioinformatic analyses of an oncogenomic profile reveal the biology of endometrial cancer and guide drug discovery

305. Integrative clinical transcriptomics analyses for new therapeutic intervention strategies: a psoriasis case study

306. Introduction: Cancer Gene Networks

307. Kinome Profiling Identifies Druggable Targets for Novel Human Cytomegalovirus (HCMV) Antivirals

308. ksRepo: a generalized platform for computational drug repositioning

309. Large-scale extraction of accurate drug-disease treatment pairs from biomedical literature for drug repurposing

310. Large-scale integration of heterogeneous pharmacogenomic data for identifying drug mechanism of action

311. Learning Opportunities for Drug Repositioning via GWAS and PheWAS Findings

312. Lessons from the Fourth Metronomic and Anti-angiogenic Therapy Meeting, 24-25 June 2014, Milan

313. Linking drug target and pathway activation for effective therapy using multi-task learning

314. Linking molecular feature space and disease terms for the immunosuppressive drug rapamycin

315. Liraglutide modulates gut microbiota and reduces NAFLD in obese mice

316. Literature-based prediction of novel drug indications considering relationships between entities

317. Loperamide Restricts Intracellular Growth of Mycobacterium tuberculosis in Lung Macrophages

318. Low-dose salinomycin induces anti-leukemic responses in AML and MLL

319. Luteolin Impacts on the DNA Damage Pathway in Oral Squamous Cell Carcinoma

320. Lysine Deacetylase Inhibitors in Parasites: Past, Present, and Future Perspectives

321. Managing Bardet-Biedl Syndrome-Now and in the Future

322. Mantra 2.0: an online collaborative resource for drug mode of action and repurposing by network analysis

323. Master Regulators Connectivity Map: A Transcription Factors-Centered Approach to Drug Repositioning

324. Matrix Factorization-Based Prediction of Novel Drug Indications by Integrating Genomic Space

325. MD-Miner: a network-based approach for personalized drug repositioning

326. Mechanistic insights into epigenetic modulation of ethanol consumption

327. Medical genetics-based drug repurposing for Alzheimer's disease

328. Memantine induces apoptosis and inhibits cell cycle progression in LNCaP prostate cancer cells

329. Meta-analysis of human gene expression in response to Mycobacterium tuberculosis infection reveals potential therapeutic targets

330. Metabolic reprogramming in clear cell renal cell carcinoma

331. Metabolic switch during adipogenesis: From branched chain amino acid catabolism to lipid synthesis

332. Metformin Use in Relation With Survival Outcomes of Patients With Renal Cell Carcinoma

333. Mevalonate Pathway Antagonist Suppresses Formation of Serous Tubal Intraepithelial Carcinoma and Ovarian Carcinoma in Mouse Models

334. Mevalonate pathway blockage enhances the efficacy of mTOR inhibitors with the activation of retinoblastoma protein in renal cell carcinoma

335. Mining Exosomal Genes for Pancreatic Cancer Targets

336. Mining the transcriptome for rare disease therapies: a comparison of the efficiencies of two data mining approaches and a targeted cell-based drug screen

337. miREFRWR: a novel disease-related microRNA-environmental factor interactions prediction method

338. Mode of action and resistance studies unveil new roles for tropodithietic acid as an anticancer agent and the gamma-glutamyl cycle as a proton sink

339. Model-based unsupervised learning informs metformin-induced cell-migration inhibition through an AMPK-independent mechanism in breast cancer

340. Molecular mechanisms underlying variations in lung function: a systems genetics analysis

341. Molecular property diagnostic suite for diabetes mellitus (MPDSDM): An integrated web portal for drug discovery and drug repurposing

342. Monocyte-macrophage differentiation of acute myeloid leukemia cell lines by small molecules identified through interrogation of the Connectivity Map database

343. Mood, stress and longevity: convergence on ANK3

344. MPGraph: multi-view penalised graph clustering for predicting drug-target interactions

345. Multi-aspect candidates for repositioning: data fusion methods using heterogeneous information sources

346. Multi-target drug repositioning by bipartite block-wise sparse multi-task learning

347. Multi-target pharmacology: possibilities and limitations of the "skeleton key approach" from a medicinal chemist perspective

348. Multiscale modelling of relationships between protein classes and drug behavior across all diseases using the CANDO platform

349. Myotonic dystrophy: candidate small molecule therapeutics

350. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo

351. Network analysis of immunotherapy-induced regressing tumours identifies novel synergistic drug combinations

352. Network and matrix analysis of the respiratory disease interactome

353. Network approaches to drug discovery

354. Network biology concepts in complex disease comorbidities

355. Network-based analysis of transcriptional profiles from chemical perturbations experiments

356. Network-based approach to prediction and population-based validation of in silico drug repurposing

357. Network-based drug repositioning: A novel strategy for discovering potential antidepressants and their mode of action

358. Network-based in silico drug efficacy screening

359. Network-based prediction and knowledge mining of disease genes

360. NetwoRx: connecting drugs to networks and phenotypes in Saccharomyces cerevisiae

361. Neuroblastoma, a Paradigm for Big Data Science in Pediatric Oncology

362. New drug candidates for treatment of atypical meningiomas: An integrated approach using gene expression signatures for drug repurposing

363. New pathogenic insights into rheumatoid arthritis

364. Niclosamide Exhibits Potent Anticancer Activity and Synergizes with Sorafenib in Human Renal Cell Cancer Cells

365. NMR spectroscopy-based metabolic profiling of drug-induced changes in vitro can discriminate between pharmacological classes

366. Novel modeling of cancer cell signaling pathways enables systematic drug repositioning for distinct breast cancer metastases

367. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis

368. Novel therapeutic strategy for cancer and autoimmune conditions: Modulating cell metabolism and redox capacity

369. Novel therapeutics for coronary artery disease from genome-wide association study data

370. Novel Therapeutics Identification for Fibrosis in Renal Allograft Using Integrative Informatics Approach

371. Nuclear matrix, nuclear envelope and premature aging syndromes in a translational research perspective

372. Nucleosome Repositioning: A Novel Mechanism for Nicotine- and Cocaine-Induced Epigenetic Changes

373. Objective assessment of cancer genes for drug discovery

374. Olaparib protects cardiomyocytes against oxidative stress and improves graft contractility during the early phase after heart transplantation in rats

375. Olfactory drug effects approached from human-derived data

376. Omics studies: their use in diagnosis and reclassification of SLE and other systemic autoimmune diseases

377. Oncogenic targets Mmp7, S100a9, Nppb and Aldh1a3 from transcriptome profiling of FAP and Pirc adenomas are downregulated in response to tumor suppression by Clotam

378. Opportunities in systems biology to discover mechanisms and repurpose drugs for CNS diseases

379. Pancreas Cancer Precision Treatment Using Avatar Mice from a Bioinformatics Perspective

380. Pathway analysis for drug repositioning based on public database mining

381. Pathway and network-based strategies to translate genetic discoveries into effective therapies

382. Pathway-based Bayesian inference of drug-disease interactions

383. PATIENT-SPECIFIC DATA FUSION FOR CANCER STRATIFICATION AND PERSONALISED TREATMENT

384. Personalised drug repositioning for Clear Cell Renal Cell Carcinoma using gene expression

385. Personalization of cancer treatment using predictive simulation

386. Personalizing Chinese medicine by integrating molecular features of diseases and herb ingredient information: application to acute myeloid leukemia

387. Pharmacogenomic approaches to lipid-regulating trials

388. Phenotypic identification of the redox dye methylene blue as an antagonist of heat shock response gene expression in metastatic melanoma cells

389. Phospholipase PLA2G7, associated with aggressive prostate cancer, promotes prostate cancer cell migration and invasion and is inhibited by statins

390. PISTON: Predicting drug indications and side effects using topic modeling and natural language processing

391. Polytherapy with a combination of three repurposed drugs (PXT3003) down-regulates Pmp22 over-expression and improves myelination, axonal and functional parameters in models of CMT1A neuropathy

392. Possible targets on carcinoma for bMAb retargeting of lymphocyte or drug cytotoxicity

393. Potential repositioning of exemestane as a neuroprotective agent for Parkinson's disease

394. PPARgamma agonists promote differentiation of cancer stem cells by restraining YAP transcriptional activity

395. Precision medicine for suicidality: from universality to subtypes and personalization

396. PREDICT: a method for inferring novel drug indications with application to personalized medicine

397. Predicting High-Impact Pharmacological Targets by Integrating Transcriptome and Text-Mining Features

398. Predicting new indications for approved drugs using a proteochemometric method

399. Predicting Potential Drugs for Breast Cancer based on miRNA and Tissue Specificity

400. Prediction of Candidate Drugs for Treating Pancreatic Cancer by Using a Combined Approach

401. Prediction of drug-target interactions for drug repositioning only based on genomic expression similarity

402. Prediction of drugs having opposite effects on disease genes in a directed network

403. Prediction of new drug indications based on clinical data and network modularity

404. Prediction of Non-coding RNAs as Drug Targets

405. Prediction of novel drug indications using network driven biological data prioritization and integration

406. Prediction of Novel Drugs and Diseases for Hepatocellular Carcinoma Based on Multi-Source Simulated Annealing Based Random Walk

407. Prediction of Novel Drugs for Hepatocellular Carcinoma Based on Multi-Source Random Walk

408. Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing

409. Prevention of skin carcinogenesis by the beta-blocker carvedilol

410. Prioritizing therapeutics for lung cancer: an integrative meta-analysis of cancer gene signatures and chemogenomic data

411. Probabilistic drug connectivity mapping

412. Proximal Pathway Enrichment Analysis for Targeting Comorbid Diseases via Network Endopharmacology

413. Pyrvinium Sensitizes Clear Cell Renal Cell Carcinoma Response to Chemotherapy Via Casein Kinase 1alpha-Dependent Inhibition of Wnt/beta-Catenin

414. Quantitative high-throughput phenotypic screening of pediatric cancer cell lines identifies multiple opportunities for drug repurposing

415. Radiation protective effects of baclofen predicted by a computational drug repurposing strategy

416. Rational drug repurposing using sscMap analysis in a HOX-TALE model of leukemia

417. Rationale for an experimental treatment of retinitis pigmentosa: 140-month test of hypothesis with one patient

418. RDF SKETCH MAPS - KNOWLEDGE COMPLEXITY REDUCTION FOR PRECISION MEDICINE ANALYTICS

419. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective

420. Registered report: Discovery and preclinical validation of drug indications using compendia of public gene expression data

421. Replication Study: Discovery and preclinical validation of drug indications using compendia of public gene expression data

422. Repositioning chloroquine and metformin to eliminate cancer stem cell traits in pre-malignant lesions

423. Repositioning drugs by targeting network modules: a Parkinson's disease case study

424. Repositioning FDA-Approved Drugs in Combination with Epigenetic Drugs to Reprogram Colon Cancer Epigenome

425. Repositioning of drugs using open-access data portal DTome: A test case with probenecid (Review

426. Repositioning of Memantine as a Potential Novel Therapeutic Agent against Meningitic E. coli-Induced Pathogenicities through Disease-Associated Alpha7 Cholinergic Pathway and RNA Sequencing-Based Transcriptome Analysis of Host Inflammatory Responses

427. Repositioning of the anthelmintic drug mebendazole for the treatment for colon cancer

428. Repurpose terbutaline sulfate for amyotrophic lateral sclerosis using electronic medical records

429. Repurposed Drugs as Potential Therapeutic Candidates for the Management of Alzheimer's Disease

430. Repurposed FDA-Approved drug sorafenib reduces replication of Venezuelan equine encephalitis virus and other alphaviruses

431. RepurposeVS: A Drug Repurposing-Focused Computational Method for Accurate Drug-Target Signature Predictions

432. Repurposing an orally available drug for the treatment of geographic atrophy

433. Repurposing Drugs in Oncology (ReDO)-itraconazole as an anti-cancer agent

434. Repurposing drugs to target the malaria parasite unfolding protein response

435. Repurposing FDA-approved drugs as therapeutics to treat Rift Valley fever virus infection

436. Repurposing FDA-approved drugs for anti-aging therapies

437. Repurposing itraconazole as an anticancer agent

438. Repurposing of anticancer drugs: in vitro and in vivo activities against Schistosoma mansoni

439. Repurposing of Potent Drug Candidates for Multiparasite Targeting

440. Repurposing of the antihistamine chlorcyclizine and related compounds for treatment of hepatitis C virus infection

441. Repurposing old drugs in oncology: Opportunities with clinical and regulatory challenges ahead

442. Repurposing propranolol as a drug for the treatment of retinal haemangioblastomas in von Hippel-Lindau disease

443. Repurposing salicylanilide anthelmintic drugs to combat drug resistant Staphylococcus aureus

444. Repurposing the anti-malarial drug artesunate as a novel therapeutic agent for metastatic renal cell carcinoma due to its attenuation of tumor growth, metastasis, and angiogenesis

445. Repurposing the clinically approved calcium antagonist manidipine dihydrochloride as a new early inhibitor of human cytomegalovirus targeting the Immediate-Early 2 (IE2) protein

446. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease

447. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

448. Repurposing tofacitinib as an anti-myeloma therapeutic to reverse growth-promoting effects of the bone marrow microenvironment

449. Resistance to Thiacetazone Derivatives Active against Mycobacterium abscessus Involves Mutations in the MmpL5 Transcriptional Repressor MAB_4384

450. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist

451. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia

452. Revisiting Connectivity Map from a gene co-expression network analysis

453. Ribavirin suppresses bacterial virulence by targeting LysR-type transcriptional regulators

454. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

455. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox

456. Roles of the RANKL-RANK axis in antitumour immunity - implications for therapy

457. Schizophrenia interactome with 504 novel protein-protein interactions

458. Screening and personalizing nootropic drugs and cognitive modulator regimens in silico

459. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

460. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing

461. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing

462. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association

463. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients

464. Shared genetic origin of asthma, hay fever and eczema elucidates allergic disease biology

465. Short communication: Nitazoxanide inhibits HIV viral replication in monocyte-derived macrophages

466. Significance and suppression of redundant IL17 responses in acute allograft rejection by bioinformatics based drug repositioning of fenofibrate

467. Similarity-based prediction for Anatomical Therapeutic Chemical classification of drugs by integrating multiple data sources

468. SIRT1 activation by methylene blue, a repurposed drug, leads to AMPK-mediated inhibition of steatosis and steatohepatitis

469. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

470. SPIDR: small-molecule peptide-influenced drug repurposing

471. SRSF6-regulated alternative splicing that promotes tumour progression offers a therapy target for colorectal cancer

472. Statistically controlled identification of differentially expressed genes in one-to-one cell line comparisons of the CMAP database for drug repositioning

473. Stress-Activated Kinase Mitogen-Activated Kinase Kinase-7 Governs Epigenetics of Cardiac Repolarization for Arrhythmia Prevention

474. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

475. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation

476. Structure Investigation, Enrichment Analysis and Structure-based Repurposing of FDA-approved Drugs as Inhibitors of BET-BRD4

477. Study protocol of a phase IB/II clinical trial of metformin and chloroquine in patients with IDH1-mutated or IDH2-mutated solid tumours

478. Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis

479. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

480. Synergistic drug combinations from electronic health records and gene expression

481. Synthetic lethality reveals mechanisms of Mycobacterium tuberculosis resistance to beta-lactams

482. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

483. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data

484. Systematic drug safety evaluation based on public genomic expression (Connectivity Map) data: myocardial and infectious adverse reactions as application cases

485. Systematic Identification and Assessment of Therapeutic Targets for Breast Cancer Based on Genome-Wide RNA Interference Transcriptomes

486. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer

487. Systematic integration of biomedical knowledge prioritizes drugs for repurposing

488. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes

489. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification

490. Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis

491. Systems Pharmacology-Based Approach of Connecting Disease Genes in Genome-Wide Association Studies with Traditional Chinese Medicine

492. Targeting epithelial-mesenchymal plasticity in cancer: clinical and preclinical advances in therapy and monitoring

493. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress

494. Targeting Phosphatidylinositol 4-Kinase IIIalpha for Radiosensitization: A Potential Model of Drug Repositioning Using an Anti-Hepatitis C Viral Agent

495. Targeting the schizophrenia genome: a fast track strategy from GWAS to clinic

496. Tezosentan inhibits uptake of proinflammatory endothelin-1 in stenotic aortic valves

497. The anthelmintic niclosamide inhibits colorectal cancer cell lines via modulation of the canonical and noncanonical Wnt signaling pathway

498. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death

499. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells

500. The combination astemizole-gefitinib as a potential therapy for human lung cancer

501. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

502. The druggable genome and support for target identification and validation in drug development

503. The extraction of drug-disease correlations based on module distance in incomplete human interactome

504. The functional therapeutic chemical classification system

505. The HIV integrase inhibitor raltegravir inhibits felid alphaherpesvirus 1 (FeHV-1) replication by targeting both DNA replication and late gene expression

506. The human disease network in terms of dysfunctional regulatory mechanisms

507. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs

508. The neuroimmune transcriptome and alcohol dependence: potential for targeted therapies

509. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma

510. The opportunities of mining historical and collective data in drug discovery

511. The pain interactome: connecting pain-specific protein interactions

512. The prescribable drugs with efficacy in experimental epilepsies (PDE3) database for drug repurposing research in epilepsy

513. The role of drug profiles as similarity metrics: applications to repurposing, adverse effects detection and drug-drug interactions

514. The Significance of Hypothiocyanite Production via the Pendrin/DUOX/Peroxidase Pathway in the Pathogenesis of Asthma

515. The spatial organization of intra-tumour heterogeneity and evolutionary trajectories of metastases in hepatocellular carcinoma

516. The Src/c-Abl pathway is a potential therapeutic target in amyotrophic lateral sclerosis

517. The use of a gene expression signature and connectivity map to repurpose drugs for bipolar disorder

518. Therapeutic Effect of Repurposed Temsirolimus in Lung Adenocarcinoma Model

519. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

520. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

521. Thioridazine inhibits autophagy and sensitizes glioblastoma cells to temozolomide

522. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function

523. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

524. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

525. Towards building a disease-phenotype knowledge base: extracting disease-manifestation relationship from literature

526. Towards precision medicine-based therapies for glioblastoma: interrogating human disease genomics and mouse phenotypes

527. Transcriptional data: a new gateway to drug repositioning

528. Transcriptomic Analysis of the Host Response and Innate Resilience to Enterotoxigenic Escherichia coli Infection in Humans

529. Transcriptomic changes induced by mycophenolic acid in gastric cancer cells

530. Transcriptomic characterization of the novel avian-origin influenza A (H7N9) virus: specific host response and responses intermediate between avian (H5N1 and H7N7) and human (H3N2) viruses and implications for treatment options

531. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

532. Transcriptomic RNAseq drug screen in cerebrocortical cultures: toward novel neurogenetic disease therapies

533. Transcriptomic-Guided Drug Repositioning Supported by a New Bioinformatics Search Tool: geneXpharma

534. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants

535. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation

536. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer

537. Trimodal Therapy: Combining Hyperthermia with Repurposed Bexarotene and Ultrasound for Treating Liver Cancer

538. Tuberculosis--advances in development of new drugs, treatment regimens, host-directed therapies, and biomarkers

539. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin

540. Use of attenuated paramyxoviruses for cancer therapy

541. Use of genome-wide association studies for cancer research and drug repositioning

542. Using Big Data to Discover Diagnostics and Therapeutics forGastrointestinal and Liver Diseases

543. Using functional signatures to identify repositioned drugs for breast, myelogenous leukemia and prostate cancer

544. Using gene expression signatures to identify novel treatment strategies in gulf war illness

545. Utilizing Cancer - Functional Gene Set - Compound Networks to Identify Putative Drugs for Breast Cancer

546. Valproic Acid Promotes Apoptosis and Cisplatin Sensitivity Through Downregulation of H19 Noncoding RNA in Ovarian A2780 Cells

547. Verteporfin inhibits gastric cancer cell growth by suppressing adhesion molecule FAT1

548. Vinorelbine rescue therapy for dogs with primary urinary bladder carcinoma

549. Virtual screening-driven repositioning of etoposide as CD44 antagonist in breast cancer cells

550. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

551. Vitamin K and hepatocellular carcinoma: The basic and clinic

552. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

553. Zafirlukast inhibits complexation of Lsr2 with DNA and growth of Mycobacterium tuberculosis

554. ZikaVR: An Integrated Zika Virus Resource for Genomics, Proteomics, Phylogenetic and Therapeutic Analysis

FACTOR 3. Antiviral Protease Inhibitors for Cancer Therapy

1. A conceptually new treatment approach for relapsed glioblastoma: coordinated undermining of survival paths with nine repurposed drugs (CUSP9) by the International Initiative for Accelerated Improvement of Glioblastoma Care

2. A perspective on targeting non-structural proteins to combat neglected tropical diseases: Dengue, West Nile and Chikungunya viruses

3. Aldo-Keto Reductase (AKR) 1C3 inhibitors: a patent review

4. Alendronate inhalation ameliorates elastase-induced pulmonary emphysema in mice by induction of apoptosis of alveolar macrophages

5. Anti-inflammatory effects of dabrafenib in vitro and in vivo

6. Anti-inflammatory effects of dabrafenib on polyphosphate-mediated vascular disruption

7. Anti-inflammatory effects of methylthiouracil in vitro and in vivo

8. Auranofin induces apoptosis by ROS-mediated ER stress and mitochondrial dysfunction and displayed synergistic lethality with piperlongumine in gastric cancer

9. Auranofin induces lethal oxidative and endoplasmic reticulum stress and exerts potent preclinical activity against chronic lymphocytic leukemia

10. Autophagy in HIV-induced T cell death

11. Cadherin-11 in poor prognosis malignancies and rheumatoid arthritis: common target, common therapies

12. Carfilzomib is an effective anticancer agent in anaplastic thyroid cancer

13. CK2 inhibition confers functional protection to young and aging axons against ischemia by differentially regulating the CDK5 and AKT signaling pathways

14. Coming full circle: 70 years of chronic lymphocytic leukemia cell redistribution, from glucocorticoids to inhibitors of B-cell receptor signaling

15. Comparison of Quantitative Mass Spectrometry Platforms for Monitoring Kinase ATP Probe Uptake in Lung Cancer

16. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

17. Computer-Aided Structure Based Drug Design Approaches for the Discovery of New Anti-CHIKV Agents

18. Could the FDA-approved anti-HIV PR inhibitors be promising anticancer agents? An answer from enhanced docking approach and molecular dynamics analyses

19. Covalent inhibitors of EGFR family protein kinases induce degradation of human Tribbles 2 (TRIB2) pseudokinase in cancer cells

20. Creating a unique, multi-stakeholder Paediatric Oncology Platform to improve drug development for children and adolescents with cancer

21. Current issues concerning drug development for pediatric hematologic malignancies

22. Direct-acting antivirals and host-targeting strategies to combat enterovirus infections

23. Discovering proteasomal deubiquitinating enzyme inhibitors for cancer therapy: lessons from rational design, nature and old drug reposition

24. Distinct effects of HIV protease inhibitors and ERAD inhibitors on zygote to ookinete transition of the malaria parasite

25. Disulfiram/copper causes redox-related proteotoxicity and concomitant heat shock response in ovarian cancer cells that is augmented by auranofin-mediated thioredoxin inhibition

26. Drug Repurposing of the Anthelmintic Niclosamide to Treat Multidrug-Resistant Leukemia

27. Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology

28. Effects of repurposed drug candidates nitroxoline and nelfinavir as single agents or in combination with erlotinib in pancreatic cancer cells

29. Evaluation of the efficacy of valproic acid and suberoylanilide hydroxamic acid (vorinostat) in enhancing the effects of first-line tuberculosis drugs against intracellular Mycobacterium tuberculosis

30. Exploiting large-scale drug-protein interaction information for computational drug repurposing

31. Exploring old drugs for the treatment of hematological malignancies

32. Expression of DRD2 Is Increased in Human Pancreatic Ductal Adenocarcinoma and Inhibitors Slow Tumor Growth in Mice

33. Fine-tuning PERK signaling for neuroprotection

34. From laptop to benchtop to bedside: structure-based drug design on protein targets

35. Generating Gene Ontology-Disease Inferences to Explore Mechanisms of Human Disease at the Comparative Toxicogenomics Database

36. Genetics of rheumatoid arthritis contributes to biology and drug discovery

37. Genome-wide association studies of cancer: current insights and future perspectives

38. Glutamate release inhibitor, Riluzole, inhibited proliferation of human hepatocellular carcinoma cells by elevated ROS production

39. High-Throughput Flow Cytometry Identifies Small-Molecule Inhibitors for Drug Repurposing in T-ALL

40. Hydralazine-valproate: a repositioned drug combination for the epigenetic therapy of cancer

41. Identification of an old antibiotic clofoctol as a novel activator of unfolded protein response pathways and an inhibitor of prostate cancer

42. Identification of endoplasmic reticulum stress-inducing agents by antagonizing autophagy: a new potential strategy for identification of anti-cancer therapeutics in B-cell malignancies

43. In silico drug repurposing of FDA-approved drugs to predict new inhibitors for drug resistant T315I mutant and wild-type BCR-ABL1: A virtual screening and molecular dynamics study

44. In silico identification of novel kinase inhibitors targeting wild-type and T315I mutant ABL1 from FDA-approved drugs

45. Inhibiting Drivers of Non-mutational Drug Tolerance Is a Salvage Strategy for Targeted Melanoma Therapy

46. LEDGIN-mediated Inhibition of Integrase-LEDGF/p75 Interaction Reduces Reactivation of Residual Latent HIV

47. Linking PharmGKB to phenotype studies and animal models of disease for drug repurposing

48. Lysine Deacetylase Inhibitors in Parasites: Past, Present, and Future Perspectives

49. Metformin and epithelial ovarian cancer therapeutics

50. Metformin use and gynecological cancers: A novel treatment option emerging from drug repositioning

51. Misfolded proteins: from little villains to little helpers in the fight against cancer

52. Nelfinavir and lopinavir impair Trypanosoma cruzi trypomastigote infection in mammalian host cells and show anti-amastigote activity

53. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo

54. Nelfinavir, a new anti-cancer drug with pleiotropic effects and many paths to autophagy

55. New derivatives of the antimalarial drug Pyrimethamine in the control of melanoma tumor growth: an in vitro and in vivo study

56. New HSP27 inhibitors efficiently suppress drug resistance development in cancer cells

57. New sources of drugs for hematologic malignancies

58. Nitazoxanide: a first-in-class broad-spectrum antiviral agent

59. Old drug, new trick: repurposing metformin for gynecologic cancers

60. Old-School Chemotherapy in Immunotherapeutic Combination in Cancer, A Low-cost Drug Repurposed

61. Pancreas Cancer Precision Treatment Using Avatar Mice from a Bioinformatics Perspective

62. Perspectives on Advances in Tuberculosis Diagnostics, Drugs, and Vaccines

63. Pharmacological targeting of p38 MAP-Kinase 6 (MAP2K6) inhibits the growth of esophageal adenocarcinoma

64. Pharmacophore anchor models of flaviviral NS3 proteases lead to drug repurposing for DENV infection

65. Predicting new indications for approved drugs using a proteochemometric method

66. Prediction of Candidate Drugs for Treating Pancreatic Cancer by Using a Combined Approach

67. Process Pharmacology: A Pharmacological Data Science Approach to Drug Development and Therapy

68. Recent Developments and Future Opportunities in the Treatment of Tuberculosis in Children

69. Repositioning approved drugs for the treatment of problematic cancers using a screening approach

70. Repositioning Drugs for Rare Immune Diseases: Hopes and Challenges for a Precision Medicine

71. Repositioning FDA-Approved Drugs in Combination with Epigenetic Drugs to Reprogram Colon Cancer Epigenome

72. Repositioning of amprenavir as a novel extracellular signal-regulated kinase-2 inhibitor and apoptosis inducer in MCF-7 human breast cancer

73. Repurposing existing medications as cancer therapy: design and feasibility of a randomized pilot investigating propranolol administration in patients receiving hematopoietic cell transplantation

74. Repurposing itraconazole for the treatment of cancer

75. Repurposing ospemifene for potentiating an antigen-specific immune response

76. Repurposing psychiatric drugs as anti-cancer agents

77. Ritonavir blocks AKT signaling, activates apoptosis and inhibits migration and invasion in ovarian cancer cells

78. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

79. Roles of the RANKL-RANK axis in antitumour immunity - implications for therapy

80. Structural insight into selectivity and resistance profiles of ROS1 tyrosine kinase inhibitors

81. Suppressive effects of methylthiouracil on polyphosphate-mediated vascular inflammatory responses

82. Sustained Complete Response to Metronomic Chemotherapy in a Child with Refractory Atypical Teratoid Rhabdoid Tumor: A Case Report

83. Targeting the off-targets: a computational bioinformatics approach to understanding the polypharmacology of nelfinavir

84. Targeting the ubiquitin-proteasome system for cancer treatment: discovering novel inhibitors from nature and drug repurposing

85. The Glucose Transporter PfHT1 Is an Antimalarial Target of the HIV Protease Inhibitor Lopinavir

86. The HIV integrase inhibitor raltegravir inhibits felid alphaherpesvirus 1 (FeHV-1) replication by targeting both DNA replication and late gene expression

87. The human immunodeficiency virus protease inhibitor ritonavir is potentially active against urological malignancies

88. The potential to treat lung cancer via inhalation of repurposed drugs

89. The repositioning of the anti-fungal agent ciclopirox olamine as a novel therapeutic agent for the treatment of haematologic malignancy

90. Therapeutic Approaches to Type I Interferonopathies

91. Therapeutic Effect of Quinacrine, an Antiprotozoan Drug, by Selective Suppression of p-CHK1/2 in p53-Negative Malignant Cancers

92. Totally drug-resistant tuberculosis and adjunct therapies

93. Tuberculosis: From an incurable scourge to a curable disease - journey over a millennium

94. Use of minocycline in viral infections

95. Use of monoclonal antibody-IRDye800CW bioconjugates in the resection of breast cancer

96. Using HIV drugs to target human papilloma virus

97. Valproic acid in the complex therapy of malignant tumors

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FACTOR 4. Neurodegenerative Diseases Biomarkers for Repurposing Targets

1. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

2. A bidirectional drug repositioning approach for Parkinson's disease through network-based inference

3. A Combination of Three Repurposed Drugs Administered at Reperfusion as a Promising Therapy for Postischemic Brain Injury

4. A Computational Drug Repositioning Approach for Targeting Oncogenic Transcription Factors

5. A Critical Review of Repurposing Apomorphine for Smoking Cessation

6. A reprofiled drug, auranofin, is effective against metronidazole-resistant Giardia lamblia

7. A review of drugs for treatment of Alzheimer's disease in clinical trials: main trends

8. A screen for Fli-1 transcriptional modulators identifies PKC agonists that induce erythroid to megakaryocytic differentiation and suppress leukemogenesis

9. A structure- and chemical genomics-based approach for repositioning of drugs against VCP/p97 ATPase

10. A Topical Zinc Ionophore Blocks Tumorigenic Progression in UV-exposed SKH-1 High-risk Mouse Skin

11. Acetaminophen attenuates dopamine neuron degeneration in animal models of Parkinson's disease

12. Activation of MyD88-dependent TLR1/2 signaling by misfolded alpha-synuclein, a protein linked to neurodegenerative disorders

13. Activation of RXR/PPARgamma underlies neuroprotection by bexarotene in ischemic stroke

14. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

15. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

16. Adrenergic regulation of innate immunity: a review

17. Advanced neuroprotection for brain ischemia: an alternative approach to minimize stroke damage

18. Advances in drug development for Parkinson's disease: present status

19. Albendazole as a promising molecule for tumor control

20. alpha-Methyl-alpha-phenylsuccinimide ameliorates neurodegeneration in a C. elegans model of TDP-43 proteinopathy

21. AlzhCPI: A knowledge base for predicting chemical-protein interactions towards Alzheimer's disease

22. Alzheimer's Disease (AD) therapeutics - 1: Repeated clinical failures continue to question the amyloid hypothesis of AD and the current understanding of AD causality

23. Alzheimer's disease master regulators analysis: search for potential molecular targets and drug repositioning candidates

24. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

25. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

26. Approaches for discovering anti-prion compounds: lessons learned and challenges ahead

27. Auranofin: repurposing an old drug for a golden new age

28. Azithromycin protects mice against ischemic stroke injury by promoting macrophage transition towards M2 phenotype

29. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

30. beta-Caryophyllene protects against alcoholic steatohepatitis by attenuating inflammation and metabolic dysregulation in mice

31. Biomarker repurposing: Therapeutic drug monitoring of serum theophylline offers a potential diagnostic biomarker of Parkinson's disease

32. Bromide supplementation exacerbated the renal dysfunction, injury and fibrosis in a mouse model of Alport syndrome

33. Can an FDA-Approved Alzheimer's Drug Be Repurposed for Alleviating Neuronal Symptoms of Zika Virus

34. Can commonly prescribed drugs be repurposed for the prevention or treatment of Alzheimer's and other neurodegenerative diseases? Protocol for an observational cohort study in the UK Clinical Practice Research Datalink

35. Candesartan stimulates reparative angiogenesis in ischemic retinopathy model: role of hemeoxygenase-1 (HO-1

36. Cell specificity dictates similarities in gene expression in multiple sclerosis, Parkinson's disease, and Alzheimer's disease

37. Checking the STEP-Associated Trafficking and Internalization of Glutamate Receptors for Reduced Cognitive Deficits: A Machine Learning Approach-Based Cheminformatics Study and Its Application for Drug Repurposing

38. Chromone as a Privileged Scaffold in Drug Discovery: Recent Advances

39. Clinical utility of neuroprotective agents in neurodegenerative diseases: current status of drug development for Alzheimer's, Parkinson's and Huntington's diseases, and amyotrophic lateral sclerosis

40. CNS repurposing - Potential new uses for old drugs: Examples of screens for Alzheimer's disease, Parkinson's disease and spasticity

41. Combination of acamprosate and baclofen as a promising therapeutic approach for Parkinson's disease

42. Combining Human Disease Genetics and Mouse Model Phenotypes towards Drug Repositioning for Parkinson's disease

43. Combining in vitro and in silico Approaches to Find New Candidate Drugs Targeting the Pathological Proteins Related to the Alzheimer's Disease

44. Comparing structural and transcriptional drug networks reveals signatures of drug activity and toxicity in transcriptional responses

45. Computational repositioning and experimental validation of approved drugs for HIF-prolyl hydroxylase inhibition

46. Copper Complexes in Cancer Therapy

47. Current and upcoming pharmacotherapy for non-alcoholic fatty liver disease

48. Cyclin dependent kinase 5: A novel avenue for Alzheimer's disease

49. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

50. Developmental toxicity of auranofin in zebrafish embryos

51. Dexpramipexole improves bioenergetics and outcome in experimental stroke

52. Discovering new treatments for Alzheimer's disease by repurposing approved medications

53. Discovery of drug mode of action and drug repositioning from transcriptional responses

54. Discovery of Surface Target Proteins Linking Drugs, Molecular Markers, Gene Regulation, Protein Networks, and Disease by Using a Web-Based Platform Targets-search

55. Discovery of the neuroprotective effects of alvespimycin by computational prioritization of potential anti-Parkinson agents

56. Do Cancer Drugs Counteract Neurodegeneration? Repurposing forAlzheimer's Disease

57. Dopamine antagonists for treatment resistance in autism spectrum disorders: review and focus on BDNF stimulators loxapine and amitriptyline

58. Dopaminergic Regulation of Innate Immunity: a Review

59. Doxycycline counteracts neuroinflammation restoring memory in Alzheimer's disease mouse models

60. Doxycycline is an NF-kappaB inhibitor that induces apoptotic cell death in malignant T-cells

61. Drug delivery for the treatment of endometriosis and uterine fibroids

62. Drug discovery using chemical systems biology: repositioning the safe medicine Comtan to treat multi-drug and extensively drug resistant tuberculosis

63. Drug Repositioning for Alzheimer's Disease Based on Systematic 'omics' Data Mining

64. Drug Repositioning for Effective Prostate Cancer Treatment

65. Drug repositioning for treatment of movement disorders: from serendipity to rational discovery strategies

66. Drug Repurposing Approach Identifies Inhibitors of the Prototypic Viral Transcription Factor IE2 that Block Human Cytomegalovirus Replication

67. Drug Repurposing for Duchenne Muscular Dystrophy: The Monoamine Oxidase B Inhibitor Safinamide Ameliorates the Pathological Phenotype in mdx Mice and in Myogenic Cultures From DMD Patients

68. Drug repurposing for immune modulation in acute ischemic stroke

69. Drug repurposing for Leishmania. Molecular basis of the leishmanicidal activity of the antidepressant sertraline

70. Drug Repurposing in Parkinson's Disease

71. Drug Repurposing Screen Identifies Foxo1-Dependent Angiopoietin-2 Regulation in Sepsis

72. Drug Repurposing Screening Identifies Novel Compounds That Effectively Inhibit Toxoplasma gondii Growth

73. Drug repurposing: a systematic approach to evaluate candidate oral neuroprotective interventions for secondary progressive multiple sclerosis

74. Drug-Repositioning Screening for Keap1-Nrf2 Binding Inhibitors using Fluorescence Correlation Spectroscopy

75. Drugs in Clinical Trials for Alzheimer's Disease: The Major Trends

76. Emerging amyloid and tau targeting treatments for Alzheimer's disease

77. Emerging treatments for Alzheimer's disease for non-amyloid and non-tau targets

78. Epigenetic Drug Repositioning for Alzheimer's Disease Based on Epigenetic Targets in Human Interactome

79. Estrogen receptor antagonists are anti-cryptococcal agents that directly bind EF hand proteins and synergize with fluconazole in vivo

80. Examining the potential preventative effects of minocycline prescribed for acne on the incidence of severe mental illnesses: A historical cohort study

81. Exenatide and the treatment of patients with Parkinson's disease

82. Exendin-4 ameliorates traumatic brain injury-induced cognitive impairment in rats

83. Exploiting the therapeutic potential of ready-to-use drugs: Repurposing antibiotics against amyloid aggregation in neurodegenerative diseases

84. Exploring the nexus of Alzheimer's disease and related dementias with cancer and cancer therapies: A convening of the Alzheimer's Association & Alzheimer's Drug Discovery Foundation

85. Fast, non-competitive and reversible inhibition of NMDA-activated currents by 2-BFI confers neuroprotection

86. Fibrosis in systemic sclerosis: common and unique pathobiology

87. Fine-tuning PERK signaling for neuroprotection

88. Folic Acid Exerts Post-Ischemic Neuroprotection In Vitro Through HIF-1alpha Stabilization

89. FoxO3a Mediates the Inhibitory Effects of the Antiepileptic Drug Lamotrigine on Breast Cancer Growth

90. From ancient herb to modern drug: Artemisia annua and artemisinin for cancer therapy

91. From stroke to neurodegenerative diseases: The multi-target neuroprotective effects of 3-n-butylphthalide and its derivatives

92. gene2drug: a computational tool for pathway-based rational drug repositioning

93. Histamine-2 receptor antagonist famotidine modulates cardiac stem cell characteristics in hypertensive heart disease

94. Identification and Validation of an Antivirulence Agent Targeting HlyU-Regulated Virulence in Vibrio vulnificus

95. Identification of an old antibiotic clofoctol as a novel activator of unfolded protein response pathways and an inhibitor of prostate cancer

96. Identification of common biological pathways and drug targets across multiple respiratory viruses based on human host gene expression analysis

97. Identification of known drugs that act as inhibitors of NF-kappaB signaling and their mechanism of action

98. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs

99. Identifying and Tackling Emergent Vulnerability in Drug-Resistant Mycobacteria

100. In silico drug screening by using genome-wide association study data repurposed dabrafenib, an anti-melanoma drug, for Parkinson's disease

101. Inferring new indications for approved drugs via random walk on drug-disease heterogenous networks

102. Inhibition of ACE Retards Tau Hyperphosphorylation and Signs of Neuronal Degeneration in Aged Rats Subjected to Chronic Mild Stress

103. Intelligent and effective informatic deconvolution of "Big Data" and its future impact on the quantitative nature of neurodegenerative disease therapy

104. Interactions of Selective Serotonin Reuptake Inhibitors with beta-Amyloid

105. Lansoprazole Upregulates Polyubiquitination of the TNF Receptor-Associated Factor 6 and Facilitates Runx2-mediated Osteoblastogenesis

106. Latest treatment options for Alzheimer's disease, Parkinson's disease dementia and dementia with Lewy bodies

107. Laying in silico pipelines for drug repositioning: a paradigm in ensemble analysis for neurodegenerative diseases

108. Lethal action of the nitrothiazolyl-salicylamide derivative nitazoxanide via induction of oxidative stress in Leishmania (L.) infantum

109. Linked clinical trials--the development of new clinical learning studies in Parkinson's disease using screening of multiple prospective new treatments

110. Liraglutide attenuates the depressive- and anxiety-like behaviour in the corticosterone induced depression model via improving hippocampal neural plasticity

111. Loxapine add-on for adolescents and adults with autism spectrum disorders and irritability

112. Mechanistic insights into epigenetic modulation of ethanol consumption

113. Meta-analysis of human gene expression in response to Mycobacterium tuberculosis infection reveals potential therapeutic targets

114. Metformin as a geroprotector: experimental and clinical evidence

115. Metformin treatment ameliorates diabetes-associated decline in hippocampal neurogenesis and memory via phosphorylation of insulin receptor substrate 1

116. Minocycline repurposing in critical illness: focus on stroke

117. Mitigation of carbon tetrachloride-induced hepatic injury by methylene blue, a repurposed drug, is mediated by dual inhibition of GSK3beta downstream of PKA

118. Mmp-9 inhibition: a therapeutic strategy in ischemic stroke

119. Modeling cerebrovascular pathophysiology in amyloid-beta metabolism using neural-crest-derived smooth muscle cells

120. Molecular investigations of protriptyline as a multi-target directed ligand in Alzheimer's disease

121. Monocyte-macrophage differentiation of acute myeloid leukemia cell lines by small molecules identified through interrogation of the Connectivity Map database

122. Mood, stress and longevity: convergence on ANK3

123. Mucuna pruriens (L.) DC chemo sensitize human breast cancer cells via downregulation of prolactin-mediated JAK2/STAT5A signaling

124. Myelination induction by a histamine H3 receptor antagonist in a mouse model of preterm white matter injury

125. Neuroprotective and immunomodulatory effects of raloxifene in the myenteric plexus of a mouse model of Parkinson's disease

126. Neuroprotective Drug for Nerve Trauma Revealed Using Artificial Intelligence

127. Neurotrophin strategies for neuroprotection: are they sufficient

128. New applications for known drugs: Human glycogen synthase kinase 3 inhibitors as modulators of Aspergillus fumigatus growth

129. New developments in the management of neurogenic orthostatic hypotension

130. Niclosamide, a Drug with Many (Re)purposes

131. Nilotinib - Differentiating the Hope fromtheHype

132. Nitrosylation of GAPDH augments pathological tau acetylation upon exposure to amyloid-beta

133. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis

134. Nrf2 inhibition reverses the resistance of cisplatin-resistant head and neck cancer cells to artesunate-induced ferroptosis

135. Nutrients, neurogenesis and brain ageing: From disease mechanisms to therapeutic opportunities

136. Olaparib protects cardiomyocytes against oxidative stress and improves graft contractility during the early phase after heart transplantation in rats

137. Old Drugs as New Treatments for Neurodegenerative Diseases

138. Old wines in new bottles: Repurposing opportunities for Parkinson's disease

139. One for All? Hitting Multiple Alzheimer's Disease Targets with One Drug

140. Opportunities for the repurposing of PARP inhibitors for the therapy of non-oncological diseases

141. Overcoming obstacles to repurposing for neurodegenerative disease

142. Oxidative stress during acetaminophen hepatotoxicity: Sources, pathophysiological role and therapeutic potential

143. Parkinson's Disease, Diabetes and Cognitive Impairment

144. Pharmacological approach for drug repositioning against cardiorenal diseases

145. Pharmacological targeting of dopamine D3 receptors: Possible clinical applications of selective drugs

146. Pharmacological targeting of GSK-3 and NRF2 provides neuroprotection in a preclinical model of tauopathy

147. Pharmacological targeting of p38 MAP-Kinase 6 (MAP2K6) inhibits the growth of esophageal adenocarcinoma

148. Pharmacological treatment and prevention of cerebral small vessel disease: a review of potential interventions

149. Pharmacology and Clinical Drug Candidates in Redox Medicine

150. Phenotypic screening of the Prestwick library for treatment of Parkinson's tremor symptoms using a humanized quantitative systems pharmacology platform

151. Platelet Hyperreactivity in Diabetes: Focus on GPVI Signaling-Are Useful Drugs Already Available

152. Poly(ADP-ribose) polymerase is not involved in the neuroprotection exerted by azithromycin against ischemic stroke in mice

153. Polytherapy with a combination of three repurposed drugs (PXT3003) down-regulates Pmp22 over-expression and improves myelination, axonal and functional parameters in models of CMT1A neuropathy

154. Post-ischemic treatment with azithromycin protects ganglion cells against retinal ischemia/reperfusion injury in the rat

155. Posttranslational Regulation of O(6)-Methylguanine-DNA Methyltransferase (MGMT) and New Opportunities for Treatment of Brain Cancers

156. Potential repositioning of exemestane as a neuroprotective agent for Parkinson's disease

157. Potential repurposing of oncology drugs for the treatment of Alzheimer's disease

158. Preclinical Evidence Supporting Early Initiation of Citalopram Treatment in Machado-Joseph Disease

159. Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing

160. Propofol post-conditioning alleviates hepatic ischaemia reperfusion injury via BRG1-mediated Nrf2/HO-1 transcriptional activation in human and mice

161. Protein Kinases and Parkinson's Disease

162. Re-engineering a neuroprotective, clinical drug as a procognitive agent with high in vivo potency and with GABAA potentiating activity for use in dementia

163. Recent Advances in Drug Repurposing for Parkinson's Disease

164. Reduction of amyloid-beta deposition and attenuation of memory deficits by tolfenamic acid

165. Repackaging FDA-approved drugs for degenerative diseases: promises and challenges

166. Repositioning drugs by targeting network modules: a Parkinson's disease case study

167. Repositioning Microtubule Stabilizing Drugs for Brain Disorders

168. Repositioning of bromocriptine for treatment of acute myeloid leukemia

169. Repositioning of Omarigliptin as a once-weekly intranasal Anti-parkinsonian Agent

170. Repositioning tolcapone as a potent inhibitor of transthyretin amyloidogenesis and associated cellular toxicity

171. Repurposed Drugs as Potential Therapeutic Candidates for the Management of Alzheimer's Disease

172. Repurposed drugs targeting eIF2α-P-mediated translational repression prevent neurodegeneration in mice

173. Repurposing an established drug: an emerging role for methylene blue in L-DOPA-induced dyskinesia

174. Repurposing an orally available drug for the treatment of geographic atrophy

175. Repurposing and repositioning neurosteroids in the treatment of traumatic brain injury: A report from the trenches

176. Repurposing and Rescuing of Mibefradil, an Antihypertensive, for Cancer: A Case Study

177. Repurposing atovaquone: targeting mitochondrial complex III and OXPHOS to eradicate cancer stem cells

178. Repurposing auranofin for the treatment of cutaneous staphylococcal infections

179. Repurposing doxycycline for synucleinopathies: remodelling of alpha-synuclein oligomers towards non-toxic parallel beta-sheet structured species

180. Repurposing Drugs in Oncology (ReDO)-clarithromycin as an anti-cancer agent

181. Repurposing drugs to treat l-DOPA-induced dyskinesia in Parkinson's disease

182. Repurposing ebselen for treatment of multidrug-resistant staphylococcal infections

183. Repurposing of Copper(II)-chelating Drugs for the Treatment of Neurodegenerative Diseases

184. Repurposing ospemifene for potentiating an antigen-specific immune response

185. Repurposing sex steroids and related drugs as potential treatment for Parkinson's disease

186. Repurposing the clinically approved calcium antagonist manidipine dihydrochloride as a new early inhibitor of human cytomegalovirus targeting the Immediate-Early 2 (IE2) protein

187. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease

188. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

189. Research and development of anti-Alzheimer's disease drugs: an update from the perspective of technology flows

190. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist

191. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

192. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

193. Senicapoc: Repurposing a Drug to Target Microglia KCa3.1 in Stroke

194. Six psychotropics for pre-symptomatic & early Alzheimer's (MCI), Parkinson's, and Huntington's disease modification

195. Small Molecules in Development for the Treatment of Spinal Muscular Atrophy

196. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

197. Sulforaphane Prevents Neuronal Apoptosis and Memory Impairment in Diabetic Rats

198. SUMOylation in brain ischemia: Patterns, targets, and translational implications

199. Suppressive effects of methylthiouracil on polyphosphate-mediated vascular inflammatory responses

200. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

201. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification

202. T3D-959: A Multi-Faceted Disease Remedial Drug Candidate for the Treatment of Alzheimer's Disease

203. Tacrine-deferiprone hybrids as multi-target-directed metal chelators against Alzheimer's disease: a two-in-one drug

204. Tamoxifen Provides Structural and Functional Rescue in Murine Models of Photoreceptor Degeneration

205. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

206. Targeting Mevalonate Pathway in Cancer Treatment: Repurposing of Statins

207. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress

208. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases

209. Tecfidera(): an approach for repurposing

210. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

211. The Linked Clinical Trials Initiative (LCT) for Parkinson's disease

212. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C

213. The possible repositioning of an oral anti-arthritic drug, auranofin, for Nrf2-activating therapy: The demonstration of Nrf2-dependent anti-oxidative action using a zebrafish model

214. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs

215. The use of a gene expression signature and connectivity map to repurpose drugs for bipolar disorder

216. Therapeutic Approaches to Prion Diseases

217. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5

218. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

219. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin

220. Understanding fibrosis in systemic sclerosis: shifting paradigms, emerging opportunities

221. Understanding organellar protein folding capacities and assessing their pharmacological modulation by small molecules

222. Ursocholanic acid rescues mitochondrial function in common forms of familial Parkinson's disease

223. Using Drugs as Molecular Probes: AComputational Chemical Biology Approach in Neurodegenerative Diseases

224. Utility of Induced Pluripotent Stem Cells for the Study and Treatment of Genetic Diseases: Focus on Childhood Neurological Disorders

225. Validating the Predicted Effect of Astemizole and Ketoconazole Using a Drosophila Model of Parkinson's Disease

226. Valproic acid mediates miR-124 to down-regulate a novel protein target, GNAI1

227. Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors

228. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

FACTOR 5a. Antifungal Applications of Non-Antifungal Drugs

1. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research

2. A repurposing approach identifies off-patent drugs with fungicidal cryptococcal activity, a common structural chemotype, and pharmacological properties relevant to the treatment of cryptococcosis

3. Anticancer Drugs as Antibiofilm Agents in Candida albicans: Potential Targets

4. Antifungal adjuvants: Preserving and extending the antifungal arsenal

5. Antifungal amphiphilic kanamycins: new life for an old drug

6. Antifungal application of nonantifungal drugs

7. Antifungal Phenothiazines: Optimization, Characterization of Mechanism, and Modulation of Neuroreceptor Activity

8. Antifungal properties of the anti-hypertensive drug: aliskiren

9. Antifungals

10. Antiviral activity of micafungin against enterovirus 71

11. Antiviral, antifungal, and antiparasitic activities of fluoroquinolones optimized for treatment of bacterial infections: a puzzling paradox or a logical consequence of their mode of action

12. Artemisinins, new miconazole potentiators resulting in increased activity against Candida albicans biofilms

13. Atorvastatin as a promising anticryptococcal agent

14. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

15. Calcineurin-NFAT signalling in myeloid leucocytes: new prospects and pitfalls in immunosuppressive therapy

16. Cancer drugs inhibit morphogenesis in the human fungal pathogen, Candida albicans

17. Candidiasis and the impact of flow cytometry on antifungal drug discovery

18. Combined analysis of gene expression and genome binding profiles identified potential therapeutic targets of ciclopirox in Ewing sarcoma

19. Cross-species discovery of syncretic drug combinations that potentiate the antifungal fluconazole

20. CYP51 as drug targets for fungi and protozoan parasites: past, present and future

21. Development of anti-fungal pesticides from protein kinase inhibitor-based anticancer agents

22. Development of inhalable hyaluronan/mannitol composite dry powders for flucytosine repositioning in local therapy of lung infections

23. Drug Repurposing Approach Identifies a Synergistic Drug Combination of an Antifungal Agent and an Experimental Organometallic Drug for Melanoma Treatment

24. Drug repurposing as an alternative for the treatment of recalcitrant bacterial infections

25. Drug Repurposing Screening Identifies Tioconazole as an ATG4 Inhibitor that Suppresses Autophagy and Sensitizes Cancer Cells to Chemotherapy

26. Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology

27. Drugs currently under investigation for the treatment of invasive candidiasis

28. Estrogen receptor antagonists are anti-cryptococcal agents that directly bind EF hand proteins and synergize with fluconazole in vivo

29. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC

30. Future perspectives for cryptococcosis treatment

31. Gene-set analysis based on the pharmacological profiles of drugs to identify repurposing opportunities in schizophrenia

32. Glybenclamide: an antidiabetic with in vivo antithrombotic activity

33. High-throughput screening of a collection of known pharmacologically active small compounds for identification of Candida albicans biofilm inhibitors

34. Identification of Small-Molecule Inhibitors of Human Golgi Mannosidase via a Drug Repositioning Screen

35. Imidazole Antifungal Drugs Inhibit the Cell Proliferation and Invasion of Human Breast Cancer Cells

36. Imidazolium salts as innovative agents against Leishmania amazonensis

37. In vitro activity of the antifungal azoles itraconazole and posaconazole against Leishmania amazonensis

38. In vitro analysis of finasteride activity against Candida albicans urinary biofilm formation and filamentation

39. In vitro and in vivo studies of the antiparasitic activity of sterol 14alpha-demethylase (CYP51) inhibitor VNI against drug-resistant strains of Trypanosoma cruzi

40. Mapping Protein Targets of Bioactive Small Molecules Using Lipid-Based Chemical Proteomics

41. Molecular docking studies on thirteen fluoroquinolines with human topoisomerase II a and b

42. New applications for known drugs: Human glycogen synthase kinase 3 inhibitors as modulators of Aspergillus fumigatus growth

43. New pharmacological treatment strategies for relapse prevention

44. Newer patents in antimycotic therapy

45. Novel Antifungal Compounds Discovered in Medicines for Malaria Venture's Malaria Box

46. Pathogenicity phenomena in three model systems: from network mining to emerging system-level properties

47. Pharmacologic treatments for pulmonary hypertension: exploring pharmacogenomics

48. Pharmacotherapeutic Targeting of G Protein-Coupled Receptors in Oncology: Examples of Approved Therapies and Emerging Concepts

49. Quinacrine inhibits Candida albicans growth and filamentation at neutral pH

50. Rapid identification of antifungal compounds against Exserohilum rostratum using high throughput drug repurposing screens

51. Repositioning of Endonuclear Receptors Binders as Potential Antibacterial and Antifungal Agents. Eptyloxim: A Potential and Novel Gyrase B and Cytochrome Cyp51 Inhibitor

52. Repurposing antipsychotic drugs into antifungal agents: Synergistic combinations of azoles and bromperidol derivatives in the treatment of various fungal infections

53. Repurposing Approach Identifies Auranofin with Broad Spectrum Antifungal Activity That Targets Mia40-Erv1 Pathway

54. Repurposing as a means to increase the activity of amphotericin B and caspofungin against Candida albicans biofilms

55. Repurposing auranofin as an antifungal: In vitro activity against a variety of medically important fungi

56. Repurposing drugs to fast-track therapeutic agents for the treatment of cryptococcosis

57. Repurposing FDA approved drugs against the human fungal pathogen, Candida albicans

58. Repurposing of Aspirin and Ibuprofen as Candidate Anti-Cryptococcus Drugs

59. Repurposing ospemifene for potentiating an antigen-specific immune response

60. Repurposing Resveratrol and Fluconazole To Modulate Human Cytochrome P450-Mediated Arachidonic Acid Metabolism

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64. Screening a Repurposing Library for Inhibitors of Multidrug-Resistant Candida auris Identifies Ebselen as a Repositionable Candidate for Antifungal Drug Development

65. Statins: antimicrobial resistance breakers or makers

66. Strategies in the discovery of novel antifungal scaffolds

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75. The triphenylethylenes, a novel class of antifungals

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78. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

79. Treatment of Disseminated Leishmaniasis With Liposomal Amphotericin B

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FACTOR 5b. Network-Based Approaches to Drug Repositioning

1. A disease similarity matrix based on the uniqueness of shared genes

2. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge

3. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis

4. A miRNA-driven inference model to construct potential drug-disease associations for drug repositioning

5. A network integration approach for drug-target interaction prediction and computational drug repositioning from heterogeneous information

6. A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer

7. A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes

8. A review of network-based approaches to drug repositioning

9. A Systematic Framework for Drug Repositioning from Integrated Omics and Drug Phenotype Profiles Using Pathway-Drug Network

10. A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case

11. Advances in epilepsy gene discovery and implications for epilepsy diagnosis and treatment

12. Application of Atlas of Cancer Signalling Network in preclinical studies

13. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

14. Cancer Drug Response Profile scan (CDRscan): A Deep Learning Model That Predicts Drug Effectiveness from Cancer Genomic Signature

15. Combining in vitro and in silico Approaches to Find New Candidate Drugs Targeting the Pathological Proteins Related to the Alzheimer's Disease

16. Compensating for literature annotation bias when predicting novel drug-disease relationships through Medical Subject Heading Over-representation Profile (MeSHOP) similarity

17. Computational approaches for innovative antiepileptic drug discovery

18. Computational drug repositioning for peripheral arterial disease: prediction of anti-inflammatory and pro-angiogenic therapeutics

19. Computational drug repositioning through heterogeneous network clustering

20. Computational drug repositioning using low-rank matrix approximation and randomized algorithms

21. Computational drug repositioning with random walk on a heterogeneous network

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23. Deep-Learning-Based Drug-Target Interaction Prediction

24. DenguePredict: An Integrated Drug Repositioning Approach towards Drug Discovery for Dengue

25. Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference

26. Detecting drug promiscuity using Gaussian ensemble screening

27. Discovery and preclinical validation of drug indications using compendia of public gene expression data

28. Disease classification: from phenotypic similarity to integrative genomics and beyond

29. DR2DI: a powerful computational tool for predicting novel drug-disease associations

30. dRiskKB: a large-scale disease-disease risk relationship knowledge base constructed from biomedical text

31. DrPOCS: Drug repositioning based on projection onto convex sets

32. Drug repositioning based on comprehensive similarity measures and Bi-Random walk algorithm

33. Drug repositioning based on triangularly balanced structure for tissue-specific diseases in incomplete interactome

34. Drug Repositioning by Integrating Known Disease-Gene and Drug-Target Associations in a Semi-supervised Learning Model

35. Drug repositioning by integrating target information through a heterogeneous network model

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37. Drug repositioning for orphan genetic diseases through Conserved Anticoexpressed Gene Clusters (CAGCs

38. Drug repositioning for prostate cancer: using a data-driven approach to gain new insights

39. Drug repurposing based on drug-drug interaction

40. Drug target prediction and repositioning using an integrated network-based approach

41. Drug-disease association and drug-repositioning predictions in complex diseases using causal inference-probabilistic matrix factorization

42. DrugNet: network-based drug-disease prioritization by integrating heterogeneous data

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44. Elucidating the modes of action for bioactive compounds in a cell-specific manner by large-scale chemically-induced transcriptomics

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47. Finding the targets of a drug by integration of gene expression data with a protein interaction network

48. From drug response profiling to target addiction scoring in cancer cell models

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51. Heter-LP: A heterogeneous label propagation algorithm and its application in drug repositioning

52. Identification of drug candidates and repurposing opportunities through compound-target interaction networks

53. In silico prediction of chemical mechanism of action via an improved network-based inference method

54. Individualized network-based drug repositioning infrastructure for precision oncology in the panomics era

55. Inferring drug-disease associations based on known protein complexes

56. Inferring drug-disease associations from integration of chemical, genomic and phenotype data using network propagation

57. Inferring new indications for approved drugs via random walk on drug-disease heterogenous networks

58. Inferring novel indications of approved drugs via a learning method with local and global consistency

59. Large-scale extraction of accurate drug-disease treatment pairs from biomedical literature for drug repurposing

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71. Network-based drug repositioning

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97. Prediction of Novel Drugs for Hepatocellular Carcinoma Based on Multi-Source Random Walk

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101. RANKS: a flexible tool for node label ranking and classification in biological networks

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105. RepurposeVS: A Drug Repurposing-Focused Computational Method for Accurate Drug-Target Signature Predictions

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118. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

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120. Using predicate and provenance information from a knowledge graph for drug efficacy screening

121. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

FACTOR 6. Antimicrobial Applications of Repurposed Drugs

1. 3, 5, 3'-Triiodothyroacetic acid (TRIAC) is an anti-inflammatory drug that targets toll-like receptor 2

2. A Biologically-Based Computational Approach to Drug Repurposing for Anthrax Infection

3. A combined systems and structural modeling approach repositions antibiotics for Mycoplasma genitalium

4. A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors

5. A Drug Repositioning Approach Reveals that Streptococcus mutans Is Susceptible to a Diverse Range of Established Antimicrobials and Nonantibiotics

6. A drug-repositioning screening identifies pentetic acid as a potential therapeutic agent for suppressing the elastase-mediated virulence of Pseudomonas aeruginosa

7. A reprofiled drug, auranofin, is effective against metronidazole-resistant Giardia lamblia

8. A signalome screening approach in the autoinflammatory disease TNF receptor associated periodic syndrome (TRAPS) highlights the anti-inflammatory properties of drugs for repurposing

9. A systematic screen of FDA-approved drugs for inhibitors of biological threat agents

10. Activity of anti-cancer protein kinase inhibitors against Leishmania spp

11. Aerosolized gentamicin reduces the burden of tuberculosis in a murine model

12. Alternative clinical indications for novel antibiotics licensed for skin and soft tissue infection

13. Alternative screening approaches for discovery of Middle East respiratory syndrome coronavirus inhibitors

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15. An invitro and invivo evaluation of new potential trans-sialidase inhibitors of Trypanosoma cruzi predicted by a computational drug repositioning method

16. An optimized background regimen for treatment of active tuberculosis with the next-generation benzothiazinone Macozinone (PBTZ169

17. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens

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22. Antibacterial effects of antiretrovirals, potential implications for microbiome studies in HIV

23. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

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26. Anticancer Drugs as Antibiofilm Agents in Candida albicans: Potential Targets

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29. Antifungal application of nonantifungal drugs

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31. Antiviral activity of doxycycline against vesicular stomatitis virus in vitro

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72. Drug repurposing for the treatment of staphylococcal infections

73. Drug repurposing of minocycline against dengue virus infection

74. Drug repurposing of quinine as antiviral against dengue virus infection

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83. EMUDRA: Ensemble of Multiple Drug Repositioning Approaches to improve prediction accuracy

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166. Repurposing an old drug to improve the use and safety of tissue plasminogen activator for acute ischemic stroke: minocycline

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187. Repurposing of Existing Statin drugs for treatment of Microbial Infections: How much Promising

188. Repurposing of gallium-based drugs for antibacterial therapy

189. Repurposing of nitroxoline as a potential anticancer agent against human prostate cancer: a crucial role on AMPK/mTOR signaling pathway and the interplay with Chk2 activation

190. Repurposing of nucleoside- and nucleobase-derivative drugs as antibiotics and biofilm inhibitors

191. Repurposing salicylanilide anthelmintic drugs to combat drug resistant Staphylococcus aureus

192. Repurposing screens identify rifamycins as potential broad-spectrum therapy for multidrug-resistant Acinetobacter baumannii and select agent microorganisms

193. Repurposing Strategy of Atorvastatin against Trypanosoma cruzi: In Vitro Monotherapy and Combined Therapy with Benznidazole Exhibit Synergistic Trypanocidal Activity

194. Repurposing the anthelmintic drug niclosamide to combat Helicobacter pylori

195. Repurposing the anticancer drug mitomycin C for the treatment of persistent Acinetobacter baumannii infections

196. Repurposing the antihistamine terfenadine for antimicrobial activity against Staphylococcus aureus

197. Repurposing the antimycotic drug flucytosine for suppression of Pseudomonas aeruginosa pathogenicity

198. Repurposing the Nonsteroidal Anti-inflammatory Drug Diflunisal as an Osteoprotective, Antivirulence Therapy for Staphylococcus aureus Osteomyelitis

199. Repurposing Toremifene for Treatment of Oral Bacterial Infections

200. Repurposing Zidovudine in combination with Tigecycline for treating carbapenem-resistant Enterobacteriaceae infections

201. Repurposing-a ray of hope in tackling extensively drug resistance in tuberculosis

202. Resistance-resistant antibiotics

203. Reversal of Azole Resistance in Candida albicans by Sulfa Antibacterial Drugs

204. Ribavirin suppresses bacterial virulence by targeting LysR-type transcriptional regulators

205. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain

206. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox

207. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides

208. Screening a Commercial Library of Pharmacologically Active Small Molecules against Staphylococcus aureus Biofilms

209. Screening a repurposing library for potentiators of antibiotics against Staphylococcus aureus biofilms

210. Screening of a Drug Library Identifies Inhibitors of Cell Intoxication by CNF1

211. Simvastatin increases the in vivo activity of the first-line tuberculosis regimen

212. Sphingolipids as targets for inhalation treatment of cystic fibrosis

213. Statins and Antimicrobial Effects: Simvastatin as a Potential Drug against Staphylococcus aureus Biofilm

214. Statins: antimicrobial resistance breakers or makers

215. Strategies to overcome the action of aminoglycoside-modifying enzymes for treating resistant bacterial infections

216. Structural Basis of Metallo-beta-Lactamase Inhibition by Captopril Stereoisomers

217. Synthetic lethality reveals mechanisms of Mycobacterium tuberculosis resistance to beta-lactams

218. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine

219. Tackling tuberculosis: Insights from an international TB Summit in London

220. Tamoxifen Provides Structural and Functional Rescue in Murine Models of Photoreceptor Degeneration

221. Target mechanism-based whole-cell screening identifies bortezomib as an inhibitor of caseinolytic protease in mycobacteria

222. Targeting intracellular p-aminobenzoic acid production potentiates the anti-tubercular action of antifolates

223. Tedizolid Activity Against Clinical Mycobacterium abscessus Complex Isolates-An in vitro Characterization Study

224. Teicoplanin inhibits Ebola pseudovirus infection in cell culture

225. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

226. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

227. The combination effects of licl and the active leflunomide metabolite, A771726, on viral-induced interleukin 6 production and EV-A71 replication

228. The epidemiology, pathogenesis, transmission, diagnosis, and management of multidrug-resistant, extensively drug-resistant, and incurable tuberculosis

229. The fatty acid synthase inhibitor triclosan: repurposing an anti-microbial agent for targeting prostate cancer

230. The Immunomodulatory Drug Glatiramer Acetate is Also an Effective Antimicrobial Agent that Kills Gram-negative Bacteria

231. The potential role of trimethoprim-sulfamethoxazole in the treatment of drug-resistant tuberculosis

232. The repositioning of the anti-fungal agent ciclopirox olamine as a novel therapeutic agent for the treatment of haematologic malignancy

233. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs

234. The role of moxifloxacin in tuberculosis therapy

235. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

236. Therapeutic synergy between tigecycline and venetoclax in a preclinical model of MYC/BCL2 double-hit B cell lymphoma

237. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function

238. Totally drug-resistant tuberculosis and adjunct therapies

239. Toward Repositioning Niclosamide for Antivirulence Therapy of Pseudomonas aeruginosa Lung Infections: Development of Inhalable Formulations through Nanosuspension Technology

240. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

241. Transcriptomic Analysis of the Host Response and Innate Resilience to Enterotoxigenic Escherichia coli Infection in Humans

242. Treatment of experimental autoimmune uveoretinitis with peroxisome proliferator-activated receptor alpha agonist fenofibrate

243. Triclosan Is an Aminoglycoside Adjuvant for Eradication of Pseudomonas aeruginosa Biofilms

244. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation

245. Tuberculosis clinical trial update and the current anti-tuberculosis drug portfolio

246. Tuberculosis--advances in development of new drugs, treatment regimens, host-directed therapies, and biomarkers

247. Use of minocycline in viral infections

248. Virtual screen for repurposing approved and experimental drugs for candidate inhibitors of EBOLA virus infection

249. Zafirlukast inhibits complexation of Lsr2 with DNA and growth of Mycobacterium tuberculosis

FACTOR 7. Repurposed Drugs or Antifungal Applications

1. A disease similarity matrix based on the uniqueness of shared genes

2. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis

3. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research

4. A miRNA-driven inference model to construct potential drug-disease associations for drug repositioning

5. A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer

6. A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes

7. A repurposing approach identifies off-patent drugs with fungicidal cryptococcal activity, a common structural chemotype, and pharmacological properties relevant to the treatment of cryptococcosis

8. A review of network-based approaches to drug repositioning

9. A Systematic Framework for Drug Repositioning from Integrated Omics and Drug Phenotype Profiles Using Pathway-Drug Network

10. A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case

11. Advances in epilepsy gene discovery and implications for epilepsy diagnosis and treatment

12. Anticancer Drugs as Antibiofilm Agents in Candida albicans: Potential Targets

13. Antifungal adjuvants: Preserving and extending the antifungal arsenal

14. Antifungal amphiphilic kanamycins: new life for an old drug

15. Antifungal application of nonantifungal drugs

16. Antifungal Phenothiazines: Optimization, Characterization of Mechanism, and Modulation of Neuroreceptor Activity

17. Antifungal properties of the anti-hypertensive drug: aliskiren

18. Antifungals

19. Antiviral activity of micafungin against enterovirus 71

20. Antiviral, antifungal, and antiparasitic activities of fluoroquinolones optimized for treatment of bacterial infections: a puzzling paradox or a logical consequence of their mode of action

21. Application of Atlas of Cancer Signalling Network in preclinical studies

22. Artemisinins, new miconazole potentiators resulting in increased activity against Candida albicans biofilms

23. Atorvastatin as a promising anticryptococcal agent

24. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

25. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

26. Calcineurin-NFAT signalling in myeloid leucocytes: new prospects and pitfalls in immunosuppressive therapy

27. Cancer Drug Response Profile scan (CDRscan): A Deep Learning Model That Predicts Drug Effectiveness from Cancer Genomic Signature

28. Cancer drugs inhibit morphogenesis in the human fungal pathogen, Candida albicans

29. Candidiasis and the impact of flow cytometry on antifungal drug discovery

30. Combined analysis of gene expression and genome binding profiles identified potential therapeutic targets of ciclopirox in Ewing sarcoma

31. Combining in vitro and in silico Approaches to Find New Candidate Drugs Targeting the Pathological Proteins Related to the Alzheimer's Disease

32. Compensating for literature annotation bias when predicting novel drug-disease relationships through Medical Subject Heading Over-representation Profile (MeSHOP) similarity

33. Computational approaches for innovative antiepileptic drug discovery

34. Computational drug repositioning for peripheral arterial disease: prediction of anti-inflammatory and pro-angiogenic therapeutics

35. Computational drug repositioning using low-rank matrix approximation and randomized algorithms

36. Constructing Disease Similarity Networks Based on Disease Module Theory

37. Cross-species discovery of syncretic drug combinations that potentiate the antifungal fluconazole

38. CYP51 as drug targets for fungi and protozoan parasites: past, present and future

39. DenguePredict: An Integrated Drug Repositioning Approach towards Drug Discovery for Dengue

40. Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference

41. Development of anti-fungal pesticides from protein kinase inhibitor-based anticancer agents

42. Development of inhalable hyaluronan/mannitol composite dry powders for flucytosine repositioning in local therapy of lung infections

43. Disease classification: from phenotypic similarity to integrative genomics and beyond

44. DR2DI: a powerful computational tool for predicting novel drug-disease associations

45. dRiskKB: a large-scale disease-disease risk relationship knowledge base constructed from biomedical text

46. DrPOCS: Drug repositioning based on projection onto convex sets

47. Drug repositioning based on comprehensive similarity measures and Bi-Random walk algorithm

48. Drug repositioning based on triangularly balanced structure for tissue-specific diseases in incomplete interactome

49. Drug Repositioning by Integrating Known Disease-Gene and Drug-Target Associations in a Semi-supervised Learning Model

50. Drug repositioning for enzyme modulator based on human metabolite-likeness

51. Drug repositioning for orphan genetic diseases through Conserved Anticoexpressed Gene Clusters (CAGCs

52. Drug repositioning for prostate cancer: using a data-driven approach to gain new insights

53. Drug Repurposing Approach Identifies a Synergistic Drug Combination of an Antifungal Agent and an Experimental Organometallic Drug for Melanoma Treatment

54. Drug repurposing as an alternative for the treatment of recalcitrant bacterial infections

55. Drug Repurposing Screening Identifies Tioconazole as an ATG4 Inhibitor that Suppresses Autophagy and Sensitizes Cancer Cells to Chemotherapy

56. Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology

57. Drug target prediction and repositioning using an integrated network-based approach

58. Drug-disease association and drug-repositioning predictions in complex diseases using causal inference-probabilistic matrix factorization

59. DrugNet: network-based drug-disease prioritization by integrating heterogeneous data

60. Drugs currently under investigation for the treatment of invasive candidiasis

61. DT-Web: a web-based application for drug-target interaction and drug combination prediction through domain-tuned network-based inference

62. Elucidating the modes of action for bioactive compounds in a cell-specific manner by large-scale chemically-induced transcriptomics

63. Estrogen receptor antagonists are anti-cryptococcal agents that directly bind EF hand proteins and synergize with fluconazole in vivo

64. Exploration of the Anti-Inflammatory Drug Space Through Network Pharmacology: Applications for Drug Repurposing

65. Exploring anti-malarial potential of FDA approved drugs: an in silico approach

66. Finding the targets of a drug by integration of gene expression data with a protein interaction network

67. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC

68. From drug response profiling to target addiction scoring in cancer cell models

69. Functional genetics-directed identification of novel pharmacological inhibitors of FAS- and TNF-dependent apoptosis that protect mice from acute liver failure

70. Fusing literature and full network data improves disease similarity computation

71. Future perspectives for cryptococcosis treatment

72. Gene-set analysis based on the pharmacological profiles of drugs to identify repurposing opportunities in schizophrenia

73. Glybenclamide: an antidiabetic with in vivo antithrombotic activity

74. Heter-LP: A heterogeneous label propagation algorithm and its application in drug repositioning

75. High-throughput screening of a collection of known pharmacologically active small compounds for identification of Candida albicans biofilm inhibitors

76. Identification of drug candidates and repurposing opportunities through compound-target interaction networks

77. Identification of Small-Molecule Inhibitors of Human Golgi Mannosidase via a Drug Repositioning Screen

78. Imidazole Antifungal Drugs Inhibit the Cell Proliferation and Invasion of Human Breast Cancer Cells

79. Imidazolium salts as innovative agents against Leishmania amazonensis

80. In silico prediction of chemical mechanism of action via an improved network-based inference method

81. In vitro activity of the antifungal azoles itraconazole and posaconazole against Leishmania amazonensis

82. In vitro analysis of finasteride activity against Candida albicans urinary biofilm formation and filamentation

83. In vitro and in vivo studies of the antiparasitic activity of sterol 14alpha-demethylase (CYP51) inhibitor VNI against drug-resistant strains of Trypanosoma cruzi

84. Individualized network-based drug repositioning infrastructure for precision oncology in the panomics era

85. Inferring drug-disease associations based on known protein complexes

86. Inferring drug-disease associations from integration of chemical, genomic and phenotype data using network propagation

87. Inferring new indications for approved drugs via random walk on drug-disease heterogenous networks

88. Inferring novel indications of approved drugs via a learning method with local and global consistency

89. Link prediction in drug-target interactions network using similarity indices

90. Linking biochemical pathways and networks to adverse drug reactions

91. Linking PharmGKB to phenotype studies and animal models of disease for drug repurposing

92. LRSSL: predict and interpret drug-disease associations based on data integration using sparse subspace learning

93. Mapping Protein Targets of Bioactive Small Molecules Using Lipid-Based Chemical Proteomics

94. Matrix Factorization-Based Prediction of Novel Drug Indications by Integrating Genomic Space

95. MD-Miner: a network-based approach for personalized drug repositioning

96. Mitochondrial biogenesis is required for the anchorage-independent survival and propagation of stem-like cancer cells

97. Molecular docking studies on thirteen fluoroquinolines with human topoisomerase II a and b

98. Multi-target drug repositioning by bipartite block-wise sparse multi-task learning

99. Network-based approach to prediction and population-based validation of in silico drug repurposing

100. Network-based drug repositioning

101. Network-based drug repositioning: A novel strategy for discovering potential antidepressants and their mode of action

102. Network-based in silico drug efficacy screening

103. Network-based inference methods for drug repositioning

104. Network-based machine learning and graph theory algorithms for precision oncology

105. Neuroblastoma, a Paradigm for Big Data Science in Pediatric Oncology

106. New applications for known drugs: Human glycogen synthase kinase 3 inhibitors as modulators of Aspergillus fumigatus growth

107. New drug candidates for treatment of atypical meningiomas: An integrated approach using gene expression signatures for drug repurposing

108. New pharmacological treatment strategies for relapse prevention

109. Newer patents in antimycotic therapy

110. Novel Antifungal Compounds Discovered in Medicines for Malaria Venture's Malaria Box

111. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis

112. Novel therapeutic strategy for cancer and autoimmune conditions: Modulating cell metabolism and redox capacity

113. On the Integration of In Silico Drug Design Methods for Drug Repurposing

114. One reporter for in-cell activity profiling of majority of protein kinase oncogenes

115. Pathogenicity phenomena in three model systems: from network mining to emerging system-level properties

116. Pathway and network-based strategies to translate genetic discoveries into effective therapies

117. PATIENT-SPECIFIC DATA FUSION FOR CANCER STRATIFICATION AND PERSONALISED TREATMENT

118. Pharmacologic treatments for pulmonary hypertension: exploring pharmacogenomics

119. Pharmacotherapeutic Targeting of G Protein-Coupled Receptors in Oncology: Examples of Approved Therapies and Emerging Concepts

120. Polypharmacology in Drug Discovery: A Review from Systems Pharmacology Perspective

121. Predicting drug-disease associations and their therapeutic function based on the drug-disease association bipartite network

122. Predicting drug-disease interactions by semi-supervised graph cut algorithm and three-layer data integration

123. Predicting drug-target interactions using restricted Boltzmann machines

124. Predicting Drug-Target Interactions With Multi-Information Fusion

125. Predicting new indications for approved drugs using a proteochemometric method

126. Predicting Potential Drugs for Breast Cancer based on miRNA and Tissue Specificity

127. Prediction of chemical-protein interactions network with weighted network-based inference method

128. Prediction of drug-target interaction by label propagation with mutual interaction information derived from heterogeneous network

129. Prediction of drug-target interactions and drug repositioning via network-based inference

130. Prediction of drugs having opposite effects on disease genes in a directed network

131. Prediction of new drug indications based on clinical data and network modularity

132. Prediction of Novel Drugs and Diseases for Hepatocellular Carcinoma Based on Multi-Source Simulated Annealing Based Random Walk

133. Prediction of Novel Drugs for Hepatocellular Carcinoma Based on Multi-Source Random Walk

134. PROMISCUOUS: a database for network-based drug-repositioning

135. ProphTools: general prioritization tools for heterogeneous biological networks

136. Protein localization vector propagation: a method for improving the accuracy of drug repositioning

137. Quinacrine inhibits Candida albicans growth and filamentation at neutral pH

138. RANKS: a flexible tool for node label ranking and classification in biological networks

139. Rapid identification of antifungal compounds against Exserohilum rostratum using high throughput drug repurposing screens

140. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective

141. Recent advances in the machine learning-based drug-target interaction prediction

142. Repositioning of Endonuclear Receptors Binders as Potential Antibacterial and Antifungal Agents. Eptyloxim: A Potential and Novel Gyrase B and Cytochrome Cyp51 Inhibitor

143. Repurpose terbutaline sulfate for amyotrophic lateral sclerosis using electronic medical records

144. RepurposeVS: A Drug Repurposing-Focused Computational Method for Accurate Drug-Target Signature Predictions

145. Repurposing antipsychotic drugs into antifungal agents: Synergistic combinations of azoles and bromperidol derivatives in the treatment of various fungal infections

146. Repurposing Approach Identifies Auranofin with Broad Spectrum Antifungal Activity That Targets Mia40-Erv1 Pathway

147. Repurposing as a means to increase the activity of amphotericin B and caspofungin against Candida albicans biofilms

148. Repurposing atovaquone: targeting mitochondrial complex III and OXPHOS to eradicate cancer stem cells

149. Repurposing auranofin as an antifungal: In vitro activity against a variety of medically important fungi

150. Repurposing drugs to fast-track therapeutic agents for the treatment of cryptococcosis

151. Repurposing FDA approved drugs against the human fungal pathogen, Candida albicans

152. Repurposing of Aspirin and Ibuprofen as Candidate Anti-Cryptococcus Drugs

153. Repurposing ospemifene for potentiating an antigen-specific immune response

154. Repurposing Resveratrol and Fluconazole To Modulate Human Cytochrome P450-Mediated Arachidonic Acid Metabolism

155. Repurposing the Clinically Efficacious Antifungal Agent Itraconazole as an Anticancer Chemotherapeutic

156. Reversal of Azole Resistance in Candida albicans by Sulfa Antibacterial Drugs

157. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox

158. Scoring multiple features to predict drug disease associations using information fusion and aggregation

159. Screening a Repurposing Library for Inhibitors of Multidrug-Resistant Candida auris Identifies Ebselen as a Repositionable Candidate for Antifungal Drug Development

160. SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drug-target interactions and drug repositioning

161. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association

162. Some Remarks on Prediction of Drug-Target Interaction with Network Models

163. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

164. Statins: antimicrobial resistance breakers or makers

165. Strategies in the discovery of novel antifungal scaffolds

166. Substrate-driven mapping of the degradome by comparison of sequence logos

167. Synergistic combinations of antifungals and anti-virulence agents to fight against Candida albicans

168. Synergy testing of FDA-approved drugs identifies potent drug combinations against Trypanosoma cruzi

169. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data

170. Targeting calcium homeostasis as the therapy of Chagas' disease and leishmaniasis - a review

171. The Amide Local Anesthetic Lidocaine in Cancer Surgery-Potential Antimetastatic Effects and Preservation of Immune Cell Function? A Narrative Review

172. The anti-Aspergillus drug pipeline: Is the glass half full or empty

173. The Anti-helminthic Compound Mebendazole Has Multiple Antifungal Effects against Cryptococcus neoformans

174. The antidepressant 5-HT2A receptor antagonists pizotifen and cyproheptadine inhibit serotonin-enhanced platelet function

175. The extraction of drug-disease correlations based on module distance in incomplete human interactome

176. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs

177. The Tissue-Reconstructing Ability of Colon CSCs Is Enhanced by FK506 and Suppressed by GSK3 Inhibition

178. The triphenylethylenes, a novel class of antifungals

179. Therapeutic Effect of Repurposed Temsirolimus in Lung Adenocarcinoma Model

180. Topical delivery of ebselen encapsulated in biopolymeric nanocapsules: drug repurposing enhanced antifungal activity

181. Toward improved anti-cryptococcal drugs: Novel molecules and repurposed drugs

182. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

183. Towards drug repositioning: a unified computational framework for integrating multiple aspects of drug similarity and disease similarity

184. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

185. Treatment of Disseminated Leishmaniasis With Liposomal Amphotericin B

186. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation

187. Updates on drug-target network; facilitating polypharmacology and data integration by growth of DrugBank database

188. Virtual screening and drug repositioning as strategies for the discovery of new antifungal inhibitors of oxidosqualene cyclase

189. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

FACTOR 8a. Use of Cellular Signatures Library to Provide Gene Expression Profiles for Drug Repurposing Prediction

1. A comparative study of disease genes and drug targets in the human protein interactome

2. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning

3. Drug repurposing to target Ebola virus replication and virulence using structural systems pharmacology

4. Drug repurposing: An approach to tackle drug resistance in S. typhimurium

5. Elucidating the modes of action for bioactive compounds in a cell-specific manner by large-scale chemically-induced transcriptomics

6. Exploration of the Anti-Inflammatory Drug Space Through Network Pharmacology: Applications for Drug Repurposing

7. Exploring the anti-proliferative activity of Pelargonium sidoides DC with in silico target identification and network pharmacology

8. Fenoprofen -- an old drug rediscovered as a biased allosteric enhancer for melanocortin receptors

9. Human pathway-based disease network

10. Identification of key pathways and drug repurposing for anaplastic thyroid carcinoma by integrated bioinformatics analysis

11. Identification of Potential Therapeutics to Conquer Drug Resistance in Salmonella typhimurium: Drug Repurposing Strategy

12. Multi-target drug repositioning by bipartite block-wise sparse multi-task learning

13. Neighbours of cancer-related proteins have key influence on pathogenesis and could increase the drug target space for anticancer therapies

14. Network-based machine learning and graph theory algorithms for precision oncology

15. New drug candidates for treatment of atypical meningiomas: An integrated approach using gene expression signatures for drug repurposing

16. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis

17. Old drugs with new skills: fenoprofen as an allosteric enhancer at melanocortin receptor 3

18. Repositioning drugs by targeting network modules: a Parkinson's disease case study

19. The extraction of drug-disease correlations based on module distance in incomplete human interactome

20. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

21. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

22. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

FACTOR 8b. Ligand-Based Target Inference

1. Application of drug repositioning strategy to TOFISOPAM

2. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

3. Cascade Ligand- and Structure-Based Virtual Screening to Identify New Trypanocidal Compounds Inhibiting Putrescine Uptake

4. Chemical-induced disease extraction via recurrent piecewise convolutional neural networks

5. Computational profiling of bioactive compounds using a target-dependent composite workflow

6. Disease classification: from phenotypic similarity to integrative genomics and beyond

7. Docking of a novel DNA methyltransferase inhibitor identified from high-throughput screening: insights to unveil inhibitors in chemical databases

8. Drug repurposing for chronic myeloid leukemia: in silico and in vitro investigation of DrugBank database for allosteric Bcr-Abl inhibitors

9. Expediting the Design, Discovery and Development of Anticancer Drugs using Computational Approaches

10. Exploring polypharmacology using a ROCS-based target fishing approach

11. High-throughput identification of off-targets for the mechanistic study of severe adverse drug reactions induced by analgesics

12. Hit Recycling: Discovery of a Potent Carbonic Anhydrase Inhibitor by in Silico Target Fishing

13. How good are publicly available web services that predict bioactivity profiles for drug repurposing

14. In Silico target fishing: addressing a "Big Data" problem by ligand-based similarity rankings with data fusion

15. MOST: most-similar ligand based approach to target prediction

16. Pharmacophore-Based Repositioning of Approved Drugs as Novel Staphylococcus aureus NorA Efflux Pump Inhibitors

17. Polypharmacological Drug-target Inference for Chemogenomics

18. Predicting targeted polypharmacology for drug repositioning and multi- target drug discovery

19. Prediction of Human Drug Targets and Their Interactions Using Machine Learning Methods: Current and Future Perspectives

20. Protein-ligand-based pharmacophores: generation and utility assessment in computational ligand profiling

21. Research advance in the drug target prediction based on chemoinformatics

22. Reverse docking: a powerful tool for drug repositioning and drug rescue

23. Reverse Screening Methods to Search for the Protein Targets of Chemopreventive Compounds

24. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison

25. TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database

26. TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds

27. Tools for in silico target fishing

28. Using reverse docking for target identification and its applications for drug discovery

FACTOR 9. Binding Site Analysis for Drug Repurposing

1. 2-acylamino-5-nitro-1,3-thiazoles: preparation and in vitro bioevaluation against four neglected protozoan parasites

2. 3, 5, 3'-Triiodothyroacetic acid (TRIAC) is an anti-inflammatory drug that targets toll-like receptor 2

3. A Biologically-Based Computational Approach to Drug Repurposing for Anthrax Infection

4. A combined systems and structural modeling approach repositions antibiotics for Mycoplasma genitalium

5. A comparative study of disease genes and drug targets in the human protein interactome

6. A computational approach to finding novel targets for existing drugs

7. A cross-species analysis method to analyze animal models' similarity to human's disease state

8. A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors

9. A disease similarity matrix based on the uniqueness of shared genes

10. A Drug Screen using Human iPSC-Derived Hepatocyte-like Cells Reveals Cardiac Glycosides as a Potential Treatment for Hypercholesterolemia

11. A drug target slim: using gene ontology and gene ontology annotations to navigate protein-ligand target space in ChEMBL

12. A dual drug regimen synergistically blocks human parainfluenza virus infection

13. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge

14. A large-scale computational approach to drug repositioning

15. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning

16. A machine learning-based method to improve docking scoring functions and its application to drug repurposing

17. A Multilayer Network Approach for Guiding Drug Repositioning in Neglected Diseases

18. A network integration approach for drug-target interaction prediction and computational drug repositioning from heterogeneous information

19. A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes

20. A New Method for Computational Drug Repositioning Using Drug Pairwise Similarity

21. A new niclosamide derivatives-B17 can inhibit urological cancers growth through apoptosis-related pathway

22. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia

23. A novel multi-modal drug repurposing approach for identification of potent ACK1 inhibitors

24. A perspective on targeting non-structural proteins to combat neglected tropical diseases: Dengue, West Nile and Chikungunya viruses

25. A phase Ib multiple ascending dose study of the safety, tolerability, and central nervous system availability of AZD0530 (saracatinib) in Alzheimer's disease

26. A physarum-inspired prize-collecting steiner tree approach to identify subnetworks for drug repositioning

27. A potential target of Tanshinone IIA for acute promyelocytic leukemia revealed by inverse docking and drug repurposing

28. A profound computational study to prioritize the disease-causing mutations in PRPS1 gene

29. A protein folding molecular imaging biosensor monitors the effects of drugs that restore mutant p53 structure and its downstream function in glioblastoma cells

30. A quality alert and call for improved curation of public chemistry databases

31. A rapid and affordable screening platform for membrane protein trafficking

32. A Receptor Tyrosine Kinase Inhibitor, Dovitinib (TKI-258), Enhances BMP-2-Induced Osteoblast Differentiation In Vitro

33. A reprofiled drug, auranofin, is effective against metronidazole-resistant Giardia lamblia

34. A review of drugs for treatment of Alzheimer's disease in clinical trials: main trends

35. A review of MED-SuMo applications

36. A screen for Fli-1 transcriptional modulators identifies PKC agonists that induce erythroid to megakaryocytic differentiation and suppress leukemogenesis

37. A screening cascade to identify ERbeta ligands

38. A Semi-Supervised Approach for Refining Transcriptional Signatures of Drug Response and Repositioning Predictions

39. A signalome screening approach in the autoinflammatory disease TNF receptor associated periodic syndrome (TRAPS) highlights the anti-inflammatory properties of drugs for repurposing

40. A structure- and chemical genomics-based approach for repositioning of drugs against VCP/p97 ATPase

41. A tool to utilize adverse effect profiles to identify brain-active medications for repurposing

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725. Repurposing the clinically approved calcium antagonist manidipine dihydrochloride as a new early inhibitor of human cytomegalovirus targeting the Immediate-Early 2 (IE2) protein

726. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease

727. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

728. Repurposing Toremifene for Treatment of Oral Bacterial Infections

729. Rescue of cell death and inflammation of a mouse model of complex 1-mediated vision loss by repurposed drug molecules

730. Research and development of anti-Alzheimer's disease drugs: an update from the perspective of technology flows

731. Resistance-resistant antibiotics

732. Reverse docking: a powerful tool for drug repositioning and drug rescue

733. Reverse Screening Methods to Search for the Protein Targets of Chemopreventive Compounds

734. Review and comparative assessment of similarity-based methods for prediction of drug-protein interactions in the druggable human proteome

735. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia

736. Revisiting Connectivity Map from a gene co-expression network analysis

737. Rho-associated kinase signalling and the cancer microenvironment: novel biological implications and therapeutic opportunities

738. Ribavirin as a tri-targeted antitumor repositioned drug

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740. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain

741. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

742. Roles of the RANKL-RANK axis in antitumour immunity - implications for therapy

743. Schizophrenia interactome with 504 novel protein-protein interactions

744. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides

745. Screening a repurposing library, the Medicines for Malaria Venture Stasis Box, against Schistosoma mansoni

746. Screening of a composite library of clinically used drugs and well-characterized pharmacological compounds for cystathionine beta-synthase inhibition identifies benserazide as a drug potentially suitable for repurposing for the experimental therapy of colon cancer

747. Screening of FDA-Approved Drugs for Inhibitors of Japanese Encephalitis Virus Infection

748. Second medical use in Turkey

749. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

750. SELF-BLM: Prediction of drug-target interactions via self-training SVM

751. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association

752. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients

753. Similarity-based prediction for Anatomical Therapeutic Chemical classification of drugs by integrating multiple data sources

754. Simultaneous blockade of IL-6 and CCL5 signaling for synergistic inhibition of triple-negative breast cancer growth and metastasis

755. Simvastatin offers new prospects for the treatment of Duchenne muscular dystrophy

756. SIS3, a specific inhibitor of Smad3 reverses ABCB1- and ABCG2-mediated multidrug resistance in cancer cell lines

757. Small Molecules in Development for the Treatment of Spinal Muscular Atrophy

758. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison

759. Some Remarks on Prediction of Drug-Target Interaction with Network Models

760. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

761. SPIDR: small-molecule peptide-influenced drug repurposing

762. SPILLO-PBSS: detecting hidden binding sites within protein 3D-structures through a flexible structure-based approach

763. SRSF6-regulated alternative splicing that promotes tumour progression offers a therapy target for colorectal cancer

764. Statin and rottlerin small-molecule inhibitors restrict colon cancer progression and metastasis via MACC1

765. Statins: antimicrobial resistance breakers or makers

766. Steroids-specific target library for steroids target prediction

767. Structural analysis of dihydrofolate reductases enables rationalization of antifolate binding affinities and suggests repurposing possibilities

768. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

769. Structural basis for inactivation of Giardia lamblia carbamate kinase by disulfiram

770. Structural basis for the hepatoprotective effects of antihypertensive 1,4-dihydropyridine drugs

771. Structural basis for the resilience of efavirenz (DMP-266) to drug resistance mutations in HIV-1 reverse transcriptase

772. Structural Basis of Antisickling Effects of Selected FDA Approved Drugs: A Drug Repurposing Study

773. Structural Basis of Metallo-beta-Lactamase Inhibition by Captopril Stereoisomers

774. Structural insight into selectivity and resistance profiles of ROS1 tyrosine kinase inhibitors

775. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

776. Structure based discovery of clomifene as a potent inhibitor of cancer-associated mutant IDH1

777. Structure based drug discovery for designing leads for the non-toxic metabolic targets in multi drug resistant Mycobacterium tuberculosis

778. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation

779. Structure Investigation, Enrichment Analysis and Structure-based Repurposing of FDA-approved Drugs as Inhibitors of BET-BRD4

780. Structure-based discovery of the novel antiviral properties of naproxen against the nucleoprotein of influenza A virus

781. Structure-based identification of a NEDD8-activating enzyme inhibitor via drug repurposing

782. Structure-based repurposing of FDA-approved drugs as inhibitors of NEDD8-activating enzyme

783. Substrate-driven mapping of the degradome by comparison of sequence logos

784. SUMOylation in brain ischemia: Patterns, targets, and translational implications

785. Suppressive effects of dabrafenibon endothelial protein C receptor shedding

786. SWEETLEAD: an in silico database of approved drugs, regulated chemicals, and herbal isolates for computer-aided drug discovery

787. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

788. Synergistic combination of flavopiridol and carfilzomib targets commonly dysregulated pathways in adrenocortical carcinoma and has biomarkers of response

789. Systematic analyses of drugs and disease indications in RepurposeDB reveal pharmacological, biological and epidemiological factors influencing drug repositioning

790. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine

791. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

792. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data

793. Systematic Identification and Assessment of Therapeutic Targets for Breast Cancer Based on Genome-Wide RNA Interference Transcriptomes

794. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach

795. Systemic amyloidosis: novel therapies and role of biomarkers

796. Systems Pharmacology Links GPCRs with Retinal Degenerative Disorders

797. Target mechanism-based whole-cell screening identifies bortezomib as an inhibitor of caseinolytic protease in mycobacteria

798. Target-Based Drug Repositioning Using Large-Scale Chemical-Protein Interactome Data

799. Target-similarity search using Plasmodium falciparum proteome identifies approved drugs with anti-malarial activity and their possible targets

800. TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database

801. Targeting ADAM17 Sheddase Activity in Cancer

802. Targeting calcium homeostasis as the therapy of Chagas' disease and leishmaniasis - a review

803. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

804. Targeting Gliomas: Can a New Alkylating Hybrid Compound Make a Difference

805. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases

806. Targeting the off-targets: a computational bioinformatics approach to understanding the polypharmacology of nelfinavir

807. Targeting the schizophrenia genome: a fast track strategy from GWAS to clinic

808. TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds

809. Tegaserod mimics the neurostimulatory glycan polysialic acid and promotes nervous system repair

810. Tetracycline hydrochloride: A potential clinical drug for radioprotection

811. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

812. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo

813. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death

814. The antineoplastic properties of FTY720: evidence for the repurposing of fingolimod

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817. The bitter pill: clinical drugs that activate the human bitter taste receptor TAS2R14

818. The CARLSBAD database: a confederated database of chemical bioactivities

819. The combination astemizole-gefitinib as a potential therapy for human lung cancer

820. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

821. The druggable genome and support for target identification and validation in drug development

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827. The Hippo pathway in normal development and cancer

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829. The Horizon of a Therapy for Rare Genetic Diseases: A "Druggable" Future for Fibrodysplasia Ossificans Progressiva

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831. The human disease network in terms of dysfunctional regulatory mechanisms

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833. The Importance of Bioactivation in Computer-Guided Drug Repositioning. Why the Parent Drug is Not Always Enough

834. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

835. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs

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847. The sodium channel-blocking antiepileptic drug phenytoin inhibits breast tumour growth and metastasis

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FACTOR 10. Antiinflammatory Applications for Repurposed Drugs

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483. S100A4 in Cancer Metastasis: Wnt Signaling-Driven Interventions for Metastasis Restriction

484. Screening of a composite library of clinically used drugs and well-characterized pharmacological compounds for cystathionine beta-synthase inhibition identifies benserazide as a drug potentially suitable for repurposing for the experimental therapy of colon cancer

485. Screening of a Drug Library Identifies Inhibitors of Cell Intoxication by CNF1

486. SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drug-target interactions and drug repositioning

487. Senicapoc: Repurposing a Drug to Target Microglia KCa3.1 in Stroke

488. Serological biochemical markers of surrogate efficacy and safety as a novel approach to drug repositioning

489. Simultaneous blockade of IL-6 and CCL5 signaling for synergistic inhibition of triple-negative breast cancer growth and metastasis

490. Sphingolipids as targets for inhalation treatment of cystic fibrosis

491. Statin and rottlerin small-molecule inhibitors restrict colon cancer progression and metastasis via MACC1

492. Statins in conditions other than hypocholesterolemic effects for chronic subdural hematoma therapy, old drug, new tricks

493. Strategy for identifying repurposed drugs for the treatment of cerebral cavernous malformation

494. Stromal microenvironment in type VII collagen-deficient skin: The ground for squamous cell carcinoma development

495. Structure based discovery of clomifene as a potent inhibitor of cancer-associated mutant IDH1

496. Structure-based discovery of the novel antiviral properties of naproxen against the nucleoprotein of influenza A virus

497. Suppressive effects of dabrafenibon endothelial protein C receptor shedding

498. Suppressive effects of methylthiouracil on polyphosphate-mediated vascular inflammatory responses

499. Sustained Complete Response to Metronomic Chemotherapy in a Child with Refractory Atypical Teratoid Rhabdoid Tumor: A Case Report

500. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

501. Synergistic combination of flavopiridol and carfilzomib targets commonly dysregulated pathways in adrenocortical carcinoma and has biomarkers of response

502. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

503. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer

504. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach

505. Systemic amyloidosis: novel therapies and role of biomarkers

506. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes

507. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification

508. Systems medicine: evolution of systems biology from bench to bedside

509. Tamoxifen Provides Structural and Functional Rescue in Murine Models of Photoreceptor Degeneration

510. Targeted therapy for Epstein-Barr virus-associated gastric carcinoma using low-dose gemcitabine-induced lytic activation

511. Targeting Abl kinases to regulate vascular leak during sepsis and acute respiratory distress syndrome

512. Targeting ADAM17 Sheddase Activity in Cancer

513. Targeting cancer stem cells with dietary phytochemical - Repositioned drug combinations

514. Targeting Gliomas: Can a New Alkylating Hybrid Compound Make a Difference

515. Targeting Hypoxia-Inducible Factors for Antiangiogenic Cancer Therapy

516. Targeting Mevalonate Pathway in Cancer Treatment: Repurposing of Statins

517. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress

518. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases

519. Targeting the ubiquitin-proteasome system for cancer treatment: discovering novel inhibitors from nature and drug repurposing

520. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

521. Tezosentan inhibits uptake of proinflammatory endothelin-1 in stenotic aortic valves

522. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

523. The Amide Local Anesthetic Lidocaine in Cancer Surgery-Potential Antimetastatic Effects and Preservation of Immune Cell Function? A Narrative Review

524. The Anthelmintic Drug Niclosamide Inhibits the Proliferative Activity of Human Osteosarcoma Cells by Targeting Multiple Signal Pathways

525. The anti-fibrotic agent pirfenidone synergizes with cisplatin in killing tumor cells and cancer-associated fibroblasts

526. The Antiarrhythmic Drug, Amiodarone, Decreases AKT Activity and Sensitizes Human Acute Myeloid Leukemia Cells to Apoptosis by ABT-263

527. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo

528. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death

529. The antiparasitic drug, potassium antimony tartrate, inhibits tumor angiogenesis and tumor growth in nonsmall-cell lung cancer

530. The Architecture and Function of Monoclonal Antibody-Functionalized Mesoporous Silica Nanoparticles Loaded with Mifepristone: Repurposing Abortifacient for Cancer Metastatic Chemoprevention

531. The CARMA3-Bcl10-MALT1 Signalosome Drives NFkappaB Activation and Promotes Aggressiveness in Angiotensin II Receptor-Positive Breast Cancer

532. The clinically used PARP inhibitor olaparib improves organ function, suppresses inflammatory responses and accelerates wound healing in a murine model of third-degree burn injury

533. The combination effects of licl and the active leflunomide metabolite, A771726, on viral-induced interleukin 6 production and EV-A71 replication

534. The Concept of Hormesis in Cancer Therapy - Is Less More

535. The druggable genome and support for target identification and validation in drug development

536. The Emerging Facets of Non-Cancerous Warburg Effect

537. The EYA tyrosine phosphatase activity is pro-angiogenic and is inhibited by benzbromarone

538. The heterogeneity of cancer stem-like cells at the invasive front

539. The Hippo pathway in normal development and cancer

540. The human immunodeficiency virus protease inhibitor ritonavir is potentially active against urological malignancies

541. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

542. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs

543. The novel JNK inhibitor AS602801 inhibits cancer stem cells in vitro and in vivo

544. The pain interactome: connecting pain-specific protein interactions

545. The photosensitizer verteporfin has light-independent anti-leukemic activity for Ph-positive acute lymphoblastic leukemia and synergistically works with dasatinib

546. The potent Cdc7-Dbf4 (DDK) kinase inhibitor XL413 has limited activity in many cancer cell lines and discovery of potential new DDK inhibitor scaffolds

547. The repurposed anthelmintic mebendazole in combination with trametinib suppresses refractory NRASQ61K melanoma

548. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs

549. The role of statins in inflammatory vasculitides

550. The Significance of Hypothiocyanite Production via the Pendrin/DUOX/Peroxidase Pathway in the Pathogenesis of Asthma

551. The use of transcriptomic biomarkers for personalized medicine

552. Therapeutic compositions and uses of alpha1-antitrypsin: a patent review (2012 - 2015

553. Therapeutic drug repositioning using personalized proteomics of liquid biopsies

554. Therapeutic Effect of Repurposed Temsirolimus in Lung Adenocarcinoma Model

555. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

556. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

557. Therapeutic Effects of Repurposed Therapies in Non-Small Cell Lung Cancer: What Is Old Is New Again

558. Therapeutic Manipulation of Ageing: Repurposing Old Dogs and Discovering New Tricks

559. Therapeutic modulators of peroxisome proliferator-activated receptors (PPAR): a patent review (2008-present

560. Therapeutic Strategies for the Treatment of Alcoholic Hepatitis

561. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment

562. Therapeutic synergy between tigecycline and venetoclax in a preclinical model of MYC/BCL2 double-hit B cell lymphoma

563. Therapeutical approaches under investigation for treatment of Chagas disease

564. Thiopurine Drugs Repositioned as Tyrosinase Inhibitors

565. Thioridazine inhibits autophagy and sensitizes glioblastoma cells to temozolomide

566. Third-generation sequencing techniques and applications to drug discovery

567. Three-Dimensional Cell Culture-Based Screening Identifies the Anthelmintic Drug Nitazoxanide as a Candidate for Treatment of Colorectal Cancer

568. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function

569. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5

570. Toward drug repurposing in epigenetics: olsalazine as a hypomethylating compound active in a cellular context

571. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

572. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

573. Transforming Cancer Prevention through Precision Medicine and Immune-oncology

574. Transplantomics: Toward Precision Medicine in Transplantation Research

575. Treating Influenza Infection, From Now and Into the Future

576. Treatment of Disseminated Leishmaniasis With Liposomal Amphotericin B

577. Treatment of experimental autoimmune uveoretinitis with peroxisome proliferator-activated receptor alpha agonist fenofibrate

578. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer

579. Trimodal Therapy: Combining Hyperthermia with Repurposed Bexarotene and Ultrasound for Treating Liver Cancer

580. Tuberculosis--advances in development of new drugs, treatment regimens, host-directed therapies, and biomarkers

581. Tuberculosis: From an incurable scourge to a curable disease - journey over a millennium

582. Tumor deconstruction as a tool for advanced drug screening and repositioning

583. Tumor progression: the neuronal input

584. Tumor selective cytotoxic action of a thiomorpholin hydroxamate inhibitor (TMI-1) in breast cancer

585. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin

586. Understanding fibrosis in systemic sclerosis: shifting paradigms, emerging opportunities

587. Use of attenuated paramyxoviruses for cancer therapy

588. Use of minocycline in viral infections

589. Use of monoclonal antibody-IRDye800CW bioconjugates in the resection of breast cancer

590. Validating drug repurposing signals using electronic health records: a case study of metformin associated with reduced cancer mortality

591. Valproic acid in the complex therapy of malignant tumors

592. Vinorelbine rescue therapy for dogs with primary urinary bladder carcinoma

593. Vitamin K and hepatocellular carcinoma: The basic and clinic

594. Warfarin Blocks Gas6-Mediated Axl Activation Required for Pancreatic Cancer Epithelial Plasticity and Metastasis

595. What's new in dermatology

596. YAP/TAZ Are Mechanoregulators of TGF-beta-Smad Signaling and Renal Fibrogenesis

FACTOR 11a. Biomarkers for Repurposed Drug-Enhanced Apoptosis of Cancer Cells

1. A Blockade of IGF Signaling Sensitizes Human Ovarian Cancer Cells to the Anthelmintic Niclosamide-Induced Anti-Proliferative and Anticancer Activities

2. A comparative study of disease genes and drug targets in the human protein interactome

3. A convenient synthesis of lubeluzole and its enantiomer: evaluation as chemosensitizing agents on human ovarian adenocarcinoma and lung carcinoma cells

4. A new niclosamide derivatives-B17 can inhibit urological cancers growth through apoptosis-related pathway

5. A novel anti-cancer role of beta-apopicropodophyllin against non-small cell lung cancer cells

6. A protein folding molecular imaging biosensor monitors the effects of drugs that restore mutant p53 structure and its downstream function in glioblastoma cells

7. A selective mitochondrial-targeted chlorambucil with remarkable cytotoxicity in breast and pancreatic cancers

8. A Small-molecule Kinase Inhibitor, CEP-1347, Inhibits Survivin Expression and Sensitizes Ovarian Cancer Stem Cells to Paclitaxel

9. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

10. Albumin nanoparticles increase the anticancer efficacy of albendazole in ovarian cancer xenograft model

11. Angiotensin II type 1 receptor blocker telmisartan induces apoptosis and autophagy in adult T-cell leukemia cells

12. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin

13. ANTENNA, a Multi-Rank, Multi-Layered Recommender System for Inferring Reliable Drug-Gene-Disease Associations: Repurposing Diazoxide as a Targeted Anti-Cancer Therapy

14. Anthelmintic mebendazole enhances cisplatin's effect on suppressing cell proliferation and promotes differentiation of head and neck squamous cell carcinoma (HNSCC

15. Antifibrotic effect of pirfenidone in a mouse model of human nonalcoholic steatohepatitis

16. Antimalarial activity of novel 4-cyano-3-methylisoquinoline inhibitors against Plasmodium falciparum: design, synthesis and biological evaluation

17. Artemisinin and Its Derivatives as a Repurposing Anticancer Agent: What Else Do We Need to Do

18. Assessment of the antitumor potential of Bithionol in vivo using a xenograft model of ovarian cancer

19. Bioinformatics and in vitro experimental analyses identify the selective therapeutic potential of interferon gamma and apigenin against cervical squamous cell carcinoma and adenocarcinoma

20. Bithionol inhibits ovarian cancer cell growth in vitro - studies on mechanism(s) of action

21. Buformin inhibits the stemness of erbB-2-overexpressing breast cancer cells and premalignant mammary tissues of MMTV-erbB-2 transgenic mice

22. Carfilzomib is an effective anticancer agent in anaplastic thyroid cancer

23. Case-specific potentiation of glioblastoma drugs by pterostilbene

24. Characterization of drug-induced transcriptional modules: towards drug repositioning and functional understanding

25. Chloroquine upregulates TRAIL/TRAILR2 expression and potentiates doxorubicin anti-tumor activity in thioacetamide-induced hepatocellular carcinoma model

26. Clustering based drug-drug interaction networks for possible repositioning of drugs against EGFR mutations: Clustering based DDI networks for EGFR mutations

27. Clustering drug-drug interaction networks with energy model layouts: community analysis and drug repurposing

28. Combination of cationic dexamethasone derivative and STAT3 inhibitor (WP1066) for aggressive melanoma: a strategy for repurposing a phase I clinical trial drug

29. Comparative oncology approach to drug repurposing in osteosarcoma

30. Complex-disease networks of trait-associated single-nucleotide polymorphisms (SNPs) unveiled by information theory

31. Computational Cell Cycle Profiling of Cancer Cells for Prioritizing FDA-Approved Drugs with Repurposing Potential

32. Computational Prediction of Drug?Target Interactions Using Chemical, Biological, and Network Features

33. Cross-species discovery of syncretic drug combinations that potentiate the antifungal fluconazole

34. Cyclic AMP efflux inhibitors as potential therapeutic agents for leukemia

35. Data integration to prioritize drugs using genomics and curated data

36. Delineation of biological and molecular mechanisms underlying the diverse anticancer activities of mycophenolic acid

37. DenguePredict: An Integrated Drug Repositioning Approach towards Drug Discovery for Dengue

38. Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference

39. Discovering drugs to overcome chemoresistance in ovarian cancers based on the cancer genome atlas tumor transcriptome profile

40. Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues

41. Discovery of rafoxanide as a dual CDK4/6 inhibitor for the treatment of skin cancer

42. Disulfiram is a direct and potent inhibitor of human O6-methylguanine-DNA methyltransferase (MGMT) in brain tumor cells and mouse brain and markedly increases the alkylating DNA damage

43. Disulfiram/copper causes redox-related proteotoxicity and concomitant heat shock response in ovarian cancer cells that is augmented by auranofin-mediated thioredoxin inhibition

44. Down-regulating IL-6/GP130 targets improved the anti-tumor effects of 5-fluorouracil in colon cancer

45. Drug repositioning based on triangularly balanced structure for tissue-specific diseases in incomplete interactome

46. Drug repositioning for gynecologic tumors: a new therapeutic strategy for cancer

47. Drug repositioning of mevalonate pathway inhibitors as antitumor agents for ovarian cancer

48. Drug repositioning using disease associated biological processes and network analysis of drug targets

49. Drug Repurposing by Simulating Flow Through Protein-Protein Interaction Networks

50. Drug repurposing screen identifies lestaurtinib amplifies the ability of the poly (ADP-ribose) polymerase 1 inhibitor AG14361 to kill breast cancer associated gene-1 mutant and wild type breast cancer cells

51. Drug repurposing screening identifies bortezomib and panobinostat as drugs targeting cancer associated fibroblasts (CAFs) by synergistic induction of apoptosis

52. Drug repurposing: a better approach for infectious disease drug discovery

53. Drug-dependent functionalization of wild-type and mutant p53 in cisplatin-resistant human ovarian tumor cells

54. Effects of digitoxin on cell migration in ovarian cancer inflammatory microenvironment

55. Effects of repurposed drug candidates nitroxoline and nelfinavir as single agents or in combination with erlotinib in pancreatic cancer cells

56. eMatchSite: sequence order-independent structure alignments of ligand binding pockets in protein models

57. Emerging roles of Myc in stem cell biology and novel tumor therapies

58. Evaluation of Effects of Metformin in Primary Ovarian Cancer Cells

59. Ex vivo drug response profiling detects recurrent sensitivity patterns in drug-resistant acute lymphoblastic leukemia

60. Exendin-4 ameliorates traumatic brain injury-induced cognitive impairment in rats

61. Exploring the anti-proliferative activity of Pelargonium sidoides DC with in silico target identification and network pharmacology

62. Expression of DRD2 Is Increased in Human Pancreatic Ductal Adenocarcinoma and Inhibitors Slow Tumor Growth in Mice

63. Expression Profiling Identifies Bezafibrate as Potential Therapeutic Drug for Lung Adenocarcinoma

64. Folate Receptor-Targeted Polymeric Micellar Nanocarriers for Delivery of Orlistat as a Repurposed Drug against Triple-Negative Breast Cancer

65. FTY720 inhibits mesothelioma growth in vitro and in a syngeneic mouse model

66. Functional genomics of pain in analgesic drug development and therapy

67. Functional Module Connectivity Map (FMCM): a framework for searching repurposed drug compounds for systems treatment of cancer and an application to colorectal adenocarcinoma

68. Glutamate release inhibitor, Riluzole, inhibited proliferation of human hepatocellular carcinoma cells by elevated ROS production

69. Growth-suppressive activity of raloxifene on liver cancer cells by targeting IL-6/GP130 signaling

70. High-throughput drug library screening identifies colchicine as a thyroid cancer inhibitor

71. Human disease-drug network based on genomic expression profiles

72. Hydroxyurea synergizes with valproic acid in wild-type p53 acute myeloid leukaemia

73. Ibuprofen and diclofenac treatments reduce proliferation of pancreatic acinar cells upon inflammatory injury and mitogenic stimulation

74. Identification of a new pharmacological activity of the phenylpiperazine derivative naftopidil: tubulin-binding drug

75. Identification of an old antibiotic clofoctol as a novel activator of unfolded protein response pathways and an inhibitor of prostate cancer

76. Identification of FDA-approved drugs as novel allosteric inhibitors of human executioner caspases

77. Identification of novel small-molecule inhibitors targeting menin-MLL interaction, repurposing the antidiarrheal loperamide

78. Identification of repaglinide as a therapeutic drug for glioblastoma multiforme

79. Identification of small-molecule inhibitors of Zika virus infection and induced neural cell death via a drug repurposing screen

80. Identification of thiazolo[5,4-d]pyrimidine derivatives as potent antiproliferative agents through the drug repurposing strategy

81. Identifying candidate agents for lung adenocarcinoma by walking the human interactome

82. Imidazole Antifungal Drugs Inhibit the Cell Proliferation and Invasion of Human Breast Cancer Cells

83. In Silico Identification and In Vitro and In Vivo Validation of Anti-Psychotic Drug Fluspirilene as a Potential CDK2 Inhibitor and a Candidate Anti-Cancer Drug

84. In vivo loss-of-function screens identify KPNB1 as a new druggable oncogene in epithelial ovarian cancer

85. Integrating systems biology sources illuminates drug action

86. Interaction and localization diversities of global and local hubs in human protein-protein interaction networks

87. Kinase scaffold repurposing for neglected disease drug discovery: discovery of an efficacious, lapatinib-derived lead compound for trypanosomiasis

88. Kinome Profiling Identifies Druggable Targets for Novel Human Cytomegalovirus (HCMV) Antivirals

89. Licofelone Enhances the Efficacy of Paclitaxel in Ovarian Cancer by Reversing Drug Resistance and Tumor Stem-like Properties

90. Loss of BRCA1 in the Cells of Origin of Ovarian Cancer Induces Glycolysis: A Window of Opportunity for Ovarian Cancer Chemoprevention

91. Lymphoma and myeloma cells are highly sensitive to growth arrest and apoptosis induced by artesunate

92. Mechanism-informed Repurposing of Minocycline Overcomes Resistance to Topoisomerase Inhibition for Peritoneal Carcinomatosis

93. Memantine induces apoptosis and inhibits cell cycle progression in LNCaP prostate cancer cells

94. Metformin and epithelial ovarian cancer therapeutics

95. Metformin repositioning as antitumoral agent: selective antiproliferative effects in human glioblastoma stem cells, via inhibition of CLIC1-mediated ion current

96. Mevalonate Pathway Antagonist Suppresses Formation of Serous Tubal Intraepithelial Carcinoma and Ovarian Carcinoma in Mouse Models

97. Molecular mimicry-based repositioning of nutlin-3 to anti-apoptotic Bcl-2 family proteins

98. Mucuna pruriens (L.) DC chemo sensitize human breast cancer cells via downregulation of prolactin-mediated JAK2/STAT5A signaling

99. Multiple effects of digoxin on subsets of cancer-associated genes through the alternative splicing pathway

100. Nelfinavir, A lead HIV protease inhibitor, is a broad-spectrum, anticancer agent that induces endoplasmic reticulum stress, autophagy, and apoptosis in vitro and in vivo

101. Network approaches to drug discovery

102. Network insights into the genes regulated by hepatocyte nuclear factor 4 in response to drug induced perturbations: a review

103. Network-based machine learning and graph theory algorithms for precision oncology

104. New derivatives of the antimalarial drug Pyrimethamine in the control of melanoma tumor growth: an in vitro and in vivo study

105. Niclosamide and its analogs are potent inhibitors of Wnt/beta-catenin, mTOR and STAT3 signaling in ovarian cancer

106. Niclosamide Exhibits Potent Anticancer Activity and Synergizes with Sorafenib in Human Renal Cell Cancer Cells

107. Niclosamide Induces Epiboly Delay During Early Zebrafish Embryogenesis

108. Novel strategies of ovarian cancer treatment

109. Novel therapeutic strategy for cancer and autoimmune conditions: Modulating cell metabolism and redox capacity

110. Olanzapine, an Atypical Antipsychotic, Inhibits Survivin Expression and Sensitizes Cancer Cells to Chemotherapeutic Agents

111. Old drug, new trick: repurposing metformin for gynecologic cancers

112. Oncogenic targets Mmp7, S100a9, Nppb and Aldh1a3 from transcriptome profiling of FAP and Pirc adenomas are downregulated in response to tumor suppression by Clotam

113. Ormeloxifene efficiently inhibits ovarian cancer growth

114. P-gp Inhibition by the Anti-psychotic Drug Pimozide Increases Apoptosis, as well as Expression of pRb and pH2AX in Highly Drug-resistant KBV20C Cells

115. Patient-Customized Drug Combination Prediction and Testing for T-cell Prolymphocytic Leukemia Patients

116. PATIENT-SPECIFIC DATA FUSION FOR CANCER STRATIFICATION AND PERSONALISED TREATMENT

117. PEGylated chitosan nanoparticles potentiate repurposing of ormeloxifene in breast cancer therapy

118. Phosphorylation of Single Stranded RNA Virus Proteins and Potential for Novel Therapeutic Strategies

119. Piperazine-based Alpha-1 AR Blocker, Naftopidil, Selectively Suppresses Malignant Human Bladder Cells via Induction of Apoptosis

120. Preclinical Evaluation of Vemurafenib as Therapy for BRAFV600E Mutated Sarcomas

121. Predicting drug-target interactions using probabilistic matrix factorization

122. Predicting Drug-Target Interactions With Multi-Information Fusion

123. Quantitative high-throughput drug screening identifies novel classes of drugs with anticancer activity in thyroid cancer cells: opportunities for repurposing

124. Rationale for an experimental treatment of retinitis pigmentosa: 140-month test of hypothesis with one patient

125. Re-purposing clinical kinase inhibitors to enhance chemosensitivity by overriding checkpoints

126. Recycling drug screen repurposes hydroxyurea as a sensitizer of glioblastomas to temozolomide targeting de novo DNA synthesis, irrespective of molecular subtype

127. Repositioning chlorpromazine for treating chemoresistant glioma through the inhibition of cytochrome c oxidase bearing the COX4-1 regulatory subunit

128. Repositioning of anti-viral drugs as therapy for cervical cancer

129. Repurposing itraconazole for the treatment of cancer

130. Repurposing of nitroxoline as a potential anticancer agent against human prostate cancer: a crucial role on AMPK/mTOR signaling pathway and the interplay with Chk2 activation

131. Repurposing of phentolamine as a potential anticancer agent against human castration-resistant prostate cancer: A central role on microtubule stabilization and mitochondrial apoptosis pathway

132. Repurposing the anti-epileptic drug sodium valproate as an adjuvant treatment for diffuse intrinsic pontine glioma

133. Repurposing the anti-malarial drug artesunate as a novel therapeutic agent for metastatic renal cell carcinoma due to its attenuation of tumor growth, metastasis, and angiogenesis

134. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist

135. Revisiting old drugs as novel agents for retinoblastoma: in vitro and in vivo antitumor activity of cardenolides

136. Ritonavir blocks AKT signaling, activates apoptosis and inhibits migration and invasion in ovarian cancer cells

137. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

138. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

139. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

140. Sulforaphane Prevents Neuronal Apoptosis and Memory Impairment in Diabetic Rats

141. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine

142. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer

143. Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis

144. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

145. Targeting the ubiquitin-proteasome system for cancer treatment: discovering novel inhibitors from nature and drug repurposing

146. The Anthelmintic Drug Niclosamide Inhibits the Proliferative Activity of Human Osteosarcoma Cells by Targeting Multiple Signal Pathways

147. The anti-fibrotic agent pirfenidone synergizes with cisplatin in killing tumor cells and cancer-associated fibroblasts

148. The anti-hypertensive drug prazosin inhibits glioblastoma growth via the PKCdelta-dependent inhibition of the AKT pathway

149. The Antiarrhythmic Drug, Amiodarone, Decreases AKT Activity and Sensitizes Human Acute Myeloid Leukemia Cells to Apoptosis by ABT-263

150. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells

151. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

152. The fatty acid synthase inhibitor triclosan: repurposing an anti-microbial agent for targeting prostate cancer

153. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma

154. The novel JNK inhibitor AS602801 inhibits cancer stem cells in vitro and in vivo

155. The potent Cdc7-Dbf4 (DDK) kinase inhibitor XL413 has limited activity in many cancer cell lines and discovery of potential new DDK inhibitor scaffolds

156. The repurposed anthelmintic mebendazole in combination with trametinib suppresses refractory NRASQ61K melanoma

157. Therapeutic Effect of Quinacrine, an Antiprotozoan Drug, by Selective Suppression of p-CHK1/2 in p53-Negative Malignant Cancers

158. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

159. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment

160. Transcriptomic changes induced by mycophenolic acid in gastric cancer cells

161. Transcriptomic characterization of the novel avian-origin influenza A (H7N9) virus: specific host response and responses intermediate between avian (H5N1 and H7N7) and human (H3N2) viruses and implications for treatment options

162. Transforming Cancer Prevention through Precision Medicine and Immune-oncology

163. Trypanocidal Effect of Isotretinoin through the Inhibition of Polyamine and Amino Acid Transporters in Trypanosoma cruzi

164. Tumor selective cytotoxic action of a thiomorpholin hydroxamate inhibitor (TMI-1) in breast cancer

165. Use of an anti-viral drug, Ribavirin, as an anti-glioblastoma therapeutic

166. Using a novel computational drug-repositioning approach (DrugPredict) to rapidly identify potent drug candidates for cancer treatment

167. Valproic acid in the complex therapy of malignant tumors

168. Valproic Acid Promotes Apoptosis and Cisplatin Sensitivity Through Downregulation of H19 Noncoding RNA in Ovarian A2780 Cells

FACTOR 11b. Repurposed Drugs for Oxidative Stress Reduction

1. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

2. A conceptually new treatment approach for relapsed glioblastoma: coordinated undermining of survival paths with nine repurposed drugs (CUSP9) by the International Initiative for Accelerated Improvement of Glioblastoma Care

3. A reprofiled drug, auranofin, is effective against metronidazole-resistant Giardia lamblia

4. A Topical Zinc Ionophore Blocks Tumorigenic Progression in UV-exposed SKH-1 High-risk Mouse Skin

5. Acetaminophen attenuates dopamine neuron degeneration in animal models of Parkinson's disease

6. Activity of imidazole compounds on Leishmania (L.) infantum chagasi: reactive oxygen species induced by econazole

7. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

8. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

9. Albendazole as a promising molecule for tumor control

10. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin

11. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

12. Antibacterial activity and mechanism of action of auranofin against multi-drug resistant bacterial pathogens

13. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

14. Antihelminthic drug niclosamide inhibits CIP2A and reactivates tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells

15. Artemisinin analogues as potent inhibitors of in vitro hepatitis C virus replication

16. Atorvastatin as a promising anticryptococcal agent

17. Auranofin and its Analogues Show Potent Antimicrobial Activity Covering Multiresistant Pathogens: Structure-Activity Relationships

18. Auranofin inactivates Trichomonas vaginalis thioredoxin reductase and is effective against trichomonads in vitro and in vivo

19. Auranofin induces apoptosis by ROS-mediated ER stress and mitochondrial dysfunction and displayed synergistic lethality with piperlongumine in gastric cancer

20. Auranofin induces lethal oxidative and endoplasmic reticulum stress and exerts potent preclinical activity against chronic lymphocytic leukemia

21. Auranofin is highly efficacious against Toxoplasma gondii in vitro and in an in vivo experimental model of acute toxoplasmosis

22. Auranofin-mediated inhibition of PI3K/AKT/mTOR axis and anticancer activity in non-small cell lung cancer cells

23. Auranofin: repurposing an old drug for a golden new age

24. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

25. beta-Caryophyllene protects against alcoholic steatohepatitis by attenuating inflammation and metabolic dysregulation in mice

26. Beyond multiple mechanisms and a unique drug: Defective autophagy as pivotal player in cerebral cavernous malformation pathogenesis and implications for targeted therapies

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35. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

36. Developmental toxicity of auranofin in zebrafish embryos

37. Discovery of the neuroprotective effects of alvespimycin by computational prioritization of potential anti-Parkinson agents

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55. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs

56. Identifying and Tackling Emergent Vulnerability in Drug-Resistant Mycobacteria

57. Imidazolium salts as innovative agents against Leishmania amazonensis

58. In silico and in vitro drug screening identifies new therapeutic approaches for Ewing sarcoma

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64. Mitigation of carbon tetrachloride-induced hepatic injury by methylene blue, a repurposed drug, is mediated by dual inhibition of GSK3beta downstream of PKA

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77. Platelet Hyperreactivity in Diabetes: Focus on GPVI Signaling-Are Useful Drugs Already Available

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82. Reactions of model proteins with aurothiomalate, a clinically established gold(I) drug: The comparison with auranofin

83. Recent Advances in Antabuse (Disulfiram): The Importance of its Metal-binding Ability to its Anticancer Activity

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87. Repurposing auranofin as a lead candidate for treatment of lymphatic filariasis and onchocerciasis

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105. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C

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FACTOR 12. Repurposed Drugs that Increase or Decrease ROS for Different Applications

1. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

2. A Blockade of IGF Signaling Sensitizes Human Ovarian Cancer Cells to the Anthelmintic Niclosamide-Induced Anti-Proliferative and Anticancer Activities

3. A cellular genetics approach identifies gene-drug interactions and pinpoints drug toxicity pathway nodes

4. A chemical-genetic interaction map of small molecules using high-throughput imaging in cancer cells

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7. A cross-species analysis method to analyze animal models' similarity to human's disease state

8. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

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10. A drug-repositioning screen for primary pancreatic ductal adenocarcinoma cells identifies 6-thioguanine as an effective therapeutic agent for TPMT-low cancer cells

11. A High-Content Screening of Anticancer Compounds Suggests the Multiple Tyrosine Kinase Inhibitor Ponatinib for Repurposing in Neuroblastoma Therapy

12. A network based approach to drug repositioning identifies plausible candidates for breast cancer and prostate cancer

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15. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia

16. A novel chemoradiation targeting stem and nonstem pancreatic cancer cells by repurposing disulfiram

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74. Bioinformatics and in vitro experimental analyses identify the selective therapeutic potential of interferon gamma and apigenin against cervical squamous cell carcinoma and adenocarcinoma

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100. Comparative oncology approach to drug repurposing in osteosarcoma

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106. Computational repositioning and experimental validation of approved drugs for HIF-prolyl hydroxylase inhibition

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110. Copper Complexes in Cancer Therapy

111. Current and upcoming pharmacotherapy for non-alcoholic fatty liver disease

112. Cyclic AMP efflux inhibitors as potential therapeutic agents for leukemia

113. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer

114. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

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123. Discovery of alkyl bis(oxy)dibenzimidamide derivatives as novel protein arginine methyltransferase 1 (PRMT1) inhibitors

124. Discovery of drug mode of action and drug repositioning from transcriptional responses

125. Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues

126. Discovery of rafoxanide as a dual CDK4/6 inhibitor for the treatment of skin cancer

127. Discovery of the neuroprotective effects of alvespimycin by computational prioritization of potential anti-Parkinson agents

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129. Disulfiram's Anticancer Activity: Evidence and Mechanisms

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136. Doxycycline or how to create new with the old

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138. Drug Intervention Response Predictions with PARADIGM (DIRPP) identifies drug resistant cancer cell lines and pathway mechanisms of resistance

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140. Drug repositioning for gynecologic tumors: a new therapeutic strategy for cancer

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148. Drug repurposing in cancer

149. Drug repurposing of quinine as antiviral against dengue virus infection

150. Drug Repurposing of the Anthelmintic Niclosamide to Treat Multidrug-Resistant Leukemia

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157. Drug-Repositioning Screens Identify Triamterene as a Selective Drug for the Treatment of DNA Mismatch Repair Deficient Cells

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164. Erythropoietin, a novel repurposed drug: an innovative treatment for wound healing in patients with diabetes mellitus

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166. Evaluating New Compounds to Treat Burkholderia pseudomallei Infections

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212. Identification of known drugs that act as inhibitors of NF-kappaB signaling and their mechanism of action

213. Identification of Mitoxantrone as a TRAIL-sensitizing agent for Glioblastoma Multiforme

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215. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs

216. Identification of Novel Cdc7 Kinase Inhibitors as Anti-Cancer Agents that Target the Interaction with Dbf4 by the Fragment Complementation and Drug Repositioning Approach

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64. Predicting new indications for approved drugs using a proteochemometric method

65. Predicting targeted polypharmacology for drug repositioning and multi- target drug discovery

66. Prediction of drug-target interactions for drug repositioning only based on genomic expression similarity

67. Prediction of Human Drug Targets and Their Interactions Using Machine Learning Methods: Current and Future Perspectives

68. ProBiS-ligands: a web server for prediction of ligands by examination of protein binding sites

69. Protein-ligand-based pharmacophores: generation and utility assessment in computational ligand profiling

70. Recent progress in repositioning Alzheimer's disease drugs based on a multitarget strategy

71. Repositioning of the anthelmintic drug mebendazole for the treatment for colon cancer

72. Repurposing Lesogaberan to Promote Human Islet Cell Survival and beta-Cell Replication

73. Research advance in the drug target prediction based on chemoinformatics

74. Reverse docking: a powerful tool for drug repositioning and drug rescue

75. Reverse Screening Methods to Search for the Protein Targets of Chemopreventive Compounds

76. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison

77. SPIDR: small-molecule peptide-influenced drug repurposing

78. Steroids-specific target library for steroids target prediction

79. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

80. Structural basis for the hepatoprotective effects of antihypertensive 1,4-dihydropyridine drugs

81. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation

82. Structure Investigation, Enrichment Analysis and Structure-based Repurposing of FDA-approved Drugs as Inhibitors of BET-BRD4

83. Tacrine-deferiprone hybrids as multi-target-directed metal chelators against Alzheimer's disease: a two-in-one drug

84. TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database

85. TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds

86. The bitter pill: clinical drugs that activate the human bitter taste receptor TAS2R14

87. The Hippo pathway in normal development and cancer

88. Therapeutic modulators of peroxisome proliferator-activated receptors (PPAR): a patent review (2008-present

89. Thiopurine Drugs Repositioned as Tyrosinase Inhibitors

90. Tools for in silico target fishing

91. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5

92. Using reverse docking for target identification and its applications for drug discovery

FACTOR 14. AMPK Activation for Cancer Treatment, Emphasizing Anti-Diabetic Drug Metformin

1. A cross-species analysis method to analyze animal models' similarity to human's disease state

2. A glucagon-like peptide-1 receptor agonist reduces intracranial pressure in a rat model of hydrocephalus

3. A phase Ib multiple ascending dose study of the safety, tolerability, and central nervous system availability of AZD0530 (saracatinib) in Alzheimer's disease

4. A phenome-wide association study of a lipoprotein-associated phospholipase A2 loss-of-function variant in 90 000 Chinese adults

5. A therapy for FXS

6. A two-step drug repositioning method based on a protein-protein interaction network of genes shared by two diseases and the similarity of drugs

7. A two-tiered unsupervised clustering approach for drug repositioning through heterogeneous data integration

8. Advances in epilepsy gene discovery and implications for epilepsy diagnosis and treatment

9. Advances in the therapeutic use of mammalian target of rapamycin (mTOR) inhibitors in dermatology

10. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

11. Anti-obesogenic and hypolipidemic effects of a glucagon-like peptide-1 receptor agonist derived from the saliva of the Gila monster

12. Application of computer-aided drug repurposing in the search of new cruzipain inhibitors: discovery of amiodarone and bromocriptine inhibitory effects

13. Baseline Regularization for Computational Drug Repositioning with Longitudinal Observational Data

14. Benserazide, a dopadecarboxylase inhibitor, suppresses tumor growth by targeting hexokinase 2

15. beta3-Adrenoceptor agonists for overactive bladder syndrome: Role of translational pharmacology in a repositioning clinical drug development project

16. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

17. Buformin inhibits the stemness of erbB-2-overexpressing breast cancer cells and premalignant mammary tissues of MMTV-erbB-2 transgenic mice

18. Calcium channel blockers as drug repurposing candidates for gestational diabetes: Mining large scale genomic and electronic health records data to repurpose medications

19. Can commonly prescribed drugs be repurposed for the prevention or treatment of Alzheimer's and other neurodegenerative diseases? Protocol for an observational cohort study in the UK Clinical Practice Research Datalink

20. Cancer Prevention and Interception: A New Era for Chemopreventive Approaches

21. Cancer: fundamentals behind pH targeting and the double-edged approach

22. Capsaicin: Current Understanding of Its Mechanisms and Therapy of Pain and Other Pre-Clinical and Clinical Uses

23. Cell-based screening identifies paroxetine as an inhibitor of diabetic endothelial dysfunction

24. Chromone as a Privileged Scaffold in Drug Discovery: Recent Advances

25. CK2 inhibition confers functional protection to young and aging axons against ischemia by differentially regulating the CDK5 and AKT signaling pathways

26. Clozapine Improves Memory Impairment and Reduces Abeta Level in the Tg-APPswe/PS1dE9 Mouse Model of Alzheimer's Disease

27. Combination of acamprosate and baclofen as a promising therapeutic approach for Parkinson's disease

28. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

29. Computational Drug Repositioning Using Continuous Self-Controlled Case Series

30. Construction of drug network based on side effects and its application for drug repositioning

31. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer

32. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

33. Designing novel therapies against sarcomas in the era of personalized medicine and economic crisis

34. Development of therapies for autoimmune disease at Stanford: a tale of multiple shots and one goal

35. Disulfiram with or without metformin inhibits oesophageal squamous cell carcinoma invivo

36. Dopamine antagonists for treatment resistance in autism spectrum disorders: review and focus on BDNF stimulators loxapine and amitriptyline

37. DPP-4 inhibitors promote proliferation and migration of rat brain microvascular endothelial cells under hypoxic/high-glucose conditions, potentially through the SIRT1/HIF-1/VEGF pathway

38. Drug repositioning for diabetes based on 'omics' data mining

39. Drug repositioning for gynecologic tumors: a new therapeutic strategy for cancer

40. Drug repurposing for vascular protection after acute ischemic stroke

41. Drug repurposing in kidney disease

42. Drug Repurposing of Metabolic Agents in Malignant Glioma

43. Drug repurposing: In-vitro anti-glycation properties of 18 common drugs

44. Drug target prediction and repositioning using an integrated network-based approach

45. Drug-disease association and drug-repositioning predictions in complex diseases using causal inference-probabilistic matrix factorization

46. Drug-repurposing identified the combination of Trolox C and Cytisine for the treatment of type 2 diabetes

47. Evaluation of Effects of Metformin in Primary Ovarian Cancer Cells

48. Exenatide and the treatment of patients with Parkinson's disease

49. Exendin-4 ameliorates traumatic brain injury-induced cognitive impairment in rats

50. Exploration of alpha1-antitrypsin treatment protocol for islet transplantation: dosing plan and route of administration

51. Exploring novel pharmacotherapeutic applications and repurposing potential of sodium glucose CoTransporter 2 inhibitors

52. Exploring the potential of adjunct therapy in tuberculosis

53. Fenofibrate Suppresses Oral Tumorigenesis via Reprogramming Metabolic Processes: Potential Drug Repurposing for Oral Cancer

54. Fluvastatin activates sirtuin 6 to regulate sterol regulatory element-binding proteins and AMP-activated protein kinase in HepG2 cells

55. Fluvoxamine, an anti-depressant, inhibits human glioblastoma invasion by disrupting actin polymerization

56. Folic Acid Exerts Post-Ischemic Neuroprotection In Vitro Through HIF-1alpha Stabilization

57. From ancient herb to modern drug: Artemisia annua and artemisinin for cancer therapy

58. Glipizide suppresses prostate cancer progression in the TRAMP model by inhibiting angiogenesis

59. Glycogen phosphorylase inhibition improves beta cell function

60. Hiding in plain view: the potential for commonly used drugs to reduce breast cancer mortality

61. High-throughput screening of FDA-approved drugs using oxygen biosensor plates reveals secondary mitofunctional effects

62. Histone Deacetylase Inhibitors and Diabetic Kidney Disease

63. Identification and validation of uterine stimulant methylergometrine as a potential inhibitor of caspase-1 activation

64. Identification of circadian clock modulators from existing drugs

65. Identification of novel therapeutics for complex diseases from genome-wide association data

66. Identification of repaglinide as a therapeutic drug for glioblastoma multiforme

67. Identification of thioridazine, an antipsychotic drug, as an antiglioblastoma and anticancer stem cell agent using public gene expression data

68. Immune Cell Metabolism in Tumor Microenvironment

69. In silico drug screening by using genome-wide association study data repurposed dabrafenib, an anti-melanoma drug, for Parkinson's disease

70. In vivo phenotypic screening: clinical proof of concept for a drug repositioning approach

71. Inhibition of effector antigen-specific T cells by intradermal administration of heme oxygenase-1 inducers

72. Inhibition of PI4K IIIalpha radiosensitizes in human tumor xenograft and immune-competent syngeneic murine tumor model

73. Inhibition of the insulin-like growth factor system is a potential therapy for rheumatoid arthritis

74. Insights into the Link Between Obesity and Cancer

75. Interplay of DDP4 and IP-10 as a Potential Mechanism for Cell Recruitment to Tuberculosis Lesions

76. Lessons from the Fourth Metronomic and Anti-angiogenic Therapy Meeting, 24-25 June 2014, Milan

77. Leveraging Population-Based Clinical Quantitative Phenotyping for Drug Repositioning

78. Liraglutide attenuates the depressive- and anxiety-like behaviour in the corticosterone induced depression model via improving hippocampal neural plasticity

79. Liraglutide modulates gut microbiota and reduces NAFLD in obese mice

80. LIRAGUTIDE AT A DOSE OF 3.0 MG (SAXENDA): NEW INDICATION FOR THE TREATMENT OF OBESITY

81. Management of drug-resistant tuberculosis in special sub-populations including those with HIV co-infection, pregnancy, diabetes, organ-specific dysfunction, and in the critically ill

82. MATE2 Expression Is Associated with Cancer Cell Response to Metformin

83. Memantine induces apoptosis and inhibits cell cycle progression in LNCaP prostate cancer cells

84. MeSHDD: Literature-based drug-drug similarity for drug repositioning

85. Metabolic reprogramming in clear cell renal cell carcinoma

86. Metformin - The Drug for the Treatment of Autoimmune Diseases; A New Use of a Known Anti-Diabetic Drug

87. Metformin and epithelial ovarian cancer therapeutics

88. Metformin and propranolol combination prevents cancer progression and metastasis in different breast cancer models

89. Metformin as a geroprotector: experimental and clinical evidence

90. Metformin as a repurposed therapy in advanced non-small cell lung cancer (NSCLC): results of a phase II trial

91. Metformin directly acts on mitochondria to alter cellular bioenergetics

92. Metformin for non-small cell lung cancer patients: Opportunities and pitfalls

93. Metformin for Prevention and Treatment of Colon Cancer: A Reappraisal of Experimental and Clinical Data

94. Metformin in patients with advanced pancreatic cancer: a double-blind, randomised, placebo-controlled phase 2 trial

95. Metformin inhibits hepatitis B virus protein production and replication in human hepatoma cells

96. Metformin repositioning as antitumoral agent: selective antiproliferative effects in human glioblastoma stem cells, via inhibition of CLIC1-mediated ion current

97. Metformin treatment ameliorates diabetes-associated decline in hippocampal neurogenesis and memory via phosphorylation of insulin receptor substrate 1

98. Metformin use and gynecological cancers: A novel treatment option emerging from drug repositioning

99. Metformin Use in Relation With Survival Outcomes of Patients With Renal Cell Carcinoma

100. Metformin: its emerging role in oncology

101. METFORMIN: NONGLYCEMIC EFFECTS AND POTENTIAL NOVEL INDICATIONS

102. Mitigation of carbon tetrachloride-induced hepatic injury by methylene blue, a repurposed drug, is mediated by dual inhibition of GSK3beta downstream of PKA

103. Mitochondria-Targeted Analogues of Metformin Exhibit Enhanced Antiproliferative and Radiosensitizing Effects in Pancreatic Cancer Cells

104. Mitochondria-targeted metformins: anti-tumour and redox signalling mechanisms

105. Model-based unsupervised learning informs metformin-induced cell-migration inhibition through an AMPK-independent mechanism in breast cancer

106. Modified Metformin as a More Potent Anticancer Drug: Mitochondrial Inhibition, Redox Signaling, Antiproliferative Effects and Future EPR Studies

107. Modulating the metabolism by trimetazidine enhances myoblast differentiation and promotes myogenesis in cachectic tumor-bearing c26 mice

108. Molecular property diagnostic suite for diabetes mellitus (MPDSDM): An integrated web portal for drug discovery and drug repurposing

109. Neuropathic Pain Creates an Enduring Prefrontal Cortex Dysfunction Corrected by the Type II Diabetic Drug Metformin But Not by Gabapentin

110. New culture medium concepts for cell transplantation

111. New perspectives for metformin in cancer therapy

112. Niclosamide, a Drug with Many (Re)purposes

113. No association between metformin use and survival in patients with pancreatic cancer: An observational cohort study

114. Non-diabetic clinical applications of insulin

115. Novel strategies of ovarian cancer treatment

116. Nutraceuticals and "repurposed" drugs of phytochemical origin in prevention and interception of chronic degenerative disease and cancer

117. Olaparib protects cardiomyocytes against oxidative stress and improves graft contractility during the early phase after heart transplantation in rats

118. Old drug, new trick: repurposing metformin for gynecologic cancers

119. One-carbon metabolism: an aging-cancer crossroad for the gerosuppressant metformin

120. Osteoprotegerin and Denosumab Stimulate Human Beta Cell Proliferation through Inhibition of the Receptor Activator of NF-kappaB Ligand Pathway

121. Paradoxical strategy for treating chronic diseases where the therapeutic effect is derived from compensatory response rather than drug effect

122. Parkinson's Disease, Diabetes and Cognitive Impairment

123. Pharmacological approach for drug repositioning against cardiorenal diseases

124. Platelet Hyperreactivity in Diabetes: Focus on GPVI Signaling-Are Useful Drugs Already Available

125. Potentiating the effects of radiotherapy in rectal cancer: the role of aspirin, statins and metformin as adjuncts to therapy

126. Pre-clinical effects of metformin and aspirin on the cell lines of different breast cancer subtypes

127. Precision medicine for suicidality: from universality to subtypes and personalization

128. Predicting and characterizing selective multiple drug treatments for metabolic diseases and cancer

129. Proximal Pathway Enrichment Analysis for Targeting Comorbid Diseases via Network Endopharmacology

130. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective

131. Repositioning chloroquine and metformin to eliminate cancer stem cell traits in pre-malignant lesions

132. Repositioning drugs for inflammatory disease - fishing for new anti-inflammatory agents

133. Repositioning metformin in cancer: genetics, drug targets, and new ways of delivery

134. Repositioning of bromocriptine for treatment of acute myeloid leukemia

135. Repositioning of Drugs in Cardiometabolic Disorders: Importance and Current Scenario

136. Repositioning therapy for thyroid cancer: new insights on established medications

137. Reprofiling of Troglitazone Towards More Active and Less Toxic Derivatives: A New Hope for Cancer Treatment

138. Repurposing diabetes drugs for brain insulin resistance in Alzheimer disease

139. Repurposing Drugs for Cancer Prevention

140. Repurposing Drugs to Target the Diabetes Epidemic

141. Repurposing existing drugs for new AMPK activators as a strategy to extend lifespan: a computer-aided drug discovery study

142. Repurposing itraconazole as an anticancer agent

143. Repurposing Lesogaberan to Promote Human Islet Cell Survival and beta-Cell Replication

144. Repurposing matrine for the treatment of hepatosteatosis and associated disorders in glucose homeostasis in mice

145. Repurposing Metformin as Therapy for Prostate Cancer within the STAMPEDE Trial Platform

146. Repurposing metformin for the prevention of cancer and cancer recurrence

147. Repurposing metformin: an old drug with new tricks in its binding pockets

148. Repurposing of Copper(II)-chelating Drugs for the Treatment of Neurodegenerative Diseases

149. Repurposing of metformin and aspirin by targeting AMPK-mTOR and inflammation for pancreatic cancer prevention and treatment

150. Repurposing of nitroxoline as a potential anticancer agent against human prostate cancer: a crucial role on AMPK/mTOR signaling pathway and the interplay with Chk2 activation

151. Repurposing old drugs in oncology: Opportunities with clinical and regulatory challenges ahead

152. Repurposing old drugs to chemoprevention: the case of metformin

153. Repurposing phenformin for the targeting of glioma stem cells and the treatment of glioblastoma

154. Repurposing the anti-malarial drug dihydroartemisinin suppresses metastasis of non-small-cell lung cancer via inhibiting NF-kappaB/GLUT1 axis

155. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

156. SIRT1 activation by methylene blue, a repurposed drug, leads to AMPK-mediated inhibition of steatosis and steatohepatitis

157. Statistically controlled identification of differentially expressed genes in one-to-one cell line comparisons of the CMAP database for drug repositioning

158. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

159. Study protocol of a phase IB/II clinical trial of metformin and chloroquine in patients with IDH1-mutated or IDH2-mutated solid tumours

160. Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis

161. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

162. Systematic drug repositioning based on clinical side-effects

163. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes

164. Systems pharmacology of adverse event mitigation by drug combinations

165. T3D-959: A Multi-Faceted Disease Remedial Drug Candidate for the Treatment of Alzheimer's Disease

166. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

167. Targeting Phosphatidylinositol 4-Kinase IIIalpha for Radiosensitization: A Potential Model of Drug Repositioning Using an Anti-Hepatitis C Viral Agent

168. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

169. The dual targeting of EGFR and ErbB2 with the inhibitor Lapatinib corrects high glucose-induced apoptosis and vascular dysfunction by opposing multiple diabetes-induced signaling changes

170. The Glucose Transporter PfHT1 Is an Antimalarial Target of the HIV Protease Inhibitor Lopinavir

171. The human disease network in terms of dysfunctional regulatory mechanisms

172. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

173. The Role of Common Pharmaceutical Agents on the Prevention and Treatment of Pancreatic Cancer

174. The susceptibility of trypanosomatid pathogens to PI3/mTOR kinase inhibitors affords a new opportunity for drug repurposing

175. Therapeutic Effects of Repurposed Therapies in Non-Small Cell Lung Cancer: What Is Old Is New Again

176. Therapeutic modulators of peroxisome proliferator-activated receptors (PPAR): a patent review (2008-present

177. Three-Dimensional Cell Culture-Based Screening Identifies the Anthelmintic Drug Nitazoxanide as a Candidate for Treatment of Colorectal Cancer

178. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5

179. Totally drug-resistant tuberculosis and adjunct therapies

180. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

181. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

182. Transforming Cancer Prevention through Precision Medicine and Immune-oncology

183. Treating the dysfunctional placenta

184. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin

185. Unexploited Antineoplastic Effects of Commercially Available Anti-Diabetic Drugs

186. Unveiling anticancer potential of glibenclamide: Its synergistic cytotoxicity with doxorubicin on cancer cells

187. Use of metformin and survival of patients with high-grade glioma

188. Using genetics to inform new therapeutics for diabetes

189. Validating drug repurposing signals using electronic health records: a case study of metformin associated with reduced cancer mortality

FACTOR 15. Repurposing of Cholesterol-Lowering Drugs for Chronic and Infectious Diseases

1. A Biologically-Based Computational Approach to Drug Repurposing for Anthrax Infection

2. A common rejection module (CRM) for acute rejection across multiple organs identifies novel therapeutics for organ transplantation

3. A Computational Systems Biology Approach for Identifying Candidate Drugs for Repositioning for Cardiovascular Disease

4. A profound computational study to prioritize the disease-causing mutations in PRPS1 gene

5. Activity of mefloquine and mefloquine derivatives against Echinococcus multilocularis

6. An optimized background regimen for treatment of active tuberculosis with the next-generation benzothiazinone Macozinone (PBTZ169

7. Anti-obesogenic and hypolipidemic effects of a glucagon-like peptide-1 receptor agonist derived from the saliva of the Gila monster

8. Anticancer Properties of Fenofibrate: A Repurposing Use

9. Antileishmanial Activity of Ezetimibe: Inhibition of Sterol Biosynthesis, In Vitro Synergy with Azoles, and Efficacy in Experimental Cutaneous Leishmaniasis

10. Atorvastatin as a promising anticryptococcal agent

11. Balance and circumstance: The renin angiotensin system in wound healing and fibrosis

12. Bioinformatics approach to prioritize known drugs towards repurposing for tuberculosis

13. Bisphosphonates inactivate human EGFRs to exert antitumor actions

14. Characterization of drug-induced transcriptional modules: towards drug repositioning and functional understanding

15. Computational Drug Repositioning by Target Hopping: A Use Case in Chagas Disease

16. Computational drugs repositioning identifies inhibitors of oncogenic PI3K/AKT/P70S6K-dependent pathways among FDA-approved compounds

17. Development of therapies for autoimmune disease at Stanford: a tale of multiple shots and one goal

18. Do statins, ACE inhibitors or sartans improve outcome in primary glioblastoma

19. Drug repositioning of mevalonate pathway inhibitors as antitumor agents for ovarian cancer

20. Drug repurposing for drug development in stroke

21. Drug repurposing for vascular protection after acute ischemic stroke

22. Drug repurposing may generate novel approaches to treating depression

23. Drug Repurposing of Metabolic Agents in Malignant Glioma

24. Drug Repurposing Screen Identifies Foxo1-Dependent Angiopoietin-2 Regulation in Sepsis

25. Drug repurposing screen reveals FDA-approved inhibitors of human HMG-CoA reductase and isoprenoid synthesis that block Cryptosporidium parvum growth

26. Drugs that reverse disease transcriptomic signatures are more effective in a mouse model of dyslipidemia

27. Effects of nutrition intervention for pressure ulcer patients--healing rate and speed of wound size and nutrition

28. Erythropoietin, a novel repurposed drug: an innovative treatment for wound healing in patients with diabetes mellitus

29. Evaluating a novel treatment for coronary artery inflammation in acute Kawasaki disease: A Phase I/IIa trial of atorvastatin

30. Exploring simvastatin, an antihyperlipidemic drug, as a potential topical antibacterial agent

31. Feedback Activation of STAT3 as a Cancer Drug-Resistance Mechanism

32. Fluvastatin activates sirtuin 6 to regulate sterol regulatory element-binding proteins and AMP-activated protein kinase in HepG2 cells

33. Fluvastatin inhibits FLT3 glycosylation in human and murine cells and prolongs survival of mice with FLT3/ITD leukemia

34. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC

35. Hiding in plain view: the potential for commonly used drugs to reduce breast cancer mortality

36. HMG-CoA Reductase Inhibition Delays DNA Repair and Promotes Senescence After Tumor Irradiation

37. Host-directed antimicrobial drugs with broad-spectrum efficacy against intracellular bacterial pathogens

38. Identification of potential anti-hepatitis C virus agents targeting non structural protein 5B using computational techniques

39. In Silico-Based Repositioning of Phosphinothricin as a Novel Technetium-99m Imaging Probe with Potential Anti-Cancer Activity

40. In vitro antibacterial effects of statins against bacterial pathogens causing skin infections

41. Inhibiting Mycobacterium tuberculosis within and without

42. Innovations in asthma therapy: is there a role for inhaled statins

43. Insights from Second-Line Treatments for Idiopathic Dilated Cardiomyopathy

44. Integrating systems biology sources illuminates drug action

45. Is There Potential for Repurposing Statins as Novel Antimicrobials

46. Ketanserin, an antidepressant, exerts its antileishmanial action via inhibition of 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGR) enzyme of Leishmania donovani

47. Metabolic switch during adipogenesis: From branched chain amino acid catabolism to lipid synthesis

48. Metastasis and chemoresistance in CD133 expressing pancreatic cancer cells are dependent on their lipid raft integrity

49. Mevalonate Pathway Antagonist Suppresses Formation of Serous Tubal Intraepithelial Carcinoma and Ovarian Carcinoma in Mouse Models

50. Mevalonate pathway blockage enhances the efficacy of mTOR inhibitors with the activation of retinoblastoma protein in renal cell carcinoma

51. Molecular therapies for inherited epidermolysis bullosa

52. Mutational patterns in the HIV genome and cross-resistance following nucleoside and nucleotide analogue drug exposure

53. New drug candidates for depression - a nationwide population-based study

54. Niacin as a drug repositioning candidate for hyperphosphatemia management in dialysis patients

55. Non-diabetic clinical applications of insulin

56. Pharmacogenomic approaches to lipid-regulating trials

57. Phenytoin repositioned in wound healing: clinical experience spanning 60 years

58. Phospholipase PLA2G7, associated with aggressive prostate cancer, promotes prostate cancer cell migration and invasion and is inhibited by statins

59. Potentiating the effects of radiotherapy in rectal cancer: the role of aspirin, statins and metformin as adjuncts to therapy

60. Prediction of drug-target interactions and drug repositioning via network-based inference

61. Repositioning "old" drugs for new causes: identifying new inhibitors of prostate cancer cell migration and invasion

62. Repositioning of drugs for intervention in tumor progression and metastasis: Old drugs for new targets

63. Repositioning of Tak-475 In Mevalonate Kinase Disease: Translating Theory Into Practice

64. Repurposing of approved cardiovascular drugs

65. Repurposing of Existing Statin drugs for treatment of Microbial Infections: How much Promising

66. Repurposing of statins via inhalation to treat lung inflammatory conditions

67. Repurposing Strategy of Atorvastatin against Trypanosoma cruzi: In Vitro Monotherapy and Combined Therapy with Benznidazole Exhibit Synergistic Trypanocidal Activity

68. Simvastatin increases the in vivo activity of the first-line tuberculosis regimen

69. Simvastatin offers new prospects for the treatment of Duchenne muscular dystrophy

70. Simvastatin Therapy for Drug Repositioning to Reduce the Risk of Prostate Cancer Mortality in Patients With Hyperlipidemia

71. Statins and Antimicrobial Effects: Simvastatin as a Potential Drug against Staphylococcus aureus Biofilm

72. Statins in conditions other than hypocholesterolemic effects for chronic subdural hematoma therapy, old drug, new tricks

73. Statins: antimicrobial resistance breakers or makers

74. Stromal microenvironment in type VII collagen-deficient skin: The ground for squamous cell carcinoma development

75. Targeting Mevalonate Pathway in Cancer Treatment: Repurposing of Statins

76. The clinically used PARP inhibitor olaparib improves organ function, suppresses inflammatory responses and accelerates wound healing in a murine model of third-degree burn injury

77. The Linked Clinical Trials Initiative (LCT) for Parkinson's disease

78. The poor design of clinical trials of statins in oncology may explain their failure - Lessons for drug repurposing

79. The potential to treat lung cancer via inhalation of repurposed drugs

80. The Role of Common Pharmaceutical Agents on the Prevention and Treatment of Pancreatic Cancer

81. The role of statins in inflammatory vasculitides

82. Therapeutic Advances and Future Prospects in Progressive Forms of Multiple Sclerosis

83. Therapeutic Effects of Repurposed Therapies in Non-Small Cell Lung Cancer: What Is Old Is New Again

84. Topical mevastatin promotes wound healing by inhibiting the transcription factor c-Myc via the glucocorticoid receptor and the long non-coding RNA Gas5

85. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

86. Treating Influenza Infection, From Now and Into the Future

87. Treating the dysfunctional placenta

FACTOR 16. Similarity-Based Methods for Drug Repurposing

1. A cross-species analysis method to analyze animal models' similarity to human's disease state

2. A disease similarity matrix based on the uniqueness of shared genes

3. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge

4. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning

5. A New Method for Computational Drug Repositioning Using Drug Pairwise Similarity

6. A novel computational approach for drug repurposing using systems biology

7. A novel multi-modal drug repurposing approach for identification of potent ACK1 inhibitors

8. A physarum-inspired prize-collecting steiner tree approach to identify subnetworks for drug repositioning

9. A Semi-Supervised Approach for Refining Transcriptional Signatures of Drug Response and Repositioning Predictions

10. A tool to utilize adverse effect profiles to identify brain-active medications for repurposing

11. A two-step drug repositioning method based on a protein-protein interaction network of genes shared by two diseases and the similarity of drugs

12. Advances in the Development of Shape Similarity Methods and Their Application in Drug Discovery

13. alpha-Methyl-alpha-phenylsuccinimide ameliorates neurodegeneration in a C. elegans model of TDP-43 proteinopathy

14. An integrated structure- and system-based framework to identify new targets of metabolites and known drugs

15. Analysis and assay of oseltamivir-resistant mutants of influenza neuraminidase via direct observation of drug unbinding and rebinding in simulation

16. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens

17. Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach

18. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

19. Assessing protein kinase target similarity: Comparing sequence, structure, and cheminformatics approaches

20. Assessing relative bioactivity of chemical substances using quantitative molecular network topology analysis

21. Back to the Roots: Prediction of Biologically Active Natural Products from Ayurveda Traditional Medicine

22. BioGPS: navigating biological space to predict polypharmacology, off-targeting, and selectivity

23. BioGPS: The Music for the Chemo- and Bioinformatics Walzer

24. Bioinformatics methods in drug repurposing for Alzheimer's disease

25. C-SPADE: a web-tool for interactive analysis and visualization of drug screening experiments through compound-specific bioactivity dendrograms

26. Can sodium/hydrogen exchange inhibitors be repositioned for treating attention deficit hyperactivity disorder? An in silico approach

27. CANDO and the infinite drug discovery frontier

28. CellFateScout - a bioinformatics tool for elucidating small molecule signaling pathways that drive cells in a specific direction

29. Characterizing protein domain associations by Small-molecule ligand binding

30. Characterizing the pocketome of Mycobacterium tuberculosis and application in rationalizing polypharmacological target selection

31. ChemMapper: a versatile web server for exploring pharmacology and chemical structure association based on molecular 3D similarity method

32. Classifying cancer genome aberrations by their mutually exclusive effects on transcription

33. Community-driven roadmap for integrated disease maps

34. Comparing Drug Images and Repurposing Drugs with BioGPS and FLAPdock: The Thymidylate Synthase Case

35. Complex-disease networks of trait-associated single-nucleotide polymorphisms (SNPs) unveiled by information theory

36. Computational Cell Cycle Profiling of Cancer Cells for Prioritizing FDA-Approved Drugs with Repurposing Potential

37. Computational drug repositioning through heterogeneous network clustering

38. Computational drug repurposing to predict approved and novel drug-disease associations

39. Computational Drug Target Screening through Protein Interaction Profiles

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41. Constructing Disease Similarity Networks Based on Disease Module Theory

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FACTOR 17. Machine Learning-Based Drug Repurposing Prediction

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2. A Network-Biology Informed Computational Drug Repositioning Strategy to Target Disease Risk Trajectories and Comorbidities of Peripheral Artery Disease

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141. Repurposing of bisphosphonates for the prevention and therapy of nonsmall cell lung and breast cancer

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145. Scoring multiple features to predict drug disease associations using information fusion and aggregation

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FACTOR 18. Tyrosine Kinase Inhibitors Repurposed for Cancer Treatment

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FACTOR 22. Drug Repurposing for Anti-Parasitic Applications

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134. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment

135. Therapeutical approaches under investigation for treatment of Chagas disease

136. Thiopurine Drugs Repositioned as Tyrosinase Inhibitors

137. Trypanocidal Effect of Isotretinoin through the Inhibition of Polyamine and Amino Acid Transporters in Trypanosoma cruzi

138. Virtual screen for repurposing approved and experimental drugs for candidate inhibitors of EBOLA virus infection

139. Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors

140. Virtual screening and drug repositioning as strategies for the discovery of new antifungal inhibitors of oxidosqualene cyclase

141. Virtual target screening: validation using kinase inhibitors

142. West Nile virus drug discovery

FACTOR 23. Phosphodiesterase Inhibitors Repurposed from Predicitions of Drug Response Signatures

1. A machine learning-based method to improve docking scoring functions and its application to drug repurposing

2. A multicenter, randomized, placebo-controlled trial for cilostazol in patients with mild cognitive impairment: The COMCID study protocol

3. Aging-related Repositioned Drugs, Donepezil and Sildenafil Citrate, Increase Apoptosis of Anti-mitotic Drug-resistant KBV20C Cells Through Different Molecular Mechanisms

4. Application of drug repositioning strategy to TOFISOPAM

5. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

6. Computational identification of multi-omic correlates of anticancer therapeutic response

7. Computational profiling of bioactive compounds using a target-dependent composite workflow

8. Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors

9. Could the FDA-approved anti-HIV PR inhibitors be promising anticancer agents? An answer from enhanced docking approach and molecular dynamics analyses

10. Delivering drugs to the lungs: The history of repurposing in the treatment of respiratory diseases

11. Design, Synthesis, and Biological Evaluation of Orally Available First-Generation Dual-Target Selective Inhibitors of Acetylcholinesterase (AChE) and Phosphodiesterase 5 (PDE5) for the Treatment of Alzheimer's Disease

12. Docking-based inverse virtual screening: methods, applications, and challenges

13. Drug Repositioning for Preeclampsia Therapeutics by In Vitro Screening: Phosphodiesterase-5 Inhibitor Vardenafil Restores Endothelial Dysfunction via Induction of Placental Growth Factor

14. Drug repositioning for schizophrenia and depression/anxiety disorders: A machine learning approach leveraging expression data

15. Drug repurposing and the prior art patents of competitors

16. Drug Targeting and Biomarkers in Head and Neck Cancers: Insights from Systems Biology Analyses

17. Explicit Drug Re-positioning: Predicting Novel Drug-Target Interactions of the Shelved Molecules with QM/MM Based Approaches

18. Formalizing drug indications on the road to therapeutic intent

19. Fragile Histidine Triad (FHIT), a Novel Modifier Gene in Pulmonary Arterial Hypertension

20. Generation and application of drug indication inference models using typed network motif comparison analysis

21. Homology modelling and molecular docking of MDR1 with chemotherapeutic agents in non-small cell lung cancer

22. Identify drug repurposing candidates by mining the protein data bank

23. In silico drug repositioning: what we need to know

24. In silico prediction of chemical mechanism of action via an improved network-based inference method

25. Inhalation of repurposed drugs to treat pulmonary hypertension

26. Large-Scale Off-Target Identification Using Fast and Accurate Dual Regularized One-Class Collaborative Filtering and Its Application to Drug Repurposing

27. Link prediction in drug-target interactions network using similarity indices

28. Novel Tadalafil Derivatives Ameliorates Scopolamine-Induced Cognitive Impairment in Mice via Inhibition of Acetylcholinesterase (AChE) and Phosphodiesterase 5 (PDE5

29. p73 as a pharmaceutical target for cancer therapy

30. Pharmacologic treatments for pulmonary hypertension: exploring pharmacogenomics

31. Pharmacological treatment and prevention of cerebral small vessel disease: a review of potential interventions

32. Prediction of drugs having opposite effects on disease genes in a directed network

33. Reactivation of cAMP Pathway by PDE4D Inhibition Represents a Novel Druggable Axis for Overcoming Tamoxifen Resistance in ER-positive Breast Cancer

34. Repositioning of molsidomine for its efficacy in diabetes induced erectile dysfunction in rats: In silico, in vitro and in vivo approach

35. Repositioning organohalogen drugs: a case study for identification of potent B-Raf V600E inhibitors via docking and bioassay

36. Repurposing drugs as inhaled therapies in asthma

37. Repurposing drugs in oncology (ReDO)-selective PDE5 inhibitors as anti-cancer agents

38. Repurposing existing drugs for new AMPK activators as a strategy to extend lifespan: a computer-aided drug discovery study

39. Repurposing human PDE4 inhibitors for neglected tropical diseases. Evaluation of analogs of the human PDE4 inhibitor GSK-256066 as inhibitors of PDEB1 of Trypanosoma brucei

40. Repurposing human PDE4 inhibitors for neglected tropical diseases: design, synthesis and evaluation of cilomilast analogues as Trypanosoma brucei PDEB1 inhibitors

41. SPIDR: small-molecule peptide-influenced drug repurposing

42. Successful shortening of tuberculosis treatment using adjuvant host-directed therapy with FDA-approved phosphodiesterase inhibitors in the mouse model

43. Targeting phosphodiesterase 5 as a therapeutic option against myocardial ischaemia/reperfusion injury and for treating heart failure

44. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

45. The genome of Onchocerca volvulus, agent of river blindness

46. Therapeutic Advances and Future Prospects in Progressive Forms of Multiple Sclerosis

47. Three-dimensional models of Mycobacterium tuberculosis proteins Rv1555, Rv1554 and their docking analyses with sildenafil, tadalafil, vardenafil drugs, suggest interference with quinol binding likely to affect protein's function

48. Treating the dysfunctional placenta

49. Virtual target screening: validation using kinase inhibitors

FACTOR 24. Inhibiting NF-KappaB Signaling for Cancer and Inflammation Treatment

1. 3, 5, 3'-Triiodothyroacetic acid (TRIAC) is an anti-inflammatory drug that targets toll-like receptor 2

2. A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors

3. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis

4. A signalome screening approach in the autoinflammatory disease TNF receptor associated periodic syndrome (TRAPS) highlights the anti-inflammatory properties of drugs for repurposing

5. A systematic screen of FDA-approved drugs for inhibitors of biological threat agents

6. A Zebrafish Drug-Repurposing Screen Reveals sGC-Dependent and sGC-Independent Pro-Inflammatory Activities of Nitric Oxide

7. Activation of MyD88-dependent TLR1/2 signaling by misfolded alpha-synuclein, a protein linked to neurodegenerative disorders

8. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

9. An invitro and invivo evaluation of new potential trans-sialidase inhibitors of Trypanosoma cruzi predicted by a computational drug repositioning method

10. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens

11. Anti-protozoal and anti-bacterial antibiotics that inhibit protein synthesis kill cancer subtypes enriched for stem cell-like properties

12. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

13. Antibiotic drug rifabutin is effective against lung cancer cells by targeting the eIF4E-beta-catenin axis

14. Antibiotic resistance breakers: can repurposed drugs fill the antibiotic discovery void

15. Antifibrotic effect of pirfenidone in a mouse model of human nonalcoholic steatohepatitis

16. Antimalarial drug mefloquine inhibits nuclear factor kappa B signaling and induces apoptosis in colorectal cancer cells

17. Antiviral activity of doxycycline against vesicular stomatitis virus in vitro

18. Antiviral activity of gemcitabine against human rhinovirus invitro and invivo

19. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis

20. Approaches for discovering anti-prion compounds: lessons learned and challenges ahead

21. Auranofin and its Analogues Show Potent Antimicrobial Activity Covering Multiresistant Pathogens: Structure-Activity Relationships

22. Azithromycin protects mice against ischemic stroke injury by promoting macrophage transition towards M2 phenotype

23. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

24. beta-Caryophyllene protects against alcoholic steatohepatitis by attenuating inflammation and metabolic dysregulation in mice

25. beta-catenin and PI3Kdelta inhibition expands precursor Th17 cells with heightened stemness and antitumor activity

26. Bioinformatics analysis reveals transcriptome and microRNA signatures and drug repositioning targets for IBD and other autoimmune diseases

27. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

28. Bromide supplementation exacerbated the renal dysfunction, injury and fibrosis in a mouse model of Alport syndrome

29. Buformin inhibits the stemness of erbB-2-overexpressing breast cancer cells and premalignant mammary tissues of MMTV-erbB-2 transgenic mice

30. Cancer drug discovery by repurposing: teaching new tricks to old dogs

31. Cancer Prevention and Interception: A New Era for Chemopreventive Approaches

32. Carbamazepine alone and in combination with doxycycline attenuates isoproterenol-induced cardiac hypertrophy

33. Cascade Ligand- and Structure-Based Virtual Screening to Identify New Trypanocidal Compounds Inhibiting Putrescine Uptake

34. Characterization of a Francisella tularensis-Caenorhabditis elegans Pathosystem for the Evaluation of Therapeutic Compounds

35. Chemoprevention of head and neck squamous cell carcinoma through inhibition of NF-kappaB signaling

36. Clobetasol promotes remyelination in a mouse model of neuromyelitis optica

37. Combined chemical genetics and data-driven bioinformatics approach identifies receptor tyrosine kinase inhibitors as host-directed antimicrobials

38. Competitive Kinase Enrichment Proteomics Reveals that Abemaciclib Inhibits GSK3beta and Activates WNT Signaling

39. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

40. Computational repositioning and experimental validation of approved drugs for HIF-prolyl hydroxylase inhibition

41. Connectivity mapping (ssCMap) to predict A20-inducing drugs and their antiinflammatory action in cystic fibrosis

42. Cooperative recognition of T:T mismatch by echinomycin causes structural distortions in DNA duplex

43. Cryo-EM structure of the Plasmodium falciparum 80S ribosome bound to the anti-protozoan drug emetine

44. Current and Future Use of Chloroquine and Hydroxychloroquine in Infectious, Immune, Neoplastic, and Neurological Diseases: A Mini-Review

45. Current and upcoming pharmacotherapy for non-alcoholic fatty liver disease

46. Cystic fibrosis transmembrane conductance regulator modulators in cystic fibrosis: current perspectives

47. Designing drugs that combat kidney damage

48. Development of inhalable hyaluronan/mannitol composite dry powders for flucytosine repositioning in local therapy of lung infections

49. Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues

50. Doxycycline and therapeutic targeting of the DNA damage response in cancer cells: old drug, new purpose

51. Doxycycline counteracts neuroinflammation restoring memory in Alzheimer's disease mouse models

52. Doxycycline inhibits proliferation and induces apoptosis of both human papillomavirus positive and negative cervical cancer cell lines

53. Doxycycline inhibits the cancer stem cell phenotype and epithelial-to-mesenchymal transition in breast cancer

54. Doxycycline is an NF-kappaB inhibitor that induces apoptotic cell death in malignant T-cells

55. Doxycycline or how to create new with the old

56. Drug Repositioning for Effective Prostate Cancer Treatment

57. Drug Repositioning through Systematic Mining of Gene Coexpression Networks in Cancer

58. Drug Repurposing by Simulating Flow Through Protein-Protein Interaction Networks

59. Drug repurposing may generate novel approaches to treating depression

60. Drug Repurposing of Histone Deacetylase Inhibitors That Alleviate Neutrophilic Inflammation in Acute Lung Injury and Idiopathic Pulmonary Fibrosis via Inhibiting Leukotriene A4 Hydrolase and Blocking LTB4 Biosynthesis

61. Drug Repurposing Screen Identifies Foxo1-Dependent Angiopoietin-2 Regulation in Sepsis

62. Drug repurposing screen identifies lestaurtinib amplifies the ability of the poly (ADP-ribose) polymerase 1 inhibitor AG14361 to kill breast cancer associated gene-1 mutant and wild type breast cancer cells

63. Effects of digitoxin on cell migration in ovarian cancer inflammatory microenvironment

64. Emerging roles of Myc in stem cell biology and novel tumor therapies

65. EMUDRA: Ensemble of Multiple Drug Repositioning Approaches to improve prediction accuracy

66. Evaluating a novel treatment for coronary artery inflammation in acute Kawasaki disease: A Phase I/IIa trial of atorvastatin

67. Evaluating New Compounds to Treat Burkholderia pseudomallei Infections

68. Evaluation of a systems biology approach to identify pharmacological correctors of the mutant CFTR chloride channel

69. Examining the potential preventative effects of minocycline prescribed for acne on the incidence of severe mental illnesses: A historical cohort study

70. Exploiting the therapeutic potential of ready-to-use drugs: Repurposing antibiotics against amyloid aggregation in neurodegenerative diseases

71. Exploration of the Anti-Inflammatory Drug Space Through Network Pharmacology: Applications for Drug Repurposing

72. Extensive impact of non-antibiotic drugs on human gut bacteria

73. Fenofibrate Attenuates Neutrophilic Inflammation in Airway Epithelia: Potential Drug Repurposing for Cystic Fibrosis

74. Fenoprofen -- an old drug rediscovered as a biased allosteric enhancer for melanocortin receptors

75. Finding off-targets, biological pathways, and target diseases for chymase inhibitors via structure-based systems biology approach

76. From ancient herb to modern drug: Artemisia annua and artemisinin for cancer therapy

77. From the era of genome analysis to the era of genomic drug discovery: a pioneering example of rheumatoid arthritis

78. Functional genetics-directed identification of novel pharmacological inhibitors of FAS- and TNF-dependent apoptosis that protect mice from acute liver failure

79. Genetic Mechanisms of Asthma and the Implications for Drug Repositioning

80. Host-directed antimicrobial drugs with broad-spectrum efficacy against intracellular bacterial pathogens

81. Host-Directed Therapies for Tackling Multi-Drug Resistant Tuberculosis: Learning From the Pasteur-Bechamp Debates

82. Ibuprofen and diclofenac treatments reduce proliferation of pancreatic acinar cells upon inflammatory injury and mitogenic stimulation

83. Identification and Validation of an Antivirulence Agent Targeting HlyU-Regulated Virulence in Vibrio vulnificus

84. Identification of Chemical Inhibitors of beta-Catenin-Driven Liver Tumorigenesis in Zebrafish

85. Identification of common biological pathways and drug targets across multiple respiratory viruses based on human host gene expression analysis

86. Identification of known drugs that act as inhibitors of NF-kappaB signaling and their mechanism of action

87. Identification of Mitoxantrone as a TRAIL-sensitizing agent for Glioblastoma Multiforme

88. Identification of Niclosamide as a Novel Anticancer Agent for Adrenocortical Carcinoma

89. Immunomodulatory tetracyclines shape the intestinal inflammatory response inducing mucosal healing and resolution

90. In vitro activity of the antiasthmatic drug zafirlukast against the oral pathogens Porphyromonas gingivalis and Streptococcus mutans

91. In Vitro and Intracellular Activity of Imipenem Combined with Rifabutin and Avibactam against Mycobacterium abscessus

92. In vitro antimicrobial activity of monensin against common clinical isolates associated with canine otitis externa

93. Increasing procaspase 8 expression using repurposed drugs to induce HIV infected cell death in ex vivo patient cells

94. Inflammatory pathway network-based drug repositioning and molecular phenomics

95. Inhaled mannitol in patients with cystic fibrosis: A randomised open-label dose response trial

96. Inhibition of Fosfomycin Resistance Protein FosA by Phosphonoformate (Foscarnet) in Multidrug-Resistant Gram-Negative Pathogens

97. Inhibition of the insulin-like growth factor system is a potential therapy for rheumatoid arthritis

98. Inhibitors of Cancer Stem Cells

99. Innovations in asthma therapy: is there a role for inhaled statins

100. Interleukin-6, A Cytokine Critical to Mediation of Inflammation, Autoimmunity and Allograft Rejection: Therapeutic Implications of IL-6 Receptor Blockade

101. Investigating Drug Repositioning Approach to Design Novel Prodrugs for Colon-specific Release of Fexofenadine for Ulcerative Colitis

102. Is There Potential for Repurposing Statins as Novel Antimicrobials

103. L-Captopril and its derivatives as potential inhibitors of microbial enzyme DapE: A combined approach of drug repurposing and similarity screening

104. Lansoprazole Upregulates Polyubiquitination of the TNF Receptor-Associated Factor 6 and Facilitates Runx2-mediated Osteoblastogenesis

105. Mechanism-informed Repurposing of Minocycline Overcomes Resistance to Topoisomerase Inhibition for Peritoneal Carcinomatosis

106. Metabolic Dysfunction in Alzheimer's Disease: From Basic Neurobiology to Clinical Approaches

107. Metabolome analysis of effect of aspirin on Drosophila lifespan extension

108. Metformin - The Drug for the Treatment of Autoimmune Diseases; A New Use of a Known Anti-Diabetic Drug

109. Metformin as a geroprotector: experimental and clinical evidence

110. Minocycline repurposing in critical illness: focus on stroke

111. Mitochondrial biogenesis is required for the anchorage-independent survival and propagation of stem-like cancer cells

112. Mode of action and resistance studies unveil new roles for tropodithietic acid as an anticancer agent and the gamma-glutamyl cycle as a proton sink

113. Modulating Innate and Adaptive Immunity by (R)-Roscovitine: Potential Therapeutic Opportunity in Cystic Fibrosis

114. N-bromotaurine surrogates for loss of antiproliferative response and enhances cisplatin efficacy in cancer cells with impaired glucocorticoid receptor

115. Nanoliposomal Buparvaquone Immunomodulates Leishmania infantum-Infected Macrophages and Is Highly Effective in a Murine Model

116. Neuroprotective and immunomodulatory effects of raloxifene in the myenteric plexus of a mouse model of Parkinson's disease

117. New Antimicrobial Approaches: Reuse of Old Drugs

118. New drug candidates for depression - a nationwide population-based study

119. New frontiers for anti-biofilm drug development

120. New Role for FDA-Approved Drugs in Combating Antibiotic-Resistant Bacteria

121. Niclosamide and its analogs are potent inhibitors of Wnt/beta-catenin, mTOR and STAT3 signaling in ovarian cancer

122. Niclosamide, a Drug with Many (Re)purposes

123. Nonantibiotic properties of macrolides and their role in modulation of the inflammatory reaction

124. Novel insight into drug repositioning: Methylthiouracil as a case in point

125. Novel Polymyxin Combination With Antineoplastic Mitotane Improved the Bacterial Killing Against Polymyxin-Resistant Multidrug-Resistant Gram-Negative Pathogens

126. Novel Therapeutics Identification for Fibrosis in Renal Allograft Using Integrative Informatics Approach

127. Nucleoside reverse transcriptase inhibitors possess intrinsic anti-inflammatory activity

128. Nutraceuticals and "repurposed" drugs of phytochemical origin in prevention and interception of chronic degenerative disease and cancer

129. Oncogenic targets Mmp7, S100a9, Nppb and Aldh1a3 from transcriptome profiling of FAP and Pirc adenomas are downregulated in response to tumor suppression by Clotam

130. Oral delivery of ivermectin using a fast dissolving oral film: Implications for repurposing ivermectin as a pharmacotherapy for alcohol use disorder

131. Osteoprotegerin and Denosumab Stimulate Human Beta Cell Proliferation through Inhibition of the Receptor Activator of NF-kappaB Ligand Pathway

132. Pentosan Polysulfate: a Novel Glycosaminoglycan-Like Molecule for Effective Treatment of Alphavirus-Induced Cartilage Destruction and Inflammatory Disease

133. Pharmacogenomic approaches to lipid-regulating trials

134. Pharmacologically active metabolites, combination screening and target identification-driven drug repositioning in antituberculosis drug discovery

135. Poly(ADP-ribose) polymerase is not involved in the neuroprotection exerted by azithromycin against ischemic stroke in mice

136. Post-ischemic treatment with azithromycin protects ganglion cells against retinal ischemia/reperfusion injury in the rat

137. Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing

138. Promoting oligodendroglial-oriented differentiation of glioma stem cell: a repurposing of quetiapine for the treatment of malignant glioma

139. Pyrvinium Sensitizes Clear Cell Renal Cell Carcinoma Response to Chemotherapy Via Casein Kinase 1alpha-Dependent Inhibition of Wnt/beta-Catenin

140. Raloxifene attenuates Pseudomonas aeruginosa pyocyanin production and virulence

141. Rationale for an experimental treatment of retinitis pigmentosa: 140-month test of hypothesis with one patient

142. Real-Time" High-Throughput Drug and Synergy Testing for Multidrug-Resistant Bacterial Infection: A Case Report

143. Repositioning drugs for inflammatory disease - fishing for new anti-inflammatory agents

144. Repositioning of antibiotic levofloxacin as a mitochondrial biogenesis inhibitor to target breast cancer

145. Repositioning of Memantine as a Potential Novel Therapeutic Agent against Meningitic E. coli-Induced Pathogenicities through Disease-Associated Alpha7 Cholinergic Pathway and RNA Sequencing-Based Transcriptome Analysis of Host Inflammatory Responses

146. Repositioning of Tak-475 In Mevalonate Kinase Disease: Translating Theory Into Practice

147. Repurposing an old drug to improve the use and safety of tissue plasminogen activator for acute ischemic stroke: minocycline

148. Repurposing an old drug to improve the use and safety of tissue plasminogen activator for acute ischemic stroke: minocycline

149. Repurposing an orally available drug for the treatment of geographic atrophy

150. Repurposing an Osteoporosis Drug for beta Cell Regeneration in Diabetic Patients

151. Repurposing atovaquone: targeting mitochondrial complex III and OXPHOS to eradicate cancer stem cells

152. Repurposing auranofin for the treatment of cutaneous staphylococcal infections

153. Repurposing doxycycline for synucleinopathies: remodelling of alpha-synuclein oligomers towards non-toxic parallel beta-sheet structured species

154. Repurposing drugs for the treatment and control of helminth infections

155. Repurposing drugs for treatment of tuberculosis: a role for non-steroidal anti-inflammatory drugs

156. Repurposing Drugs in Oncology (ReDO)-clarithromycin as an anti-cancer agent

157. Repurposing ebselen for treatment of multidrug-resistant staphylococcal infections

158. Repurposing FDA-approved drugs to combat drug-resistant Acinetobacter baumannii

159. Repurposing itraconazole as an anticancer agent

160. Repurposing niclosamide as a versatile antimicrobial surface coating against device-associated, hospital-acquired bacterial infections

161. Repurposing of Anticancer Drugs for the Treatment of Bacterial Infections

162. Repurposing of approved drugs from the human pharmacopoeia to target Wolbachia endosymbionts of onchocerciasis and lymphatic filariasis

163. Repurposing of gallium-based drugs for antibacterial therapy

164. Repurposing of metformin and aspirin by targeting AMPK-mTOR and inflammation for pancreatic cancer prevention and treatment

165. Repurposing of nitroxoline as a potential anticancer agent against human prostate cancer: a crucial role on AMPK/mTOR signaling pathway and the interplay with Chk2 activation

166. Repurposing of nucleoside- and nucleobase-derivative drugs as antibiotics and biofilm inhibitors

167. Repurposing the anti-malarial drug dihydroartemisinin suppresses metastasis of non-small-cell lung cancer via inhibiting NF-kappaB/GLUT1 axis

168. Repurposing the antimycotic drug flucytosine for suppression of Pseudomonas aeruginosa pathogenicity

169. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

170. Repurposing Toremifene for Treatment of Oral Bacterial Infections

171. Repurposing Zidovudine in combination with Tigecycline for treating carbapenem-resistant Enterobacteriaceae infections

172. Repurposing-a ray of hope in tackling extensively drug resistance in tuberculosis

173. Rescue of cell death and inflammation of a mouse model of complex 1-mediated vision loss by repurposed drug molecules

174. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain

175. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox

176. S100A4 in Cancer Metastasis: Wnt Signaling-Driven Interventions for Metastasis Restriction

177. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides

178. Screening a Commercial Library of Pharmacologically Active Small Molecules against Staphylococcus aureus Biofilms

179. Screening a repurposing library for potentiators of antibiotics against Staphylococcus aureus biofilms

180. Senicapoc: Repurposing a Drug to Target Microglia KCa3.1 in Stroke

181. Sphingolipids as targets for inhalation treatment of cystic fibrosis

182. Statins in conditions other than hypocholesterolemic effects for chronic subdural hematoma therapy, old drug, new tricks

183. Statins: antimicrobial resistance breakers or makers

184. Strategies to overcome the action of aminoglycoside-modifying enzymes for treating resistant bacterial infections

185. Stromal microenvironment in type VII collagen-deficient skin: The ground for squamous cell carcinoma development

186. Suppressive effects of dabrafenibon endothelial protein C receptor shedding

187. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

188. Synthetic lethality reveals mechanisms of Mycobacterium tuberculosis resistance to beta-lactams

189. Systemic amyloidosis: novel therapies and role of biomarkers

190. Targeting Abl kinases to regulate vascular leak during sepsis and acute respiratory distress syndrome

191. Targeting ADAM17 Sheddase Activity in Cancer

192. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases

193. Tedizolid Activity Against Clinical Mycobacterium abscessus Complex Isolates-An in vitro Characterization Study

194. Teicoplanin inhibits Ebola pseudovirus infection in cell culture

195. Tetracycline hydrochloride: A potential clinical drug for radioprotection

196. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

197. Tezosentan inhibits uptake of proinflammatory endothelin-1 in stenotic aortic valves

198. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

199. The Anthelmintic Drug Niclosamide Inhibits the Proliferative Activity of Human Osteosarcoma Cells by Targeting Multiple Signal Pathways

200. The anthelmintic niclosamide inhibits colorectal cancer cell lines via modulation of the canonical and noncanonical Wnt signaling pathway

201. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo

202. The clinically used PARP inhibitor olaparib improves organ function, suppresses inflammatory responses and accelerates wound healing in a murine model of third-degree burn injury

203. The Concept of Hormesis in Cancer Therapy - Is Less More

204. The heterogeneity of cancer stem-like cells at the invasive front

205. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

206. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma

207. The Repurposing of Anti-Psychotic Drugs, Quetiapine and Olanzapine, as Anti-Cryptococcus Drugs

208. The Significance of Hypothiocyanite Production via the Pendrin/DUOX/Peroxidase Pathway in the Pathogenesis of Asthma

209. The Tissue-Reconstructing Ability of Colon CSCs Is Enhanced by FK506 and Suppressed by GSK3 Inhibition

210. Therapeutic Effect of Quinacrine, an Antiprotozoan Drug, by Selective Suppression of p-CHK1/2 in p53-Negative Malignant Cancers

211. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

212. Therapeutic synergy between tigecycline and venetoclax in a preclinical model of MYC/BCL2 double-hit B cell lymphoma

213. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function

214. Toward Repositioning Niclosamide for Antivirulence Therapy of Pseudomonas aeruginosa Lung Infections: Development of Inhalable Formulations through Nanosuspension Technology

215. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

216. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

217. Treating Influenza Infection, From Now and Into the Future

218. Treatment of experimental autoimmune uveoretinitis with peroxisome proliferator-activated receptor alpha agonist fenofibrate

219. Triclosan Is an Aminoglycoside Adjuvant for Eradication of Pseudomonas aeruginosa Biofilms

220. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer

221. Use of minocycline in viral infections

222. Using a novel computational drug-repositioning approach (DrugPredict) to rapidly identify potent drug candidates for cancer treatment

223. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

FACTOR 25. Repurposing Based on Comprehensive Multi-Metric Similarity Measures

1. A comparative study of disease genes and drug targets in the human protein interactome

2. A cross-species analysis method to analyze animal models' similarity to human's disease state

3. A disease similarity matrix based on the uniqueness of shared genes

4. A diseasome cluster-based drug repurposing of soluble guanylate cyclase activators from smooth muscle relaxation to direct neuroprotection

5. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge

6. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning

7. A machine-learned computational functional genomics-based approach to drug classification

8. A New Method for Computational Drug Repositioning Using Drug Pairwise Similarity

9. A novel multi-modal drug repurposing approach for identification of potent ACK1 inhibitors

10. A physarum-inspired prize-collecting steiner tree approach to identify subnetworks for drug repositioning

11. A Semi-Supervised Approach for Refining Transcriptional Signatures of Drug Response and Repositioning Predictions

12. A tool to utilize adverse effect profiles to identify brain-active medications for repurposing

13. A two-step drug repositioning method based on a protein-protein interaction network of genes shared by two diseases and the similarity of drugs

14. A two-tiered unsupervised clustering approach for drug repositioning through heterogeneous data integration

15. Advances in the Development of Shape Similarity Methods and Their Application in Drug Discovery

16. alpha-Methyl-alpha-phenylsuccinimide ameliorates neurodegeneration in a C. elegans model of TDP-43 proteinopathy

17. An integrated structure- and system-based framework to identify new targets of metabolites and known drugs

18. Analysis and assay of oseltamivir-resistant mutants of influenza neuraminidase via direct observation of drug unbinding and rebinding in simulation

19. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens

20. Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach

21. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

22. Assessing protein kinase target similarity: Comparing sequence, structure, and cheminformatics approaches

23. Assessing relative bioactivity of chemical substances using quantitative molecular network topology analysis

24. Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computer-Aided Drug Repurposing

25. Back to the Roots: Prediction of Biologically Active Natural Products from Ayurveda Traditional Medicine

26. Baseline Regularization for Computational Drug Repositioning with Longitudinal Observational Data

27. BioGPS: navigating biological space to predict polypharmacology, off-targeting, and selectivity

28. BioGPS: The Music for the Chemo- and Bioinformatics Walzer

29. Bioinformatics methods in drug repurposing for Alzheimer's disease

30. Bioinformatics: Novel Insights from Genomic Information

31. C-SPADE: a web-tool for interactive analysis and visualization of drug screening experiments through compound-specific bioactivity dendrograms

32. Can sodium/hydrogen exchange inhibitors be repositioned for treating attention deficit hyperactivity disorder? An in silico approach

33. CANDO and the infinite drug discovery frontier

34. CellFateScout - a bioinformatics tool for elucidating small molecule signaling pathways that drive cells in a specific direction

35. Characterizing protein domain associations by Small-molecule ligand binding

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893. Repurposing of phentolamine as a potential anticancer agent against human castration-resistant prostate cancer: A central role on microtubule stabilization and mitochondrial apoptosis pathway

894. Repurposing of Potent Drug Candidates for Multiparasite Targeting

895. Repurposing of Proton Pump Inhibitors as first identified small molecule inhibitors of endo-beta-N-acetylglucosaminidase (ENGase) for the treatment of NGLY1 deficiency, a rare genetic disease

896. Repurposing the anti-malarial drug artesunate as a novel therapeutic agent for metastatic renal cell carcinoma due to its attenuation of tumor growth, metastasis, and angiogenesis

897. Repurposing the clinically approved calcium antagonist manidipine dihydrochloride as a new early inhibitor of human cytomegalovirus targeting the Immediate-Early 2 (IE2) protein

898. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease

899. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

900. Repurposing Toremifene for Treatment of Oral Bacterial Infections

901. Rescue of cell death and inflammation of a mouse model of complex 1-mediated vision loss by repurposed drug molecules

902. Research advance in the drug target prediction based on chemoinformatics

903. Research and development of anti-Alzheimer's disease drugs: an update from the perspective of technology flows

904. Resistance to Thiacetazone Derivatives Active against Mycobacterium abscessus Involves Mutations in the MmpL5 Transcriptional Repressor MAB_4384

905. Resistance-resistant antibiotics

906. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist

907. Reverse Screening Methods to Search for the Protein Targets of Chemopreventive Compounds

908. Review and comparative assessment of similarity-based methods for prediction of drug-protein interactions in the druggable human proteome

909. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia

910. Revisiting Connectivity Map from a gene co-expression network analysis

911. Rho-associated kinase signalling and the cancer microenvironment: novel biological implications and therapeutic opportunities

912. Ribavirin suppresses bacterial virulence by targeting LysR-type transcriptional regulators

913. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain

914. Ritonavir-Mediated Induction of Apoptosis in Pancreatic Cancer Occurs via the RB/E2F-1 and AKT Pathways

915. Role of acid responsive genes in the susceptibility of Escherichia coli to ciclopirox

916. Schistosomiasis: from drug deployment to drug development

917. Schizophrenia interactome with 504 novel protein-protein interactions

918. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides

919. Scoring multiple features to predict drug disease associations using information fusion and aggregation

920. Screening a repurposing library, the Medicines for Malaria Venture Stasis Box, against Schistosoma mansoni

921. Screening of FDA-Approved Drugs for Inhibitors of Japanese Encephalitis Virus Infection

922. SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drug-target interactions and drug repositioning

923. Selective human inhibitors of ATR and ATM render Leishmania major promastigotes sensitive to oxidative damage

924. SELF-BLM: Prediction of drug-target interactions via self-training SVM

925. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing

926. Semantic Web Ontology and Data Integration: a Case Study in Aiding Psychiatric Drug Repurposing

927. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association

928. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients

929. Shared genetic origin of asthma, hay fever and eczema elucidates allergic disease biology

930. Significance and suppression of redundant IL17 responses in acute allograft rejection by bioinformatics based drug repositioning of fenofibrate

931. Similarity-based prediction for Anatomical Therapeutic Chemical classification of drugs by integrating multiple data sources

932. Simvastatin offers new prospects for the treatment of Duchenne muscular dystrophy

933. siRNA Genome Screening Approaches to Therapeutic Drug Repositioning

934. SIRT1 activation by methylene blue, a repurposed drug, leads to AMPK-mediated inhibition of steatosis and steatohepatitis

935. Small molecule inhibition of apicomplexan FtsH1 disrupts plastid biogenesis in human pathogens

936. Small Molecules in Development for the Treatment of Spinal Muscular Atrophy

937. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison

938. Some Remarks on Prediction of Drug-Target Interaction with Network Models

939. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

940. SPILLO-PBSS: detecting hidden binding sites within protein 3D-structures through a flexible structure-based approach

941. SRSF6-regulated alternative splicing that promotes tumour progression offers a therapy target for colorectal cancer

942. Statins: antimicrobial resistance breakers or makers

943. Statistically controlled identification of differentially expressed genes in one-to-one cell line comparisons of the CMAP database for drug repositioning

944. Steroids-specific target library for steroids target prediction

945. Stress-Activated Kinase Mitogen-Activated Kinase Kinase-7 Governs Epigenetics of Cardiac Repolarization for Arrhythmia Prevention

946. Structural analysis of dihydrofolate reductases enables rationalization of antifolate binding affinities and suggests repurposing possibilities

947. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

948. Structural basis for the resilience of efavirenz (DMP-266) to drug resistance mutations in HIV-1 reverse transcriptase

949. Structural insight into selectivity and resistance profiles of ROS1 tyrosine kinase inhibitors

950. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

951. Structure based drug discovery for designing leads for the non-toxic metabolic targets in multi drug resistant Mycobacterium tuberculosis

952. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation

953. Structure Investigation, Enrichment Analysis and Structure-based Repurposing of FDA-approved Drugs as Inhibitors of BET-BRD4

954. Structure-based discovery of the novel antiviral properties of naproxen against the nucleoprotein of influenza A virus

955. Structure-based identification of a NEDD8-activating enzyme inhibitor via drug repurposing

956. Structure-based repurposing of FDA-approved drugs as inhibitors of NEDD8-activating enzyme

957. Study protocol of a phase IB/II clinical trial of metformin and chloroquine in patients with IDH1-mutated or IDH2-mutated solid tumours

958. Substrate-driven mapping of the degradome by comparison of sequence logos

959. SUMOylation in brain ischemia: Patterns, targets, and translational implications

960. Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis

961. Suppressive effects of dabrafenibon endothelial protein C receptor shedding

962. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

963. Synergistic combination of flavopiridol and carfilzomib targets commonly dysregulated pathways in adrenocortical carcinoma and has biomarkers of response

964. Synergistic drug combinations from electronic health records and gene expression

965. Synthetic lethality reveals mechanisms of Mycobacterium tuberculosis resistance to beta-lactams

966. Systematic analyses of drugs and disease indications in RepurposeDB reveal pharmacological, biological and epidemiological factors influencing drug repositioning

967. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine

968. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

969. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data

970. Systematic Identification and Assessment of Therapeutic Targets for Breast Cancer Based on Genome-Wide RNA Interference Transcriptomes

971. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer

972. Systematic integration of biomedical knowledge prioritizes drugs for repurposing

973. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach

974. Systematical analysis of lncRNA-mRNA competing endogenous RNA network in breast cancer subtypes

975. Systemic amyloidosis: novel therapies and role of biomarkers

976. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes

977. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification

978. Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis

979. Systems biology-embedded target validation: improving efficacy in drug discovery

980. Systems Medicine Approaches to Improving Understanding, Treatment, and Clinical Management of Neuroendocrine Prostate Cancer

981. Systems medicine: evolution of systems biology from bench to bedside

982. Systems Pharmacology Links GPCRs with Retinal Degenerative Disorders

983. Systems pharmacology of adverse event mitigation by drug combinations

984. Systems Pharmacology-Based Approach of Connecting Disease Genes in Genome-Wide Association Studies with Traditional Chinese Medicine

985. Target mechanism-based whole-cell screening identifies bortezomib as an inhibitor of caseinolytic protease in mycobacteria

986. Target-Based Drug Repositioning Using Large-Scale Chemical-Protein Interactome Data

987. Target-similarity search using Plasmodium falciparum proteome identifies approved drugs with anti-malarial activity and their possible targets

988. Targeting ADAM17 Sheddase Activity in Cancer

989. Targeting calcium homeostasis as the therapy of Chagas' disease and leishmaniasis - a review

990. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

991. Targeting Gliomas: Can a New Alkylating Hybrid Compound Make a Difference

992. Targeting STAT1 in Both Cancer and Insulin Resistance Diseases

993. Targeting the off-targets: a computational bioinformatics approach to understanding the polypharmacology of nelfinavir

994. Targeting the schizophrenia genome: a fast track strategy from GWAS to clinic

995. Tegaserod mimics the neurostimulatory glycan polysialic acid and promotes nervous system repair

996. Tetracycline hydrochloride: A potential clinical drug for radioprotection

997. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

998. The anthelmintic niclosamide inhibits colorectal cancer cell lines via modulation of the canonical and noncanonical Wnt signaling pathway

999. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo

1000. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death

1001. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells

1002. The CARLSBAD database: a confederated database of chemical bioactivities

1003. The combination astemizole-gefitinib as a potential therapy for human lung cancer

1004. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

1005. The druggable genome and support for target identification and validation in drug development

1006. The extraction of drug-disease correlations based on module distance in incomplete human interactome

1007. The EYA tyrosine phosphatase activity is pro-angiogenic and is inhibited by benzbromarone

1008. The genome of Onchocerca volvulus, agent of river blindness

1009. The Hippo pathway in normal development and cancer

1010. The HIV integrase inhibitor raltegravir inhibits felid alphaherpesvirus 1 (FeHV-1) replication by targeting both DNA replication and late gene expression

1011. The Horizon of a Therapy for Rare Genetic Diseases: A "Druggable" Future for Fibrodysplasia Ossificans Progressiva

1012. The human disease network in terms of dysfunctional regulatory mechanisms

1013. The human immunodeficiency virus protease inhibitor ritonavir is potentially active against urological malignancies

1014. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

1015. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs

1016. The multitargeted drug ivermectin: from an antiparasitic agent to a repositioned cancer drug

1017. The neuroimmune transcriptome and alcohol dependence: potential for targeted therapies

1018. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma

1019. The pain interactome: connecting pain-specific protein interactions

1020. The polypharmacology of natural products

1021. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C

1022. The positive inotropic agent DPI-201106 selectively reverses ABCB1-mediated multidrug resistance in cancer cell lines

1023. The prescribable drugs with efficacy in experimental epilepsies (PDE3) database for drug repurposing research in epilepsy

1024. The proteasome inhibitor bortezomib attenuates renal fibrosis in mice via the suppression of TGF-beta1

1025. The protein kinase 2 inhibitor CX-4945 regulates osteoclast and osteoblast differentiation in vitro

1026. The proton-pump inhibitor lansoprazole enhances amyloid beta production

1027. The repurposed anthelmintic mebendazole in combination with trametinib suppresses refractory NRASQ61K melanoma

1028. The role of drug profiles as similarity metrics: applications to repurposing, adverse effects detection and drug-drug interactions

1029. The sodium channel-blocking antiepileptic drug phenytoin inhibits breast tumour growth and metastasis

1030. The Src/c-Abl pathway is a potential therapeutic target in amyotrophic lateral sclerosis

1031. The susceptibility of trypanosomatid pathogens to PI3/mTOR kinase inhibitors affords a new opportunity for drug repurposing

1032. The use of a gene expression signature and connectivity map to repurpose drugs for bipolar disorder

1033. Therapeutic Approaches to Prion Diseases

1034. Therapeutic compositions and uses of alpha1-antitrypsin: a patent review (2012 - 2015

1035. Therapeutic compounds for Cushing's syndrome: a patent review (2012-2016

1036. Therapeutic drug repositioning using personalized proteomics of liquid biopsies

1037. Therapeutic Effect of Repurposed Temsirolimus in Lung Adenocarcinoma Model

1038. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

1039. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

1040. Therapeutic potential for phenytoin: targeting Na(v)1.5 sodium channels to reduce migration and invasion in metastatic breast cancer

1041. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment

1042. Three-dimensional models of Mycobacterium tuberculosis proteins Rv1555, Rv1554 and their docking analyses with sildenafil, tadalafil, vardenafil drugs, suggest interference with quinol binding likely to affect protein's function

1043. Toll-Like Receptor-4 Signaling Drives Persistent Fibroblast Activation and Prevents Fibrosis Resolution in Scleroderma

1044. Toward more realistic drug-target interaction predictions

1045. Toward repurposing ciclopirox as an antibiotic against drug-resistant Acinetobacter baumannii, Escherichia coli, and Klebsiella pneumoniae

1046. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

1047. Towards building a disease-phenotype knowledge base: extracting disease-manifestation relationship from literature

1048. Towards drug repositioning: a unified computational framework for integrating multiple aspects of drug similarity and disease similarity

1049. Towards precision medicine-based therapies for glioblastoma: interrogating human disease genomics and mouse phenotypes

1050. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

1051. Transcriptional data: a new gateway to drug repositioning

1052. Transcriptomic Analysis of the Host Response and Innate Resilience to Enterotoxigenic Escherichia coli Infection in Humans

1053. Transcriptomic changes induced by mycophenolic acid in gastric cancer cells

1054. Transcriptomic characterization of the novel avian-origin influenza A (H7N9) virus: specific host response and responses intermediate between avian (H5N1 and H7N7) and human (H3N2) viruses and implications for treatment options

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1056. Transcriptomic RNAseq drug screen in cerebrocortical cultures: toward novel neurogenetic disease therapies

1057. Transcriptomic-Guided Drug Repositioning Supported by a New Bioinformatics Search Tool: geneXpharma

1058. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants

1059. Treating Influenza Infection, From Now and Into the Future

1060. Treating the dysfunctional placenta

1061. Treatment of Schistosoma mansoni with miltefosine in vitro enhances serological recognition of defined worm surface antigens

1062. Trends of Clinical Trials for Drug Development in Rare Diseases

1063. Trypanocidal Effect of Isotretinoin through the Inhibition of Polyamine and Amino Acid Transporters in Trypanosoma cruzi

1064. Uncovering Drug Mechanism of Action by Proteome Wide- Identification of Drug-Binding Proteins

1065. Uncovering novel repositioning opportunities using the Open Targets platform

1066. Understanding organellar protein folding capacities and assessing their pharmacological modulation by small molecules

1067. Unveiling the role of network and systems biology in drug discovery

1068. Updates on drug-target network; facilitating polypharmacology and data integration by growth of DrugBank database

1069. Use of genome-wide association studies for cancer research and drug repositioning

1070. Using Big Data to Discover Diagnostics and Therapeutics forGastrointestinal and Liver Diseases

1071. Using functional signatures to identify repositioned drugs for breast, myelogenous leukemia and prostate cancer

1072. Using gene expression signatures to identify novel treatment strategies in gulf war illness

1073. Using predicate and provenance information from a knowledge graph for drug efficacy screening

1074. Utilizing Cancer - Functional Gene Set - Compound Networks to Identify Putative Drugs for Breast Cancer

1075. Valproic acid in the complex therapy of malignant tumors

1076. Valproic acid mediates miR-124 to down-regulate a novel protein target, GNAI1

1077. Verteporfin inhibits gastric cancer cell growth by suppressing adhesion molecule FAT1

1078. Virtual screening and repositioning of inconclusive molecules of beta-lactamase Bioassays-A data mining approach

1079. Virtual screening-driven repositioning of etoposide as CD44 antagonist in breast cancer cells

1080. Virtual target screening: validation using kinase inhibitors

1081. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

1082. Vitamin K and hepatocellular carcinoma: The basic and clinic

1083. Voltage-gated sodium channel as a target for metastatic risk reduction with re-purposed drugs

1084. Voltage-gated sodium channels and metastatic disease

1085. Warfarin Blocks Gas6-Mediated Axl Activation Required for Pancreatic Cancer Epithelial Plasticity and Metastasis

1086. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

1087. YAP/TAZ Are Mechanoregulators of TGF-beta-Smad Signaling and Renal Fibrogenesis

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FACTOR 27. Drug Repurposing for Brain Cancer

1. A chemical-genetic interaction map of small molecules using high-throughput imaging in cancer cells

2. A conceptually new treatment approach for relapsed glioblastoma: coordinated undermining of survival paths with nine repurposed drugs (CUSP9) by the International Initiative for Accelerated Improvement of Glioblastoma Care

3. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

4. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

5. A Drug Screen using Human iPSC-Derived Hepatocyte-like Cells Reveals Cardiac Glycosides as a Potential Treatment for Hypercholesterolemia

6. A drug-repositioning screen for primary pancreatic ductal adenocarcinoma cells identifies 6-thioguanine as an effective therapeutic agent for TPMT-low cancer cells

7. A High-Content Screening of Anticancer Compounds Suggests the Multiple Tyrosine Kinase Inhibitor Ponatinib for Repurposing in Neuroblastoma Therapy

8. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research

9. A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer

10. A novel anti-cancer role of beta-apopicropodophyllin against non-small cell lung cancer cells

11. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia

12. A novel chemoradiation targeting stem and nonstem pancreatic cancer cells by repurposing disulfiram

13. A Novel High Content Imaging-Based Screen Identifies the Anti-Helminthic Niclosamide as an Inhibitor of Lysosome Anterograde Trafficking and Prostate Cancer Cell Invasion

14. A protein folding molecular imaging biosensor monitors the effects of drugs that restore mutant p53 structure and its downstream function in glioblastoma cells

15. A rapid and affordable screening platform for membrane protein trafficking

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22. A tumor deconstruction platform identifies definitive end points in the evaluation of drug responses

23. Activity of anti-cancer protein kinase inhibitors against Leishmania spp

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25. Adaptive mitochondrial reprogramming and resistance to PI3K therapy

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27. Alcohol-abuse drug disulfiram targets cancer via p97 segregase adaptor NPL4

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30. An in vitro test system for compounds that modulate human inflammatory macrophage polarization

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32. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin

33. Angiotensin inhibition enhances drug delivery and potentiates chemotherapy by decompressing tumour blood vessels

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35. Anthelmintic mebendazole enhances cisplatin's effect on suppressing cell proliferation and promotes differentiation of head and neck squamous cell carcinoma (HNSCC

36. Anti-inflammatory effects of dabrafenib in vitro and in vivo

37. Anti-inflammatory effects of dabrafenib on polyphosphate-mediated vascular disruption

38. Anti-inflammatory effects of methylthiouracil in vitro and in vivo

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43. Antihelminthic drug niclosamide inhibits CIP2A and reactivates tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells

44. Antimalarial drug mefloquine inhibits nuclear factor kappa B signaling and induces apoptosis in colorectal cancer cells

45. Antischistosomal agents: state of art and perspectives

46. Antitubercular activity of disulfiram, an antialcoholism drug, against multidrug- and extensively drug-resistant Mycobacterium tuberculosis isolates

47. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis

48. Aripiprazole, an Antipsychotic and Partial Dopamine Agonist, Inhibits Cancer Stem Cells and Reverses Chemoresistance

49. Artemisinin and Its Derivatives as a Repurposing Anticancer Agent: What Else Do We Need to Do

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73. Chloroquine analogues in drug discovery: new directions of uses, mechanisms of actions and toxic manifestations from malaria to multifarious diseases

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80. Computational approaches for drug repositioning and combination therapy design

81. Computational Approaches for Translational Oncology: Concepts and Patents

82. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

83. Computational identification of multi-omic correlates of anticancer therapeutic response

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88. Concise Review: Cell Surface N-Linked Glycoproteins as Potential Stem Cell Markers and Drug Targets

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91. Current and Future Use of Chloroquine and Hydroxychloroquine in Infectious, Immune, Neoplastic, and Neurological Diseases: A Mini-Review

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93. Cytogenomic profiling of breast cancer brain metastases reveals potential for repurposing targeted therapeutics

94. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer

95. Data integration to prioritize drugs using genomics and curated data

96. Designing novel therapies against sarcomas in the era of personalized medicine and economic crisis

97. Development and optimization of an injectable formulation of copper diethyldithiocarbamate, an active anticancer agent

98. Diethyldithiocarbamate complex with copper: the mechanism of action in cancer cells

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107. Do statins, ACE inhibitors or sartans improve outcome in primary glioblastoma

108. Dose-dependent effect and pharmacokinetics of fexinidazole and its metabolites in a mouse model of human African trypanosomiasis

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126. Drug Repurposing in Anticancer Reagent Development

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181. Identification of Mitoxantrone as a TRAIL-sensitizing agent for Glioblastoma Multiforme

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214. Medical treatment in neurofibromatosis type 2. Review of the literature and presentation of clinical reports

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245. Neuroblastoma, a Paradigm for Big Data Science in Pediatric Oncology

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247. New derivatives of the antimalarial drug Pyrimethamine in the control of melanoma tumor growth: an in vitro and in vivo study

248. New pharmacological treatment strategies for relapse prevention

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320. Repurposing an orally available drug for the treatment of geographic atrophy

321. Repurposing and Rescuing of Mibefradil, an Antihypertensive, for Cancer: A Case Study

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328. Repurposing drugs for glioblastoma: From bench to bedside

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330. Repurposing Established Compounds to Target Pancreatic Cancer Stem Cells (CSCs

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FACTOR 28. Repurposing Anthelmintic Drugs for Cancer Treatment

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4. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

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22. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis

23. Applications and implications of heparin and protamine in tissue engineering and regenerative medicine

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492. Steroids-specific target library for steroids target prediction

493. Structural analysis of protein tyrosine phosphatase 1B reveals potentially druggable allosteric binding sites

494. Structural basis for the resilience of efavirenz (DMP-266) to drug resistance mutations in HIV-1 reverse transcriptase

495. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

496. Structure based investigation on the binding interaction of transport proteins in leishmaniasis: insights from molecular simulation

497. Structure-based identification of a NEDD8-activating enzyme inhibitor via drug repurposing

498. Structure-based repurposing of FDA-approved drugs as inhibitors of NEDD8-activating enzyme

499. Substrate-driven mapping of the degradome by comparison of sequence logos

500. Sulforaphane Prevents Neuronal Apoptosis and Memory Impairment in Diabetic Rats

501. SUMOylation in brain ischemia: Patterns, targets, and translational implications

502. Suppressive effects of dabrafenibon endothelial protein C receptor shedding

503. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

504. Synergistic combination of flavopiridol and carfilzomib targets commonly dysregulated pathways in adrenocortical carcinoma and has biomarkers of response

505. Systematic analyses of drugs and disease indications in RepurposeDB reveal pharmacological, biological and epidemiological factors influencing drug repositioning

506. Systematic discovery of drug action mechanisms by an integrated chemical genomics approach: identification of functional disparities between azacytidine and decitabine

507. Systematic dissection of dysregulated transcription factor-miRNA feed-forward loops across tumor types

508. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach

509. T3D-959: A Multi-Faceted Disease Remedial Drug Candidate for the Treatment of Alzheimer's Disease

510. Tacrine-deferiprone hybrids as multi-target-directed metal chelators against Alzheimer's disease: a two-in-one drug

511. Targeting calcium homeostasis as the therapy of Chagas' disease and leishmaniasis - a review

512. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

513. Targeting phosphodiesterase 5 as a therapeutic option against myocardial ischaemia/reperfusion injury and for treating heart failure

514. Targeting the off-targets: a computational bioinformatics approach to understanding the polypharmacology of nelfinavir

515. Tetracycline hydrochloride: A potential clinical drug for radioprotection

516. Tetracycline repurposing in neurodegeneration: focus on Parkinson's disease

517. The antihelminthic drug niclosamide effectively inhibits the malignant phenotypes of uveal melanoma in vitro and in vivo

518. The antimalarial amodiaquine causes autophagic-lysosomal and proliferative blockade sensitizing human melanoma cells to starvation- and chemotherapy-induced cell death

519. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells

520. The CARLSBAD database: a confederated database of chemical bioactivities

521. The case of galantamine: repurposing and late blooming of a cholinergic drug

522. The combination astemizole-gefitinib as a potential therapy for human lung cancer

523. The Coming of Age of the Angiotensin Hypothesis in Alzheimer's Disease: Progress Toward Disease Prevention and Treatment

524. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

525. The extraction of drug-disease correlations based on module distance in incomplete human interactome

526. The EYA tyrosine phosphatase activity is pro-angiogenic and is inhibited by benzbromarone

527. The FDA-approved natural product dihydroergocristine reduces the production of the Alzheimer's disease amyloid-beta peptides

528. The human immunodeficiency virus protease inhibitor ritonavir is potentially active against urological malignancies

529. The interleukin-6 receptor as a target for prevention of coronary heart disease: a mendelian randomisation analysis

530. The Molecular Revolution in Cutaneous Biology: Emerging Landscape in Genomic Dermatology: New Mechanistic Ideas, Gene Editing, and Therapeutic Breakthroughs

531. The multitargeted drug ivermectin: from an antiparasitic agent to a repositioned cancer drug

532. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C

533. The positive inotropic agent DPI-201106 selectively reverses ABCB1-mediated multidrug resistance in cancer cell lines

534. The protein kinase 2 inhibitor CX-4945 regulates osteoclast and osteoblast differentiation in vitro

535. The proton-pump inhibitor lansoprazole enhances amyloid beta production

536. The repurposed anthelmintic mebendazole in combination with trametinib suppresses refractory NRASQ61K melanoma

537. The role of drug profiles as similarity metrics: applications to repurposing, adverse effects detection and drug-drug interactions

538. The sodium channel-blocking antiepileptic drug phenytoin inhibits breast tumour growth and metastasis

539. The Src/c-Abl pathway is a potential therapeutic target in amyotrophic lateral sclerosis

540. The susceptibility of trypanosomatid pathogens to PI3/mTOR kinase inhibitors affords a new opportunity for drug repurposing

541. Therapeutic Approaches to Prion Diseases

542. Therapeutic compositions and uses of alpha1-antitrypsin: a patent review (2012 - 2015

543. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

544. Therapeutic potential for phenytoin: targeting Na(v)1.5 sodium channels to reduce migration and invasion in metastatic breast cancer

545. Therapeutic strategies of drug repositioning targeting autophagy to induce cancer cell death: from pathophysiology to treatment

546. Three-dimensional models of Mycobacterium tuberculosis proteins Rv1555, Rv1554 and their docking analyses with sildenafil, tadalafil, vardenafil drugs, suggest interference with quinol binding likely to affect protein's function

547. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

548. Transcriptomic Analysis of the Host Response and Innate Resilience to Enterotoxigenic Escherichia coli Infection in Humans

549. Transcriptomic changes induced by mycophenolic acid in gastric cancer cells

550. Transcriptomic RNAseq drug screen in cerebrocortical cultures: toward novel neurogenetic disease therapies

551. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants

552. Trypanocidal Effect of Isotretinoin through the Inhibition of Polyamine and Amino Acid Transporters in Trypanosoma cruzi

553. Uncovering Drug Mechanism of Action by Proteome Wide- Identification of Drug-Binding Proteins

554. Understanding organellar protein folding capacities and assessing their pharmacological modulation by small molecules

555. Unveiling the role of network and systems biology in drug discovery

556. Ursocholanic acid rescues mitochondrial function in common forms of familial Parkinson's disease

557. Using Drugs as Molecular Probes: AComputational Chemical Biology Approach in Neurodegenerative Diseases

558. Using predicate and provenance information from a knowledge graph for drug efficacy screening

559. Validating the Predicted Effect of Astemizole and Ketoconazole Using a Drosophila Model of Parkinson's Disease

560. Valproic acid in the complex therapy of malignant tumors

561. Valproic acid mediates miR-124 to down-regulate a novel protein target, GNAI1

562. Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors

563. Virtual target screening: validation using kinase inhibitors

564. Vitamin K and hepatocellular carcinoma: The basic and clinic

565. Voltage-gated sodium channels and metastatic disease

566. Warfarin Blocks Gas6-Mediated Axl Activation Required for Pancreatic Cancer Epithelial Plasticity and Metastasis

567. YAP/TAZ Are Mechanoregulators of TGF-beta-Smad Signaling and Renal Fibrogenesis

568. Zafirlukast inhibits complexation of Lsr2 with DNA and growth of Mycobacterium tuberculosis

FACTOR 30. Repurposed Drugs Targeting Glutamate Receptors

1. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

2. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

3. A screen of approved drugs and molecular probes identifies therapeutics with anti-Ebola virus activity

4. ADEPTUS: a discovery tool for disease prediction, enrichment and network analysis based on profiles from many diseases

5. Advances in epilepsy gene discovery and implications for epilepsy diagnosis and treatment

6. Advances in the therapeutic use of mammalian target of rapamycin (mTOR) inhibitors in dermatology

7. Analysis of genome-wide association data highlights candidates for drug repositioning in psychiatry

8. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

9. Anticonvulsant activity of artificial sweeteners: a structural link between sweet-taste receptor T1R3 and brain glutamate receptors

10. Antidepressants in the Treatment of Functional Dyspepsia: A Systematic Review and Meta-Analysis

11. Antidepressants, antimicrobials or both? Gut microbiota dysbiosis in depression and possible implications of the antimicrobial effects of antidepressant drugs for antidepressant effectiveness

12. Butamben derivatives enhance BMP-2-stimulated commitment of C2C12 cells into osteoblasts with induction of voltage-gated potassium channel expression

13. Case-specific potentiation of glioblastoma drugs by pterostilbene

14. CaV channels and cancer: canonical functions indicate benefits of repurposed drugs as cancer therapeutics

15. Cell-based screening identifies paroxetine as an inhibitor of diabetic endothelial dysfunction

16. Clinical validation of blood/brain glutamate grabbing in acute ischemic stroke

17. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

18. Cytokine sensitivity screening highlights BMP4 pathway signaling as a therapeutic opportunity in ER+ breast cancer

19. Discovering gene re-ranking efficiency and conserved gene-gene relationships derived from gene co-expression network analysis on breast cancer data

20. Drug discovery for the treatment of substance use disorders: novel targets, repurposing, and the need for new paradigms

21. Drug repurposing for Leishmania. Molecular basis of the leishmanicidal activity of the antidepressant sertraline

22. Drug repurposing may generate novel approaches to treating depression

23. Drug similarity search based on combined signatures in gene expression profiles

24. Dual Targeting of the Autophagic Regulatory Circuitry in Gliomas with Repurposed Drugs Elicits Cell-Lethal Autophagy and Therapeutic Benefit

25. Effects of the nicotinic agonist varenicline on the performance of tasks of cognition in aged and middle-aged rhesus and pigtail monkeys

26. Exendin-4 ameliorates traumatic brain injury-induced cognitive impairment in rats

27. Fast, non-competitive and reversible inhibition of NMDA-activated currents by 2-BFI confers neuroprotection

28. Finding the targets of a drug by integration of gene expression data with a protein interaction network

29. Fluvoxamine, an anti-depressant, inhibits human glioblastoma invasion by disrupting actin polymerization

30. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC

31. Glutamate release inhibitor, Riluzole, inhibited proliferation of human hepatocellular carcinoma cells by elevated ROS production

32. High-content drug screening for rare diseases

33. Identification of Chemical Inhibitors of beta-Catenin-Driven Liver Tumorigenesis in Zebrafish

34. In Silico-Based Repositioning of Phosphinothricin as a Novel Technetium-99m Imaging Probe with Potential Anti-Cancer Activity

35. Inhibition of ACE Retards Tau Hyperphosphorylation and Signs of Neuronal Degeneration in Aged Rats Subjected to Chronic Mild Stress

36. Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding

37. Is there a relationship between sweet taste and seizures? Anticonvulsant and proconvulsant effects of non-nutritive sweeteners

38. KCa 3.1-a microglial target ready for drug repurposing

39. Ketamine for treatment-resistant unipolar depression: current evidence

40. Ketamine: repurposing and redefining a multifaceted drug

41. Ketanserin, an antidepressant, exerts its antileishmanial action via inhibition of 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGR) enzyme of Leishmania donovani

42. Liraglutide attenuates the depressive- and anxiety-like behaviour in the corticosterone induced depression model via improving hippocampal neural plasticity

43. MD-Miner: a network-based approach for personalized drug repositioning

44. Medications for alcohol use disorders: An overview

45. Metformin use and gynecological cancers: A novel treatment option emerging from drug repositioning

46. Metformin: its emerging role in oncology

47. Microglial KCa3.1 Channels as a Potential Therapeutic Target for Alzheimer's Disease

48. Mining mouse behavior for patterns predicting psychiatric drug classification

49. Molecular investigations of protriptyline as a multi-target directed ligand in Alzheimer's disease

50. Mood, stress and longevity: convergence on ANK3

51. N-acetylcysteine prevents stress-induced anxiety behavior in zebrafish

52. Network-assisted prediction of potential drugs for addiction

53. Network-based drug repositioning

54. Network-based drug repositioning: A novel strategy for discovering potential antidepressants and their mode of action

55. New drug candidates for depression - a nationwide population-based study

56. New indications for existing drugs; repurposing in psychiatry and addiction medicine

57. New perspectives for metformin in cancer therapy

58. New pharmacological treatment strategies for relapse prevention

59. New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate

60. Pharmacological targeting of ion channels for cancer therapy: In vivo evidences

61. Potential repurposing of known drugs as potent bacterial beta-glucuronidase inhibitors

62. Predicting Potential Drugs for Breast Cancer based on miRNA and Tissue Specificity

63. Re-engineering a neuroprotective, clinical drug as a procognitive agent with high in vivo potency and with GABAA potentiating activity for use in dementia

64. Repurposing itraconazole as an anticancer agent

65. Repurposing Lesogaberan to Promote Human Islet Cell Survival and beta-Cell Replication

66. Repurposing potential of 1st generation H1-specific antihistamines as anti-filovirus therapeutics

67. Senicapoc: Repurposing a Drug to Target Microglia KCa3.1 in Stroke

68. Sertraline, Paroxetine, and Chlorpromazine Are Rapidly Acting Anthelmintic Drugs Capable of Clinical Repurposing

69. Sphingolipids as targets for inhalation treatment of cystic fibrosis

70. SPIDR: small-molecule peptide-influenced drug repurposing

71. SPILLO-PBSS: detecting hidden binding sites within protein 3D-structures through a flexible structure-based approach

72. Stress-Activated Kinase Mitogen-Activated Kinase Kinase-7 Governs Epigenetics of Cardiac Repolarization for Arrhythmia Prevention

73. Subanaesthetic dose of ketamine in intractable asthma

74. Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis

75. Systems Medicine Approaches to Improving Understanding, Treatment, and Clinical Management of Neuroendocrine Prostate Cancer

76. Targeting cyclin D3/CDK6 activity for treatment of Parkinson's disease

77. Teaching an old dog new tricks: drug repositioning in small cell lung cancer

78. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

79. The antidepressant 5-HT2A receptor antagonists pizotifen and cyproheptadine inhibit serotonin-enhanced platelet function

80. The antiparasitic drug, potassium antimony tartrate, inhibits tumor angiogenesis and tumor growth in nonsmall-cell lung cancer

81. The bitter pill: clinical drugs that activate the human bitter taste receptor TAS2R14

82. The case of galantamine: repurposing and late blooming of a cholinergic drug

83. The combination astemizole-gefitinib as a potential therapy for human lung cancer

84. The susceptibility of trypanosomatid pathogens to PI3/mTOR kinase inhibitors affords a new opportunity for drug repurposing

85. Topical phenytoin for the treatment of neuropathic pain

86. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

87. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation

88. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

89. Where do we stand in the field of anti-abuse drug discovery

FACTOR 31. Repurposing Drugs that Target Oxidative and Inflammation Biomarkers VEGF, HO-1, iNOS, Nrf2

1. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

2. A Novel High Content Imaging-Based Screen Identifies the Anti-Helminthic Niclosamide as an Inhibitor of Lysosome Anterograde Trafficking and Prostate Cancer Cell Invasion

3. A Topical Zinc Ionophore Blocks Tumorigenic Progression in UV-exposed SKH-1 High-risk Mouse Skin

4. A Zebrafish Drug-Repurposing Screen Reveals sGC-Dependent and sGC-Independent Pro-Inflammatory Activities of Nitric Oxide

5. Acetaminophen attenuates dopamine neuron degeneration in animal models of Parkinson's disease

6. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

7. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

8. Advances in intravesical therapy for urinary tract disorders

9. Albendazole as a promising molecule for tumor control

10. Albumin nanoparticles increase the anticancer efficacy of albendazole in ovarian cancer xenograft model

11. Ameliorative effect of methylthiouracil on TGFBIp-induced septic responses

12. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

13. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

14. Antiviral effects of inhibiting host gene expression

15. Auranofin: repurposing an old drug for a golden new age

16. Bedaquiline, an FDA-approved antibiotic, inhibits mitochondrial function and potently blocks the proliferative expansion of stem-like cancer cells (CSCs

17. beta-Caryophyllene protects against alcoholic steatohepatitis by attenuating inflammation and metabolic dysregulation in mice

18. Beyond standard therapy: drugs under investigation for the treatment of gastrointestinal stromal tumor

19. Bioinformatics methods in drug repurposing for Alzheimer's disease

20. Bioinformatics-driven discovery of rational combination for overcoming EGFR-mutant lung cancer resistance to EGFR therapy

21. Bisphosphonates inactivate human EGFRs to exert antitumor actions

22. Blocking IL-6/GP130 signaling inhibits cell viability/proliferation, glycolysis, and colony forming activity in human pancreatic cancer cells

23. Breast cancer cells condition lymphatic endothelial cells within pre-metastatic niches to promote metastasis

24. Candesartan stimulates reparative angiogenesis in ischemic retinopathy model: role of hemeoxygenase-1 (HO-1

25. Chemoprevention of head and neck squamous cell carcinoma through inhibition of NF-kappaB signaling

26. CK2 inhibition confers functional protection to young and aging axons against ischemia by differentially regulating the CDK5 and AKT signaling pathways

27. Clinical dosage of meclozine promotes longitudinal bone growth, bone volume, and trabecular bone quality in transgenic mice with achondroplasia

28. Combination of acamprosate and baclofen as a promising therapeutic approach for Parkinson's disease

29. Combined analysis of gene expression and genome binding profiles identified potential therapeutic targets of ciclopirox in Ewing sarcoma

30. Combined chemical genetics and data-driven bioinformatics approach identifies receptor tyrosine kinase inhibitors as host-directed antimicrobials

31. Computational Discovery of Niclosamide Ethanolamine, a Repurposed Drug Candidate That Reduces Growth of Hepatocellular Carcinoma Cells InVitro and in Mice by Inhibiting Cell Division Cycle 37 Signaling

32. Computational repositioning and experimental validation of approved drugs for HIF-prolyl hydroxylase inhibition

33. Computational-experimental approach to drug-target interaction mapping: A case study on kinase inhibitors

34. Copper Complexes in Cancer Therapy

35. Covalent inhibitors of EGFR family protein kinases induce degradation of human Tribbles 2 (TRIB2) pseudokinase in cancer cells

36. Current and upcoming pharmacotherapy for non-alcoholic fatty liver disease

37. Deciphering cellular biological processes to clinical application: a new perspective for Talpha1 treatment targeting multiple diseases

38. Designing novel therapies against sarcomas in the era of personalized medicine and economic crisis

39. Development and Characterization of Bladder Cancer Patient-Derived Xenografts for Molecularly Guided Targeted Therapy

40. Developmental toxicity of auranofin in zebrafish embryos

41. Disulfiram, a drug widely used to control alcoholism, suppresses the self-renewal of glioblastoma and over-rides resistance to temozolomide

42. DPP-4 inhibitors promote proliferation and migration of rat brain microvascular endothelial cells under hypoxic/high-glucose conditions, potentially through the SIRT1/HIF-1/VEGF pathway

43. Drug combination approach to overcome resistance to EGFR tyrosine kinase inhibitors in lung cancer

44. Drug delivery for the treatment of endometriosis and uterine fibroids

45. Drug repositioning for gynecologic tumors: a new therapeutic strategy for cancer

46. Drug Repositioning for Preeclampsia Therapeutics by In Vitro Screening: Phosphodiesterase-5 Inhibitor Vardenafil Restores Endothelial Dysfunction via Induction of Placental Growth Factor

47. Drug Repurposing for Duchenne Muscular Dystrophy: The Monoamine Oxidase B Inhibitor Safinamide Ameliorates the Pathological Phenotype in mdx Mice and in Myogenic Cultures From DMD Patients

48. Drug repurposing for Leishmania. Molecular basis of the leishmanicidal activity of the antidepressant sertraline

49. Drug Repurposing Screen Identifies Foxo1-Dependent Angiopoietin-2 Regulation in Sepsis

50. Drug-Repositioning Screening for Keap1-Nrf2 Binding Inhibitors using Fluorescence Correlation Spectroscopy

51. Fibrosis in systemic sclerosis: common and unique pathobiology

52. Folic Acid Exerts Post-Ischemic Neuroprotection In Vitro Through HIF-1alpha Stabilization

53. Fragile Histidine Triad (FHIT), a Novel Modifier Gene in Pulmonary Arterial Hypertension

54. From ancient herb to modern drug: Artemisia annua and artemisinin for cancer therapy

55. Heme Oxygenase Database (HemeOxDB) and QSAR Analysis of Isoform?1 Inhibitors

56. Histamine-2 receptor antagonist famotidine modulates cardiac stem cell characteristics in hypertensive heart disease

57. Identification of KX2-391 as an inhibitor of HBV transcription by a recombinant HBV-based screening assay

58. Identification of Non-Electrophilic Nrf2 Activators from Approved Drugs

59. Identifying and Tackling Emergent Vulnerability in Drug-Resistant Mycobacteria

60. Imidazolium salts as innovative agents against Leishmania amazonensis

61. In silico identification of potent small molecule inhibitors targeting epidermal growth factor receptor 1

62. In silico prediction and in vitro and in vivo validation of acaricide fluazuron as a potential inhibitor of FGFR3 and a candidate anticancer drug for bladder carcinoma

63. In vitro and in vivo study of hydralazine, a potential anti-angiogenic agent

64. Inhibition of effector antigen-specific T cells by intradermal administration of heme oxygenase-1 inducers

65. Inhibition of EGFR Signaling Protects from Mucormycosis

66. Inhibition of the insulin-like growth factor system is a potential therapy for rheumatoid arthritis

67. KCa 3.1-a microglial target ready for drug repurposing

68. Lethal action of the nitrothiazolyl-salicylamide derivative nitazoxanide via induction of oxidative stress in Leishmania (L.) infantum

69. Luteolin Impacts on the DNA Damage Pathway in Oral Squamous Cell Carcinoma

70. Mechanism-informed Repurposing of Minocycline Overcomes Resistance to Topoisomerase Inhibition for Peritoneal Carcinomatosis

71. Meclozine facilitates proliferation and differentiation of chondrocytes by attenuating abnormally activated FGFR3 signaling in achondroplasia

72. Medical treatment in neurofibromatosis type 2. Review of the literature and presentation of clinical reports

73. Metformin use and gynecological cancers: A novel treatment option emerging from drug repositioning

74. Microglial role in the development of chronic pain

75. Mining Retrospective Data for Virtual Prospective Drug Repurposing: L-DOPA and Age-related Macular Degeneration

76. Mitigation of carbon tetrachloride-induced hepatic injury by methylene blue, a repurposed drug, is mediated by dual inhibition of GSK3beta downstream of PKA

77. Molecular therapeutic strategies for FGFR3 gene-related skeletal dysplasia

78. Mood, stress and longevity: convergence on ANK3

79. Nelfinavir and lopinavir impair Trypanosoma cruzi trypomastigote infection in mammalian host cells and show anti-amastigote activity

80. Nelfinavir, a new anti-cancer drug with pleiotropic effects and many paths to autophagy

81. Neuroprotective and immunomodulatory effects of raloxifene in the myenteric plexus of a mouse model of Parkinson's disease

82. Nitrosylation of GAPDH augments pathological tau acetylation upon exposure to amyloid-beta

83. Nrf2 inhibition reverses the resistance of cisplatin-resistant head and neck cancer cells to artesunate-induced ferroptosis

84. Olaparib protects cardiomyocytes against oxidative stress and improves graft contractility during the early phase after heart transplantation in rats

85. Oxidative stress during acetaminophen hepatotoxicity: Sources, pathophysiological role and therapeutic potential

86. Parkinson's Disease, Diabetes and Cognitive Impairment

87. Pharmacological approach for drug repositioning against cardiorenal diseases

88. Pharmacological targeting of GSK-3 and NRF2 provides neuroprotection in a preclinical model of tauopathy

89. Pharmacological treatment and prevention of cerebral small vessel disease: a review of potential interventions

90. Pharmacological use of a novel scaffold, anomeric N,N-diarylamino tetrahydropyran: molecular similarity search, chemocentric target profiling, and experimental evidence

91. Pharmacology and Clinical Drug Candidates in Redox Medicine

92. Platelet Hyperreactivity in Diabetes: Focus on GPVI Signaling-Are Useful Drugs Already Available

93. Posttranslational Regulation of O(6)-Methylguanine-DNA Methyltransferase (MGMT) and New Opportunities for Treatment of Brain Cancers

94. Potential repositioning of exemestane as a neuroprotective agent for Parkinson's disease

95. PPARgamma agonists sensitize PTEN-deficient resistant lung cancer cells to EGFR tyrosine kinase inhibitors by inducing autophagy

96. Pre-clinical effects of metformin and aspirin on the cell lines of different breast cancer subtypes

97. Promethazine Hydrochloride Inhibits Ectopic Fat Cell Formation in Skeletal Muscle

98. Propofol post-conditioning alleviates hepatic ischaemia reperfusion injury via BRG1-mediated Nrf2/HO-1 transcriptional activation in human and mice

99. Re-engineering a neuroprotective, clinical drug as a procognitive agent with high in vivo potency and with GABAA potentiating activity for use in dementia

100. Repositioning of molsidomine for its efficacy in diabetes induced erectile dysfunction in rats: In silico, in vitro and in vivo approach

101. Repurposing an established drug: an emerging role for methylene blue in L-DOPA-induced dyskinesia

102. Repurposing an orally available drug for the treatment of geographic atrophy

103. Repurposing atovaquone: targeting mitochondrial complex III and OXPHOS to eradicate cancer stem cells

104. Repurposing cationic amphiphilic drugs as adjuvants to induce lysosomal siRNA escape in nanogel transfected cells

105. Repurposing Drugs in Oncology (ReDO)-nitroglycerin as an anti-cancer agent

106. Repurposing FDA-approved drugs as therapeutics to treat Rift Valley fever virus infection

107. Repurposing of bisphosphonates for the prevention and therapy of nonsmall cell lung and breast cancer

108. Repurposing propranolol as a drug for the treatment of retinal haemangioblastomas in von Hippel-Lindau disease

109. Repurposing the anti-malarial drug, quinacrine: new anti-colitis properties

110. Repurposing the NRF2 Activator Dimethyl Fumarate as Therapy Against Synucleinopathy in Parkinson's Disease

111. Retinal Neuroprotective Effects of Flibanserin, an FDA-Approved Dual Serotonin Receptor Agonist-Antagonist

112. Ribavirin as a tri-targeted antitumor repositioned drug

113. Rifampin inhibits Toll-like receptor 4 signaling by targeting myeloid differentiation protein 2 and attenuates neuropathic pain

114. Ritonavir blocks AKT signaling, activates apoptosis and inhibits migration and invasion in ovarian cancer cells

115. Role of TGFbeta in regulation of the tumor microenvironment and drug delivery (review

116. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients

117. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

118. Systemic hemin therapy attenuates blood-brain barrier disruption after intracerebral hemorrhage

119. T3D-959: A Multi-Faceted Disease Remedial Drug Candidate for the Treatment of Alzheimer's Disease

120. Tacrine-deferiprone hybrids as multi-target-directed metal chelators against Alzheimer's disease: a two-in-one drug

121. Targeting ADAM17 Sheddase Activity in Cancer

122. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress

123. Targeting transcriptional control of soluble guanylyl cyclase via NOTCH for prevention of cardiovascular disease

124. The antifungal compound butenafine eliminates promastigote and amastigote forms of Leishmania (Leishmania) amazonensis and Leishmania (Viannia) braziliensis

125. The dual targeting of EGFR and ErbB2 with the inhibitor Lapatinib corrects high glucose-induced apoptosis and vascular dysfunction by opposing multiple diabetes-induced signaling changes

126. The neuroimmune transcriptome and alcohol dependence: potential for targeted therapies

127. The polysialic acid mimetics idarubicin and irinotecan stimulate neuronal survival and neurite outgrowth and signal via protein kinase C

128. The possible repositioning of an oral anti-arthritic drug, auranofin, for Nrf2-activating therapy: The demonstration of Nrf2-dependent anti-oxidative action using a zebrafish model

129. Therapeutic Effect of Quinacrine, an Antiprotozoan Drug, by Selective Suppression of p-CHK1/2 in p53-Negative Malignant Cancers

130. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

131. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

132. Treating the dysfunctional placenta

133. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer

134. TUSC2(FUS1)-erlotinib Induced Vulnerabilities in Epidermal Growth Factor Receptor(EGFR) Wildtype Non-small Cell Lung Cancer(NSCLC) Targeted by the Repurposed Drug Auranofin

135. Understanding fibrosis in systemic sclerosis: shifting paradigms, emerging opportunities

136. Valproic Acid Promotes Apoptosis and Cisplatin Sensitivity Through Downregulation of H19 Noncoding RNA in Ovarian A2780 Cells

FACTOR 32. Computational Drug Repositioning Based on Similarity Networks

1. A bidirectional drug repositioning approach for Parkinson's disease through network-based inference

2. A Biologically-Based Computational Approach to Drug Repurposing for Anthrax Infection

3. A chemo-centric view of human health and disease

4. A comparative study of disease genes and drug targets in the human protein interactome

5. A Computational Drug Repositioning Approach for Targeting Oncogenic Transcription Factors

6. A computational method for clinically relevant cancer stratification and driver mutation module discovery using personal genomics profiles

7. A convenient synthesis of lubeluzole and its enantiomer: evaluation as chemosensitizing agents on human ovarian adenocarcinoma and lung carcinoma cells

8. A cross-species analysis method to analyze animal models' similarity to human's disease state

9. A curated C. difficile strain 630 metabolic network: prediction of essential targets and inhibitors

10. A disease similarity matrix based on the uniqueness of shared genes

11. A diseasome cluster-based drug repurposing of soluble guanylate cyclase activators from smooth muscle relaxation to direct neuroprotection

12. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

13. A framework for the targeted selection of herbs with similar efficacy by exploiting drug repositioning technique and curated biomedical knowledge

14. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis

15. A Large-Scale Gene Expression Intensity-Based Similarity Metric for Drug Repositioning

16. A miRNA-driven inference model to construct potential drug-disease associations for drug repositioning

17. A Multilayer Network Approach for Guiding Drug Repositioning in Neglected Diseases

18. A network based approach to drug repositioning identifies plausible candidates for breast cancer and prostate cancer

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390. Predicting drug-disease interactions by semi-supervised graph cut algorithm and three-layer data integration

391. Predicting drug-target interaction for new drugs using enhanced similarity measures and super-target clustering

392. Predicting drug-target interactions using probabilistic matrix factorization

393. Predicting drug-target interactions using restricted Boltzmann machines

394. Predicting Drug-Target Interactions via Within-Score and Between-Score

395. Predicting Drug-Target Interactions With Multi-Information Fusion

396. Predicting new indications of compounds with a network pharmacology approach: Liuwei Dihuang Wan as a case study

397. Predicting Potential Drugs for Breast Cancer based on miRNA and Tissue Specificity

398. Predicting targeted polypharmacology for drug repositioning and multi- target drug discovery

399. Prediction of chemical-protein interactions network with weighted network-based inference method

400. Prediction of chemical-protein interactions: multitarget-QSAR versus computational chemogenomic methods

401. Prediction of drug's Anatomical Therapeutic Chemical (ATC) code by integrating drug-domain network

402. Prediction of drug-target interaction by label propagation with mutual interaction information derived from heterogeneous network

403. Prediction of drug-target interactions and drug repositioning via network-based inference

404. Prediction of drug-target interactions for drug repositioning only based on genomic expression similarity

405. Prediction of drugs having opposite effects on disease genes in a directed network

406. Prediction of new drug indications based on clinical data and network modularity

407. Prediction of Non-coding RNAs as Drug Targets

408. Prediction of novel drug indications using network driven biological data prioritization and integration

409. Prediction of Novel Drugs and Diseases for Hepatocellular Carcinoma Based on Multi-Source Simulated Annealing Based Random Walk

410. Prediction of Novel Drugs for Hepatocellular Carcinoma Based on Multi-Source Random Walk

411. Prediction of off-target drug effects through data fusion

412. Prediction of polypharmacological profiles of drugs by the integration of chemical, side effect, and therapeutic space

413. Prediction of structure of human WNT-CRD (FZD) complex for computational drug repurposing

414. PROMISCUOUS: a database for network-based drug-repositioning

415. ProphTools: general prioritization tools for heterogeneous biological networks

416. Protein localization vector propagation: a method for improving the accuracy of drug repositioning

417. Protein-ligand-based pharmacophores: generation and utility assessment in computational ligand profiling

418. Proximal Pathway Enrichment Analysis for Targeting Comorbid Diseases via Network Endopharmacology

419. Pyrvinium Sensitizes Clear Cell Renal Cell Carcinoma Response to Chemotherapy Via Casein Kinase 1alpha-Dependent Inhibition of Wnt/beta-Catenin

420. RANKS: a flexible tool for node label ranking and classification in biological networks

421. Rare Diseases: Drug Discovery and Informatics Resource

422. Rational drug repositioning guided by an integrated pharmacological network of protein, disease and drug

423. Re-positioning protein-kinase inhibitors against schistosomiasis

424. Recent Advances in the Development of Pharmaceutical Agents for Metabolic Disorders: A Computational Perspective

425. Recent advances in the machine learning-based drug-target interaction prediction

426. Recommendation Techniques for Drug-Target Interaction Prediction and Drug Repositioning

427. Rectifying cancer drug discovery through network pharmacology

428. Registered report: Discovery and preclinical validation of drug indications using compendia of public gene expression data

429. Relating anatomical therapeutic indications by the ensemble similarity of drug sets

451. Research and development of anti-Alzheimer's disease drugs: an update from the perspective of technology flows

452. Review and comparative assessment of similarity-based methods for prediction of drug-protein interactions in the druggable human proteome

453. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia

454. Revisiting Connectivity Map from a gene co-expression network analysis

455. Ribavirin as a tri-targeted antitumor repositioned drug

456. Roles of the RANKL-RANK axis in antitumour immunity - implications for therapy

457. SCMBYK: prediction and characterization of bacterial tyrosine-kinases based on propensity scores of dipeptides

458. Scoring multiple features to predict drug disease associations using information fusion and aggregation

459. SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drug-target interactions and drug repositioning

460. SELF-BLM: Prediction of drug-target interactions via self-training SVM

461. SemFunSim: a new method for measuring disease similarity by integrating semantic and gene functional association

462. SIS3, a specific inhibitor of Smad3 reverses ABCB1- and ABCG2-mediated multidrug resistance in cancer cell lines

463. SMAP-WS: a parallel web service for structural proteome-wide ligand-binding site comparison

464. Some Remarks on Prediction of Drug-Target Interaction with Network Models

465. Sorafenib Impedes Rift Valley Fever Virus Egress by Inhibiting Valosin-Containing Protein Function in the Cellular Secretory Pathway

466. SPIDR: small-molecule peptide-influenced drug repurposing

467. Statistically controlled identification of differentially expressed genes in one-to-one cell line comparisons of the CMAP database for drug repositioning

468. Steroids-specific target library for steroids target prediction

469. Structural analysis of dihydrofolate reductases enables rationalization of antifolate binding affinities and suggests repurposing possibilities

470. Structural re-positioning, in silico molecular modelling, oxidative degradation, and biological screening of linagliptin as adenosine 3 receptor (ADORA3) modulators targeting hepatocellular carcinoma

471. Substrate-driven mapping of the degradome by comparison of sequence logos

472. Synergistic drug combinations from electronic health records and gene expression

473. Systematic drug repositioning for a wide range of diseases with integrative analyses of phenotypic and molecular data

474. Systematic Identification of Druggable Epithelial-Stromal Crosstalk Signaling Networks in Ovarian Cancer

475. Systematic integration of biomedical knowledge prioritizes drugs for repurposing

476. Systematic Prioritization of Druggable Mutations in 5000 Genomes Across 16 Cancer Types Using a Structural Genomics-based Approach

477. Systematical analysis of lncRNA-mRNA competing endogenous RNA network in breast cancer subtypes

478. Systems approach to the pharmacological actions of HDAC inhibitors reveals EP300 activities and convergent mechanisms of regulation in diabetes

479. Systems biological understanding of the regulatory network and the possible therapeutic strategies for vascular calcification

480. Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis

481. Systems biology-embedded target validation: improving efficacy in drug discovery

482. Systems Medicine Approaches to Improving Understanding, Treatment, and Clinical Management of Neuroendocrine Prostate Cancer

483. Systems medicine: evolution of systems biology from bench to bedside

484. Systems pharmacology of adverse event mitigation by drug combinations

485. Systems Pharmacology-Based Approach of Connecting Disease Genes in Genome-Wide Association Studies with Traditional Chinese Medicine

486. Target-Based Drug Repositioning Using Large-Scale Chemical-Protein Interactome Data

487. Target-similarity search using Plasmodium falciparum proteome identifies approved drugs with anti-malarial activity and their possible targets

488. TargetHunter: an in silico target identification tool for predicting therapeutic potential of small organic molecules based on chemogenomic database

489. Targeting epithelial-mesenchymal plasticity in cancer: clinical and preclinical advances in therapy and monitoring

490. Targeting nasopharyngeal carcinoma by artesunate through inhibiting Akt/mTOR and inducing oxidative stress

491. Targeting Phosphatidylinositol 4-Kinase IIIalpha for Radiosensitization: A Potential Model of Drug Repositioning Using an Anti-Hepatitis C Viral Agent

492. The antineoplastic properties of FTY720: evidence for the repurposing of fingolimod

493. The aryl hydrocarbon receptor is required for induction of p21cip1/waf1 expression and growth inhibition by SU5416 in hepatoma cells

494. The cyclic GMP/protein kinase G pathway as a therapeutic target in head and neck squamous cell carcinoma

495. The extraction of drug-disease correlations based on module distance in incomplete human interactome

496. The human disease network in terms of dysfunctional regulatory mechanisms

497. The neuroimmune transcriptome and alcohol dependence: potential for targeted therapies

498. The neuroleptic drug pimozide inhibits stem-like cell maintenance and tumorigenicity in hepatocellular carcinoma

499. The pain interactome: connecting pain-specific protein interactions

500. The polypharmacology of natural products

501. The positive inotropic agent DPI-201106 selectively reverses ABCB1-mediated multidrug resistance in cancer cell lines

502. The role of drug profiles as similarity metrics: applications to repurposing, adverse effects detection and drug-drug interactions

503. The spatial organization of intra-tumour heterogeneity and evolutionary trajectories of metastases in hepatocellular carcinoma

504. Therapeutic compounds for Cushing's syndrome: a patent review (2012-2016

505. Therapeutic effects of antibiotic drug tigecycline against cervical squamous cell carcinoma by inhibiting Wnt/beta-catenin signaling

506. Therapeutic effects of artesunate in hepatocellular carcinoma: repurposing an ancient antimalarial agent

507. Thiopurine Drugs Repositioned as Tyrosinase Inhibitors

508. Tigecycline targets nonsmall cell lung cancer through inhibition of mitochondrial function

509. Tools for in silico target fishing

510. Toward drug repurposing in epigenetics: olsalazine as a hypomethylating compound active in a cellular context

511. Toward more realistic drug-target interaction predictions

512. Toward Repurposing Metformin as a Precision Anti-Cancer Therapy Using Structural Systems Pharmacology

513. Towards drug repositioning: a unified computational framework for integrating multiple aspects of drug similarity and disease similarity

514. Transcription Factor NRF2 as a Therapeutic Target for Chronic Diseases: A Systems Medicine Approach

515. Transcriptional data: a new gateway to drug repositioning

516. Transcriptomic-Guided Drug Repositioning Supported by a New Bioinformatics Search Tool: geneXpharma

517. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants

518. Trends of Clinical Trials for Drug Development in Rare Diseases

519. Trimodal Therapy: Combining Hyperthermia with Repurposed Bexarotene and Ultrasound for Treating Liver Cancer

520. Tuberculosis: From an incurable scourge to a curable disease - journey over a millennium

521. Unveiling the role of network and systems biology in drug discovery

522. Updates on drug-target network; facilitating polypharmacology and data integration by growth of DrugBank database

523. Utilizing Cancer - Functional Gene Set - Compound Networks to Identify Putative Drugs for Breast Cancer

524. Vinorelbine rescue therapy for dogs with primary urinary bladder carcinoma

525. Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors

526. Virtual screening and repositioning of inconclusive molecules of beta-lactamase Bioassays-A data mining approach

527. VisANT 4.0: Integrative network platform to connect genes, drugs, diseases and therapies

528. Vitamin K and hepatocellular carcinoma: The basic and clinic

529. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

530. Word-of-Mouth Innovation: Hypothesis Generation for Supplement Repurposing based on Consumer Reviews

FACTOR 33. Repurposing Antipsychotic Drugs

1. A chemical genomics approach to drug reprofiling in oncology: Antipsychotic drug risperidone as a potential adenocarcinoma treatment

2. A comparative study of disease genes and drug targets in the human protein interactome

3. A Critical Review of Repurposing Apomorphine for Smoking Cessation

4. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

5. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

6. A genomics-based systems approach towards drug repositioning for rheumatoid arthritis

7. A History of Drug Discovery for Treatment of Nausea and Vomiting and the Implications for Future Research

8. A rapid and affordable screening platform for membrane protein trafficking

9. A screen of approved drugs and molecular probes identifies therapeutics with anti-Ebola virus activity

10. A systems-level analysis of drug-target-disease associations for drug repositioning

11. A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case

12. Acetaminophen attenuates dopamine neuron degeneration in animal models of Parkinson's disease

13. Activation of PP2A by perphenazine induces apoptosis in T-ALL

14. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

15. Adjunct treatments for schizophrenia and bipolar disorder: what to try when you are out of ideas

16. Analysis of genome-wide association data highlights candidates for drug repositioning in psychiatry

17. Antidepressants in the Treatment of Functional Dyspepsia: A Systematic Review and Meta-Analysis

18. Antidepressants, antimicrobials or both? Gut microbiota dysbiosis in depression and possible implications of the antimicrobial effects of antidepressant drugs for antidepressant effectiveness

19. Antifungal Phenothiazines: Optimization, Characterization of Mechanism, and Modulation of Neuroreceptor Activity

20. Approaches for establishing the function of regulatory genetic variants involved in disease

21. Aripiprazole, an Antipsychotic and Partial Dopamine Agonist, Inhibits Cancer Stem Cells and Reverses Chemoresistance

22. Buspirone Counteracts MK-801-Induced Schizophrenia-Like Phenotypes through Dopamine D3 Receptor Blockade

23. Calcium channel blockers as drug repurposing candidates for gestational diabetes: Mining large scale genomic and electronic health records data to repurpose medications

24. Cancer based pharmacogenomics network supported with scientific evidences: from the view of drug repurposing

25. Case-specific potentiation of glioblastoma drugs by pterostilbene

26. Cell-based screening identifies paroxetine as an inhibitor of diabetic endothelial dysfunction

27. Chapter 7: Pharmacogenomics

28. Citalopram Reduces Aggregation of ATXN3 in a YAC Transgenic Mouse Model of Machado-Joseph Disease

29. Clinical Trials and Therapeutic Rationale for Drug Repurposing in Schizophrenia

30. Clomipramine kills Trypanosoma brucei by apoptosis

31. Combating Multidrug-Resistant Pathogens with Host-Directed Nonantibiotic Therapeutics

32. Complex-disease networks of trait-associated single-nucleotide polymorphisms (SNPs) unveiled by information theory

33. Connecting genetics and gene expression data for target prioritisation and drug repositioning

34. Discovery of antiandrogen activity of nonsteroidal scaffolds of marketed drugs

35. Discovery of novel polyamine analogs with anti-protozoal activity by computer guided drug repositioning

36. DiseaseConnect: a comprehensive web server for mechanism-based disease-disease connections

37. Dopamine antagonists for treatment resistance in autism spectrum disorders: review and focus on BDNF stimulators loxapine and amitriptyline

38. Dopaminergic Regulation of Innate Immunity: a Review

39. Drug enrichment and discovery from schizophrenia genome-wide association results: an analysis and visualisation approach

40. Drug repositioning approaches for the discovery of new therapeutics for Alzheimer's disease

41. Drug repositioning for schizophrenia and depression/anxiety disorders: A machine learning approach leveraging expression data

42. Drug repurposing and emerging adjunctive treatments for schizophrenia

43. Drug repurposing for Leishmania. Molecular basis of the leishmanicidal activity of the antidepressant sertraline

44. Drug repurposing may generate novel approaches to treating depression

45. Drug Repurposing Screening Identifies Novel Compounds That Effectively Inhibit Toxoplasma gondii Growth

46. Drug Side Effect Profiles as Molecular Descriptors for Predictive Modeling of Target Bioactivity

47. Dual Targeting of the Autophagic Regulatory Circuitry in Gliomas with Repurposed Drugs Elicits Cell-Lethal Autophagy and Therapeutic Benefit

48. Effects of lorcaserin and buspirone, administered alone and as a mixture, on cocaine self-administration in male and female rhesus monkeys

49. Enhancing the Promise of Drug Repositioning through Genetics

50. Evaluation of Crimean-Congo hemorrhagic fever virus in vitro inhibition by chloroquine and chlorpromazine, two FDA approved molecules

51. Experimental confirmation of new drug-target interactions predicted by Drug Profile Matching

52. Expression of DRD2 Is Increased in Human Pancreatic Ductal Adenocarcinoma and Inhibitors Slow Tumor Growth in Mice

53. FDA-approved drugs selected using virtual screening bind specifically to G-quadruplex DNA

54. Filling the gap in CNS drug development: evaluation of the role of drug repurposing

55. Fluvoxamine, an anti-depressant, inhibits human glioblastoma invasion by disrupting actin polymerization

56. From Bench to Bedside: Attempt to Evaluate Repositioning of Drugs in the Treatment of Metastatic Small Cell Lung Cancer (SCLC

57. From the era of genome analysis to the era of genomic drug discovery: a pioneering example of rheumatoid arthritis

58. Future Directions of Genomics Research in Rheumatic Diseases

59. Gene expression-based chemical genomics identifies potential therapeutic drugs in hepatocellular carcinoma

60. Gene-set analysis based on the pharmacological profiles of drugs to identify repurposing opportunities in schizophrenia

61. Genetic and molecular aspects of hypertension

62. Genetics of rheumatoid arthritis contributes to biology and drug discovery

63. Genome-wide association analyses for lung function and chronic obstructive pulmonary disease identify new loci and potential druggable targets

64. Genome-wide association studies of cancer: current insights and future perspectives

65. GWAS of Rheumatoid Arthritis and Drug Discovery

66. High-throughput screen of drug repurposing library identifies inhibitors of Sarcocystis neurona growth

67. Histamine H1-receptor antagonists against Leishmania (L.) infantum: an in vitro and in vivo evaluation using phosphatidylserine-liposomes

68. Human Pluripotent Stem Cell-derived Cortical Neurons for High Throughput Medication Screening in Autism: A Proof of Concept Study in SHANK3 Haploinsufficiency Syndrome

69. Identification of antipsychotic drug fluspirilene as a potential anti-glioma stem cell drug

70. Identification of Chemical Inhibitors of beta-Catenin-Driven Liver Tumorigenesis in Zebrafish

71. Identification of novel therapeutics for complex diseases from genome-wide association data

72. Identification of ST3AGL4, MFHAS1, CSNK2A2 and CD226 as loci associated with systemic lupus erythematosus (SLE) and evaluation of SLE genetics in drug repositioning

73. Identification of thioridazine, an antipsychotic drug, as an antiglioblastoma and anticancer stem cell agent using public gene expression data

74. In silico drug screening by using genome-wide association study data repurposed dabrafenib, an anti-melanoma drug, for Parkinson's disease

75. In Silico Receptorome Screening of Antipsychotic Drugs

76. In silico repurposing of antipsychotic drugs for Alzheimer's disease

77. Insights into the Modulation of Dopamine Transporter Function by Amphetamine, Orphenadrine, and Cocaine Binding

78. Integrating systems biology sources illuminates drug action

79. Interactions of Selective Serotonin Reuptake Inhibitors with beta-Amyloid

80. Ketamine for treatment-resistant unipolar depression: current evidence

81. Ketamine: repurposing and redefining a multifaceted drug

82. Ketanserin, an antidepressant, exerts its antileishmanial action via inhibition of 3-hydroxy-3-methylglutaryl coenzyme A reductase (HMGR) enzyme of Leishmania donovani

83. Learning Opportunities for Drug Repositioning via GWAS and PheWAS Findings

84. Liraglutide attenuates the depressive- and anxiety-like behaviour in the corticosterone induced depression model via improving hippocampal neural plasticity

85. Low Dose Loxapine: Neuromotor Side Effects and Tolerability in Autism Spectrum Disorders

86. Loxapine add-on for adolescents and adults with autism spectrum disorders and irritability

87. Medication discovery for addiction: translating the dopamine D3 receptor hypothesis

88. Medications for alcohol use disorders: An overview

89. Meta-analysis of human gene expression in response to Mycobacterium tuberculosis infection reveals potential therapeutic targets

90. Mining mouse behavior for patterns predicting psychiatric drug classification

91. Molecular investigations of protriptyline as a multi-target directed ligand in Alzheimer's disease

92. Molecular mechanisms underlying variations in lung function: a systems genetics analysis

93. Mood, stress and longevity: convergence on ANK3

94. Mucuna pruriens (L.) DC chemo sensitize human breast cancer cells via downregulation of prolactin-mediated JAK2/STAT5A signaling

95. Multiple Sclerosis-Secondary Progressive Multi-Arm Randomisation Trial (MS-SMART): a multiarm phase IIb randomised, double-blind, placebo-controlled clinical trial comparing the efficacy of three neuroprotective drugs in secondary progressive multiple sclerosis

96. Network-based drug repositioning: A novel strategy for discovering potential antidepressants and their mode of action

97. Neuroleptic drugs in the treatment of tuberculosis: Minimal inhibitory concentrations of different phenothiazines against Mycobacterium tuberculosis

98. Neuron-specific regulation of class I PI3K catalytic subunits and their dysfunction in brain disorders

99. New Antimicrobial Approaches: Reuse of Old Drugs

100. New developments in the management of neurogenic orthostatic hypotension

101. New drug candidates for depression - a nationwide population-based study

102. New HSP27 inhibitors efficiently suppress drug resistance development in cancer cells

103. New indications for existing drugs; repurposing in psychiatry and addiction medicine

104. New pathogenic insights into rheumatoid arthritis

105. New Role for FDA-Approved Drugs in Combating Antibiotic-Resistant Bacteria

106. New use of an old drug: inhibition of breast cancer stem cells by benztropine mesylate

107. Novel putative drugs and key initiating genes for neurodegenerative disease determined using network-based genetic integrative analysis

108. Novel therapeutics for coronary artery disease from genome-wide association study data

109. Olanzapine, an Atypical Antipsychotic, Inhibits Survivin Expression and Sensitizes Cancer Cells to Chemotherapeutic Agents

110. Paroxetine-mediated GRK2 inhibition reverses cardiac dysfunction and remodeling after myocardial infarction

111. Pharmacological exploitation of the phenothiazine antipsychotics to develop novel antitumor agents-A drug repurposing strategy

112. Pharmacological targeting of dopamine D3 receptors: Possible clinical applications of selective drugs

113. Pharmacological targeting of GSK-3 and NRF2 provides neuroprotection in a preclinical model of tauopathy

114. PhenoPredict: A disease phenome-wide drug repositioning approach towards schizophrenia drug discovery

115. Potential repurposing of known drugs as potent bacterial beta-glucuronidase inhibitors

116. Preclinical Evidence Supporting Early Initiation of Citalopram Treatment in Machado-Joseph Disease

117. Prediction of polypharmacological profiles of drugs by the integration of chemical, side effect, and therapeutic space

118. Promoting oligodendroglial-oriented differentiation of glioma stem cell: a repurposing of quetiapine for the treatment of malignant glioma

119. Reduced emergence of isoniazid resistance with concurrent use of thioridazine against acute murine tuberculosis

120. Repositioning antipsychotic chlorpromazine for treating colorectal cancer by inhibiting sirtuin 1

121. Repositioning chlorpromazine for treating chemoresistant glioma through the inhibition of cytochrome c oxidase bearing the COX4-1 regulatory subunit

122. Repositioning drugs by targeting network modules: a Parkinson's disease case study

123. Repositioning Microtubule Stabilizing Drugs for Brain Disorders

124. Repositioning of the antipsychotic trifluoperazine: Synthesis, biological evaluation and in silico study of trifluoperazine analogs as anti-glioblastoma agents

125. Repurposed drugs for the treatment of schizophrenia and bipolar disorders

126. Repurposing Drugs for Cognition in Schizophrenia

127. Repurposing of clinically developed drugs for treatment of Middle East respiratory syndrome coronavirus infection

128. Repurposing of prochlorperazine for use against dengue virus infection

129. Repurposing psychiatric drugs as anti-cancer agents

130. Repurposing Thioridazine (TDZ) as an anti-inflammatory agent

131. Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia

132. Schizophrenia interactome with 504 novel protein-protein interactions

133. Sequence Analysis of Drug Target Genes with Suicidal Behavior in Bipolar Disorder Patients

134. Sertraline, Paroxetine, and Chlorpromazine Are Rapidly Acting Anthelmintic Drugs Capable of Clinical Repurposing

135. Shared genetic origin of asthma, hay fever and eczema elucidates allergic disease biology

136. Sphingolipids as targets for inhalation treatment of cystic fibrosis

137. Spironolactone is an antagonist of NRG1-ERBB4 signaling and schizophrenia-relevant endophenotypes in mice

138. Sulforaphane Prevents Neuronal Apoptosis and Memory Impairment in Diabetic Rats

139. Sympathoadrenergic modulation of hematopoiesis: a review of available evidence and of therapeutic perspectives

140. Symposium 2-1The autoimmunome: Similarities and differences among genetic susceptibility to common immune-related diseases

141. Symptomatic thinking: the current state of Phase III and IV clinical trials for cognition in schizophrenia

142. Synergy testing of FDA-approved drugs identifies potent drug combinations against Trypanosoma cruzi

143. Targeting the schizophrenia genome: a fast track strategy from GWAS to clinic

144. Teaching an old dog new tricks: drug repositioning in small cell lung cancer

145. Tegaserod mimics the neurostimulatory glycan polysialic acid and promotes nervous system repair

146. The ABC7 regimen: a new approach to metastatic breast cancer using seven common drugs to inhibit epithelial-to-mesenchymal transition and augment capecitabine efficacy

147. The antidepressant 5-HT2A receptor antagonists pizotifen and cyproheptadine inhibit serotonin-enhanced platelet function

148. The druggable genome and support for target identification and validation in drug development

149. The effects of buspirone on occupancy of dopamine receptors and the rat gambling task

150. Therapeutic Advances and Future Prospects in Progressive Forms of Multiple Sclerosis

151. Thioridazine inhibits autophagy and sensitizes glioblastoma cells to temozolomide

152. Topical phenytoin for the treatment of neuropathic pain

153. Transcriptomic profiling of human hippocampal progenitor cells treated with antidepressants and its application in drug repositioning

154. Translating Mendelian and complex inheritance of Alzheimer's disease genes for predicting unique personal genome variants

155. Tricyclic antidepressants inhibit Candida albicans growth and biofilm formation

156. Trifluoperazine, an antipsychotic agent, inhibits cancer stem cell growth and overcomes drug resistance of lung cancer

157. Use of genome-wide association studies for cancer research and drug repositioning

158. Valproic acid mediates miR-124 to down-regulate a novel protein target, GNAI1

159. What do the genetic association data say about the high risk of suicide in people with depression? A novel network-based approach to find common molecular basis for depression and suicidal behavior and related therapeutic targets

FACTOR 34. Multiple Ligand Simultaneous Docking and Drug Repositioning for Cancer Therapy

1. 2-acylamino-5-nitro-1,3-thiazoles: preparation and in vitro bioevaluation against four neglected protozoan parasites

2. 3, 5, 3'-Triiodothyroacetic acid (TRIAC) is an anti-inflammatory drug that targets toll-like receptor 2

3. 4-Acetoxyphenol Prevents RPE Oxidative Stress-Induced Necrosis by Functioning as an NRF2 Stabilizer

4. A Blockade of IGF Signaling Sensitizes Human Ovarian Cancer Cells to the Anthelmintic Niclosamide-Induced Anti-Proliferative and Anticancer Activities

5. A cellular genetics approach identifies gene-drug interactions and pinpoints drug toxicity pathway nodes

6. A Combination of Three Repurposed Drugs Administered at Reperfusion as a Promising Therapy for Postischemic Brain Injury

7. A current perspective on the oncopreventive and oncolytic properties of selective serotonin reuptake inhibitors

8. A drug repositioning approach identifies tricyclic antidepressants as inhibitors of small cell lung cancer and other neuroendocrine tumors

9. A High-Content Screening of Anticancer Compounds Suggests the Multiple Tyrosine Kinase Inhibitor Ponatinib for Repurposing in Neuroblastoma Therapy

10. A machine learning-based method to improve docking scoring functions and its application to drug repurposing

11. A new niclosamide derivatives-B17 can inhibit urological cancers growth through apoptosis-related pathway

12. A novel anti-cancer role of beta-apopicropodophyllin against non-small cell lung cancer cells

13. A novel application of furazolidone: anti-leukemic activity in acute myeloid leukemia

14. A screening cascade to identify ERbeta ligands

15. A statin-regulated microRNA represses human c-Myc expression and function

16. A systems pharmacology-oriented discovery of a new therapeutic use of the TCM formula Liuweiwuling for liver failure

17. A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case

18. Accidental interaction between PDZ domains and diclofenac revealed by NMR-assisted virtual screening

19. Acute oxidant damage promoted on cancer cells by amitriptyline in comparison with some common chemotherapeutic drugs

20. Adaptive mitochondrial reprogramming and resistance to PI3K therapy

21. Adjuvant potential of selegiline in attenuating organ dysfunction in septic rats with peritonitis

22. Advances in Developing Therapies to Combat Zika Virus: Current Knowledge and Future Perspectives

23. Aging-related Repositioned Drugs, Donepezil and Sildenafil Citrate, Increase Apoptosis of Anti-mitotic Drug-resistant KBV20C Cells Through Different Molecular Mechanisms

24. Albendazole as a promising molecule for tumor control

25. Albumin nanoparticles increase the anticancer efficacy of albendazole in ovarian cancer xenograft model

26. Alendronate inhalation ameliorates elastase-induced pulmonary emphysema in mice by induction of apoptosis of alveolar macrophages

27. An in vitro test system for compounds that modulate human inflammatory macrophage polarization

28. Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens

29. Angiotensin II type 1 receptor blocker telmisartan induces apoptosis and autophagy in adult T-cell leukemia cells

30. Angiotensin II type 1 receptor blockers increase tolerance of cells to copper and cisplatin

31. Anthelminthic drug niclosamide sensitizes the responsiveness of cervical cancer cells to paclitaxel via oxidative stress-mediated mTOR inhibition

32. Anthelmintic mebendazole enhances cisplatin's effect on suppressing cell proliferation and promotes differentiation of head and neck squamous cell carcinoma (HNSCC

33. Anti-infectious drug repurposing using an integrated chemical genomics and structural systems biology approach

34. Antibiotic drug levofloxacin inhibits proliferation and induces apoptosis of lung cancer cells through inducing mitochondrial dysfunction and oxidative damage

35. Antibiotic drug rifabutin is effective against lung cancer cells by targeting the eIF4E-beta-catenin axis

36. Anticancer Properties of Fenofibrate: A Repurposing Use

37. Antifibrotic effect of pirfenidone in a mouse model of human nonalcoholic steatohepatitis

38. Antihelminthic drug niclosamide inhibits CIP2A and reactivates tumor suppressor protein phosphatase 2A in non-small cell lung cancer cells

39. Antimalarial drug mefloquine inhibits nuclear factor kappa B signaling and induces apoptosis in colorectal cancer cells

40. Antiviral Drug Ribavirin Targets Thyroid Cancer Cells by Inhibiting the eIF4E-beta-Catenin Axis

41. Application of the 4D fingerprint method with a robust scoring function for scaffold-hopping and drug repurposing strategies

42. Appraisal of mechanisms of radioprotection and therapeutic approaches of radiation countermeasures

43. Artemisinin and Its Derivatives as a Repurposing Anticancer Agent: What Else Do We Need to Do

44. Assessing protein kinase target similarity: Comparing sequence, structure, and cheminformatics approaches

45. Assessment of the antitumor potential of Bithionol in vivo using a xenograft model of ovarian cancer

46. Auranofin induces apoptosis by ROS-mediated ER stress and mitochondrial dysfunction and displayed synergistic lethality with piperlongumine in gastric cancer

47. Auranofin induces lethal oxidative and endoplasmic reticulum stress and exerts potent preclinical activity against chronic lymphocytic leukemia

48. Auranofin-mediated inhibition of PI3K/AKT/mTOR axis and anticancer activity in non-small cell lung cancer cells

49. Auranofin: repurposing an old drug for a golden new age

50. Autophagy in HIV-induced T cell death

51. Autophagy Induced by Naftopidil Inhibits Apoptosis of Human Gastric Cancer Cells

52. Bazedoxifene as a Novel GP130 Inhibitor for Pancreatic Cancer Therapy

53. Benchmarking human protein complexes to investigate drug-related systems and evaluate predicted protein complexes

54. Benserazide, a dopadecarboxylase inhibitor, suppresses tumor growth by targeting hexokinase 2

55. beta3-Adrenoceptor agonists for overactive bladder syndrome: Role of translational pharmacology in a repositioning clinical drug development project

56. Beyond Channel Activity: Protein-Protein Interactions Involving Viroporins

57. BioGPS: The Music for the Chemo- and Bioinformatics Walzer

58. Bioinformatics and in vitro experimental analyses identify the selective therapeutic potential of interferon gamma and apigenin against cervical squamous cell carcinoma and adenocarcinoma

59. Bioinformatics-driven discovery of rational combination for overcoming EGFR-mutant lung cancer resistance to EGFR therapy

60. Bithionol inhibits ovarian cancer cell growth in vitro - studies on mechanism(s) of action

61. Blocking epithelial-to-mesenchymal transition in glioblastoma with a sextet of repurposed drugs: the EIS regimen

62. Blocking IL-6/GP130 signaling inhibits cell viability/proliferation, glycolysis, and colony forming activity in human pancreatic cancer cells

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Appendix 4: Markers from the AD Study

Four tables adapted from the AD study will be presented to show the breadth of markers included, and the directions in which they change in the presence of AD contributing factors (causes) or AD treatments.

Table A4-1 presents the impact of AD causes (contributing factors) identified in the AD study on the myriad markers identified in the study. Because these impact phrases are arranged by frequency of the AD marker, the list starts with the higher-level markers, and then proceeds to address the detailed biomarkers.

Table A4-1: IMPACTS OF AD CAUSES ON MARKERS

(arranged by # records; abbreviations as shown in software)

# RECORDS	AD CAUSES IMPACTS
80759	AD enhance
26726	ABETA incr
25423	DEMENTIA incr
24065	COGNITION degrad
12234	MEMORY degrad
7388	METABOLISM decr
6879	APOPTOSIS incr
6732	CHOLINERGIC decr
6307	BEHAVIOR degrad
5946	NEUROTOXICITY incr
5582	PLASTICITY reduc
5358	INFLAMM incr
5075	NFT incr
5011	ANTIBOD reduc
4418	OXIDATIVE STRESS incr
4403	DEPRESSION incr
3992	MMSE decr
3701	LEARNING reduc
3687	HYPERPHOSPHORYLATION incr
3652	NEURON degrad
2835	ASTROGLIOSIS incr
2669	MICROGLIAL ACTIV incr
2663	TAU PATHOLOGY incr
2610	MITOCHONDRIA degrad
2437	ANTIOXIDANT DEFENSE reduc
2328	ROS incr
2300	ALPHA-SECRETASE decr
1623	NEURODEGENERAT incr
1213	EXCITOTOXICITY incr glut
1194	NMDA enhanc
1132	NEUROGENESIS incr
1121	PHF enhanc

1081	MISFOLD incr
1062	ANXIETY incr
988	ESTROGEN reduc
979	CEREB BLOOD FLOW decr
971	CASPASE incr
856	SLEEP decr
820	NGF decr
809	AGITATION incr
770	SEROTONIN decr
761	DENDR SPINE degrad
736	BACE-1 incr
732	IL-1 incr
700	STRESS incr
683	GLUTATHIONE decr
667	TNF-alpha incr
666	AGGRESSION incr
652	COPPER incr
632	GSK-3 incr
615	NEUR NET degen
607	LTP decr
588	AGEs incr
567	APATHY incr
567	BRAIN ATROPHY incr
536	ATP decr
520	BDNF decr
497	HOMOCYSTEINE incr
487	IL-6 incr
433	PS1 incr
423	MAPK enhanc
388	NF-kappaB incr
360	Akt decr
358	Cdk5 enhanc
344	NONAMYLOIDOGENIC decr
333	ATAXIA incr
330	CALCIUM incr
327	ATTENTION decr
322	INSULIN SIGNAL reduc
317	CHOLESTEROL incr
316	MELATONIN decr
309	MAO enhanc
307	Bcl-2 decr
305	NEP decr
276	PHAGOCYTOSIS reduc
275	FOLATE degrad
273	cAMP decr
269	MULTIPLE PATHWAYS reduc
261	IDE decr
254	MOBILITY reduc

253	JNK incr
250	AXONAL DYSTROPHY incr
248	DHA decr
236	CORTISOL incr
231	NOREPINEPHRINE decr
223	iNOS incr
223	PGE2 incr
222	NAA decr
213	VIT B12 decr
211	GPX decr
204	Bax incr
196	HISTAMINE decr
194	TTR decr
185	IADL reduc
173	INSOMNIA incr
162	DOPAMINE decr
160	TESTOSTERONE decr
155	ADAM10 decr
137	PP2A decr
136	ENDOTHEL FUNCT decr
135	Hsp70 decr
134	HDAC incr
133	DNA METHYLAT decr
132	CREB decr
127	BRAIN ACTIVAT decr
122	CALCINEURIN incr
122	VEGF decr
118	ANDROGEN decr
117	BBB degrad
116	TYROSINE HYDROXYLASE decr
109	MDA incr
108	COX-1 stimulat
105	DHEA decr
104	Pgp decr
101	PROGESTERONE decr
100	HYPERLIPIDEMIA incr
96	HYPERGLYCEMIA incr
96	LRP1 decr
96	MoCA decr
96	MTOR incr
96	PGRN decr
95	IGF-1 decr
93	LEPTIN decr
93	NITROTYROSINE incr
92	CATHEPSIN-B enhanc
91	VIT B6 decr
90	LXR decr
85	ABCA1 decr

85	CMRglc decr
84	GLP-1 decr
83	Nrf2 decr
82	c-fos decr
81	LDL incr
81	SIRT1 decr
80	TrkB reduc
76	s100B incr
75	LH incr
71	CEREBROVASC DYSFUNCT incr
71	IL-4 decr
69	PPAR-gamma decr
67	MAC enhanc
63	METAL HOMEOSTAS decr
59	HMGCoAr decr
57	PICALM incr
56	O-GlcNAc decr
54	MUSCAR M1 decr
53	BrdU decr
50	QUALITY OF LIFE reduc
49	ADDL stimulat
49	AUTOPHAGY reduc
48	GELSOLIN decr
47	AMPK decr
44	SNAP-25 decr
41	HISTONE ACETYL decr
40	27-OHC incr
40	ECE decr
38	ALLOPREGNANOLONE decr
34	Beclin-1 incr
33	DCX degrad
33	Drp1 incr
32	25-OHD decr
32	PSD95 decr
31	EAAT2 decr
31	PGC-1alpha decr
31	Seladin-1 decr
30	IRS-1 incr
30	MYOINOSITOL incr
30	sAPP decr
29	PAI-1 enhanc
26	NFAT incr
26	PREGNENOLONE decr
25	ADIPONECTIN decr
25	MENOPAUSAL worsen
23	SLAI reduc
22	ABCA7 decr
22	LDH incr

20	p38MAPK incr
19	ADAM9 decr
19	LR11 decr
19	MAP1B decr
18	24-OHC incr
17	CD33 enhanc
17	GABA decr
17	HDL decr
17	Ngb decr
17	PCNA decr
17	UCH-L1 decr
16	ATF4 incr
16	HSF1 decr
16	PAK incr
15	GLUT4 decr
15	MEGALIN reduc
15	miRNA-146a incr
15	TLR-4 incr
14	CRP decr
14	Egr-1 decr
13	BH4 degrad
13	PLASMA VITAMIN E decr
12	ADMA incr
12	CLAUDIN-5 decr
12	CNPase decr
12	CX3CR1 incr
11	LYSOSOMAL ACIDIFICATION reduc
11	NAAG decr
10	CXCR2 incr
10	GSAP incr
10	Wnt3 decr
9	EphB2 decr
8	PI(4,5)P(2) decr
7	Ras ACTIVITY decr
7	SOCE incr
6	GEPHYRIN decr
6	TPI decr
5	EXCESSIVE NO incr
5	GCSF decr
5	GLYMPHATIC DRAINAGE reduc
5	iPLA2 decr
5	NEUROTROPHIN decr
5	p16 incr
5	TUBULIN reduc
4	BAG3 decr
4	C3 CONVERTASE incr
4	CXCL1 decr
4	IGFBP3 decr

4	RESOLVIN D1 decr
4	Synj1 incr
4	TERT reduc
3	B1R decr
3	CHROM MIS-SEGR incr
3	cyclinD1 decr
3	MAGNESIUM decr
3	mir-206 incr
3	Pr-SSG incr
3	SIR1 decr
3	TRPM2 incr
2	B2R decr
2	DYSPHAGIA incr
2	HSV REP prevent
2	HYPERVASCULARITY incr
2	PALMITOLEIC ACID incr
2	RLT decr
2	SREBP2 incr
2	T-MEHA decr
2	WT1 incr
1	BRN-4 decr
1	IL-12p40/p70 incr
1	METHIONONE decr
1	miR-30a-5p incr
1	miR-339-5p decr
1	S6K1 incr
1	TOMOSYN incr

Because of the chronology of conducting the AD study, identification of the AD markers and their directions of change was driven by the treatment identification process. The contributing factors identification process served to complete the identification of remaining biomarkers and their directions of change. Table A4-2 reflects the depth of the taxonomy and process used to identify the myriad AD existing markers changes resulting from the existing AD treatments identified.

Table A4-2: TAXONOMY OF BENEFITS FROM AD TREATMENT

AD TREATMENT BENEFITS
IMPROVE MAINLINE BIOMARKER DEFICITS
1. Neurotransmission modulation
1.1 Enhance cholinergic neurotransmission
1.15 Improve synapse plasticity
1.2 Antagonize NMDA receptors
1.3 GABAergic modulation
1.4 Serotonin receptor modulation
1.5 Histamine receptor modulation
1.6 Adenosine receptor modulation
1.7 Other neurotransmitter modulation
2. Tau modulation
2.1 Tau phosphorylation inhibition
2.2 Microtubule stabilization
2.3 Reducing Tau oligomerization/pathology
3. Abeta modulation
3.1 Reduce Abeta
3.2 Modulate amyloid transport
3.3 Prevent amyloid aggregation
3.4 Promote amyloid clearance
3.5 Amyloid based immunotherapy
3.6 Secretase enzymes modulation
3.7 Improve structural deficits
3.8 Other
IMPROVE METABOLISM BIOMARKERS
4. Insulin and energy metabolism
4.1 Insulin metabolism
4.2 Energy metabolism
5. Oxidative stress reduction
5.1 Augment endogenous defense
5.2 AGEs reduction
6. Mitochondrial function improvement
7. Modulation of cellular calcium homeostasis

8. Inflammation alleviation
9. Others
9.1 Hormone dyshomeostasis improvement
9.2 Lipid dyshomeostasis improvement
9.3 Growth factor restoration
9.4 Metal homeostasis improvement
9.5 Epigenetic modification
9.6 Caspase inhibition
9.7 Nitric oxide synthase modulation
9.8 Combinatorial improvements
IMPROVE PERFORMANCE DEFICITS
10. Cognition/Memory/Learning
10.1 Cognition
10.2 Memory
10.3 Learning
IMPROVE BEHAVIORAL DEFICITS
11. Behavioral problems
11.1 Behavior
11.2 Quality of Life
11.3 Agitation
11.4 Aggression
11.5 Anxiety
11.6 Depression
11.7 Attention
11.8 Apathy
11.9 Sleep
IMPROVE NEUROPATHOLOGY AND AD/DEMENTIA
12. Prevent and reverse neuropathology
12.1 ameliorate neurodegeneration
12.2 attenuate neurotoxicity
12.3 prevent apoptosis
12.4 protect neurons
12.5 promote neurogenesis
13. Prevent and reverse AD/dementia
13.1 prevent and reverse AD
13.2 prevent and reverse dementia

Table A4-3 provides the next level of detail in populating the previous taxonomy of Table A4-2.

Table A4-3: DETAILED TAXONOMY OF AD TREATMENT BENEFITS

BENEFITS FROM AD TREATMENT
IMPROVE MAINLINE BIOMARKER DEFICITS
1. Neurotransmission modulation
1.101 incr cholinergic
1.102 restor SLAI
1.15 Improve synapse plasticity
1.1501 improv PLASTICITY
1.1502 reduc SREBP2
1.1503 regen neural network
1.1504 incr PSD95
1.1505 incr Ras activity
1.1506 incr CMRglc
1.1507 incr MAP1B
1.1508 reduc TOMOSYN
1.1509 reduc myoinositol
1.151 reduc S6K1
1.1511 rescu PI(4,5)P(2)
1.1512 restor SNAP-25
1.1513 decr PAK
1.1514 amelior excessive NO
1.1515 incr magnesium
1.1516 incr EAAT2
1.1517 reduc glut excitotoxicity
1.1518 decr calcineurin
1.2 Antagonize NMDA receptors
1.201 antag NMDA
1.3 GABAergic modulation
1.301 incr GABA
1.302 restor gephyrin
1.4 Serotonin receptor modulation
1.401 incr SEROTONIN
1.402 inhibit MAO
1.5 Histamine receptor modulation
1.501 incr histamine
1.502 incr T-MEHA
1.6 Adenosine receptor modulation
1.601 incr ATP
1.7 Other neurotransmitter modulation
1.701 incr norepinephrine
1.702 activat M1
1.703 incr N-acetylaspartate
1.704 incr NAAG

1.705 incr brain activation
2. Tau modulation
2.1 Tau phosphorylation inhibition
2.101 reduc hyperphosphorylation
2.2 Microtubule stabilization
2.201 restor tubulin
2.202 decr NFT
2.203 incr glutathione
2.3 Reducing Tau oligomerization/pathology
2.301 reduc tau pathology
2.302 decr paired helical filament
2.303 inhibit Hsp90alpha
2.304 prevent hsv
2.305 incr anti-tau antibod
3. Abeta modulation
3.1 Reduce Abeta
3.101 reduc Abeta
3.102 reduc mTOR
3.103 incr AMPK
3.104 incr Brn-4
3.105 incr p75ECD
3.106 incr LR11
3.107 inhibit CatB
3.108 reduc PRAS40 phosphorylation
3.109 restor glymphatic drainage
3.2 Amyloid transport
3.201 restor BBB
3.202 incr Claudin-5
3.3 Preventing amyloid aggregation
3.302 incr iPLA2
3.303 inhibit ADDL
3.304 reduc C3 convertase
3.305 incr TTR
3.306 incr LRP1
3.307 incr NEP
3.308 incr ECE-2
3.309 incr tyrosine hydroxylase
3.4 Promoting amyloid clearance
3.401 enhanc phagocytosis
3.402 restor lysosomal acidification
3.403 incr ABCA1
3.404 incr ABCA7
3.405 inhibit CD33
3.406 incr LXR

3.407 enhanc megalin
3.408 incr gelsolin
3.409 restor Pgp
3.5 Amyloid based immunotherapy
3.501 enhanc antibod
3.6 Secretase enzymes modulation
3.601 incr alpha-secretase
3.602 incr sAPP
3.603 incr nonamyloidogenic
3.604 reduc GSAP
3.605 reduc PS1
3.606 incr ADAM10
3.607 incr ADAM9
3.608 reduc BACE1
3.609 incr SIRT1
3.61 decr PICALM
3.7 Improve structural deficits
3.701 decr brain atrophy
3.8 Other
3.801 decr homocysteine
3.802 incr methionone
IMPROVE METABOLISM BIOMARKERS
4. Insulin and Energy metabolism
4.1 Insulin metabolism
4.101 allev diabet
4.102 reduc IRS-1
4.103 improv hyperglycemia
4.104 incr IDE
4.105 incr GLP-1
4.106 incr Akt
4.107 incr BAG3
4.108 incr GLUT4
4.2 Neuronal metabolism
4.201 improv metabol
4.202 incr O-GlcNAc
5. Oxidative stress reduction
5.1 Augmenting endogenous defense
5.101 improv antioxidant defense
5.102 reduc oxidative stress
5.103 incr glutathione peroxidase
5.104 decr nitrotyrosine
5.105 incr plasma Vitamin E
5.106 reduc Pr-SSG
5.107 decr ROS

5.108 incr Nrf2
5.109 incr IGF-1
5.11 reduc ADMA
5.111 decr GSK-3
5.112 improv endotheli
5.113 restor BH4
5.114 incr cerebral blood flow
5.2 AGEs reduction
5.201 reduc AGEs
6. Mitochondrial function improvement
6.101 protect mitochondria
6.102 incr SIR1
6.103 incr PGC-1alpha
6.104 decr Drp1
7. Modulation of cellular calcium homeostasis
7.101 decr calcium
7.102 reduc SOCE
8. Inflammation alleviation
8.101 reduc inflamm
8.102 decr TNF-alpha
8.103 decr CRP
8.104 incr cAMP
8.105 decr IL-1
8.106 decr IL-6
8.107 incr IL-4
8.108 reduc NF-kappaB
8.109 decr p16
8.11 incr cyclinD1
8.111 incr PPAR-gamma
8.112 inhib cyclooxygenase-1
8.113 incr resolvin D1
8.114 reduc CXCR2
8.115 reduc TLR-4
8.116 reduc MKL1
8.117 reduc s100B
9. Others
9.1 Hormone dyshomeostasis
9.101 incr progesterone
9.102 incr testosterone
9.103 replace estrogen
9.104 incr androgen
9.105 reduc luteinizing hormone
9.106 incr DHEA
9.107 incr Allopregnanolone

9.108 incr pregnenolone
9.2 Lipid dyshomeostasis
9.201 reduc cholesterol level
9.202 decr 24-hydroxycholesterol
9.203 decr 27-hydroxycholesterol
9.204 incr HDL
9.205 decr LDL
9.206 incr HMGCoAr
9.207 reduc chromosome mis-segregation
9.208 ameliorat hyperlipidemia
9.209 incr leptin
9.3 Growth factor restoration
9.301 incr NGF
9.302 incr VEGF
9.4 Metal homeostasis improvement
9.401 restor metal homeostasis
9.402 decr copper
9.403 inhib MAPK
9.5 Epigenetic modification
9.501 incr DNA methylation
9.502 amelior B6
9.503 amelior B12
9.504 amelior folate
9.511 inhib HDAC
9.512 incr histone acetylation
9.513 incr histone H3K9
9.521 incr miR-339-5p
9.522 decr miR-30a-5p
9.523 decr mir-206
9.524 decr miRNA-146a
9.6 Caspase inhibition
9.601 reduc caspase
9.602 reduc JNK
9.603 restor IGFBP3
9.7 Nitric oxide synthase modulation
9.701 reduc iNOS
9.8 Combinatorial improvements
9.801 activat multiple pathways
IMPROVE PERFORMANCE DEFICITS
10. Cognition/Memory/Learning
10.1 Cognition
10.101 improv cogniti
10.102 amelior cerebrovascular dysfunction
10.103 revers hypervascularity

10.104 incr CXCL1
10.105 improv MoCA
10.106 improv MMSE
10.107 reduc palmitoleic acid
10.108 incr DHA
10.109 incr c-fos
10.11 incr Egr-1
10.111 incr adiponectin
10.112 incr TPI
10.2 Memory
10.201 improv memory
10.202 incr B2R
10.203 incr B1R
10.204 incr GCSF
10.205 incr LTP
10.206 incr RLT
10.207 inhib Cdk5
10.208 inhib MAC
10.209 restor TrkB
10.21 restor melatonin
10.211 reduc CX3CR1
10.212 decr ATF4
10.213 incr dopamine
10.214 incr EphB2
10.3 Learning
10.301 improv learning
10.302 decr RORgammat
IMPROVE BEHAVIORAL DEFICITS
11. Behavioral problems
11.1 Behavior
11.101 improv behavior
11.2 Quality of Life
11.201 prevent nutritional deficien
11.201 improv quality of life
11.201 improv quality-of-life
11.202 allev menopausal
11.203 amelior dysphagia
11.204 restor IADL
11.205 allev ataxia
11.206 improv mobility
11.207 incr 25-OHD
11.208 reduc reduce stress
11.3 Agitation
11.301 reduc agitat

11.302 decr cortisol
11.4 Aggression
11.401 decr aggressi
11.5 Anxiety
11.501 reduc anxiety
11.6 Depression
11.601 reduc depression
11.7 Attention
11.701 improv attention
11.8 Apathy
11.801 reduc apathy
11.9 Sleep
11.901 improv sleep
11.902 reduc insomnia
REVERSE NEUROPATHOLOGY AND AD/DEMENTIA
12. Prevent and reverse neuropathology
12.1 Ameliorate neurodegeneration
12.101 reduc neuro degenerat
12.102 reduc astrogli
12.103 suppress activation microgli
12.104 attenuat NFAT
12.105 incr CNPase
12.106 incr Bcl-2
12.107 decr Bax
12.108 decr MDA
12.109 incr BDNF
12.11 incr neurotrophin
12.111 incr UCH-L1
12.112 inhibit PAI-1
12.113 rescu TGF-beta1
12.114 decr axonal dystrophy
12.115 incr PP2A
12.116 reduc LDH
12.117 incr PGRN
12.2 Attenuate neurotoxicity
12.201 alleviat neurotoxic
12.202 incr Ngb
12.3 Prevent apoptosis
12.301 inhib apopto
12.302 rescu dendritic spine
12.303 reduc Ephexin5
12.304 incr seladin-1
12.305 incr Hsp70
12.306 reduc TRPM2

12.307 reduc WT1
12.308 restor TERT
12.309 reduc p38MAPK
12.4 Protect neurons
12.401 protect neuron
12.402 enhanc autophagy
12.403 decr Beclin-1
12.404 decr SQSTM1
12.405 reduc synj1
12.406 incr CREB
12.407 decr IL-12p40/p70
12.5 Promote neurogenesis
12.501 incr neurogenesis
12.502 restor DCX
12.503 incr PCNA
12.504 incr 5-bromo-2'-deoxyuridine
12.505 incr heat shock transcription factor
12.506 incr Wnt3
PREVENT AND REVERSE AD/DEMENTIA
13. AD and Dementia
13.1 AD/Dementia
13.101 prevent AD
13.102 reduc prostaglandin
13.103 prevent dementia

Table A4-4 offers a non-taxonomic view of markers and their directions of change resulting from AD treatments.

Table A4-4: AD TREATMENT BENEFITS

(ordered by # records; abbreviations as shown in software)

# RECORDS	AD TREATMENT BENEFIT
15766	AD prevent
8299	DEMENTIA prevent
8245	COGNITION improv
6592	ABETA reduc
3697	MEMORY improv
3557	CHOLINERGIC enhanc
2765	BEHAVIOR improv
2220	INFLAMM reduc
2053	NEURON protect
2048	NEUROTOXICITY allev
1644	METABOLISM improv
1612	APOPTOSIS inhibit
1467	OXIDATIVE STRESS reduc
1456	MMSE improv
1455	DEPRESSION reduc
1335	LEARNING improv
1331	PLASTICITY improv
1190	NEURODEGENERAT reduc
1152	ANTIBOD enhanc
924	HYPERPHOSPHORYLATION reduc
800	NFT decr
759	AGITATION reduc
752	ALPHA-SECRETASE incr
720	ROS decr
715	MICROGLIAL ACTIV suppress
648	INSULIN SIGNAL restor
562	MITOCHONDRIA protect
545	TAU PATHOLOGY reduc
532	NMDA antagon
526	ESTROGEN replac
480	ASTROGLIOSIS reduc
471	ANXIETY reduc
439	AGGRESSION decr
390	SLEEP improv
376	SEROTONIN incr
364	NEUROGENESIS incr
322	BACE-1 reduc
306	NGF incr
305	GLUTATHIONE incr
297	BDNF incr

256	CASPASE reduc
250	GSK-3 decr
239	TNF-alpha decr
237	MULTIPLE PATHWAYS activat
212	IL-1 decr
211	EXCITOTOXICITY reduc glut
207	APATHY improv
195	MELATONIN restor
190	LTP incr
190	MAO inhibit
185	CEREB BLOOD FLOW incr
185	DHA incr
163	FOLATE amelior
160	VIT B12 amelior
159	HOMOCYSTEINE decr
153	COPPER decr
152	MOBILITY improv
145	Akt incr
143	AGEs reduc
139	Bcl-2 incr
138	ATTENTION improv
134	DENDR SPINE rescu
134	NF-kappaB reduc
123	IL-6 decr
122	MDA decr
121	CHOLESTEROL lower
119	MAPK inhibit
117	INSOMNIA reduc
112	GPX incr
109	Bax decr
109	NONAMYLOIDOGENIC incr
107	NEUR NET regen
106	MISFOLD prevent
106	NEP incr
100	IADL restor
96	ATP incr
96	PHAGOCYTOSIS enhanc
93	IDE incr
93	iNOS reduc
91	QUALITY OF LIFE improv
85	TESTOSTERONE incr
80	ANTIOXIDANT DEFENSE improv
79	cAMP incr
76	CREB incr
74	JNK reduc
74	PHF inhibit
69	MUSCAR M1 activat
66	PGE2 reduc

65	VIT B6 amelior
64	HDAC inhibit
62	NOREPINEPHRINE incr
61	MTOR reduc
60	ANTI-TAU ANTIBOD incr
59	HISTAMINE incr
57	BRAIN ATROPHY reduc
56	Cdk5 inhibit
56	HMGCoAr incr
53	ADAM10 incr
51	CORTISOL decr
51	GLP-1 incr
51	sAPP incr
49	LEPTIN incr
47	COX-1 inhib
46	DHEA incr
46	PPAR-gamma incr
46	PROGESTERONE incr
42	SIRT1 incr
41	Nrf2 incr
40	IL-4 incr
39	ANDROGEN incr
39	VEGF incr
36	HYPERLIPIDEMIA ameliorat
35	Pgp restor
34	IGF-1 incr
34	NAA incr
34	TrkB restor
33	MoCA improv
31	NITROTYROSINE decr
31	PP2A incr
30	BRAIN ACTIVAT incr
29	ATAXIA allev
28	CALCIUM decr
28	TTR incr
27	DNA METHYLAT incr
27	DOPAMINE incr
27	LRP1 incr
26	AMPK incr
26	BrdU incr
25	LXR incr
23	LDL decr
22	HISTONE ACETYL incr
21	CALCINEURIN decr
21	Hsp70 incr
21	HYPERGLYCEMIA improv
21	STRESS reduc
20	ABCA1 incr

20	ENDOTHEL FUNCT improv
19	ADDL inhibit
19	CATHEPSIN-B inhibit
19	MAC inhibit
19	PS1 reduc
18	ALLOPREGNANOLONE incr
18	AUTOPHAGY enhanc
18	DCX restor
18	METAL HOMEOSTAS restore
18	PSD95 incr
17	Seladin-1 incr
17	SLAI restor
16	25-OHD incr
16	GELSOLIN incr
16	LH reduc
15	c-fos incr
15	LDH reduc
15	PGRN incr
14	IRS-1 reduc
14	PGC-1alpha incr
14	s100B reduc
13	CMRglc incr
12	AXONAL DYSTROPHY decr
12	Beclin-1 decr
11	ADIPONECTIN incr
11	PAI-1 inhibit
11	SNAP-25 restor
10	GABA incr
10	p38MAPK reduc
10	PREGNENOLONE incr
10	TYROSINE HYDROXYLASE incr
9	ADAM9 incr
9	Drp1 decr
8	HDL incr
7	BBB restor
7	ECE incr
7	Egr-1 incr
7	NFAT attenuat
7	PICALM decr
7	TLR-4 reduc
6	NEUROTROPHIN incr
6	Ngb incr
6	PLASMA VITAMIN E incr
5	27-OHC decr
5	GCSF incr
5	HSF1 incr
5	MENOPAUSAL allev
5	O-GlcNAc incr

5	PCNA incr
5	Ras ACTIVITY incr
5	RESOLVIN D1 incr
4	ATF4 decr
4	CD33 inhibit
4	EAAT2 incr
4	GSAP reduc
4	iPLA2 incr
4	LR11 incr
4	MEGALIN enhanc
4	PAK decr
3	24-OHC decr
3	ABCA7 incr
3	ADMA reduc
3	CNPase incr
3	HSV REP prevent
3	IGFBP3 restor
3	LYSOSOMAL ACIDIFICATION restor
3	miR-339-5p incr
3	miRNA-146a decr
3	MYOINOSITOL reduc
3	SIR1 incr
3	Synj1 decr
3	TERT restor
3	TUBULIN restor
3	Wnt3 incr
2	BH4 restor
2	CHROM MIS-SEGR reduc
2	CLAUDIN-5 incr
2	CRP decr
2	CXCR2 reduc
2	cyclinD1 incr
2	DYSPHAGIA amelior
2	EphB2 incr
2	GLYMPHATIC DRAINAGE restor
2	MAGNESIUM incr
2	mir-206 decr
2	NAAG incr
2	p75ECD incr
2	PI(4,5)P(2) rescu
2	PRAS40 reduc
2	S6K1 reduc
2	SOCE reduc
2	TGF-beta1 rescu
2	UCH-L1 incr
1	B1R incr
1	B2R incr
1	BAG3 incr

1	BRN-4 incr
1	C3 CONVERTASE reduc
1	CEREBROVASC DYSFUNCT amelior
1	CX3CR1 reduc
1	CXCL1 incr
1	Ephexin5 reduc
1	EXCESSIVE NO amelior
1	GEPHYRIN restor
1	GLUT4 incr
1	HISTONE H3K9 incr
1	HSP90ALPHA inhibit
1	HYPERVASCULARITY revers
1	IL-12p40/p70 decr
1	MAP1B incr
1	METHIONONE incr
1	miR-30a-5p decr
1	MKL1 reduc
1	p16 decr
1	PALMITOLEIC ACID reduc
1	Pr-SSG reduc
1	RLT incr
1	RORgammat decr
1	SQSTM1 decr
1	SREBP2 reduc
1	T-MEHA incr
1	TOMOSYN reduc
1	TPI incr
1	TRPM2 reduc
1	WT1 reduc

The present TR approach has the benefit that TR discovery can be generated from searching the e.g. Medline database alone. Any combination of the myriad classes of markers (illustrated above for AD) can be used for the query. However, the present TR approach is not restricted to stand-alone. It can be used as part of a hybrid approach that would impose additional conditions on TR candidates, perhaps requiring additional types of information from additional databases.

Chapter 4 - Treatment Repurposing Bibliography

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