GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. _____

Project No. G-33-669 (Q5356-0A0) ~~GTRC~~/GIT DATE 2/19/86

Project Director: R. A. Pierotti School/~~Lab~~ CHEM

Sponsor: DHHS/PHS/NIH/DRR

Type Agreement: Grant No. 1 S10 RR02846-01

Award Period: From 2/1/86 To 1/31/87 (Performance) 4/30/87 (Reports)

Sponsor Amount:	This Change	Total to Date
Estimated: $		$ 300,000
Funded: $		$ 300,000

Cost Sharing Amount: $ 50,000 Cost Sharing No: G-33-313

Title: Shared Mass Spectrometer System

ADMINISTRATIVE DATA

OCA Contact John B. Schonk X 4820

1) Sponsor Technical Contact:

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301/496-6743

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Defense Priority Rating: N/A Military Security Classification: N/A

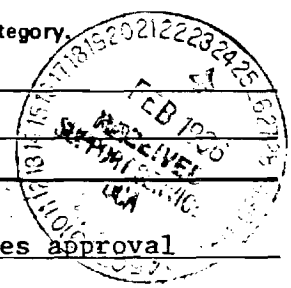
(or) Company/Industrial Proprietary: N/Z

RESTRICTIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with GIT



COMMENTS:

This grant is for instrumentation specified, any deviation requires approval from the Division of Research Resources.

COPIES TO:

SPONSOR'S I. D. NO. 02,010,136.86

Project Director	Procurement/EES Supply Services	GTRC
Research Administrative Network	Research Security Services	Library
Research Property Management	Reports Coordinator (OCA)	Project File
Accounting	Research Communications (2)	Other A. Jones; LEGAL

GEORGIA INSTITUTE OF TECHNOLOGY OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 3/2/87

Project No. G-33-669 School/~~Lab~~ Chem

Includes Subproject No.(s) N/A

Project Director(s) R. A. Pierotti ~~GTRC~~/ GIT

Sponsor DHHS/PHS/NIH/DRR

Title Shared Mass Spectrometer System

Effective Completion Date: 1/31/87 (Performance) 4/30/87 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [X] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [X] Final Report of Inventions - Patent Questionnaire to P.I.
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other _____

Continues Project No. _____ Continued by Project No. _____

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Project File
Other Ina Lashley
Angela Dubois
~~Russ Embry~~

FORM OCA 69.285

G-33-669

FINAL REPORT

SHARED MASS SPECTROMETER SYSTEM GRANT

AWARDED TO THE SCHOOL OF CHEMISTRY

GEORGIA INSTITUTE OF TECHNOLOGY

FROM

BIOMEDICAL RESEARCH SUPPORT PROGRAM

DIVISION OF RESEARCH RESOURCES

NATIONAL INSTITUTES OF HEALTH

Funds awarded to the School of Chemistry for a shared mass spectrometer system have been used to purchase a VG Analytical VG-7070SE complete mass spectrometer system. The specification of the system is given in Attachment A which is a copy of the bid specifications. The total cost of the system was $338,975.00. The Biomedical Research Support Program contributed $300,000.00 to the cost of the system and Georgia Institute of Technology contributed $38,975.00 to the cost of the mass spectrometer system.

During the time between placing the order for this instrument and its delivery, a laboratory to house this instrument in the School of Chemistry was completely renovated with funds from the Georgia Institute of Technology. This laboratory was renovated and equipped with additional power, additional air conditioning capacity, a new refrigeration system to supply recirculated chilled water for spectrometer diffusion pumps, new gas and water service, computer network lines, roughing pump exhaust lines, furniture, and compressed gas facilities. The newly renovated mass spectrometry laboratory includes a consultation office, a preparative lab with hood, the main instruments room, and a parts storage/repair room.

The VG-7070SE was delivered early fall and installation started shortly thereafter. During the installation period, Mr. Larry Abbey, of our mass spectrometry laboratory staff, has been continually involved in the installation and operation of the new mass spectrometer system. As each new subsystem and mass spectrometry technique was brought up to full specification, it was made available to NIH supported investigations in our Department. We are now able to obtain mass spectral analysis that were impossible for our investigators to obtain prior to delivery of this new mass spectrometer system.

APPENDIX A

Description of the mass spectrometer embodied in the bid accepted by VG Analytical is given below. The high resolution magnetic sector mass spectrometer system with extended mass range and mass spectrometer data system is described by the following specifications:

Direct inlet - heatable from 25-400°C temperature controlled manually, linear programmed and total ion current controlled; with temperature display and vacuum lock.

Heated batch inlet for reference compounds and volatile samples - heatable to 200°C, with temperature display and heater control.

Desorption chemical ionization probe - temperature controlled manually and by linear programming; with temperature or current display, and replaceable element.

Gas Chromatograph (HP5890A) arranged for capillary column operation, capillary split/splitless injection, capillary on-column injection, GC/MS interface including open split capillary column interface with solvent diverter, direct capillary column interface. The GC/MS interface shall be heated and include temperature display and heater control. The GC column oven temperature shall be controlled by a multiramp temperature programmer. A GC table shall be provided.

Moving Belt Liquid Chromatograph/Mass Spectrometer Interface - complete with moving belt chamber and drive mechanism, sample depositor for moving

belt FAB, sample nebulizer for EI/CI operation, all necessary desorption heaters, desolvation heaters, cleanup heaters, cleanup squeegee, heater controls and temperature display. Two rotary pumps for the interface, flanges for mounting, all necessary electronics for control and monitoring of heaters and belt speed, and a blank probe for sealing source vacuum when the belt is not in use shall be included. A complete ion source as required for use with moving belt system for EI/CI/DCI and FAB operation shall be provided.

Combined Electron Impact/Chemical Ionization Ion Source - In EI mode the electron beam shall be trap regulated with the electron energy continuously variable from 0-100 eV. Dual ion source controls for optimizing two settings, i.e. EI and CI, high resolution and low resolution, shall be provided. A triple gas inlet system for automatic EI/CI changeover and manual override, with metering values and pumpout shall be included. When using isobutane as a CI gas at normal operating pressure, the ratio $57^{+}/43^{+}$ shall be at least 2.

Alternating EI/CI (ACE) under data system control. Changeover in < 1 sec.

Fast Atom Bombardment Source - including fast atom gun and power supply, mounting flange and hardware, sample introduction probe, FAB ion source and associated electronics and controls.

Alternating FAB probe - for admission of FAB sample and reference compound for precise mass measurement. Alternately positioning dual sample stages on the center line of the ion source under peak matcher or data system

control, with associated electronics and control.

Field Desorption/Field Ionization/Electron Impact Ion Source - with associated electronics and high voltage power supply; with display for emitter temperature or current. Additional flange, vacumm lock and sample probe, if required.

The Analyzer shall consist of a magnetically scanned, double focused system.

- The mass range at rated accelerating voltage > 2100 daltons
- resolution (10% valley) > 70,000
- negative ion operation with +/- changeover and vice versa manually or under computer control. Changeover time at mass 500 < 400 ms.
- A collision cell shall be fitted in the frist field free region for collisional activation of the primary ion beam. A gas manifold for metering and removing the collision gas shall be included.
- A total ion current monitor and amplifier shall be included.
- Continuously variable, remotely controlled source and collector slit assemblies with rapid selection of two presettable widths.
- laminated magnet for high scan speed, fast reset, and high stability. Maximum scan speed = 0.1 s/mass decade; scan between 25-500 and reset in < 0.3 sec, magnet power supply to produce linear or exponential scans and field regulated or current regulated mode. Field control by means of Hall probe.
- linked scanning for daughter or precursor ions
- peak matching unit for accurate mass determination and instrument set-up

- oscilloscope display unit for display of peaks
- scan modes shall include:
    a) linear and exponential magnet scans in field or current mode
    b) linear voltage scan
    c) B/E linked scan
    d) B^2/E linked scan
    e) B/E 1-E (constant neutral loss) linked scan
- Detection system including off-axis discrete dynode electron multiplier with variable ±20 kV conversion dynode and all associated power supplies, preamplifier, amplifier, filter and controls for multiplier signal processing.
- necessary equipment shall be included for the connection of a Honeywell 1508C Visicorder oscillographic recorder for the recording of mass spectra. Provision shall be made for recording of signal and mass marker. The 1508C Visicorder will be supplied by the customer.
- Digital mass marker display.

Mass Spectrometer data system for the simultaneous acquisition, processing and output of data.

- The processor shall be a Digital Equipment Corp. Micro PDP-11/73 or equivalent with no less than 1 Mbyte of random access memory (16 Bit word) with multiuser, multitasking, real-time operating system.
- mass storage will be provided for a total capacity of not less than 100 Mbytes, including not less than 60 Mbytes on a disk drive of high access speed.
- The processor shall be arranged to provide ports for a total of not less than 5 terminals (at least 3 of these ports shall be serial ports).

- The serial ports shall be software configurable, RS232 ports.
- Two terminals shall be provided for mass spectrometer control and data system operation.
- A 150 line/minute printer/plotter (Printronix MVP-2 or equivalent) shall be provided.
- Mass spectrometer interface shall be provided with a signal digitization rate > 200 kHz. Microprocessor based mass spectrometer/data system interfacing equipment will provide data system control of all mass spectrometer scan functions including mass range, scan rate, linked scan functions, and multiple ion detection as well as control of the gas chromatograph including temperature programming.
- Complete software including programs for:
    - Full GC/MS acquisition of spectra
    - high resolution
    - elemental composition
    - library searching
    - GC control
    - linked scanning
    - multiple ion detection and quantitation
    - multichannel analyzer
    - printing and plotting
    - spectrum averaging
    - spectrum subtraction
    - automatic peak matching
    - calibration
    - instrument set-up
    - operating system and utilities

- system generation programs for system configuration
- diagnostics and test programs for all computer equipment
- library for use with searching routines
- programmer package including:
- sources for application software
- compilers for high level and intermediate level languages used in:
  - applications software
  - documentation of sources and compilers

- Appropriate acquisition microcodes shall be included to allow data acquisition under data system control of multiply charged ions which have undergone charge exchange reactions in the first field free region. In the case of doubly charged ions, it will be necessary to set the accelerating voltage to 1/2 normal while maintaining the electrostatic sector voltage at normal value.

Pumping System

- each high vacuum pump shall be backed up by a separate direct drive rotary pump
- a separate direct drive rotary pump shall be supplied for roughing
- all necessary pumps shall be provided for the moving belt LC/MS system
- an isolation valve shall be provided between the source housing and the analyzer; and, if required for rapid source changeover, a valve shall be provided between the source housing and the source pump.
- the ion source housing shall be differentially pumped with respect to the analyzer
- low and high vacuum monitoring equipment shall be provided
- Fail safe protection for the high vacuum pumps and electronics shall be

provided. Protection should include vacuum failure, power failure, and coolant failure.

- all equipment necessary for bake out of the instrument shall be provided including a bake out timer switch

Operating and service manuals should be provided for all equipment incuding mass spectrometer and associated attachments, gas chromatograph, data system, including full documentation of any special designed unit such as acquisition processor or mass spectrometer interface; manuals shall also be included for the computer operating system and utilities. The format for all microporcessor microcodes shall be documented for use in diagnostics and troubleshooting.

Vibration mounts shall be provided.

Extender boards or cables shall be provided wherever necessary to allow full maintenance of the complete system to the component level.