

PROJECT ADMINISTRATION DATA SHEET

ORIGINAL REVISION NO. _____

Project No. C-33-614 GTRC/~~GRX~~ DATE 9 / 13 / 85

Project Director: F. L. Suddath School/~~GRX~~ Chemistry

Sponsor: DHHS/PHS/NIH/NIGMS

Type Agreement: Grant No. 7 R01 GM36610-01

Award Period: From 8/1/85 To 4/30/86 (Performance) 7/30/86 (Reports)

Sponsor Amount: This Change Total to Date

Estimated: \$ _____ \$ 96,056

Funded: \$ _____ \$ 96,056

Cost Sharing Amount: \$ 5,058 Cost Sharing No: G-33-395

Title: High Resolution Structures of Pisum Sativum Lectin

ADMINISTRATIVE DATA

OCA Contact John B. Schonk X4820

1) Sponsor Technical Contact: John Norvell 2) Sponsor Admin/Contractual Matters: Diana O'Donovan

National Institute of Health National Institute of Health

NIGMS NIGMS

Program Administration Grants Management

Bethesda, MD 20205 Bethesda, MD 20205

301/496-7260 301/496-7746

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

(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

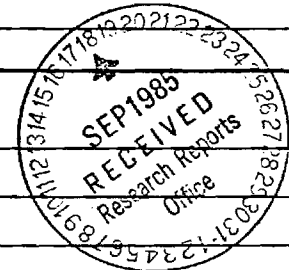
See Attached NIH Supplemental Information Sheet for Additional Requirements.

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:

No funds may be expended after 4/30/86.



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- GTRC
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- Project File
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SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date 5/15/86

Project No. G-33-614

School ~~XXX~~ Chem

Includes Subproject No.(s) N/A

Project Director(s) Fred Suddath GTRI/~~XXX~~

Sponsor DHHS/PHS/NIH/NIGMS

Title - High Resolution Structures of Pisum Sativum Lectin

Effective Completion Date: 4/30/86 (Performance) 7/30/86 (Reports)

Grant/Contract Closeout Actions Remaining:

Note: Annual report submitted as a part of renewal application for G33-684.

- None
- ~~Final Fiscal Report~~ Final Fiscal Report
- Closing Documents
- Final Report of Inventions
- Govt. Property Inventory & Related Certificate
- Classified Material Certificate
- Other _____

Continues Project No. _____

Continued by Project No. G-33-684

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- R. Embry

SECTION IV PROGRESS REPORT SUMMARY		GRANT NUMBER R01 GM36610-02	
PRINCIPAL INVESTIGATOR OR PROGRAM DIRECTOR Suddath, Fred L		PERIOD COVERED BY THIS REPORT	
NAME OF ORGANIZATION Georgia Tech Research Corporation		FROM 08/01/85	THROUGH 04/30/86
TITLE (Repeat title shown in item 1 on first page) High-Resolution Structure of Pisum Sativum Lectin			

(SEE INSTRUCTIONS)

Publications

1. The Location of Manganese and Calcium Ion Cofactors in Pea Lectin Crystals by Use of Anomalous Dispersion and Tuneable Synchrotron X-Radiation. H. Einspahr, K. Suguna, F. L. Suddath, G. Ellis, J. R. Helliwell, and M. Z. Papiz. Acta Cryst. 91985) B41, 336-341.
2. The Crystal Structure of Pea Lectin at 3.0 Å Resolution. Howard Einspahr, Elizabeth H. Parks, Kaza Suguna, E. Subramanian, and F. L. Suddath. (Submitted to Journal of Biological Chemistry).

Progress Report

1. No change in scientific goals.
2. The model of pea lectin based on partial interpretation of a 3.0 Å electron density map was subjected to CORELS refinement with each amino acid residue taken as a rigid domain. After six cycles, the R value for the partial model was reduced from 0.54 to 0.37 (7.0-3.0 Å data). This was followed by two cycles of restrained least squares refined to improve the geometry of the model. Phases were calculated from the refinement model and were combined with MIR phases by use of Bricogne's modification of the Sim weighting scheme. The combined phases and observed structure factors were input to Wang's density-modification system of programs. All residues including side chains were fit to the map except residues 235-239 in one monomer due to absence of electron density in the region. This model was then subjected to restrained least squares refinement with an overall isotropic temperature factor. The R value was reduced from 0.40 to 0.27 in eight cycles (7.0-3.0 Å data with 3σ cutoff). An effort was made to calculate a map in which bias due to the model was eliminated or minimized in a local area by leaving a slab of density out of the map (slab set to zero). The modified asymmetric unit was backtransformed to obtain new calculated F 's and phases. Calculated and observed structure factor were scaled together. Calculated phases were combined with MIR phases as before. The coefficients $2F_{\text{comb}} F_{\text{obs}} - F_{\text{calc}}$ and the combined phases were used to calculate the map within the slab described above. This process was repeated with successive slabs until the entire asymmetric unit had been constructed. The model was adjusted to fit this new map and refined for 16 cycles to a R value of 0.24 (7.0-3.0 σ cutoff).

The model at 3.0 Å resolution was used to calculate phases at successively higher resolutions in 4 steps to 2.48 Å. Observed structure factors from film data were carefully added to the refinement data set. After numerous cycles the R value is 0.27 (5.0-2.48 Å 3σ cutoff). This model must now be reexamined vs the electron density map and solvent molecules added.

During the budget period we established a collaborative arrangement with Dr. Jeremy Carver of the University of Toronto. Dr. Carver and his colleagues have prepared crystals of pea lectin complexed with methyl 3,6-Di-O- (α -O-Manno-

pyranosyl)- α -D-Mannopyranoside. Data were collected at UAB from numerous crystals of the complex to 2.5 Å resolution. The structure has been solved by Carver and colleagues by molecular replacement methods.

Specific objectives of the coming year.

- (1) Complete the refinement at 2.48 Å resolution.
- (2) Extend the resolution to the limit of film data (1.83 Å)
- (3) Collect high resolution data at Daresbury to 1.2 Å
- (4) Assess the structure of pea lectin in terms of the structure of the carbohydrate complex determined by Carver et al.