

1976 - 1977
ANNUAL REPORT

RESOURCE-RELATED RESEARCH
COMPUTERS AND CHEMISTRY

Grant No. RR-00612

BIOTECHNOLOGY RESOURCES PROGRAM
OF THE
NATIONAL INSTITUTES OF HEALTH

February, 1977

COMPUTER SCIENCE DEPARTMENT
STANFORD UNIVERSITY

SECTION 1

DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE PUBLIC HEALTH SERVICE APPLICATION FOR CONTINUATION GRANT	REVIEW GROUP	TYPE	PROGRAM	GRANT NUMBER (insert on all pages)
	SSS	5	R24	RR-00612
	TOTAL PROJECT PERIOD			
	From: 5/1/74		Through: 4/30/77	
REQUESTED BUDGET PERIOD				
From: 8/1/76		Through: 4/30/77		

1. TITLE
Resource-Related Research Computers and Chemistry

2A. PRINCIPAL INVESTIGATOR OR PROGRAM DIRECTOR
(Name and Address, Street, City, State, Zip Code)
DJERASSI, CARL
STANFORD UNIVERSITY
DEPT. OF CHEMISTRY
STANFORD, CALIF. 94305

4. APPLICANT ORGANIZATION (Name and Address-Street, City, State, Zip Code)

STANFORD UNIVERSITY

2B. DEGREE
PH.D.

2C. SOCIAL SECURITY NO.

5. PHS ACCOUNT NUMBER
1941156365A1

2D. DEPARTMENT, SERVICE, LABORATORY OR EQUIPMENT
CHEMISTRY

6. TITLE AND ADDRESS OF OFFICIAL IN BUSINESS OFFICE OF APPLICANT ORGANIZATION

DEPUTY V. P. FOR BUSINESS & FINANCE
STANFORD UNIVERSITY
STANFORD, CALIF. 94305

2E. MAJOR SUBDIVISION
SCH. OF HUMANITIES AND SCIENCES

3. ORGANIZATIONAL COMPONENT TO RECEIVE CREDIT FOR INSTITUTIONAL GRANT PURPOSES
20 OTHER

7. RESEARCH INVOLVING HUMAN SUBJECTS (See Instructions)

No Yes APPROVED

Date

8. INVENTIONS (See Instructions)

No

Yes-not previously reported

Yes previously reported

9. PERFORMANCE SITE(S)

STANFORD UNIVERSITY
DEPARTMENT OF CHEMISTRY
COMPUTER SCIENCE DEPARTMENT
DEPARTMTNE OF GENETICS
STANFORD, CALIF. 94305

TELEPHONE INFORMATION

	Area code	Tele. No. & Ext.
11A. PRINCIPAL INVESTIGATOR OR PROGRAM DIRECTOR (Item 2a)	415	497-2783
11B. Name of business official (Item 6)	415	497-2251
11C. Name and title of administrative official (Item 15b)	415	497-2883

10. DIRECT COSTS REQUESTED FOR BUDGET PERIOD

\$129,931.00

12A. CONGRESSIONAL DISTRICT OF APPLICANT ORGANIZATION SHOWN IN ITEM 4

TWELFTH

D'Ann B. Downey,
Sponsored Projects Dir.

12B. COUNTY OF APPLICANT ORGANIZATION SHOWN IN ITEM 4

SANTA CLARA

13. DO NOT USE THIS SPACE

14. CERTIFICATION AND ACCEPTANCE. We, the undersigned, certify that the statements herein are true and complete to the best of our knowledge and accept, as to any grant awarded, the obligation to comply with Public Health Service terms and conditions in effect at the time of the award.

15. SIGNATURES

(Signatures required on original copy only. Use ink. "Per" signatures not acceptable.)

15A. PRINCIPAL INVESTIGATOR OR PROGRAM DIRECTOR

DATE

15B. OFFICIAL SIGNING FOR APPLICANT ORGANIZATION

DATE

SECTION II

SECTION II—BUDGET (USUALLY 12 MONTHS)

FROM
May, 1977

THROUGH
April, 1978

GRANT NUMBER
RR-00612

A. ITEMIZE DIRECT COSTS REQUESTED FOR NEXT BUDGET PERIOD

PERSONNEL		TIME OR EFFORT %/HRS (c)	SALARY REQUESTED (d)	FRINGE BENEFITS (See Instructions) (e)	TOTAL (f)
NAME (Last, First, Initial) (a)	TITLE OF POSITION (b)				
	PRINCIPAL INVESTIGATOR				
See Proposal for Continued Research 1977-80 Submitted May, 1976					
Subtotals			\$	\$	
(Indicate cost of each item listed below)					\$
TOTAL (Columns (d) and (e))					\$
CONSULTANT COSTS (See Instructions)					\$
EQUIPMENT					\$
SUPPLIES					\$
TRAVEL	DOMESTIC				\$
	FOREIGN				\$
PATIENT COSTS (See instructions)					\$
ALTERATIONS AND RENOVATIONS					\$
OTHER EXPENSES (Itemize)					\$
TOTAL DIRECT COST (Enter on Page 1, Item 10)					\$

INDIRECT COST (See Instructions)

% S&W*
% TDC*
*if this is a special rate (e.g. off-site), explain.

Date of DHEW Agreement:

() Not Requested
() Under negotiation with

SECTION II—BUDGET (Continued)

Grant Number

RR-00612

B. Supplemental information regarding ITEMS in the proposed budget for the next period which require explanation or justification. (See instructions)

See Proposal for Continued Research

1977-80

submitted May, 1976

SECTION III

SECTION III—FISCAL DATA FOR CURRENT BUDGET PERIOD (USUALLY 12 MONTHS)	FROM	THROUGH	GRANT NUMBER
	8/1/76	4/30/77	RR-00612

The following pertains to your CURRENT PHS budget. Do not include cost sharing funds. This information in conjunction with that provided on Page 2 will be used in determining the amount of support for the NEXT budget period.

A. BUDGET CATEGORIES		CURRENT BUDGET (As approved by awarding unit) (1)	ACTUAL EXPENDITURES THRU 1/31/77 (Insert Date) (2)	ESTIMATED ADDITIONAL EXPENDITURES AND OBLIGATIONS FOR REMAINDER OF CURRENT BUDGET PERIOD (3)	TOTAL ESTIMATED EXPENDITURES AND OBLIGATIONS (Col. 2 plus Col. 3) (4)	ESTIMATED UNOBLIGATED BALANCE (Subtract Col. 4 from Col. 1) (5)
Personnel (Salaries)		100,761	59,784	36,593	96,377	4,384
Fringe Benefits		18,943	11,144	6,953	18,097	846
Consultant Costs		-	-	-	-	-
Equipment		-	-	-	-	-
Supplies		-	50	10	60	(60)
TRAVEL	Domestic	1,400	1,509	1,741	3,250	(1,850)
	Foreign					
Patient Costs						
Alterations and Renovations						
*Other		8,827	7,355	4,585	11,940	(3,113)
Total Direct Costs		129,931	79,842	49,882	129,724	207
Indirect Costs (If included in award)						
TOTALS →		\$ 129,931	\$ 79,842	\$ 49,882	\$ 129,724	\$ 207

Use space below to:

- B. List all items of equipment purchased or expected to be purchased during this budget period which have a unit cost of \$1000 or more.
 C. Explain any significant balance or deficit shown in any category of Column 5.
 D. List all other research support for Principal Investigator by source, project title, and annual amount.

B. Equipment Purchased

Terminal Rental	3,587	3,957	1,800		
Telephone	2,100	2,340	1,080		
Publications and Technical services	2,900	984	1,600		
Postage	240	74	105	11,940	(3,113)

D. Research Support for Principal Investigator

NIH AM04257	Mass Spectrometry in Organic Biochemistry	\$ 67,700
NIH GM06840	Marine chemistry with special Emphasis on Steroids	101,490
NIH GM20276	Applications of Magnetic Circular Dichroism	40,834

SECTION IV

APPLICANT: REPEAT GRANT NUMBER SHOWN ON PAGE 1 →		GRANT NUMBER	
SECTION IV—SUMMARY PROGRESS REPORT		RR-00612	
PRINCIPAL INVESTIGATOR OR PROGRAM DIRECTOR (Last, First, Initial)		PERIOD COVERED BY THIS REPORT	
NAME OF ORGANIZATION		FROM	THROUGH
		8/1/76	4/30/77

TITLE (Repeat title shown in Item 1 on first page)

1. List publications: (a) published and not previously reported; (b) in press. Provide five reprints if not previously submitted.
2. List all additions and deletions in professional personnel and any changes in effort.
3. Progress Report. (See Instructions)

Progress Report Follows

program was tested to see if it could rediscover the rules of mass spectrometry for two classes of chemical compounds that were already well understood (amines and estrogenic steroids). Then it was applied to three classes of compounds whose behavior in a mass spectrometer was not as well known (mono-, di-, and tri-ketoandrostanes). The program produced three sets of rules that explained much of the significant data for these classes. The time for manual rule formation for these data was estimated to be several months.

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