DR. LEDERBERG

RESOURCE-RELATED RESEARCH
COMPUTERS AND CHEMISTRY
(RR-00612 RENEWAL APPLICATION)

Submitted to the

BIOTECHNOLOGY RESOURCES BRANCH

OF THE

NATIONAL INSTITUTES OF HEALTH

December, 1973

School of Medicine
Stanford University

SECTION I

Form Approved
Budget Bureau No. 68-R0249

DEPARTMENT OF
HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

GRANT APPLICATION

LEAVE BLANK		
TYPE	PROGRAM	NUMBER
REVIEW GROUP		FORMERLY
COUNCIL *(Month, Year)*		DATE RECEIVED

TO BE COMPLETED BY PRINCIPAL INVESTIGATOR *(Items 1 through 7 and 15A)*

1. TITLE OF PROPOSAL *(Do not exceed 53 typewriter spaces)*

Resource Related Research - Computers and Chemistry (RR-00612 renewal)

2. PRINCIPAL INVESTIGATOR

2A. NAME *(Last, First, Initial)*

Djerassi, Carl

2B. TITLE OF POSITION

Professor of Chemistry

2C. MAILING ADDRESS *(Street, City, State, Zip Code)*

Department of Chemistry
Stanford University
Stanford, California 94305

2D. DEGREE

Ph.D.

2E. SOCIAL SECURITY NO.

[redacted]

2F. TELEPHONE DATA — Area Code: 415 — TELEPHONE NUMBER AND EXTENSION: 321-2300, Ext. 2783

2G. DEPARTMENT, SERVICE, LABORATORY OR EQUIVALENT *(See Instructions)*

Department of Chemistry

2H. MAJOR SUBDIVISION *(See Instructions)*

School of Humanities and Sciences

3. DATES OF ENTIRE PROPOSED PROJECT PERIOD *(This application)*

FROM: 5/1/74 THROUGH: 4/31/79

4. TOTAL DIRECT COSTS REQUESTED FOR PERIOD IN ITEM 3

$1,350,795.00

5. DIRECT COSTS REQUESTED FOR FIRST 12-MONTH PERIOD

$276,197.00

6. PERFORMANCE SITE(S) *(See Instructions)*

Department of Genetics,
Department of Chemistry, and
Department of Computer Science
Stanford University

7. Research Involving Human Subjects *(See Instructions)*

A. ☐ NO B. ☒ YES Approved: _____ Date

C. ☒ YES — Pending Review

8. Inventions *(Renewal Applicants Only - See Instructions)*

A. ☒ NO B. ☐ YES — Not previously reported

C. ☐ YES — Previously reported

TO BE COMPLETED BY RESPONSIBLE ADMINISTRATIVE AUTHORITY *(Items 8 through 13 and 15B)*

9. APPLICANT ORGANIZATION(S) *(See Instructions)*

Stanford University
Stanford, California 94305
IRS No. 94-1156365
Congressional District No. 17

11. TYPE OF ORGANIZATION *(Check applicable item)*

☐ FEDERAL ☐ STATE ☐ LOCAL ☒ OTHER *(Specify)*

Private, non-profit University

12. NAME, TITLE, ADDRESS, AND TELEPHONE NUMBER OF OFFICIAL IN BUSINESS OFFICE WHO SHOULD ALSO BE NOTIFIED IF AN AWARD IS MADE

K. D. Creighton
Deputy Vice Pres. for Business & Finance
Stanford University
Stanford, California 94305

Telephone Number (415)321-2300,X2551

10. NAME, TITLE, AND TELEPHONE NUMBER OF OFFICIAL(S) SIGNING FOR APPLICANT ORGANIZATION(S)

c/o Sponsored Projects Office
Telephone Number (s) (415) 321-2300, X2883

13. IDENTIFY ORGANIZATIONAL COMPONENT TO RECEIVE CREDIT FOR INSTITUTIONAL GRANT PURPOSES *(See Instructions)*

20 School of Humanities and Sciences

14. ENTITY NUMBER (Formerly PHS Account Number)

458210

15. 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.

SIGNATURES (Signatures required on original copy only. *Use ink, "Per" signatures not acceptable)*	A. SIGNATURE OF PERSON NAMED IN ITEM 2A	DATE
	B. SIGNATURE(S) OF PERSON(S) NAMED IN ITEM 10	DATE

NIH 398 (FORMERLY PHS 398
Rev. 1/73

SECTION 1

DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

RESEARCH OBJECTIVES

LEAVE BLANK

PROJECT NUMBER

NAME AND ADDRESS OF APPLICANT ORGANIZATION

Stanford University
Stanford, California 94305

NAME, SOCIAL SECURITY NUMBER, OFFICIAL TITLE, AND DEPARTMENT OF ALL PROFESSIONAL PERSONNEL ENGAGED ON PROJECT. BEGINNING WITH PRINCIPAL INVESTIGATOR

Carl Djerassi [redacted] Professor of Chemistry, Department of Chemistry; Joshua Lederberg, [redacted] Professor of Genetics, Department of Genetics; Edward Feigenbaum [redacted] rofessor of Computer Science, Department of Computer Science; Bruce Buchanan, [redacted] Research Computer Scientist, Department of Computer Science; Alan Duffield, [redacted], Research Associate, Department of Genetics; Dennis Smith, [redacted], Research Associate, Department of Genetics; Natesa Sridharan, [redacted], Research Associate, Department of Computer Science; Harold Brown [redacted], Research Associate, Department of Computer Science; Geoff Dromey, SS# applied for-to be supplied at a later date, Department of Computer Science.

TITLE OF PROJECT

Resource-Related Research -- Computer and Chemistry

USE THIS SPACE TO ABSTRACT YOUR PROPOSED RESEARCH. OUTLINE OBJECTIVES AND METHODS. UNDERSCORE THE KEY WORDS (NOT TO EXCEED 10) IN YOUR ABSTRACT.

The objectives of this research program are the development of innovative computer and biochemical analysis techniques for application in medical research and closely related aspects of investigative patient care. We will apply the unique analytical capabilities of gas chromatography/mass spectrometry (GC/MS) with the assistance of data interpreting computer programs utilizing artificial intelligence techniques, to investigate the chemical constituents of human body fluids in a variety of clinical contexts. Specific subtasks of this program include; 1) the application of artificial intelligence (AI) techniques to programs capable of interpreting mass spectra from basic principles as well as extending mass spectral theory by analysis of solved spectrum-structure examples, 2) the extension of GC/MS data systems to provide stand-alone capabilities for collecting low and high resolution mass spectral and metastable ion data, 3) the application of GC/MS and AI techniques to analysis of biomolecular structure elucidation problems of a large number of collaborators, and 4) the extension of artificial intelligence techniques to an interactive system for computer assisted structure elucidation based on a variety of data.

LEAVE BLANK

SECTION II – PRIVILEGED COMMUNICATION

DETAILED BUDGET FOR FIRST 12-MONTH PERIOD

FROM 5/1/74 THROUGH 4/31/75

DESCRIPTION (Itemize)		TIME OR EFFORT %/HRS.	AMOUNT REQUESTED (Omit cents)		
PERSONNEL					
NAME	TITLE OF POSITION		SALARY	FRINGE BENEFITS	TOTAL
	PRINCIPAL INVESTIGATOR				
DETAILED SALARY DATA LISTED SEPARATELY ON ATTACHED SHEET					
			163,935	28,962	192,897
CONSULTANT COSTS					-0-
EQUIPMENT					
Equipment Purchase (First Year Items Only):					
DEC GT-40 Display Terminal					13,400
PDP 11/20 Upgrade					34,000
Equipment Maintenance:					
PDP-11 (DEC Contract)					4,200
MAT-711 (Parts, etc.)					6,500
SUPPLIES Electronics Supplies					4,400
GC Supplies (Columns, gases, etc.)					1,000
Liquid Nitrogen					1,000
Chemicals, glassware, stock, etc.					1,500
Data Recording Media					1,000
Minicomputer Supplies					700
TRAVEL DOMESTIC					1,200
TRAVEL FOREIGN					-0-
PATIENT COSTS (See instructions)					-0-
ALTERATIONS AND RENOVATIONS					-0-
OTHER EXPENSES (Itemize)					
Publications, telephone, office supplies, postage					4,000
Computer Terminal Lease (4)					5,400
Computer Usage - 370/158 (First Year Item Only)					5,000
TOTAL DIRECT COST (Enter on Page 1, Item 5) →					276,197

INDIRECT COST (See Instructions)

DATE OF DHEW AGREEMENT:

_____ % S&W*

47 % ~~TDC~~ NTDC - June 26, 1973

☐ WAIVED

☐ UNDER NEGOTIATION WITH: _____

*IF THIS IS A SPECIAL RATE (e.g. off-site), SO INDICATE.

DETAILED SALARY DATA
NIH GRANT #RR-00612
5/1/74-4/31/75

	% Effort	Salary	Fringe Benefits	Total
PRINCIPAL INVESTIGATORS:				
C. Djerassi	10	-0-	-0-	-0-
J. Lederberg	10	-0-	-0-	-0-
E. Feigenbaum	10	2,910	514	3,424
RESEARCH ASSOCIATES:				
B. Buchanan (1)	50	7,000	1,237	8,237
A. Duffield	25	6,195	1,094	7,289
D. Smith	100	16,200	2,862	19,062
N. Sridharan	100	16,050	2,835	18,885
H. Brown	100	16,200	2,862	19,062
G. Dromey	100	15,500	2,738	18,238
PROGRAMMERS:				
W. White	100	14,400	2,545	16,945
R. Tucker	100	14,100	2,491	16,591
SENIOR RESEARCH ASSISTANT:				
A. Wegmann	100	15,000	2,650	17,650
ELECTRONICS ENGINEER:				
N. Veizades	60	11,670	2,062	13,732
GLASS BLOWER/MACHINEST:				
E. Steed	25	4,410	779	5,189
RESEARCH ASSISTANTS:				
L. Masinter	100	5,070	895	5,965
M. Stefik	100	4,915	868	5,783
To Be Appointed	100	4,915	868	5,783
SECRETARIAL SUPPORT:				
K. Wharton	100	9,400	1,662	11,062
TOTAL:		$163,935	$28,962	$192,897

(1)Dr. Buchanan's salary charges do not begin until 9/1/74 at which time his NIH Research Career Development Award expires.

SECTION II – PRIVILEGED COMMUNICATION

BUDGET ESTIMATES FOR ALL YEARS OF SUPPORT REQUESTED FROM PUBLIC HEALTH SERVICE
DIRECT COSTS ONLY (Omit Cents)

DESCRIPTION		1ST PERIOD (SAME AS DETAILED B)	ADDITIONAL YEARS SUPPORT REQUESTED *(This application only)*					
			2ND YEAR	3RD YEAR	4TH YEAR	5TH YEAR	~~XXXXXX~~ TOTAL	7TH YEAR
PERSONNEL COSTS		192,897	210,611	225,129	240,630	257,383	1,126,650	
CONSULTANT COSTS *(Include fees, travel, etc.)*		-0-	-0-	-0-	-0-	-0-	-0-	
EQUIPMENT		58,100	11,770	12,947	14,241	15,665	112,723	
SUPPLIES		9,600	6,920	7,612	8,370	9,207	41,709	
TRAVEL	DOMESTIC	1,200	1,320	1,452	1,597	1,757	7,326	
	FOREIGN	-0-	-0-	-0-	-0-	-0-	-0-	
PATIENT COSTS		-0-	-0-	-0-	-0-	-0-	-0-	
ALTERATIONS AND RENOVATIONS		-0-	-0-	-0-	-0-	-0-	-0-	
OTHER EXPENSES		14,400	10,340	11,374	12,511	13,762	62,387	
TOTAL DIRECT COSTS		276,197	240,961	258,514	277,349	297,774	1,350,795	

TOTAL FOR ENTIRE PROPOSED PROJECT PERIOD *(Enter on Page 1, Item 4)* ⟶ $ 1,350,795

REMARKS: *Justify all costs for the first year for which the need may not be obvious. For future years, justify equipment costs, as well as any significant increases in any other category. If a recurring annual increase in personnel costs is requested, give percentage. (Use continuation page if needed.)*

See following pages for budget justification.

Budget Justification

The availability of existing equipment - including the mass spectrometer and SUMEX computer - avoids the need for requesting funds for major laboratory items and substantial computing costs. Thus, the major expense in the resulting budget is for personnel. We feel that the personnel listed here are necessary to carry out the research, as justified below. Recurring costs are about $227,000 per year. First year expenditures are higher to provide the instrumentation necessary for mass spectrometry service in the first year.

We are requesting funds for five years to coincide with the funding of the AIM-SUMEX resource, to which we hope to make significant constributions.

This budget overlaps slightly with the budget for the Genetics Research Center (J. Lederberg, Principal Investigator). Dr. Alan Duffield's 25% salary budgeted here is covered by the other budget (where 100% of his salary is budgeted). 10% of Ms. Annemarie Wegmann's salary is covered there (with 100% of her salary budgeted here). These are the only overlapping items. We have no official notification of Genetics Center funding; if the present proposal is successful, the Genetics Center budget will be adjusted accordingly.

In the five-year budget, salaries are increased by 6% per year and staff benefits are computed at 17% for the period 5/74-8/74, 18% for the period 9/74-8/75, and are increased 1% per year thereafter, based on current University projections. Other budget categories are increased by 10% per year to account for inflation.

Personnel:

BRUCE G. BUCHANAN
Dr. Bruce Buchanan holds an NIH Research Career Development Award to work on applications of artificial intelligence to health-related problems, including theory formation by computer. His work on those aspects of this grant is thus consistent with the Development Award. Half-time support is requested after the third year of the Development Award (starting September, 1974) to cover the contingency that the award will not be extended to the full five years. These funds will be returned if the Award is extended.

DENNIS H. SMITH
Dr. Dennis H. Smith has been a member of the DENDRAL project since July, 1971. He has been responsible for the MS and its computer support, and has been involved in the application of the AI programs to structural studies of biomedically important compounds, primarily steroids. These responsibilities will continue in the future, with particular emphasis on providing the mass spectrometer/AI program link to the user community and its mass spectrometry and general structure elucidation needs, and in providing the necessary chemical knowledge and input for development of the computer programs and user interfaces for the proposed computer assisted structure elucidation effort.

ALAN DUFFIELD
Dr. Alan Duffield is the senior scientist in charge of the mass spectrometry facilities of the GRC. Because of his expertise in the analysis of mass spectra from various fractions of human body fluids, he will provide the link between the structure elucidation techniques of this proposal and other scientists with similar problems. The GC/HRMS facilities are also expected to provide service to the Genetics Center for high resolution analysis of compounds isolated from body fluids.

NATESA SRIDHARAN
Dr. Sridharan will be responsible for developing interface routines that allow new researchers to make use of the structure elucidation programs. We expect these routines to accept information about a research problem, in semi-formal terms, and translate it into a format the program can use. They should be complete enough so that individual researchers do not need to know about the inner workings of the programs. In addition, he will continue to help Dr. Brown and Mr. Masinter with development of the cyclic generator program. (Within a few days of this writing, Dr. Sridharan has decided to take a leave of absence. During his absence we will recruit another Research Associate to perform his duties.)

HAROLD BROWN
Dr. Harold Brown's knowledge of graph theory and combinatorial mathematics is essential to the development of the cyclic structure generator. Many problems with development and implementation of this program have required sophisticated, new mathematical solutions worked out by Dr. Brown. For example, generating the dictionary of cyclic graphs and assembling substructures involve problems in graph theory that Dr. Brown is currently working on.

Dr. Brown has submitted a proposal to the NSF to cover his salary for this research. If that grant is awarded, funds requested here for his salary will not be needed.

P. GEOFF DROMEY
Dr. Geoff Dromey is a chemist with strong computer science interests who has been associated with the project since September, 1973. He has become familiar with many aspects of the DENDRAL performance programs and will be expected to help outside researchers use those programs. In addition, he will be developing new programs, such as the program for molecular ion determination from mass spectra.

WILLIAM C. WHITE
Mr. William White provides high-level programming support for the theory formation programs, including helping to devise new programs in response to new research problems as well as implementing them. He wrote almost all of the LISP code for the INTSUM program, for example, and is currently responsible for the RULEGEN program.

MS. ANNEMARIE WEGMANN
Ms. Annemarie Wegmann is the Senior Research Assistant in charge of the GC/HRMS system. She was formerly head of Hewlett-Packard's Palo Alto gas chromatography applications laboratory and has been responsible for the operation of the GC/MS system since the

delivery to our laboratory of the MAT-711 (November, 1971). Her technical ability is absolutely essential to the continued operation and development of the mass spectrometry facility.

INSTRUMENT SUPPORT PERSONNEL

Messers. Veizades and Steed will assist part time in maintaining the GC/MS system. Mr. Veizades is an Electronics Engineer who is responsible for the electronic and mechanical systems as well as providing the necessary voltage read-out and control development for the metastable analysis data system. Mr. Steed is a Research Engineer responsible for the system glasswork and vacuum system maintenance.

ROBERT TUCKER
Mr. Robert Tucker implements and maintains the computer programs for data acquisition and reduction of MS data. This includes translating existing PL/ACME into FORTRAN and PDP-11 assembly language. In addition, he will be responsible for improving these programs for repetitive HRMS scans, implementing the multiplet resolution algorithm and the software necessary for semi-automated collection of metastable ion data.

LARRY M. MASINTER
Mr. Larry Masinter, Research Assistant, will continue to work with Drs. Lederberg and Brown on the development of the cyclic structure generator. His LISP expertise has been an invaluable resource for every member of the research team.

MARK STEFIK
Mr. Mark Stefik, Research Assistant, combines two years of experience on the ACME/MS data acquisition system with a long-term commitment to computer science. He has developed interactive library search capabilities for the mass spectrometer and will continue to improve them. His knowledge of the data acquisition computer programs will be very valuable in assisting initial translation of those programs into FORTRAN (from PL/ACME code) for the extended PDP-11/20 system.

RESEARCH ASSISTANT - unnamed
We have interviewed two prospective Research Assistants, both of whom have broad chemical experience and strong computer science interests. We request funds to hire one of them to provide additional links between computer science techniques and structure elucidation problems.

SECRETARIAL SUPPORT
One full-time secretary is necessary for the secretarial support of this number of scientists. Ms. Kathleen Wharton is now with the Computer Science group.

EQUIPMENT PURCHASE:
As discussed in the text (Section III.A), in the first year we plan to augment our existing PDP-11/20 computer (4k memory) to allow its operation as a stand-alone data system. We plan to add 16k of memory ($3,000), a floating print arithmetic unit ($7,500), an industry compatible tape drive ($9,000), a disk drive (10,500), a low speed communications interface ($1,000), and a bootstrap

loader and clock ($1,200). These devices together with state sales tax total to $34,000. The prices quoted are representations of the most cost-effective suppliers of the respective devices we have been able to locate. We will continue to review the market before implementation to maximize technical and cost performance.

As stated above, we plan to provide interface programs to provide the communication link between the users and the programs. The universal language of molecular structure is diagrammatic representation of the structures, drawn usually in two dimensions (or as two-dimensional representations of three dimensional information). Therefore, we feel that a graphics terminal such as the DEC GT-40 is necessary for effective sharing of the programs among Stanford users. The GT-40 terminal is a good choice for performing this structural display task, for a number of reasons. Programs are available for input and output of structural information which can be modified to run on a GT-40 (e.g., we have just implemented on an experimental basis routines made available to us by R. Feldman, NIH); Sophisticated structural display programs have been written especially for a GT-40 which we would hope to point; and the AIM-SUMEX resource will specifically support one GT-40 for use by the SUMEX staff. This terminal will be physically located in the MS laboratory since all of the users will interact with that laboratory.

EQUIPMENT MAINTENANCE:
Maintenance is budgeted for the proposed stand-alone PDP-11/20 system under DEC contract based on current prices. Also included is a budget for maintenance of the MAT-711 system. This estimate is based on our experience with parts replacements to date. We will provide the necessary maintenance manpower (see personnel justification) because Varian cannot provide adequate service.

SUPPLIES:
Supplies are budgeted in various categories based on our operating experience to date. Electronics supplies include parts necessary for maintaining our electronics and test equipment ($1,000) as well as parts in the first year for the metastable ion data system ($3,200). These comprise several D/A and A/D converters for accelerating voltage, ESA voltage, and magnetic field control as well as parts to upgrade the Hall probe mass marker. GC supplies include carrier gases, columns, phases, syringes, septa, etc., for GC/MS operation. The liquid nitrogen is required for cold trap operation on the MAT-711. Chemicals, glassware, etc., include the various organic chemicals, glassware, apparatus, glass tubing, etc., needed to support the GC/MS laboratory operation. Data recording media include special uv sensitive recording paper for the MAT-711, paper for GC and instrumentation recorder, and calcomp paper and pens for ion currennt and spectrum plotting. Mini-computer supplies include paper, magnetic tape, ribbons, spare disk cartridges, etc., for data system operation.

TRAVEL:
The travel budget covers estimated needs (2 east coast and 2 west coast) trips for attending related professional meetings and interfacing potential program users nationally. Domestic travel is budgeted for two East Coast trips and two California trips per year among all personnel. No foreign travel is budgeted.

OTHER:

The "Other" budget includes operating telephone, office supplies, postage, reproduction, etc., support necessary for this project based on our previous experience. The "computer usage" allocation provides a continued limited usage of the 370/158 computer during the augmentation of the PDP-11/20 system. This cost does not appear in later years. Terminal rental covers four terminals to be distributed among the MS laboratory, the Computer Science Dept., and J. Lederberg's laboratory.

BIOGRAPHICAL SKETCHES

Principal Investigator: Carl Djerassi

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Carl DJERASSI	Professor of Chemistry	October 29, 1923
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
Vienna, Austria	U.S.A.	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Kenyon College	A.B. (summa cum laude)	1942	Chemistry, Biology
University of Wisconsin	Ph.D.	1945	Organic chemistry, Biochemistry (minor)

HONORS Hon. D.Sc., Natl. Univ. of Mexico (1953), Kenyon College (1958), Worcester Polytechnic Institute (1972); Hon. Prof., Fed. Univ. Rio de Janeiro (1969). Member U.S. National Academy of Sciences, American Academy of Arts and Sciences, foreign member, Royal Swedish Academy of Sciences, German Academy of Natural Scientists (Leopoldina), Brazilian Academy of Sciences, (cont. below)

MAJOR RESEARCH INTEREST Nat. prod. chemistry (steroids, alkaloids, terpenoids, antibiotics) and chem. applications of physical methods (mass spec., optical rotatory dispersion, circular dichroism).

ROLE IN PROPOSED PROJECT

Principal Investigator

RESEARCH SUPPORT *(See instructions)*

Grant	Title	Period	Current Year	Total Budgeted	% Time Effort
NIH AM 04257	Mass Spectrometry in Organic and Biochemistry	10/1/70 to 9/30/75	$52,306	$316,016	10%
NIH GM AM 06840-15	Marine Chemistry with special emphasis on steroids	1/1/73 to 12/31/77	$75,650	578,180	18%

NSF Pending Grant Application #P3P3689, Magnetic Circular Dichroism in Organic Molecules, in the amount of $27,640.

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

Academic Experience:
Professor of Chemistry, Stanford University, 1959-present.
Associate Professor (1952-1954) and Professor (1954-1959), Wayne State University.

Industrial Research Experience:
Ciba Pharmaceutical Co., Summit, N.J.: Research Chemist, 1942-1943 and 1945-1949.
Syntex Corporation: Associate Director of Chemical Research (Mexico City) 1949-1952, Research Vice President (Mexico City) 1957-1960; (Palo Alto, California) 1960-1968, President, Syntex Research 1968-~~present~~ 1972, Zoecon Corporation (Palo Alto), President, 1968-~~present~~ 1972.

Editorial Boards:
(Current) Journal of the American Chemical Society, Steroids, Tetrahedron, Organic Mass Spectrometry.

(continued on next page)

Honors (cont.)
Mexican Academy for Scientific Investigation. Hon. Fellow of Phi Lambda Upsilon. Amer. Academy of Pharmaceutical Sciences, British Chemical Society and Mexican Chemical Society, Phi Beta Kappa. Numerous hon. lectureships including 1964 Centenary Lecturer (The British Chemical Society) and 1969 Annual Chemistry Lecturer, Royal Swedish Academy of Engineering. American Chemical Society Award in Pure Chemistry (1958), Baekeland Medal (1959), Fritzsche Award (1960). Intra-Science Research Foundation Award (1969). Freedman Patent Award of American Institute of Chemists (1971). Foreign Member, Royal Swedish Academy of Sciences (1972). D.Sc. (hon.), Worcester Poiytechnic Institute (1972). Scheele-Lecturer, Pharmaceutical Society of Sweden (1972); American Chemical Society's Award for Creative Invention (1973), National Medal of Science (1973).

U. S. GOVERNMENT PRINTING OFFICE : 1971 O - 451-736

11

RESEARCH AND/OR PROFESSIONAL EXPERIENCE (cont.)

Miscellaneous:
Chairman of the AAAS Gordon Research Conferences on Steroids and Natural Products (1952-1954); Member of American Pugwash Committee (1968 to present); Chairman of Latin America Science Board of National Academy of Sciences (1966-1968); Chairman of National Academy's Board on Science and Technology for International Development.

PUBLICATIONS

Author or co-author of six books and approximately 800 publications dealing with natural products (notably steriods, terpenoids, alkaloids and antibiotics), medicinal chemistry (primarily antihistamines, oral contraceptives and anti-inflammatory agents) and applications of physical methods (mass spectrometry, optical rotatory dispersion, magnetic circular dichroism) to organic and biochemical problems.

NAME	TITLE	BIRTHDATE (Mo., Day, Yr.)
LEDERBERG, JOSHUA	Professor and Executive Head, Department of Genetics	5-23-25
PLACE OF BIRTH (City, State, Country)	**PRESENT NATIONALITY** (If non-U.S. citizen, indicate kind of visa and expiration date)	**SEX**
Montclair, New Jersey	U.S.A.	☒ Male ☐ Female

EDUCATION: (Begin with baccalaureate training and include postdoctoral)

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Columbia College, New York	B.A.	1944	
College of Physicians & Surgeons, Columbia University, New York (1944-46)			
Yale University	Ph.D.	1947	Microbiology

HONORS

1957 - National Academy of Sciences
1958 - Nobel Prize in Medicine

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Molecular Genetics; Artificial Intelligence	PRINCIPAL INVESTIGATOR

RESEARCH SUPPORT (See instructions)

SEE ATTACHMENTS:

RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

1961-	Stanford University Director, Kennedy Laboratories for Molecular Medicine
1959-	Professor, Genetics and Biology, and Executive Head, Department of Genetics, Stanford University
1957-1959	University of Wisconsin Chairman, Department of Medical Genetics
1957	Melbourne University, Australia Fullbright Visiting Professor of Bacteriology
1950	University of California, Berkeley Visiting Professor of Bacteriology
1947-1959	University of Wisconsin Professor of Genetics
1946-1947	Yale University. Research Fellow of the Jane Coffin Childs Fund for Medical Research
1945-1946	Columbia University. Research Assistant in Zoology

Professional Activities:

1967-	NIMH: National Mental Health Advisory Council
1961-1962	President (Kennedy)'s Panel on Mental Retardation
1960-	NASA Committees: Lunar and Planetary Missions Board
1958-	National Academy of Sciences: Committees on Space Biology
1950-	President's Science Advisory Committee panels. National Institutes of Health, National Science Foundation study sections (genetics)

RESEARCH SUPPORT SUMMARY FOR JOSHUA LEDERBERG

	Grant Number	Grant Title	Current Year	Total Award	Grant Term	Budgeted % Time
1)	NASA:NGR-05-020-004	Cytochemical Studies of Planetary Micro-organisms	$150,000	$3,950,000	9/60-8/74 (Future support dubious)	4%
2)	NIH:AI-05160	Genetics of Bacteria	60,000	280,000	9/68-8/73 (Renewal Pending)	15%
3)	NIH:GM	Genetics Research Center	547,035	2,609,383	9/73-8/78 (Pending)	10%
4)	NIH:RR-00785	Stanford University Medical Experimental Computer Facility (SUMEX) Successor to #3	571,567	2,769,262	10/73-7/78	20%
5)	NIH: Computer Laboratory Health Care Resource Program	Large Scale Screening of Body Fluids for Metabolic Signs of Disease with Computer-managed Gas Chromatography and Mass Spectrometry	159,881	900,238	9/73-8/78 (Pending, Program funds impounded)	10%
6)	NIH:GM00295	Training Grant in Genetics	121,172	321,163	7/1/73-6/30/77	15%

14

SELECTED LIST OF PUBLICATIONS

Lederberg, J., 1959
A View of Genetics
Les Prix Nobel en 1958: 170-89.

Buchs, A., A. B. Delfino, A. M. Duffield, C. Djerassi, B. G. Buchanan, E. A. Feigenbaum, and J. Lederberg, 1970.
Applications of Artificial Intelligence for Chemical Inference. VI. Approach to a general method of interpreting low resolution mass spectra with a computer. Helvitia Chimica Acta 53 (6): 1394-1417.

Feigenbaum, E. A., B. G. Buchanan, J. Lederberg, 1971
On generality and problem solving: a case study using the DENDRAL program in Machine Intelligence 6, (B. Meltzer and D. Michie, eds.), Edinburgh University Press, P. 165-190.

Reynolds, W. E., V. A. Bacon, J. C. Bridges, T. C. Coburn, B. Halpern, J. Lederberg, E. C. Levinthal, E. Steed, R. B. Tucker, 1970
. A Computer Operated Mass Spectrometer System.
Analytical Chem. 42:1122-1129, September 1970.

Lederberg, J.
"Use of Computer to Identify Unknown Compounds: The Automation of Scientific Inference" in Biochemical Applications of Mass Spectrometry (G. R. Waller, ed.). John Wiley & Sons, New York (in press).

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE (Mo., Day, Yr.)
Feigenbaum, Edward A.	Principal Investigator, DENDRAL Project	1-20-36
PLACE OF BIRTH (City, State, Country)	**PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)**	**SEX**
Weehawken, New Jersey	U.S. Citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Carnegie Institute of Technology Pittsburgh, Pennsylvania	B.S. Ph.D.	1956 1959	Electrical Engineering Behavioral Sciences.

HONORS and memberships:
American Psychological Association; Association for Computing Machinery (Member of the National Council 1966-68); American Association for the Advancement of Science, SIGBIO Chairman, 11/73-present.

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Artificial Intelligence	Principal Investigator

RESEARCH SUPPORT *(See instructions)*

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1965- Stanford University, Computer Science Department Faculty
1965-1968 Stanford University, Director, Computation Center
1963 Summer Research Training Institute in Computer Simulation of Cognitive Processes (National Science Foundation)
1962 Carnegie Corporation. Summer Research Training Institute in Heuristic Programming. Faculty member.
1960-1964 University of California, Berkeley
Research-Center for Research in Management Science, 1960-1964
Research-Center for Human Learning, 1961-1964
Assistant and Associate Professor, School of Business Administration, 1960-64
1957-1960 The RAND Corporation, Santa Monica, California
1956 IBM Scientific Computing Center, New York

Selected Publications:

"Applications of Artificial Intelligence for Chemical Inference I. The Number of Possible Organic Compounds. Acyclic Structures Containing C, H, O and N", J. Am. Chem. Soc., 91, 2973 (1969). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference II. Interpretation of Low Resolution Mass Spectra of Ketones", J. Am. Chem. Soc., 91, 2977 (1969). (Co-Author).

Publications of Edward Feigenbaum

"Applications of Artificial Intelligence for Chemical Inference III. Aliphatic Ethers Diagnosed by their Low Resolution Mass Spectra and Nuclear Magnetic Resonance", J. Am. Chem. Soc., 91, 7440 (1969). (Co-Author).

"Heuristic DENDRAL: A Program for Generating Explanatory Hypotheses in Organic Chemistry", in Machine Intelligence 4, Edinburgh University Press, 1969. (Co-Author).

"Toward an Understanding of Information Processes of Scientific Inference in the Context of Organic Chemistry", in Machine Intelligence 5, Edinburgh University Press, 1970. (Co-Author).

"A Heuristic Program for Solving a Scientific Inference Problem: Summary of Motivation and Implementation", Stanford Artificial Intelligence Project Memo No. 104, November 1969. (Co-Author).

"Applications of Artificial Intelligence For Chemical Inference IV. Saturated Amines Diagnosed by Their Low Resolution Mass Spectra and Nuclear Magnetic Resonance Spectra", Journal of the American Chemical Society, 92, 6831 (1970). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference V. An Approach to the Computer Generation of Cyclic Structures. Differentiation Between All the Possible Isomeric Ketones of Composition C6H100", Organic Mass Spectrometry, 4, 493 (1970). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference VI. Approach to a General Method of Interpreting Low Resolution Mass Spectra with a Computer", Chem. Acta Helvetica, 53, 1394 (1970). (Co-Author).

"On Generality and Problem Solving: A Case Study Using the DENDRAL Program", in Machine Intelligence 6, Edinburgh University Press (1971). (Co-Author).

"A Heuristic Programming Study of Theory Formation in Science", in proceedings of the Second International Joint Conference on Artificial Intelligence, Imperial College, London (September 1971). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference VIII. An Approach to the Computer Interpretation of the High Resolution Mass Spectra of Complex Molecules. Structure Elucidation of Estrogenic Steroids", Journal of the American Chemical Society, 94, 5962-5971 (1972). (Co-Author).

"Heuristic Theory Formation: Data Interpretation and Rule Formation", in Machine Intelligence 7, Edinburgh University Press (1972). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference X. Intsum A Data Interpretation Program as Applied to the Collected Mass Spectra of Estrogenic Steroids", Tetrahedron, 29, 3117 (1973). (co-author).

SECTION II – PRIVILEGED COMMUN. TION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Buchanan, Bruce G.	Research Computer Scientist	7-7-40
PLACE OF BIRTH *(City, State, Country)*	**PRESENT NATIONALITY** *(If non-U.S. citizen, indicate kind of visa and expiration date)*	**SEX**
St. Louis, Missouri	U.S.Citizen	☒ Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Ohio Wesleyan University	B.A.	1961	Mathematics
Michigan State University	M.A., Ph.D.	1966	Philosophy

HONORS

Recipient of National Institutes of Health Career Development Award (1971-1976)

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Artificial Intelligence	Associate Investigator

RESEARCH SUPPORT *(See instructions)*

NIH Research Career Development Award, GM-29662

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1972-present Research Computer Scientist, Stanford University
1966-1971 Research Associate, Stanford Artificial Intelligence Project

Publications:

"On the Design of Inductive Systems: Some Philosophical Problems". British Journal for the Philosophy of Science 20 (1969), 311-323. (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference II. Interpretation of Low Resolution Mass Spectra of Ketones". Journal of the American Chemical Society, 91, 2977-2981 (1969). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference I. The Number of Possible Organic Compounds: Acyclic Structures Containing C, H, O and N". Journal of the American Chemical Society, 91, 2973-2976 (1969). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference III. Aliphatic Ethers Diagnosed by Their Low Resolution Mass Spectra and NMR Data". Journal of the American Chemical Society, 91, 7440-45 (1969). (Co-Author).

"Heuristic DENDRAL: A Program for Generating Explanatory Hypotheses in Organic Chemistry". Machine Intelligence.4, Edinburgh University Press (1969). (Co-Author).

Publications of Bruce Buchanan:

"Toward an Understanding of Information Processes of Scientific Inference in the Context of Organic Chemistry". Machine Intelligence 5, Edinburgh University Press (1969). (Co-Author).

"On Generality and Problem Solving: A Case Study Using the DENDRAL Program". Machine Intelligence 6, Edinburgh University Press (1969). (Co-Author).

"Some Speculation About Artificial Intelligence and Legal Reasoning". Stanford Law Review, Vol. 23, No. 1, November 1970. (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference VI. Approach to a General Method of Interpreting Low Resolution Mass Spectra with a Computer". Chemica Acta Helvetica, 53, 1394 (1970). (Co-Author).

"An Application of Artificial Intelligence to the Interpretation of Mass Spectra". Mass Spectrometry Techniques and Appliances (1970).

"Applications of Artificial Intelligence for Chemical Inference IV. Saturated Amines Diagnosed by Their Low Resolution Mass Spectra and Nuclear Magnetic Resonance Spectra". Journal of the American Chemical Society, 93, 6831 (1970). (Co-Author).

"The Heuristic DENDRAL Program for Explaining Empirical Data". Proceedings of IFIP Congress 1971, Ljubljana, Yugoslavia. (Co-Author).

"A Heuristic Programming Study of Theory Formation in Science". Proceedings of Second International Joint Conference on Artificial Intelligence, Imperial College, London (1971). (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference VIII. An Approach to the Computer Interpretation of the High Resolution Mass Spectra of Complex Molecules. Structure Elucidation of Estrogenic Steroids". Journal of the American Chemical Society, 1972. (Co-Author).

"Heuristic Theory Formation: Data Interpretation and Rule Formation". Machine Intelligence 7, Edinburgh University Press (1972). (Co-Author).

"Review of Hubert Dreyfus' 'What Computers Can't Do: A Critique of Artificial Reason'", Computing Reviews (January, 1973).

"Applications of Artificial Intelligence for Chemical Inference IX. Analysis of Mixtures Without Prior Separation as Illustrated for Estrogens". Submitted to the Journal of the American Chemical Society. (Co-Author).

"Applications of Artificial Intelligence for Chemical Inference X. Intsum A Data Interpretation Program as Applied to the Collected Mass Spectra of Estrogenic Steroids". Tetrahedron, 29, 3117 (1973). (co-author)

"Rule Formation on Non-Homogeneous Classes of Objects". In proceedings of the Third International Joint Conference on Artificial Intelligence (Stanford. 1973). (co-author).

"Current Status of the Heuristic DENDRAL Program for Applying Artificial Intelligence to the Interpretation of Mass Spectra". DENDRAL Project Memo, August 1973

Biographical Sketch of Bruce G. Buchanan

Memberships:

Association for Computing Machinery (ACM)
Philosophy of Science Association
American Association for Advancement of Science (AAAS)

Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE (Mo.-Day-Yr.)
Alan M. DUFFIELD	Research Associate	December 16 1936

PLACE OF BIRTH (City, State, Country)	PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)	SEX
Perth, Western Australia	Australian, Permanent resident Immigrant Visa	☒ Male ☐ Female

EDUCATION (Begin with baccalaureate training and include postdoctoral)

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
University of Western Australia	B. Sc(1st Class Hons)	1958	Organic Chemistry
University of Western Australia	Ph.D.	1962	Organic Chemsitry

HONORS

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Applications of mass spectrometry to Biology and Biomedical Problems	Organic Chemist/mass spectroscopist

RESEARCH SUPPORT (See instructions)

N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE (Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)

1970 -	Research Associate, Department of Genetics, Stanford University School of Medicine
1969 -	Head of the Mass Spectrometry Laboratory, Chemistry Department Stanford University
1965 - 69	Research Associate, Department of Chemistry, Stanford University
1963 - 65	Postdoctoral Fellow, Department of Chemistry, Stanford University
1962 - 63	Postdoctoral Fellow, Department of Biochemistry, Stanford University School of Medicine.

PUBLICATIONS SINCE 1971

1. An Application of Artificial Intelligence to the Interpretation of Mass Spectra. Mass Spectrometry, B.W.G. Milne, Ed., John Wiley and Sons, New York, 1971, pp. 121-178
By B. G. Buchanan, A. M. Duffield and A. V. Robertson

2. Mass Spectrometry in Structural and Stereochemical Problems. CCIV. Spectra of Hydantoins.II. Electron Impact Induced Fragmentation of some Substituted Hydantoins.
   Org. Mass Spectr., 5, 551 (1971)
   By R. A. Corral, O. O. Orazi, A. M. Duffield and C. Djerassi

3. Electron Impact Induced Hydrogen Scrambling in Cyclohexanol and Isomeric Methylcyclohexanols.
   Org. Mass Spectr., 5, 383 (1971)
   By R. H. Shapiro, S. P. Levine and A. M. Duffield

4. Derivatives of 2-Biphenylcarboxylic Acid.
   Rev. Roumain. Chem., 16, 1095 (1971)
   By A. T. Balaban and A. M. Duffield

5. Alkaloide aus Evonymus europaea L.
   Helv. Chim. Acta, 54, 2144 (1971)
   By A. Klásek, T. Reichstein, A. M. Duffield and F. Santavý

6. Studies on Indian Medicinal Plants. XXVIII. Sesquiterpene Lactones of Enhydra Fluctuans Lour. Structures of Enhydrin, Fluctuanin and Fluctuadin.
   Tetrahedron, 28, 2285 (1972).
   By E. Ali, P. P. Ghosh Dastidar, S. C. Pakrashi, L. J. Durham and A. M. Duffield

7. The Electron Impact Promoted Fragmentation of Aurone Epoxides.
   Org. Mass Spectr., 6, 199 (1972)
   By B. A. Brady, W. I. O'Sullivan and A. M. Duffield

8. The Determination of Cyclohexylamine in Aqueous Solutions of Sodium Cyclamate by Electron Capture Gas Chromatography.
   Anal. Letters, 4, 301 (1971)
   By M. D. Soloman, W. E. Pereira and A. M. Duffield

9. Computer Recognition of Metastable Ions. Nineteenth Annual Conference on Mass Spectrometry, Atlanta, 1971, p. 63
   By A. M. Duffield, W. E. Reynolds, D. A. Anderson, R. A. Stillman, Jr. and C. E. Carroll

10. Spectrometrie de Masse. VI. Fragmentation de Dimethyl-2,2-dioxolanes-1,3-Insatures.
    Org. Mass Spectr., 5, 1409 (1971)
    By J. Kossanyi, J. Chuche and A. M. Duffield

11. Chlorpromazine Metabolism in Sheep. II. In vitro Metabolism and Preparation of 3H-7-Hydroxychlorpromazine.
    Journees D'Agressologie, 12, 333 (1971)
    By L. G. Brooks, M. A. Holmes, I. S. Forrest, V. A. Bacon, A. M. Duffield and M. D. Solomon

12. Mass Spectrometry in Structural and Stereochemical Problems. CCXVII. Electron Impact Promoted Fragmentation of O-Methyl Oximes of Some α,β-Unsaturated Ketones and Methyl Substituted Cyclohexanones.
    Canadian J. Chem., 50, 2776 (1972)
    By Y. M. Sheikh, R. J. Liedtke, A. M. Duffield and C. Djerassi

13. Thermal Fragmentation of Quinoline and Isoquinoline N-Oxides in the Ion Source of a Mass Spectrometer.
Acta Chem. Scand., 26, 2423 (1972).
By A. M. Duffield and O. Buchardt

14. Applications of Artificial Intelligence for Chemical Inference. VII. An Approach to the Computer Interpretation of the High Resolution Mass Spectra of Complex Molecules. Structure Elucidation of Estrogenic Steroids.
J. Amer. Chem. Soc., 94, 5962 (1972)
By D. H. Smith, B. G. Buchanan, R. S. Englemore, A. M. Duffield, A. Yeo, E. A. Feigenbaum, J. Lederberg and C. Djerassi

15. Mass Spectrometry in Structural and Stereochemical Problems. CCXIX. Identification of a Unidirectional Quadruple Hydrogen Transfer Process in 7-Phenyl-hept-3-en-2-one O-Methyl Oxime Ether.
Org. Mass Spectr., 6,1271 (1972).
By R. J. Liedtke, Y. M. Sheikh, A. M. Duffield and C. Djerassi

16. An Automated Gas Chromatographic Analysis of Phenylalanine in Serum.
Clinical Biochem., 5, 166 (1972)
By E. Steed, W. Pereira, B. Halpern, M. D. Solomon and A. M. Duffield

17. Pyrrolizidine Alkaloids. XIX. Structure of the Alkaloid Erucifoline.
Coll. Czech. Chem. Commun., (1972)
By P. Sedmera, A. Klásek, A. M. Duffield and F. Santavý.

18. Mass Spectrometry in Structural and Stereochemical Problems. CCXXII. Delineation of Competing Fragmentation Pathways of Complex Molecules from a Study of Metastable Ion Transitions of Deuterated Derivatives.
Org. Mass Spectr., 7, (1973)
By D. H. Smith, A. M. Duffield and C. Djerassi

19. Chlorination Studies I. The Reaction of Aqueous Hypochlorous Acid with Cytosine.
Biochem. Biophys. Res. Commun., 48, 880 (1972)
By W. Patton, V. Bacon, A. M. Duffield, B. Halpern, Y. Hoyano, W. Pereira and J. Lederberg

20. A Study of the Electron Impact Fragmentation of Promazine Sulphoxide and Promazine using Specifically Deuterated Analogues.
Austral. J. Chem., 26, (1973).
By M. D. Solomon, R. Summons, W. Pereira and A. M. Duffield

21. Spectrometric de Masse. VIII. Elimination d'eau Induite par Impact Electronique dans le Tetrhydro-1,2,3,4-naphtalenediol-1,2.
Org. Mass. Spectrom., 7 (1973).
By P. Perros, J. P. Morizui, J. Kossanyi and A. M. Duffield

22. The Determination of Phenylalanine in Serum by Mass Fragmentography
Clinical Biochem., submitted for publication (1973).
By W. E. Pereira, V. A. Bacon, Y. Hoyano, R. Summons and A. M. Duffield

SECTION II – PRIVILEGED COMMUNICATION

BIOGRAPHICAL SKETCH

(Give the following information for all professional personnel listed on page 3, beginning with the Principal Investigator. Use continuation pages and follow the same general format for each person.)

NAME	TITLE	BIRTHDATE *(Mo., Day, Yr.)*
Dennis H. Smith	Research Associate	11/12/42

PLACE OF BIRTH *(City, State, Country)*	PRESENT NATIONALITY *(If non-U.S. citizen, indicate kind of visa and expiration date)*	SEX
New York	USA	X Male ☐ Female

EDUCATION *(Begin with baccalaureate training and include postdoctoral)*

INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	SCIENTIFIC FIELD
Massachusetts Inst. of Technology Cambridge, Mass.	S.B.	1964	Chemistry
University of California, Berkeley Berkeley, California	Ph.D.	1967	Chemistry

HONORS

Alfred P. Sloan Foundation Scholarship
NASA Predoctoral Traineeship
Phi Lambda Upsilon, Sigma Xi

MAJOR RESEARCH INTEREST	ROLE IN PROPOSED PROJECT
Mass Spectrometry and A.I. in Chemistry	Research Associate

RESEARCH SUPPORT *(See instructions)*

N/A

RESEARCH AND/OR PROFESSIONAL EXPERIENCE *(Starting with present position, list training and experience relevant to area of project. List all or most representative publications. Do not exceed 3 pages for each individual.)*

1971-Present Research Associate, Stanford University, Stanford,Ca.
1970-1971 Visiting Scientist, University of Bristol, Bristol, England
1967-1970 Assistant Research Chemist, University of Calif.at Berkeley, Berkeley, Ca.
1965-1967 NASA Pre-Doctoral Traineeship, University of Calif.at Berkeley,Berkeley, Ca.

Publications: See attached list.

PUBLICATIONS: D. H. SMITH

1. H. G. Langer, R. S. Gohlke and D. H. Smith, "Mass Spectrometric Differential Thermal Analysis," Anal. Chem., 37, 433 (1965).

2. S. M. Kupchan, J. M. Cassady, J. E. Kelsey, H. K. Schnoes, D. H. Smith and A. L. Burlingame, "Structural Elucidation and High Resolution Mass Spectrometry of Gaillardin, a New Cytotoxic Sesquiterpene Lactone," J. Amer. Chem. Soc., 88, 5292 (1966).

3. D. H. Smith, Ph.D. Thesis, "High Resolution Mass Spectrometry: Techniques and Applications to Molecular Structure Problems," Dept. of Chemistry, University of California, Berkeley, California (1967).

4. H. K. Schnoes, D. H. Smith, A. L. Burlingame, P. W. Jeffs and W. Döpke, "Mass Spectra of Amaryllidaceae Alkaloids: The Lycorenine Series," Tetrahedron, 24, 2825 (1968).

5. A. L. Burlingame, D. H. Smith and R. W. Olsen, "High Resolution Mass Spectrometry in Molecular Structure Studies, XIV. Real-time Data Acquisition, Processing and Display of High Resolution Mass Spectral Data," Anal. Chem., 40, 13 (1968).

6. A. L. Burlingame and D. H. Smith, "High Resolution Mass Spectrometry in Molecular Structure Studies II. Automated Heteroatomic Plotting as an Aid to the Presentation and Interpretation of High Resolution Mass Spectral Data," Tetrahedron, 24, 5749 (1968).

7. W. J. Richter, B. R. Simoneit, D. H. Smith and A. L. Burlingame, "Detection and Identification of Oxocarboxylic and Dicarboxylic Acids in Complex Mixtures by Reductive Silylation and Computer-Aided Analysis of High Resolution Mass Spectral Data," Anal. Chem., 41, 1392 (1969).

8. The Lunar Sample Preliminary Examination Team, "Preliminary Examination of Lunar Samples from Apollo 11," Science, 165, 1211 (1969).

9. S. M. Kupchan, W. K. Anderson, P. Bollinger, R. W. Doskotch, R. M. Smith, J. A. Saenz Renauld, H. K. Schnoes, A. L. Burlingame and D. H. Smith, "Tumor Inhibitors, XXXIX. Active Principles of Acnistus arborescens. Isolation and Structural and Spectral Studies of Withaferin A and Withacnistin," J. Org. Chem., 34, 3858 (1969).

10. A. L. Burlingame, D. H. Smith, T. O. Merren and R. W. Olsen, "Real-time High Resolution Mass Spectrometry," in Computers in Analytical Chemistry (Vol. 4 in Progress in Analytical Chemistry series), C. H. Orr and J. Norris, Eds., Plenum Press, New York, 1970, pp. 17-38.