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
DEPARTMENT OF
HEALTH, EDUCATION, AND WELFARE
PUBLIC HEALTH SERVICE

GRANT APPLICATION

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. NAME (Last, First, Initial)
   Djerassi, Carl

3. TITLE OF POSITION
   Professor of Chemistry

4. MAILING ADDRESS (Street, City, State, Zip Code)
   Department of Chemistry
   Stanford University
   Stanford, California 94305

5. DEGREE
   Ph.D.

6. SOCIAL SECURITY NO.

7. TELEPHONE DATA
   Area Code Telephone Number and Extension
   415 321-2300, Ext. 2783

8. DEPARTMENT, SERVICE, LABORATORY OR EQUIVALENT
   Department of Chemistry

9. MAJOR SUBDIVISION (See Instructions)
   School of Humanities and Sciences

10. INVENTIONS
    A. NO B. YES - Approved:
    C. YES - Pending Review

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

13. ENTITY NUMBER (Formerly PHS Account Number)
    458210

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.

SIGNATURES

A. SIGNATURE OF PERSON NAMED IN ITEM 2A

B. SIGNATURE(S) OF PERSON(S) NAMED IN ITEM 10

458210

Rev. 1/73
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.
### DETAILED BUDGET FOR FIRST 12-MONTH PERIOD

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

#### PERSONNEL

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE OF POSITION</th>
<th>TIME OR EFFORT</th>
<th>SALARY</th>
<th>FRINGE BENEFITS</th>
<th>TOTAL</th>
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<tr>
<td></td>
<td>Principal Investigator</td>
<td></td>
<td></td>
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**DEDICATED SALARY DATA LISTED SEPARATELY ON ATTACHED SHEET**

#### 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
- 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)

- % S&W

**DATE OF DHEW AGREEMENT:**

- 47% NTDTC - June 26, 1973

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

<table>
<thead>
<tr>
<th>Name</th>
<th>%</th>
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<tbody>
<tr>
<td>C. Djerassi</td>
<td>10</td>
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<tr>
<td>J. Lederberg</td>
<td>10</td>
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<tr>
<td>E. Feigenbaum</td>
<td>10</td>
<td>2,910</td>
<td>514</td>
<td>3,424</td>
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RESEARCH ASSOCIATES:

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<tr>
<td>B. Buchanan (1)</td>
<td>50</td>
<td>7,000</td>
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<tr>
<td>A. Duffield</td>
<td>25</td>
<td>6,195</td>
<td>1,094</td>
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<tr>
<td>D. Smith</td>
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<td>16,200</td>
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<td>G. Dromey</td>
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PROGRAMMERS:

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<td>R. Tucker</td>
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SENIOR RESEARCH ASSISTANT:

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<td>A. Wegmann</td>
<td>100</td>
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<td>17,650</td>
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ELECTRONICS ENGINEER:

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<td>N. Veizades</td>
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<td>11,670</td>
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GLASS BLOWER/MACHINIST:

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<td>E. Steed</td>
<td>25</td>
<td>4,410</td>
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RESEARCH ASSISTANTS:

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<tr>
<td>M. Stefik</td>
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<td>To Be Appointed</td>
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SECRETARIAL SUPPORT:

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<tr>
<td>K. Wharton</td>
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<td>9,400</td>
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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.
# Budget Estimates for All Years of Support Requested from Public Health Service

**DIRECT COSTS ONLY (Omit Cents)**

<table>
<thead>
<tr>
<th>DESCRIPTION</th>
<th>1ST PERIOD (SAME AS TAILORED)</th>
<th>ADDITIONAL YEARS SUPPORT REQUESTED (This application only)</th>
<th>2ND YEAR</th>
<th>3RD YEAR</th>
<th>4TH YEAR</th>
<th>5TH YEAR</th>
<th>6TH YEAR</th>
<th>7TH YEAR</th>
<th>TOTAL</th>
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<td><strong>PERSONNEL COSTS</strong></td>
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<tr>
<td></td>
<td>192,897</td>
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<td>210,611</td>
<td>225,129</td>
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<td>257,383</td>
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<td><strong>CONSULTANT COSTS</strong> (Include fees, travel, etc.)</td>
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<td>-0-</td>
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<td>-0-</td>
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<td><strong>EQUIPMENT</strong></td>
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<td>6,920</td>
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<tr>
<td>Domestic</td>
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<tr>
<td><strong>PATIENT COSTS</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td><strong>ALTERATIONS AND RENOVATIONS</strong></td>
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<td></td>
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<td>-0-</td>
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<tr>
<td><strong>OTHER EXPENSES</strong></td>
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<tr>
<td><strong>TOTAL DIRECT COSTS</strong></td>
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<td></td>
<td>240,961</td>
<td>258,514</td>
<td>277,349</td>
<td>297,774</td>
<td>1,350,795</td>
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</table>

**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 $277,000 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 ATM-SUMEX resource, to which we hope to make significant contributions.

This budget overlaps slightly with the budget for the Genetics Research Center (J. Lederberg, Principal Investigator). Dr. Alanuffield's 25% salary budgeted here is covered by the other budget (where 100% of his salary is budgeted). 10% of Ms. Annemarie Weismann'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. Those 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.

VATESA 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 DROMY
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 PULGGEN program.

MS. ANNEMAPIE 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

Messrs. 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 W. MASINTER

Mr. Larry Masinter, Research Assistant, will continue to work with Drs. Lederberg and Brown on the development of the cyclic structure generator. His LTSP 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

A 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 P. Feldman, NIH); Sophisticated structural display programs have been written especially for a GT-40 which we would hope to mount; and the ATM-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 DPC 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 ($1,200). 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 calcom paper and pens for ion current 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 370/150 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.
Principal Investigator: Carl Djerassi

NAME: Carl DJERASSI
TITLE: Professor of Chemistry
BIRTHDATE: October 29, 1923

PLACE OF BIRTH: Vienna, Austria
PRESENT NATIONALITY: U.S.A.
SEX: Male

EDUCATION:
- Kenyon College
  - A.B. (summa cum laude) 1942
  - Ph.D. Chemistry, Biology
- University of Wisconsin
  - Hon. D.Sc., Natl. Univ. of Mexico (1953), Kenyon College (1958), Worcester Polytechnic Institute (1972)
- Major Research Interests:
  - Nat. prod. chemistry (steroids, alkaloids, terpenoids, antibiotics)
  - Applications of physical methods (mass spec., optical rotatory dispersion, circular dichroism)

Grant Support:
- NIH AM 04257
  - Mass Spectrometry in Organic and Biochemistry
  - Period: 10/1/70 to 9/30/75
  - Budgeted: $316,016
  - Effort: 10%
- NIH GM AM 06840-15
  - Marine Chemistry with special emphasis on steroids
  - Period: 1/1/73 to 12/31/77
  - Budgeted: $578,180
  - Effort: 18%
- NSF Pending Grant Application #P3P3689, Magnetic Circular Dichroism in Organic Molecules, in the amount of $21,000.

RESEARCH AND/OR PROFESSIONAL EXPERIENCE:
- Academic Experience:
  - Professor of Chemistry, Stanford University, 1959-present.
  - Associate Professor (1952-1954) and Professor (1954-1959), Wayne State University.

- Industrial Research Experience:
  - 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--
  - Zocon Corporation (Palo Alto), President, 1968--

- Editorial Board:

Honors (cont.):
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 steroids, 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.
LEDERBERG, JOSHUA

Professor and Executive Head,
Department of Genetics

Montclair, New Jersey

U.S.A.

Male

Columbia College, New York B.A. 1944
College of Physicians & Surgeons, Columbia University, New York (1944-46)
Yale University Ph.D. 1947

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

Molecular Genetics; Artificial Intelligence

PRINCIPAL INVESTIGATOR

SEE ATTACHMENTS:

RESEARCH AND/OR PROFESSIONAL EXPERIENCE

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)
<table>
<thead>
<tr>
<th>Grant Number</th>
<th>Grant Title</th>
<th>Current Year</th>
<th>Total Award</th>
<th>Grant Term</th>
<th>Budgeted % Time</th>
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<tr>
<td>1) NASA:NGR-05-020-004</td>
<td>Cytochemical Studies of Planetary Micro-organisms</td>
<td>$150,000</td>
<td>$3,950,000</td>
<td>9/60-8/74</td>
<td>4%</td>
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<td></td>
<td></td>
<td></td>
<td>(Future support</td>
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<td></td>
<td></td>
<td>dubious)</td>
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<td>2) NIH:AI-05160</td>
<td>Genetics of Bacteria</td>
<td>60,000</td>
<td>280,000</td>
<td>9/68-8/73</td>
<td>15%</td>
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<td>(Renewal Pending)</td>
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<td>3) NIH:GM</td>
<td>Genetics Research Center</td>
<td>547,035</td>
<td>2,609,383</td>
<td>9/73-8/78</td>
<td>10%</td>
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<td>(Pending)</td>
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<td>4) NIH:RR-00785</td>
<td>Stanford University Medical</td>
<td>571,567</td>
<td>2,769,262</td>
<td>10/73-7/78</td>
<td>20%</td>
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<td>Experimental Computer Facility (SUMEX) Successor to #3</td>
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<td>5) NIH:GM00295</td>
<td>Large Scale Screening of Body Fluids for Metabolic Signs of Disease with</td>
<td>151,881</td>
<td>906,238</td>
<td>9/73-8/78</td>
<td>10%</td>
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<td></td>
<td>Care Resource Computer-managed Gas Chromatography and Mass Spectrometry</td>
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<td>(Pending, Program Funds impounded)</td>
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<td></td>
<td>Training Grant in Genetics</td>
<td>121,172</td>
<td>321,163</td>
<td>7/1/73-6/30/77</td>
<td>15%</td>
</tr>
</tbody>
</table>
SELECTED LIST OF PUBLICATIONS

Lederberg, J., 1959
A View of Genetics

Applications of Artificial Intelligence for Chemical Inference.

Feigenbaum, E. A., B. G. Buchanan, J. Lederberg, 1971

A Computer Operated Mass Spectrometer System.

Lederberg, J.
SECTION II - PRIVILEGED COMMUNICATION

BIографICAL 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
Feigenbaum, Edward A.

TITLE
Principal Investigator,
DENDRAL Project

BIRTHDATE (Mo. Day, Yr.)
1-20-36

PLACE OF BIRTH (City, State, Country)
Weehawken, New Jersey

PRESENT NATIONALITY /If non-U.S. citizen, indicate kind of visa and expiration date)
U.S. Citizen

SEX
M Male  F Female

EDUCATION (Begin with baccalaureate training and include postdoctoral)

INSTITUTION AND LOCATION
Carnegie Institute of Technology
Pittsburgh, Pennsylvania

DEGREE
B.S.
Ph.D.

YEAR CONFERRED
1956
1959

SCIENTIFIC FIELD
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
Artificial Intelligence

ROLE IN PROPOSED PROJECT
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:

Publications of Edward Feigenbaum


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
Buchanan, Bruce G.

TITLE
Research Computer Scientist

BIRTHDATE (Mo., Day, Yr.)
7-7-40

PLACE OF BIRTH (City, State, Country)
St. Louis, Missouri

PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)
U.S. Citizen

SEX
☑ Male ☐ Female

EDUCATION (Begin with baccalaureate training and include postdoctoral)

<table>
<thead>
<tr>
<th>INSTITUTION AND LOCATION</th>
<th>DEGREE</th>
<th>YEAR CONFERRED</th>
<th>SCIENTIFIC FIELD</th>
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<tbody>
<tr>
<td>Ohio Wesleyan University</td>
<td>B.A.</td>
<td>1961</td>
<td>Mathematics</td>
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<td>Michigan State University</td>
<td>M.A., Ph.D.</td>
<td>1966</td>
<td>Philosophy</td>
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HONORS

MAJOR RESEARCH INTEREST
Artificial Intelligence

ROLE IN PROPOSED PROJECT
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:


Publications of Bruce Buchanan:


"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).


"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)
NAME: Alan M. DUFFIELD

PLACE OF BIRTH (City, State, Country): Perth, Western Australia

PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date): Australian, Permanent resident

SEX: Male

EDUCATION (Begin with bachelor's degree training and include postdoctoral):

<table>
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<th>INSTITUTION AND LOCATION</th>
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<tbody>
<tr>
<td>University of Western Australia</td>
<td>B. Sc (1st Class Hons)</td>
<td>1958</td>
<td>Organic Chemistry</td>
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<tr>
<td>University of Western Australia</td>
<td>Ph.D.</td>
<td>1962</td>
<td>Organic Chemistry</td>
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HONORS

MAJOR RESEARCH INTEREST:
Applications of mass spectrometry to Biology and Biomedical Problems

HOLY IN PROPOSED PROJECT: Organic Chemist/mass spectrometrist

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 of 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:


By B. G. Buchanan, A. M. Duffield and A. V. Robertson
   By R. A. Corral, O. O. Orazi, A. M. Duffield and C. Djerassi

3. Electron Impact Induced Hydrogen Scrambling in Cyclohexanol and Isomeric Methylcyclohexanols.
   By R. H. Shapiro, S. P. Levine and A. M. Duffield

4. Derivatives of 2-Biphenylcarboxylic Acid.
   By A. T. Balaban and A. M. Duffield

5. Alkaloid aus Evonymus europaeus L.
   By A. Kläsek, T. Reichstein, A. M. Duffield and F. Santavy

   Tetrahedron, 28, 2289 (1972)

   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. Solomon, W. E. Pereira and A. M. Duffield

   By A. M. Duffield, W. E. Reynolds, D. A. Anderson, R. A. Stillman, Jr. and C. E. Carroll

10. Spectrometrie de Masse. VT. Fragmentation de Dimethyl-2,2-Dioxolanes-1,3-Insatures.
    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
Publications

   By A. M. Duffield and O. Buchardt

   *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

   By R. J. Liedtke, Y. M. Sheikh, A. M. Duffield and C. Djerassi

   *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.
   By P. Sedmera, A. Klasek, A. M. Duffield and F. Santavy

   *Org. Mass Spectr.*, 7, (1973)
   By D. H. Smith, A. M. Duffield and C. Djerassi

   By W. Patton, V. Bacon, A. M. Duffield, B. Halpern, Y. Hoyano, W. Pereira and J. Lederberg

   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.
   By P. Perros, J. P. Morizui, J. Kossanyi and A. M. Duffield

22. The Determination of Phenylalanine in Serum by Mass Fragmentography
   By W. E. Pereira, V. A. Bacon, Y. Hoyano, R. Summons and A. M. Duffield
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.)

<table>
<thead>
<tr>
<th>NAME</th>
<th>TITLE</th>
<th>BIRTHDATE (Mo., Day, Yr.)</th>
<th>SEX</th>
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<tbody>
<tr>
<td>Dennis H. Smith</td>
<td>Research Associate</td>
<td>11/12/42</td>
<td></td>
</tr>
</tbody>
</table>

PLACE OF BIRTH (City, State, Country)
New York USA

PRESENT NATIONALITY (If non-U.S. citizen, indicate kind of visa and expiration date)

EDUCATION (Begin with baccalaureate training and include postdoctoral)

<table>
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<th>DEGREE</th>
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<th>SCIENTIFIC FIELD</th>
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<tr>
<td>Massachusetts Inst. of Technology Cambridge, Mass.</td>
<td>S.B.</td>
<td>1964</td>
<td>Chemistry</td>
</tr>
<tr>
<td>University of California, Berkeley Berkeley, California</td>
<td>Ph.D.</td>
<td>1967</td>
<td>Chemistry</td>
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HONORS
Alfred P. Sloan Foundation Scholarship
NASA Predoctoral Traineeship
Phi Lambda Upsilon, Sigma Xi

MAJOR RESEARCH INTEREST
Mass Spectrometry and A.I. in Chemistry

ROLE IN PROPOSED PROJECT
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

Publications: See attached list.


