

**INFORMATION ABOUT PRINCIPAL INVESTIGATORS/PROJECT DIRECTORS(PI/PD) and
co-PRINCIPAL INVESTIGATORS/co-PROJECT DIRECTORS**

Submit only ONE copy of this form for each PI/PD and co-PI/PD identified on the proposal. The form(s) should be attached to the original proposal as specified in GPG Section II.B. Submission of this information is voluntary and is not a precondition of award. This information will not be disclosed to external peer reviewers. **DO NOT INCLUDE THIS FORM WITH ANY OF THE OTHER COPIES OF YOUR PROPOSAL AS THIS MAY COMPROMISE THE CONFIDENTIALITY OF THE INFORMATION.**

PI/PD Name: Chris Arumainayagam

Gender: Male Female

Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race: American Indian or Alaska Native

(Select one or more)

Asian

Black or African American

Native Hawaiian or Other Pacific Islander

White

Disability Status: Hearing Impairment

(Select one or more)

Visual Impairment

Mobility/Orthopedic Impairment

Other

None

Citizenship: (Choose one) U.S. Citizen Permanent Resident Other non-U.S. Citizen

Check here if you do not wish to provide any or all of the above information (excluding PI/PD name):

REQUIRED: Check here if you are currently serving (or have previously served) as a PI, co-PI or PD on any federally funded project

Ethnicity Definition:

Hispanic or Latino. A person of Mexican, Puerto Rican, Cuban, South or Central American, or other Spanish culture or origin, regardless of race.

Race Definitions:

American Indian or Alaska Native. A person having origins in any of the original peoples of North and South America (including Central America), and who maintains tribal affiliation or community attachment.

Asian. A person having origins in any of the original peoples of the Far East, Southeast Asia, or the Indian subcontinent including, for example, Cambodia, China, India, Japan, Korea, Malaysia, Pakistan, the Philippine Islands, Thailand, and Vietnam.

Black or African American. A person having origins in any of the black racial groups of Africa.

Native Hawaiian or Other Pacific Islander. A person having origins in any of the original peoples of Hawaii, Guam, Samoa, or other Pacific Islands.

White. A person having origins in any of the original peoples of Europe, the Middle East, or North Africa.

WHY THIS INFORMATION IS BEING REQUESTED:

The Federal Government has a continuing commitment to monitor the operation of its review and award processes to identify and address any inequities based on gender, race, ethnicity, or disability of its proposed PIs/PDs. To gather information needed for this important task, the proposer should submit a single copy of this form for each identified PI/PD with each proposal. Submission of the requested information is voluntary and will not affect the organization's eligibility for an award. However, information not submitted will seriously undermine the statistical validity, and therefore the usefulness, of information received from others. Any individual not wishing to submit some or all the information should check the box provided for this purpose. (The exceptions are the PI/PD name and the information about prior Federal support, the last question above.)

Collection of this information is authorized by the NSF Act of 1950, as amended, 42 U.S.C. 1861, et seq. Demographic data allows NSF to gauge whether our programs and other opportunities in science and technology are fairly reaching and benefiting everyone regardless of demographic category; to ensure that those in under-represented groups have the same knowledge of and access to programs and other research and educational opportunities; and to assess involvement of international investigators in work supported by NSF. The information may be disclosed to government contractors, experts, volunteers and researchers to complete assigned work; and to other government agencies in order to coordinate and assess programs. The information may be added to the Reviewer file and used to select potential candidates to serve as peer reviewers or advisory committee members. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records", 63 Federal Register 267 (January 5, 1998), and NSF-51, "Reviewer/Proposal File and Associated Records", 63 Federal Register 268 (January 5, 1998).

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PI/PD Name: David R Haines

Gender: Male Female
Ethnicity: (Choose one response) Hispanic or Latino Not Hispanic or Latino

Race:
(Select one or more)
 American Indian or Alaska Native
 Asian
 Black or African American
 Native Hawaiian or Other Pacific Islander
 White

Disability Status:
(Select one or more)
 Hearing Impairment
 Visual Impairment
 Mobility/Orthopedic Impairment
 Other
 None

Citizenship: (Choose one) U.S. Citizen Permanent Resident Other non-U.S. Citizen

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CERTIFICATION PAGE

Certification for Principal Investigators and Co-Principal Investigators:

I certify to the best of my knowledge that:

- (1) the statements herein (excluding scientific hypotheses and scientific opinions) are true and complete, and
 (2) the text and graphics herein as well as any accompanying publications or other documents, unless otherwise indicated, are the original work of the signatories or individuals working under their supervision. I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this proposal.

I understand that the willful provision of false information or concealing a material fact in this proposal or any other communication submitted to NSF is a criminal offense (U.S.Code, Title 18, Section 1001).

Name (Typed)	Signature	Social Security No.*	Date
PI/PD Chris Arumainayagam		*ON FASTLANE SUBMISSIONS* SSNs are confidential and are not displayed	
Co-PI/PD David R Haines			
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			
Co-PI/PD			

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the individual applicant or the authorized official of the applicant institution is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding Federal debt status, debarment and suspension, drug-free workplace, and lobbying activities (see below), as set forth in Grant Proposal Guide (GPG), NSF 00-2. Willful provision of false information in this application and its supporting documents or in reports required under an ensuring award is a criminal offense (U. S. Code, Title 18, Section 1001).

In addition, if the applicant institution employs more than fifty persons, the authorized official of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of Grant Policy Manual Section 510; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflict which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Debt and Debarment Certifications

(If answer "yes" to either, please provide explanation.)

Is the organization delinquent on any Federal debt?

Yes

No

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency?

Yes

No

Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding \$100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding \$150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.

(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.

(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME/TITLE (TYPED) William S. Reed/Vice President (Finance)		09/15/00
TELEPHONE NUMBER 781-283-2305	ELECTRONIC MAIL ADDRESS wreed@wellesley.edu	FAX NUMBER 781-283-3696

*SUBMISSION OF SOCIAL SECURITY NUMBERS IS VOLUNTARY AND WILL NOT AFFECT THE ORGANIZATION'S ELIGIBILITY FOR AN AWARD. HOWEVER, THEY ARE AN INTEGRAL PART OF THE INFORMATION SYSTEM AND ASSIST IN PROCESSING THE PROPOSAL. SSN SOLICITED UNDER NSF ACT OF 1950, AS AMENDED.

Project Summary – Proposal Section A

REU Site: Chemistry as the Focus of an Interdisciplinary Summer Research Program at Wellesley College

The Chemistry Department of Wellesley College requests funding for the renewal of our summer Research Experiences for Undergraduates (REU) site program for each of three summers beginning in June of 2001. The central feature of our ten-week summer program is, and will continue to be, student participation in a research project under the guidance and supervision of the Chemistry Department faculty. Undergraduate students, especially those doing research during the summer, have co-authored most of the presentations and papers that come out of this department. The research of faculty members in the Chemistry Department has appeared in numerous publications and presentations at regional, national, and international meetings, and has led to major research grants and invitations to speak at other institutions. Wellesley's supportive infrastructure, including equipment and facilities comparable to those at many research universities, contributes greatly to the strength of our research programs.

In addition to the student research project component, our summer program will build on and expand interdisciplinary connections between Chemistry and other departments (for example, Biological Sciences, Physics, Computer Science, and the social sciences) and interdepartmental programs (such as Biological Chemistry, Neuroscience and Environmental Science). The primary thrust of the interdisciplinary focus will be the inclusion of physics faculty and students in the proposed summer research program. Other examples of intellectual cooperation across disciplinary lines will include collaboration between Chemistry faculty members and those in the Biological Sciences and Art Departments, more interdisciplinary seminars especially focused on materials science and nanotechnology, student oral presentations at common forums, and a campus-wide poster session at the end of the summer.

Wellesley College has shown extraordinary commitment to the summer research program in the Chemistry Department. Most importantly, College and other funding will be used to support approximately 15 chemistry/physics summer students each year in addition to the ten to be funded by NSF-REU. The staff of the College's Office of Institutional Research will be available to perform comprehensive assessments of the proposed Chemistry summer research program. Moreover, the College will provide a nominal stipend to faculty participating as research advisors during the summer.

The goal of the Wellesley program is to encourage bright young women to pursue research careers in science and medicine through their participation in a research project as early as possible in their academic careers. We propose to maintain many aspects of our program that have proven to be so successful in the past. The key components of the program are: a student research project supervised by a Chemistry Department faculty member; weekly meetings in which students give oral presentations of their work; weekly seminars by visiting scientists; field trips to nearby industrial and academic research labs; career and graduate school panels; skills workshops in public speaking, scientific writing, and poster presentations; and a campus-wide poster session at the end of the program.

We expect a total of approximately 25 chemistry and physics students to participate in the ten-week summer research program each year. As in the past, at least five of the ten NSF-REU slots will be reserved for non-Wellesley students with preference given to participants from institutions with limited research opportunities. The point-of-contact for student recruitment will be the principal investigator, Dr. Chris Arumainayagam, who may be reached at 781-283-3326 or via email at carumainayag@wellesley.edu. Details of the 2000 summer research program, including the schedule of events, can be found at the following site: <http://www.wellesley.edu/Sumres/main/main.htm>

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J Appendix (List below.) (Include only if allowed by a specific program announcement/ solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)	<u> </u>	<u> </u>
Appendix Items:		

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

Project Description – Proposal Section C (Including Results from Prior NSF Support)

(a) Overview:

The goal of the Wellesley program is to encourage bright young women to pursue research careers in science and medicine through their participation in a research project as early as possible in their academic careers. We propose to maintain many aspects of our program that have proven to be so successful in the past. The key components of the program are: a student research project supervised by a Chemistry Department faculty member; weekly meetings in which students give oral presentations of their work; weekly seminars by visiting scientists; field trips to nearby industrial and academic research labs; career and graduate school panels; skills workshops in public speaking, scientific writing, and poster presentations; and a campus-wide poster session at the end of the program. In addition, our summer program will build on and expand interdisciplinary connections between Chemistry and other departments such as Physics and Biological Sciences.

Intellectual Focus:

The summer research program in Chemistry has developed an interdisciplinary focus during the past several years. The Chemistry and Biological Sciences departments have shared management of the seminar series and panels, choosing speakers of interest to both disciplines. The Biological Chemistry program has served as a connection between the two disciplines, and in some summers we have had journal clubs for students and faculty in biochemistry, cell and molecular biology. Within the past two years, we have begun similar overlapping programs with the Physics Department, including selection of outside speakers, student research presentations, and journal clubs. We propose a secondary emphasis on the new programs in neuroscience and environmental science, bringing in speakers whose training is in chemistry and field of research is of interest to students and faculty in these interdepartmental programs. Similarly, during the two summers that the NSF-AIRE award has funded summer research in the social sciences, chemistry and other science programs have had increasing interactions with students working on social science and multicultural projects. The poster session in August of 2000 was the high point of this collaboration, and more events are planned for the future. Skills workshops have been jointly organized, and assessment activities are being managed centrally.

The primary thrust of the interdisciplinary focus will be the inclusion of physics faculty and students in the proposed chemistry summer research program. The relatively small size of the Physics Department precludes a viable REU program of their own. Many of the research interests of the physics faculty are in fields that closely border traditional chemistry research fields. For example, this past summer two physics students worked with two faculty on the development of an atomic cooling and trapping apparatus. A third student worked on the computational modeling of the motions of colloidal suspensions in response to electric fields. The department also has an active research effort underway in the growing field of “optical tweezers,” in which there are many fascinating applications for biological systems. Finally, the newest faculty member in the Physics Department is an experimental biophysicist with an interest in the physical properties of helical ribbons. The faculty in the Physics Department see their participation in the Chemistry REU program as a wonderful opportunity for them to broaden their collaborative efforts with members of our department. Most importantly, chemistry and physics students will be able to find relationships between common concepts, and overcome the tendency to compartmentalize what they learn.

Organizational Structure:

All of the continuing members of the chemistry faculty have participated in past REU programs and have supervised undergraduate summer research students. We expect eight to ten faculty members to

participate each summer and supervise two or more students, including at least one supported by the REU program. Although the faculty participants may vary each year, they will all be tenured or tenure-track Chemistry and Physics faculty.

Professors Chris Arumainayagam and David Haines will share the duties of program director during the grant period. The program director will publicize the programs, coordinate the selection of participants, assign participants to faculty advisors, arrange seminars and field trips, oversee the day-to-day functioning of the program and the budget, and report on the program. Most of these activities will be done in consultation with the program director for the Biological Sciences summer program, the summer research coordinator for the Physics Department, the faculty director of the Science Center, and the program directors for social science and multicultural programs. The ten-week summer research program will begin the day after Memorial Day.

Institutional Commitment:

The College administration has demonstrated its strong support for the Chemistry Department's research endeavors, particularly the summer program, in a variety of ways aside from substantial budgetary support for facilities, equipment, and staff. All College facilities, including libraries, computing, and athletic and sports facilities will be available to all participants. Housing in College dormitories will be available to participants at cost. In addition to faculty research grants and an annual allowance for faculty travel to professional meetings to present their work, the College now provides stipends to faculty who supervise summer student research. The stipend is small for the amount of time invested, but is of great symbolic importance to the participating faculty, and represents a major expenditure by the College, given the large number of faculty involved. The Dean's Office also partially funds summer student travel to professional meetings, and supported summer workshops on public speaking for all research students in 2000. Following this year's all-campus poster session, the Dean's Office sponsored a celebratory dinner for all participants and their advisors representing 16 departments and programs. The College has also provided funding for assessment and evaluation activities associated with summer research. In recognition of the importance of the REU program to the education of Wellesley College students and to the research environment of the Chemistry Department, the College administration has agreed not to request an administrative allowance in this grant. Most importantly, College and other funding sources will be used to support approximately 15 chemistry and physics summer students each year in addition to the ten to be funded by NSF-REU.

(b) Nature of Student Activities:

(1) *Student Research Projects*: Each student will work for ten weeks on a specific research project in collaboration with a Wellesley College Chemistry faculty member. The program directors will coordinate the assignment of student participants to particular faculty advisers to assure an optimum match in needed background and mutual interests. All summer chemistry students and faculty will participate in weekly meetings in which each of the students will give at least one formal oral presentation during the ten-week period. Most labs hold daily or weekly group meetings at which students informally discuss results. Some of these meetings include faculty and students from collaborating labs across disciplinary lines. Several examples of student research projects are given below.

- (i) *The Synthesis and Degradation of a Unique Bacterial Polymer*: An interdisciplinary team of faculty (Professors Nancy Kolodny, Mary Allen, and Adele Wolfson) and students in chemistry, biological chemistry and biology is investigating the synthesis and degradation of the only known non-protein polymer whose function is the storage of nitrogen, cyanophycin (multi-L-arginyl poly-[L-aspartic acid]). The metabolism of this polymer is being studied by enzyme analysis and purification and by *in vivo* and *in vitro* NMR spectroscopy after labeling cyanobacteria with ¹⁵N-labeled nitrogen sources.

Nitrogen metabolism is investigated during normal growth and during growth under various conditions of nutrient stress, including nitrogen starvation, light limitation, and blocking of ribosomal protein synthesis with chloramphenicol. Experiments have been designed to determine whether cyanophycin has a dynamic role in cyanobacterial metabolism.

Little is known about the mechanisms for the synthesis and degradation of cyanophycin, although it accumulates in large amounts during nutrient stress and during nitrogen fixation. It is mobilized when cyanobacteria are starved for nitrogen. If cyanophycin is an obligatory intermediate in the flow of nitrogen into the metabolic pool, its role in cyanobacteria will be central. It is therefore important to understand regulatory strategies and how storage is integrated with intermediary metabolism. Studies of the mechanisms involved in specific environmental responses will provide new information about gene regulation and pathways leading from the sensing of environmental signals to the regulation of enzymatic activities.

Recently, a new technique has been developed by this team that utilizes ^1H NMR spectroscopy of cyanophycin isolated from small volumes of cyanobacteria to determine both the amount of cyanophycin produced and the relative extent of ^{14}N and ^{15}N labeling. This technique has been used successfully by students to study cyanobacteria grown under a variety of stressful conditions. In addition, gel electrophoresis of the cell samples has indicated the production of at least one unique protein at levels varying with time under stress. Each of these techniques holds great promise for projects that study a wide range of wild type and mutant cyanobacteria under conditions of environmental stress.

- (ii) *Electron-Induced Reactions in Halocarbon Nanoscale Thinfilms*: Students working in Professor Chris Arumainayagam's laboratory will study the interactions of low-energy electrons with halocarbons using post-irradiation temperature programmed desorption (TPD). They have recently demonstrated that the exposure of multilayers of an adsorbate to low-energy (≤ 55 eV) electrons under ultrahigh vacuum (UHV) conditions ($p \sim 1 \times 10^{-10}$ Torr) followed by temperature programmed desorption is an effective method to investigate a variety of electron-induced reactions including ion-molecule and radical-radical reactions. Their experimental protocol to study radiation chemistry has been well received by the scientific community, as evidenced by an invitation to present a plenary lecture at an international symposium organized by the Department of Energy titled Research Needs and Opportunities in Radiation Chemistry. Additional invited talks include the annual meeting of the Radiation Research Society (1996) and the Gordon Research Conference on Radiation Chemistry (1998). It is noteworthy that the basis of these invited talks is research done exclusively at Wellesley College with B.A. candidates.

Understanding the decomposition of halocarbons by low-energy electrons could provide critical new concepts of importance to the emerging cold plasma technology aimed at on-site, cost-efficient destruction of hazardous halogenated organic compounds. Although relatively high-energy (100 - 300 keV) electrons are utilized to produce the cold plasma, it is the low-energy (≤ 15 eV) secondary electrons that are postulated to initiate the decomposition of the halocarbons. Among the objectives of the proposed research are:

- Identify all of the electron-induced reaction products of each halomethane. The post-irradiation TPD method is particularly useful in identifying labile products as shown by the first identification of methoxymethanol ($\text{CH}_3\text{OCH}_2\text{OH}$) as a reaction product of electron-induced reactions of methanol (CH_3OH).
- For each reaction product, the dependence of the yield on electron fluence (electron flux multiplied by exposure time) will be probed. Such studies will yield valuable information on the optimum electron beam dose necessary for the decomposition of halocarbons.

- The dependence of the reaction cross section on initial electron energy for each reaction pathway will be investigated to obtain additional information regarding the dynamics of electron-induced dissociation of chloromethanes. Such studies will provide insight into the relative roles of electron impact ionization and dissociative electron attachment (DEA) in the decomposition of halogen containing organic molecules.

(iii) *Identification of Blue Pigments in Yoruba Painted Sculpture*: A group of chemistry and art history students working with Professor Merritt and staff members of the Wellesley College Davis Museum have initiated a project to identify the blue pigments in African wood sculptures. The overall project goal is to determine if ultramarine, the blue of 20th century painted Yoruba wood sculpture, was the pigment used by West African artists in the 19th century. Manufactured ultramarine, readily available in the form of laundry bluing traveling with British and French colonialists, has been incorporated into indigenous art globally including Yorubaland. Reckitts, the largest producer of laundry blue, began to export this product to West Africa in the late 1880's or early 1890's in a product called Bag Blue. Consequently, Yoruba art collected prior to 1880 should contain only the blue pigment used by Yoruba artists prior to contact with British traders. The work of this team seeks to answer the following questions: (1) Was ultramarine the traditional blue pigment of the Yoruba artists for painting Gelede masks and other carved wood ceremonial objects? Or did the laundry product replace the less vibrant blue of indigo, widely used in other Yoruba art and produced locally? (2) If ultramarine is found in 19th century Yoruba art, was it the form extracted from the gemstone lapis lazuli, used in European art prior to the 1850's, or was there indigenous manufacture of this pigment? Answers to these questions will provide insight into Yoruba cultural practices of the late 19th century.

In the last two years, the appropriate microscopic and infrared spectroscopic equipment has been acquired and procedures developed to remove small (< 2 mm in diameter) paint chips from art objects and to identify the pigments in these samples. Student teams have applied these procedures to a 20th century Gelede mask from the Davis Museum and other Yoruba masks obtained specifically for this project. They have identified the blue as ultramarine. Microscopic studies show that the appearance of this pigment in some masks is consistent with the form found in laundry blue, but in others, consistent with lapis lazuli-derived ultramarine. The proposed REU project will expand these preliminary studies and apply microscopic and infrared methods to 19th century Yoruba wood sculptures from other museum collections. The results will be combined with historical and archaeological data to determine the relative influence of trade and indigenous technology on Yoruba cultural practices in the 19th and early 20th century. Samples for laboratory work at Wellesley College will be collected in collaboration with museum scientists and conservators.

(2) *Seminar series*: All students will participate in the weekly seminar series that introduces them to practicing chemists, biochemists, and other scientists from outside Wellesley College. The seminar program will be open to all Wellesley College summer research students and faculty. The weekly REU seminar series will be jointly sponsored by the Chemistry/Physics and Biological Sciences programs, as was done during previous REU grants. Speakers will be chosen for their wide appeal, and there will be particular emphasis on interdisciplinary research. Since Wellesley's Reunion coincides with the first weekend of the summer research program, we have traditionally invited one of the department's recent, highly accomplished, graduates to give the first seminar of the summer. These alumnae provide identifiable role models for students and offer current career advice. Refreshments before the seminar or dinner afterwards provide additional informal opportunities for discussions with the speakers.

(3) *Career Panel*: A career panel has become a fixture of the summer program. Each year, we invite a group of professionals whose undergraduate degrees were in chemistry or other scientific fields, who are currently working in sectors other than academia or medicine, to discuss their career paths. Recent speakers have included patent attorneys, employees with dot-com start-ups, scientists at biotech or

pharmaceutical companies, high school teachers, physical therapists, management consultants, and environmental consultants.

(4) Graduate School Panel: We also plan to continue scheduling one panel each summer devoted to discussions of graduate education in the sciences: whether to go, how to apply and choose a school, and what to expect when you are there. Wellesley alumnae attending local graduate programs will be invited, as well as members of the Wellesley faculty who have recently completed their graduate training.

(5) Field trips: Two field trips each summer to local industries will also serve to expose the REU participants to career possibilities in the industrial sector as well as broaden their background in chemistry. Most recently, groups visited Boston Scientific and Creative Biomolecules. We will broaden the choice of companies to those at the interface of chemistry and physics such as Polaroid.

(6) Public speaking workshop: Beginning this past year, Wellesley College has made a major commitment to the improvement of students' public speaking skills. As part of this emphasis, the Learning and Teaching Center hired outside consultants to work with summer research students. Three sets of workshops were conducted, one each for students in the natural sciences, social sciences and multicultural programs. Chemistry students attended two two-hour workshops, where such topics as organizing and outlining a research presentation, the use of graphics, delivering a research talk, speaking apprehension, and preparing a poster presentation were discussed. Evaluations completed by students afterwards led to some suggestions that will be implemented in future workshops, including more input from faculty and more actual practice.

(7) Poster preparation workshop: Also for the first time this year, a faculty member in the Art Department offered an afternoon workshop on the visual aspects of a poster presentation and was available for consultation in the week before the final poster session. Although this activity was particularly aimed at the non-science students who had never presented data in a poster format, it was also useful for the science students, particularly the non-Wellesley participants. We propose to include this workshop in future programs, given the large number of students making off-campus presentations, especially at the spring national meeting of the ACS.

(8) Scientific writing workshop: The Writing Program at Wellesley offers a number of workshops for students and faculty during the academic year. During 1999-2000, the director of the Writing Program, together with a faculty member from the Chemistry Department, organized a series of workshops for faculty on writing in science courses. We propose that some of the ideas that emerged from these workshops – how to keep a laboratory notebook, writing for publication, review and revision, presentation of numerical data, differences in style among disciplines – be used to develop workshops for students in the summer program, one early and one later in the summer. Analogous to the public speaking and poster workshops, the writing workshops would be followed by office hours for consultation. Students will be expected to submit a paper on their research project at the beginning of the fall semester.

(9) GRE preparation: In January of 2000, Wellesley joined a group of women's colleges in proposing a large collaborative grant to develop GRE prep courses that would help to raise women's scores on the general portion of this test and thereby increase the numbers of women pursuing scientific careers. We propose to offer a course to prepare science students for the GRE as part of our summer research program. The course will be approximately eight weeks long, five evening hours of classroom time each week, and will be taught by an instructor recruited from the Wellesley faculty or staff. It will be modeled on the successful Baylor program, with pre-tests, identification of skills and weaknesses, and practice on the types of questions needing improvement. The Baylor program began during the summer in order to target students who may have had their first recognition that graduate school is what they seek because

they were enjoying research. The GRE preparation course will be offered as an optional activity to our summer research students, and they will have first priority in enrolling. The College is very interested in this project and has committed to continue it past the funding period if successful. Our interest in this pilot offering is not just the benefit that will come to the participating students, but also what the analysis of their experience will teach us about how our students perform on standardized tests in general. We propose to conduct focus groups with the students at the end of the course, and also to follow this group of students, matched with a group of similar students who did not participate. We hope that by doing this type of analysis we can apply the lessons learned from this program to other measures that may be obstacles to women's success.

(10) Poster Sessions: The final poster session is a culmination of the summer's research activities. Participants from across campus display their posters in the Science Center. A formal abstract booklet is printed and distributed. Invitations are issued to all offices on campus, as well as to the home institutions of non-Wellesley students and to local politicians. The President and Deans of the College often attend. The level of presentation and discussion is very professional, and the students' posters rival those at many national scientific meetings.

(c) Research Environment

(1) Institutional research environment:

Wellesley College is a highly-selective private liberal arts college devoted to the undergraduate education of women. The current enrollment is 2,333 with 2,282 candidates for the A.B. degree, including 120 continuing education (non-traditional) students. The student body is rich in its cultural diversity: 7 % of the full-time students identify themselves as African-American; 1 % Native American; 23 % Asian-American; and 6 % Latina. Approximately 6 % are international students. In the 1999 U.S. News & World Report Best Colleges issue, Wellesley was ranked third for diversity among all national liberal arts colleges, the only New England college to place in the top 10. Wellesley has a need-blind admissions policy, and over half of the students receive financial aid from the College. Teaching faculty include 333 members (full-time equivalent of 225); 99% of the tenured and tenure-track faculty hold doctorates or the terminal degree in their field. Fifty-three percent of the tenured faculty are women. Of the tenured faculty 17 % are members of minority groups, and of those on the tenure track, the proportion is 27 %.

The mission of Wellesley College is long-standing and widely affirmed: to provide an excellent liberal arts education for women who will make a difference in the world. Among our greatest strengths are the clear vision and central commitment of faculty to mentoring students. Wellesley has a long tradition of engaging students in course related laboratory work and collaborative research with faculty, believing that students should discover principles for themselves, start research as early as possible, and do hands-on science. A number of recent innovations and interdisciplinary connections have expanded collaborative and mentoring relationships. These activities include:

- (1) The annual Ruhlman Conference: This is a College-wide forum for presentation and celebration of student work in all fields. Classes are canceled for the day so that faculty, staff, and students can attend the talks, posters, panel discussions, and performances. Over 200 students participate each year, including many of our summer research students. A major focus of the event is interdisciplinary work.
- (2) First-Year/Sophomore Mentoring Program: To encourage more students from underrepresented groups to pursue scientific careers, Wellesley initiated a minority-mentoring program in 1994, with funding from the Howard Hughes Medical Institute, GTE and the College. The program has now been extended to admit participants based on economic and other disadvantage as well as on

our original criteria. Up to 20 first and second-year students are placed in faculty research labs. The program also includes career seminars, workshops on study skills, and oral and poster presentations. Students are enthusiastic about the experience, commenting on the confidence they have gained in doing research.

- (3) Extension of the summer research programs to areas outside of the sciences: In 1998, NSF recognized Wellesley's success in building and supporting an effective research community in the sciences with one of ten awards nationally to undergraduate institutions for the integration of research and education (AIRE). This award has allowed the establishment of a summer research program in the social sciences modeled on that in the Science Center. The director of that program, together with the director of multicultural summer research, met regularly with the PIs of the Chemistry and Biological Sciences REU site programs and the faculty director of the Science Center to coordinate summer activities in 2000. The result has been an environment of excitement about scholarship, discussions that bridge disciplines and sub-disciplines, and better understanding of the nature of research in different fields.

Wellesley's ten-year reaccreditation visiting committee report in 1999 specifically noted that, "An area in which Wellesley faculty, especially in the natural sciences, have excelled is in establishing research partnerships with students. It has become the norm at Wellesley for science faculty to do research in collaboration with students, both during the summer and during the academic year ...Long a leader among 'research colleges' in the sciences, Wellesley is now extending this model into other areas..."

The scientific environment at Wellesley appears to be not only nurturing and collaborative, but also productive in terms of the quality of research done by its faculty and students. In a recent survey of publications and their impact as measured by the number of citations, the average impact of papers produced by Wellesley authors was double the world average for all papers indexed by the Institute for Scientific Information.

(ii) Chemistry Department Research Environment

The Chemistry Department has its own traditions of strength in teaching and research going back 125 years. Members of the department have garnered many of the College's teaching awards as well as external awards related to teaching. In addition, faculty members have had and continue to have successful research programs. The research of faculty members in the Chemistry Department has appeared in numerous publications and presentations at regional, national, and international meetings, and has led to major research grants and invitations to speak at other institutions. Undergraduate students, especially those doing research during the summer, have co-authored most of the presentations and papers that come out of this department. A snapshot of such activities and events is given below.

- (1) Jim Loehlin's research, focused on alcohol/amine cocrystals involving saturated hydrogen bonding (SHB), received international recognition when a feature article in *Chemical & Engineering News*, December 11, 1995, 33-34, cited his research and that of the other three groups in the world known to be active in research on these SHB structures. In August of 2000, he delivered an invited talk at the annual meeting of the American Crystallographic Association.
- (2) Nancy Kolodny's research involving magnetic resonance imaging of ocular disorders and NMR studies of cyanobacterial metabolism resulted in her receiving the Guggenheim fellowship in 1991 for "unusually distinguished achievement in the past and exceptional promise for future accomplishment." The Camille and Henry Dreyfus Scholar award she received in 1990 enabled her to appoint a recent Ph.D. recipient as a Camille and Henry Dreyfus Fellow.
- (3) Michael Hearn's research accomplishments were recognized when he was appointed Associate Editor of *Organic Preparations and Procedures International*. Michael's research work involving

the development of new compounds for treatment of tuberculosis has been featured in numerous invited talks, including his plenary lecture at the international symposium "Academia and Industry Propelling Chemistry into the New Millennium" in Hyderabad, India, this year. Under the advice of Wellesley College counsel, he has recently held back on publication, for reasons concerning intellectual property.

- (4) Peggy Merritt's research involving the detection of chiral carbocations using chromatography and isotopic methods for establishing asymmetric solvation of these reactive species resulted in several invited lectures at academic institutions ranging from the University of Minnesota and Brandeis University to the College of Wooster where she was the 1994 James T. MacFarland Lecturer. She is one of 13 members of the Committee on Women Chemists (COACH) whose aim is to "coach women in tenured positions in academia to be leaders in the chemical sciences."
- (5) Flick Coleman's research interests over the past decade have centered on the photophysics of complexes of chromium(III), chromium(VI) and the uranyl ion. He has presented invited research talks at more than 30 Colleges and Universities since 1990.
- (6) Adele Wolfson became, in 1999, the second faculty member in the chemistry department to receive the Camille and Henry Dreyfus Scholar/Fellow award "designed to attract talented Ph.D. recipients to careers in the chemical sciences in undergraduate colleges and universities, and to recognize outstanding research accomplishments by faculty from predominantly undergraduate institutions."
- (7) David Haines' research on the synthesis of nucleoside analogs, and the development of NMR techniques for their structural and conformational analysis, has involved many students in the laboratory, and has resulted in many presentations (12 in the last three years), by the students, at National ACS meetings. His research and his research group were featured in a press release at the San Francisco ACS meeting in the spring of 2000.
- (8) Chris Arumainayagam received a Henry Dreyfus Teacher-Scholar award in 1996 that recognizes "continuing commitment to encouragement and support of undergraduates in the chemical sciences through teaching, mentorship, and research with undergraduate participation." He was recently appointed to the advisory board of the American Chemical Society Petroleum Research Fund.
- (9) Julia Miwa received in 1994 a Camille and Henry Dreyfus Faculty Start-up Grant that was first "introduced in 1993 to provide funding for new faculty members at non-Ph.D.-granting institutions at the start of their research and teaching activities."
- (10) Shane Ohline was the second faculty member in the Chemistry department to receive the Camille and Henry Dreyfus Faculty Start-up Grant in 1996. The AAUW American Fellowship she received in 1999 (one of 16 fellowships given in the arts and humanities, social sciences, and the natural sciences) is supporting her Junior Leave at the University of Oregon where she is investigating the organization of phospholipids at the oil/water interface when perturbed by proteins and antibiotics by using Sum Frequency Vibrational Spectroscopy.

Research and independent investigation pervade the chemistry curriculum, and there is no sharp division between teaching, mentoring, and research activity for faculty. The great majority of courses involve laboratories that require students to develop an experimental plan and interpret data. There is increasing emphasis on the statistical analysis of data; from the introductory level on, students are guided to ask research-related questions about the reliability of the data they obtain. Examples from faculty members' research and from the current literature are brought into the classroom, and students are encouraged to participate in research early in their Wellesley careers.

Interdisciplinary curricular programs available to Chemistry students complement the theme of this NSF-REU proposal. The major in Biological Chemistry is an interdepartmental program whose administration is shared jointly by the Chemistry and Biological Sciences Departments. In the past 10 years, the number of students graduating with a degree in Chemistry or Biological Chemistry has been between 19 and 41. Two new interdepartmental programs draw heavily from chemistry. Both Neuroscience, which has been in effect for two years, and Environmental Science, currently under review

by the College's Committee on Curriculum and Instruction, include a number of chemistry courses, and majors in these programs may carry out research with members of the chemistry faculty. Individual majors in such fields as Biotechnology, Chemical Physics, and Biophysics have been created in the recent past, and the programs of students planning such majors allow additional opportunities for interdepartmental discussion.

Although students are not required to undertake research, within the past ten years, 76 % of Chemistry majors and 42 % of Biological Chemistry majors have done research for academic credit. In some years, as many as 85 % overall have been involved in research in one form or another during the academic year or summer. The percentage of Chemistry majors participating in on-campus research and the senior thesis program is the highest of any department at Wellesley.

A recent survey of alumnae of selected classes from 1974 to 1995 indicated that 90% of natural science majors enrolled in an advanced degree program after graduation from Wellesley. Our data on Chemistry and Biological Chemistry majors during 1990-1999 suggest that many students work for one or two years before continuing their education. Immediately after graduation, 33 % of Chemistry majors and 16 % of Biological Chemistry majors go to graduate school; 30 % of Chemistry and 51 % of Biological Chemistry majors go to health professions schools; 12 % of Chemistry and 14 % of Biological Chemistry majors work in research or other science-related jobs.

(iii) Physics Department Research Environment:

The Physics Department faculty consists of six full-time equivalent professors and three full-time laboratory instructors. The department is committed to creating a challenging, academically rigorous, and supportive environment for their majors. One of their central goals is to prepare their majors interested in graduate studies with the theoretical and practical backgrounds needed for success in high-quality graduate programs in physics and other related fields. The department recognizes that an essential component of this preparation is experience in both independent and collaborative research environments. As such, the Physics Department strongly encourages physics majors to work on independent projects throughout their time at Wellesley.

Faculty research in the department spans a wide range of interests, including experimental research in atomic, optical, and molecular physics, the physics of complex fluids, experimental biophysics, and theoretical research in laser spectroscopy and cavity quantum electrodynamics. The physics department facilities were dramatically upgraded as a result of their relocation in 1990 to the new addition in the Science Center. An NSF College Science Instrumentation Program grant and a grant from the Keck Foundation made it possible to equip one of their teaching laboratories as a "quantum mechanics lab", focusing on optical spectroscopy. In that laboratory, and in the Science Center's collaborative laser laboratory, the Physics Department has access to research-grade spectroscopic instrumentation.

(iv) Chemistry Department Facilities and Support:

The Chemistry Department is housed in the Science Center, along with all of the other science departments, the Science Library, and classrooms and laboratories for teaching and research. Wellesley's supportive infrastructure contributes to the strength of our research programs. A major Science Center expansion and renovation, completed in 1991, was specifically designed to bring together in one building all of the natural science departments, allowing efficient sharing of resources and easy interaction and intellectual cooperation across disciplinary lines.

The College enjoys equipment and facilities comparable to those at many research universities. Major grants from outside funding agencies, as well as the generous support of the College, have helped to equip the department and interdepartmental programs. Grants from the Howard Hughes Medical Institute and several NSF programs have enabled the chemistry department to purchase two NMR spectrometers (300 MHz and 400 MHz), differential scanning and isothermal titration microcalorimeters, a GC-MS system, capillary electrophoresis and ion chromatography equipment, and sophisticated computer workstations and software for computational chemistry and modeling. The most recent grant from the Howard Hughes Medical Institute includes funds for a new fluorimeter, as well as equipment for image analysis to be shared with Biological Sciences. Specialized Science Center facilities likely to be used by chemistry and physics research students and faculty include two x-ray generators with single crystal cameras and a powder diffractometer, an atomic force microscope, an ultrahigh vacuum chamber (equipped with a mass spectrometer, low energy electron diffraction and Auger electron spectroscopy), a laser laboratory (equipped with a nitrogen laser, nitrogen pumped dye laser, YAG laser, YAG pumped dye laser, one meter and several 0.5 meter spectrometers, and single photon counting detection), a Cary 500 spectrometer with capabilities in the UV-VIS-NIR regions, several high-end FTIR systems (one with remote sampling capabilities), two computer laboratories (equipped with 25 400MHz Pentium PC's, one SGI Iris Indigo and two SGI O₂ molecular modeling workstations), complete animal care facilities, a well-equipped student machine shop, a high frequency direct current spot welder, laminar flow hoods, autoclaves, five walk-in environmental rooms, cold rooms, and culture rooms.

Other resources available to support the summer research experience include the Science Library that contains over 106,000 volumes and maintains subscriptions to more than 626 periodicals. On-line literature searching and on-line access to several journals is available to students and faculty through the Science Library, and from other networked computers. The professional staff of the library offers a series of training sessions each summer for the participants in the use of the library resources. A wide variety of computers are available for student use. The Information Technologies Services provide extensive computer consulting services and resources. The Science Center staff includes a full-time PhD scientist who specializes in advanced instrumentation including NMR spectrometers. Additional support personnel include an instrument technician, a toolmaker, stockroom staff, purchasing officer, a full-time director, and other office staff.

(d) Student Recruitment and Selection:

The ten students to be fully supported by the NSF-REU funds will be selected each summer on the basis of their academic record, a written application, and two letters of recommendation from science faculty members. It is expected that approximately half of the group of students fully supported by this grant will be Wellesley students, with a preference for rising sophomores or juniors. We propose that two of the REU slots be reserved for Physics students working with Physics faculty. At least half of the participants will be non-Wellesley students.

a. Wellesley Participants.

The Wellesley College participants in the REU program will all be women and will include a significant percentage of minorities, reflecting College demographics; approximately one-third of the participants in the previous REU programs have been members of minority groups. The inclusion of participants from the first-year/sophomore (minority) mentorship program should continue to increase the number of under-represented minorities in the summer research program.

The programs will be publicized at Wellesley via the Web and an electronic bulletin board early in the second semester with applications due March 1 and announcements of awards made prior to Spring Break at the end of March. At least two weeks will be given for students to make a decision regarding the

award offer. Beginning in 2000, the application was made available electronically, and a single application served for all Science Center-based programs. In addition to the general publicity for the summer research programs, Chemistry faculty members will hold several late afternoon sessions in which they briefly describe their research interests, as part of our departmental seminar program.

The College has been aggressive in seeking non-government funds to support student research stipends in the sciences. Grants from the Howard Hughes Medical Institute (three awards from 1988-2000, with a fourth award recently announced) have provided funds for approximately 16 fellowships for students working with Wellesley faculty members each summer. Approximately seven of these competitive fellowships were awarded to chemistry students each year during 1998-2000. Other College and foundation funds have provided summer stipends for an average of six additional students in chemistry each summer. In addition, Wellesley students will be encouraged to apply for external grants to support summer research at Wellesley such as the James Flack Norris Award of the Northeast Section of the ACS and those awarded by the Council on Undergraduate Research. Successful applicants, regardless of the source of their financial support, will be full participants in all NSF-REU sponsored activities including the student workshops, career panels, seminars, field trips, and final poster session.

The interactions between Chemistry and Physics within the past year have been so successful that we propose to include physics students and faculty more formally in the chemistry program. In 2000, three physics students, two of them rising sophomores, working with three physics faculty members, participated in weekly meetings and seminars with chemistry, biology, and computer science students. Although physics research has been carried out in previous years, the students were not part of an organized program and worked in relative isolation. The small number of physics students does not allow for a separate program in that field, but they can be well integrated into the chemistry program.

As summer research on campus expands, it is particularly important that the Chemistry Department maintain its own source of funding, so that we can target particular groups of students and have a strong voice in programming seminars and other events. One of the strengths of the Chemistry Department's program and its success in attracting and retaining outstanding students in chemistry-related research has been its inclusion of talented rising sophomores in its summer research program. Most College-sponsored summer fellowships are not often awarded to these less experienced students. Similarly, the Chemistry Department has been a strong proponent of including students who are not chemistry majors in our research programs. During the past three years of NSF support, students from nine majors other than Chemistry and Biological Chemistry have participated in summer research in the department, and most of these students have continued in science after their graduation from Wellesley College. We feel strongly that the inclusion of both non-majors and highly promising, but inexperienced research students is crucial to the success of our program, and to the education of future citizens. REU funding has allowed us the flexibility to choose students according to these criteria.

b. Non-Wellesley Participants.

All of the participating faculty members at Wellesley College have expressed a commitment to take non-Wellesley, as well as Wellesley, students into their research laboratories. Our major focus in soliciting outside applicants has been, and will continue to be, to attract students from other women's colleges and from institutions with limited facilities for on-site research. However, the non-Wellesley students will not be limited to women. The most effective means of publicity appears to be the Web, through both the NSF site and our own. The Science Center, Chemistry, and Physics web sites will showcase recent student research activities. In addition, we will continue to send mailings to local chemistry departments, and will now include physics departments. Education departments with science teacher training programs will also be targeted. All application materials will be available either on-line or as paper versions. For non-Wellesley students, spending the summer at a women's college where the

science faculty is approximately 50% female will be an important component of their experience. Not only will women science faculty provide positive role models for those students who may not be exposed to women scientists on a daily basis, but the institutional support that Wellesley provides to women in science will serve as an example which visiting students can take back to their own colleges.

(e) Project Evaluation and Reporting:

Assessment and evaluation of the summer research program will be done in consultation with Wellesley's Office of Institutional Research (OIR). In addition to its primary function to provide the College administration with institutional information that can be used in making policy decisions, the office works with other campus groups that are conducting surveys on institutional functions, analyzing institutional data, or evaluating programs. Staffed by two FTE professionals, an administrator and student interns, OIR often calls upon advisory groups of faculty, administrators, and outside consultants to work with them in posing the most fruitful research questions and interpreting the findings.

Extensive non-REU funding will be available to perform comprehensive assessment of the proposed Chemistry summer research program. Grinnell, Hope, Harvey Mudd and Wellesley College have just received a grant from the ROLE program at NSF in the Division of Research, Evaluation and Communication for Dr. Elaine Seymour (University of Colorado) and Dr. David Lopatto (professor of psychology at Grinnell) to do a "Pilot study to establish the nature and impact of effective undergraduate research experiences on learning, attitude and career choice." As a prelude to this project, Dr. Seymour conducted in-depth interviews this past summer with rising seniors in chemistry and biology and their faculty supervisors. Mandatory evaluations, to be done electronically, will include a section requesting narrative comments in addition to a section that asks about specific skills gained during the summer research experience. As in past years, student evaluations will be used to shape and refine the program in such areas as the seminar speakers and journal clubs. In addition to performing evaluations and obtaining student demographic data, we will also follow outcomes such as career plans and majors.

Faculty were also asked this summer to complete a confidential assessment of the research program. Their comments will be collected and summarized with help from the Office of Institutional Research, and may help in recruiting more faculty for research programs, especially outside of the sciences.

(f) Results from Prior Support (1998-2000) NSF Grant CHE-9732409 (\$171,000)

The NSF-REU grant provided funds that fully supported a total of 29 (13 Wellesley and 16 non-Wellesley) chemistry student fellowships during three summer sessions of ten-weeks' duration during the period 1998-2000. An additional 37 chemistry summer research fellowships were funded from other sources over this three-year period. Because some students participated in more than one year, a total of 55 different students took part in summer programs in the Chemistry department over this period. All chemistry students, regardless of the source of funding for their stipends, participated equally in all of the various programs and activities supported by the NSF-REU grant. Eleven of the twelve continuing members of the regular Chemistry Department faculty served as a faculty advisor for at least one summer during this grant period. Some details of the 2000 summer research program, including the schedule of events and photographs of the student participants, can be found at the following site:
<http://www.wellesley.edu/Sumres/main/main.htm>.

Wellesley College student participants were recruited by announcements in chemistry classes, posters, electronic conferences, and a web site: <http://www.wellesley.edu/Chemistry/insidereu.html>. An analogous web site for non-Wellesley students greatly facilitated recruitment of students outside the New England area. Students from New England were also recruited by letters to the Chairs of Chemistry

Departments of approximately 50 colleges and universities. Each year, 25-30 non-Wellesley students completed applications. Our success rate in recruiting the accepted non-Wellesley students has been approximately 90 %.

Of the 55 undergraduates carrying out summer research in the Chemistry Department in this period, eight worked for two or more summers; two were male (both REU participants), 5 had just completed their first year (three REU participants), eight were black (African, African-American or Caribbean) (two REU participants), and twelve were Asian or Asian-American (six REU participants). Two high school teachers did summer research in chemistry with funding from the Howard Hughes Medical Institute. Sixteen of the Wellesley participants did senior honors research following their summer experience, an additional 6 did other research for academic credit, and others continued their work for pay or on an informal basis. Of the 23 Wellesley students who have graduated since their summer research, 5 are currently in medical school, 5 are in graduate school in chemistry or biochemistry, and 7 are working in scientific fields. An additional three non-Wellesley students are known to be in graduate school, and two in medical school. The Wellesley students who participated in our summer programs in this period have garnered a number of College and national awards, including one Goldwater Scholarship, one Beckman Fellowship, three Phi Beta Kappa elections, the first student summer prize from the Sequella Global Tuberculosis Foundation, one NCAA post-graduate student-athlete award, five of the highest awards given by the chemistry and biology departments at the College, and one Schiff Fellowship, granted to seniors carrying out senior honors research. A non-Wellesley REU participant was the recipient of a Luce Fellowship.

Several social events and many lunches were scheduled to enhance the sense of community. The outside students, who would welcome even more orientation and social programming, especially appreciated these events.

Student participants completed an electronic and written evaluation of the program during the last week of the program. Almost all aspects of the program appear to have improved over the three years of this grant period, judging from student comments. In the past, students found that the outside speakers were not useful or misjudged their audience, but the most recent evaluations indicated that the outside seminars were excellent. Faculty guidance with projects also appears to be more appropriate than in the past. The least valuable aspect of the program was found to be the poster skills workshops, and we will work with the Learning and Teaching Center to improve this presentation. Students also asked for more interaction with biology students in this last year, when there was more formal programming with physics, and for more field trips.

Listed below are publications and presentations with student co-authors during the award period (1998-2000). All students are indicated with an asterisk; summer research students are underlined; the two high school teachers are not starred):

Publications:

1. K.T. Queeney, **C.R. Arumainayagam**, *A. Balaji, and C.M. Friend, "Carbon-Carbon Coupling from Formaldehyde Reaction on Mo(110)," *Surface Sci.*, **418** (1998) L31-L38.
2. *Elizabeth Ferrenz, *Andinet Amare, and **Christopher R. Arumainayagam**; "An improved method to spot-weld difficult junctions." Submitted, *Review of Scientific Instruments* (2000).
3. **James H. Loehlin**, *Katherine J. Franz, *Lauren Gist and *Rebecca H. Moore; "Supramolecular Alcohol-Amine Crystals and Their Hydrogen-Bond Patterns," *Acta Crystallographica*, **B54**, 695-704(1998).
4. Lawrence, B.L., Suarez, C., *DePina, A., *Click, E., **Kolodny, N.H.** and Allen, M.M., "Two Internal pools of soluble polyphosphate in the cyanobacterium Synechocystis sp. strain PCC 6308: an *in vivo* ³¹P NMR spectroscopic study", *Arch. Microbiol.* 169, 195-200 (1998).

5. **Kolodny, N.H., Goode, S.T.***, Ryan, W., Freddo, T.F., "Evaluation of Therapeutic Effectiveness by MR Imaging in Rabbit Model of Anterior Uveitis," submitted, *Investigative Ophthalmology and Visual Science* (2000).
6. ***Erickson, N.A., Kolodny, N.H.** and Allen, M.M., "A Rapid and Sensitive Method for the Analysis of Cyanophycin," submitted, *Applied and Environmental Microbiology* (2000).
7. **Shane M. Ohline, *Mary L. Campbell,** Marilyn T. Turnbull and Susan J. Kohler; "Differential Scanning Calorimetric Study of Bilayer Membrane Phase Transitions: A Biophysical Chemistry Experiment." Submitted *J. Chem. Ed* (2000).
8. ***Erika Cervasio, *Cynthia Soroos, *Jennifer Williams, and William F. Coleman;** "Cr(VI)-Cr(III) Energy Transfer in $[\text{Cr}(\text{NH}_3)_6]_2[\text{Cr}_2\text{O}_7]_3$ ", accepted *J. Luminescence* (2000).

Presentations:

1. ***T.D. Harris, *D.H. Lee, *M.Q. Blumberg, and C.R. Arumainayagam;** "Radiation Chemistry Studies Using Surface Science Techniques" Research Needs and Opportunities in Radiation Chemistry Workshop, Chesterton, In. Department of Energy, Office of Basic Energy Sciences (1998).
2. ***T.D. Harris, *D.H. Lee, *M.Q. Blumberg, and C.R. Arumainayagam;** "Radiation Chemistry Studies Using Surface Science Techniques." Gordon Research Conference on Radiation Chemistry, Newport, RI (1998).
3. Katie T. Queeney, ***Khanh Nguyen, Christopher R. Arumainayagam** and Cynthia M. Friend; "Carbon-carbon coupling from formaldehyde reaction on Mo(110)." 217th ACS National Meeting, Anaheim, CA (1999).
4. Katie T. Queeney, ***Khanh Nguyen, Christopher R. Arumainayagam** and Cynthia M. Friend; "Carbon-carbon coupling from formaldehyde reaction on Mo(110)." American Vacuum Society National Meeting, Seattle WA (1999).
5. ***Elizabeth Ferrenz, *Andinet Amare, and Christopher R. Arumainayagam;** "An improved method to spot-weld difficult junctions." 219th ACS National Meeting, San Francisco, CA (2000).
6. **David R. Haines, *Lisa D. Heyden, *Pauline Johnston and *Jennifer Huang;** "Synthetic studies of imidazotriazole nucleoside analogs," 215th ACS National Meeting, Dallas, Texas (1998).
7. **David R. Haines, *Emily A. Milsovic and *Rayane Moriera;** "Carbon-Carbon bond formation: Strategies for an inosine analog," 215th ACS National Meeting, Dallas, Texas (1998).
8. **David R. Haines, *Junko Takeshita, *Kyleigh Geissler, *Tim Briggs, *Meghana Hate and *Suzanne Johnston;** "Imidazotriazoles as adenosine and inosine nucleoside analogs," 215th ACS National Meeting, Dallas, Texas (1998).
9. **David R. Haines, *Caroline B. Faris, *Junko Takeshita, *Kyleigh Geissler and *Mary E. Harris;** "Synthesis and ribosidation of chlorotriazole," 215th ACS National Meeting, Dallas, Texas (1998).
10. ***Katherine Doerr and David R. Haines;** "Formation of carbon-carbon bonds at the C3 position of 1,2,4-tiazoles." 217th ACS National Meeting, Anaheim, CA (1999).
11. **David R. Haines, *Yoori Lee and *Amanda Doran;** "Direct cyanation of 4-phenyl-[1,2,4]-triazole using electrophilic cyanating agents." 219th ACS National Meeting, San Francisco CA (2000).
12. **David R. Haines, *Lisa M. Wittenhagen and *Katherine A. Doerr;** "Synthesis of a xanthosine analog through C3 triazole substituted intermediates." 219th ACS National Meeting, San Francisco, CA (2000).
13. **David R. Haines, *Nancy L. Kesek, *Suzanne Johnston and *Karlene Boswell;** "Synthesis of 3-substituted-7-phenyl-[1,2,4]-triazolo-(4,3-b)-triazoles." 219th ACS National Meeting, San Francisco, CA (2000).
14. **David R. Haines, *Amanda C. Doran, *Yoori Lee and *Lisa M. Wittenhagen;** "Relative reactivities of N-1 and N-4 phenyl-[1,2,4]-triazoles." 219th ACS National Meeting, San Francisco, CA (2000).
15. **David R. Haines, *Angelyn K. Larkin, *Amanda Doran, *Lisa M. Wittenhagen, *Meghana Hate, and *Elizabeth Harris;** "Synthesis of selectively ribosidated [1,2,4]-triazoles." 219th ACS National Meeting, San Francisco CA (2000).

16. *Meghana Hate, **David R. Haines** and *Lisa Wittenhagen; "Synthesis of an adenosine analog via a cyanotriazole intermediate." 217th ACS National Meeting, Anaheim, CA (1999).
17. *Irene M. Lee, **David R. Haines** and *Margaret Lippincott; "Halogenation of heterocyclic compounds with halo-succinimides." 217th ACS National Meeting, Anaheim, CA (1999).
18. *Connie Chang and **Shane Ohline**; "Surface orientation of dye molecules adsorbed on quartz using second harmonic generation and atomic force microscopy." 217th ACS National Meeting, Anaheim, CA (1999).
19. **Shane M. Ohline**, *Sunyoung Lee, *Connie Chang, and Stacie Williams; "Dye Aggregation on Quartz Surfaces: Quantification by UV-Vis Spectroscopy and Atomic Force Microscopy." 220th National ACS meeting, Washington D.C. (2000).
20. **Shane M. Ohline**, *Mary L. Campbell, Marilyn T. Turnbull and Susan J. Kohler; "Differential scanning calorimetric study of phospholipid bilayer phase transitions: A biophysical chemistry experiment." NSF Symposium on for ILI and CCLI catalyzed work, 220th National ACS meeting, Washington D.C., (2000).
21. *Stephanie Goode, Anne Sheffield and **Shane Ohline**; "Towards imaging biomembranes: Atomic force microscopy." 217th ACS National Meeting, Anaheim, CA (1999).
22. **Jean Fuller-Stanley** and *Rachel Gershman; "Si-29 and C-13 NMR studies of some diisopropylsilanes." 217th ACS National Meeting, Anaheim, CA (1999).
23. Mona L. Hall, *Christine A. Guth, Susan J. Kohler and **Adele J. Wolfson**; "Advanced instrumentation projects for first-semester biochemistry laboratory." Amer. Soc. Biochem. and Molec. Biol., Boston MA, Abs. 1497 (2000).
24. *Tsui, C. and **Wolfson, A. J.** "Activation of endopeptidase EC 3.4.24.15 by cadmium ions;" Amer. Soc. Biochem. and Molec. Biol. Annual Meeting, Washington DC, Abs. 696 (1998).
25. *Hieronymus, H.V. and **Wolfson, A. J.** "Kinetic analysis of calcium-mediated activation of Endopeptidase 24.15," Amer. Soc. Biochem. and Molec. Biol. Annual Meeting, San Francisco CA, (1999).
26. **Nancy H. Kolodny**, *Stephanie Goode, W. Ryan and T.F. Freddo; "Evaluation of therapeutic effectiveness by MR imaging in rabbit model of anterior uveitis." Invest. Ophthalmol. Sci. 40 (1999).
27. *Erickson, N.A., **Kolodny, N.H.** and Allen, M.M.; "A rapid and sensitive method for the analysis of cyanophycin." International Society for Phototropic Prokaryotes 2000, Barcelona, Spain (2000).
28. *Medeiros, L., Erickson, N.A., *Bang, S., Allen, M.M and **Kolodny, N.H.**; "1H NMR spectroscopic studies of the formation and degradation of cyanophycin in environmentally stressed Synechocystis sp. strain PCC 6308." International Soc. for Phototropic Prokaryotes 2000, Barcelona, Spain (2000).
29. Kohler, S., Bao, T.*, **Kolodny, N.H.** and Allen, M.M., "NMR analysis of cyanophycin synthesized by the cyanobacterium Synechocystis sp. PCC 6308," Abstracts of the 99th Annual Meeting, American Society for Microbiology (1999).
30. *Heidi M. Curtiss, *Ayla C. Aygun, *Abigail E. Dennis, *Stephanie Goode and **Margaret V. Merritt**; "Blue eyes of Africa: Diffuse reflectance infrared spectral analysis of blue pigment of a Yoruba Gelede mask." Eastern Analytical Symposium, Somerset, NJ (1999).
31. *Ann M. Meyer and **Julia Miwa**; "Synthesis of thiopeptides of varying length." 217th ACS National Meeting, Anaheim, CA (1999).
32. *Sarah Popek and **Julia H. Miwa**; "Synthesis of a thioamide substituted 12-residue peptide." 219th ACS National Meeting, San Francisco, CA (2000).
33. *Olivia Sementi and **Julia H. Miwa** "Synthesis of β -Aspartyl-Arginine," 219th ACS National Meeting, San Francisco, CA (2000).
34. *Laura Margarida and **Julia H. Miwa**, "Substitution of a thioamide into an eight residue peptide via solid-phase synthesis" 219th ACS National Meeting, San Francisco, CA (2000).
35. *Ian Mangion, *Anita Tsai, and **Julia H. Miwa**, "Synthesis of a thioamide inhibitor of endopeptidase EP 24.15," 219th ACS National Meeting, San Francisco, CA (2000).
36. *Michelle Farkas and **Julia H. Miwa**, "Substituent and dihedral angle effects on carbonyl stretching frequency in oxamides" 219th ACS National Meeting, San Francisco, CA (2000).

REFERENCES CITED

References Cited
Not Applicable

Biographical Sketches – Proposal Section E

Chris R. Arumainayagam

Associate Professor of Chemistry

Field: Physical Chemistry

Research interests: Applications of surface and radiation chemistry to environmental problems.

A.B. 1985 Harvard University (Chemistry and Physics)

Ph.D. 1990 Stanford University (Chemical Physics)

Graduate Advisor: Dr. Robert J. Madix

Recent publications (limited to 5) (*indicates undergraduate student co-author):

1. T.D. Harris,* D.H. Lee,* M.Q. Blumberg,* and C.R. Arumainayagam, "Electron-Induced Reactions in Methanol Ultrathin Films Studied by Temperature-Programmed Desorption: A Useful Method to Study Radiation Chemistry," *J. Phys. Chem.*, **99** (1995) 9530.
2. K.L. Queeney, C.R. Arumainayagam, M.K. Weldon, C.M. Friend, and M.Q. Blumberg,* "Differential Reactivity and Structure of Mono- and Di-alkoxides: the Reactions of Ethylene Glycol on Mo(110)," *J. Am. Chem. Soc.*, **118** (1996) 3896.
3. C.E. Tripa, C.R. Arumainayagam, J.T. Yates, Jr., "Kinetics Measurements of CO Photooxidation on Pt(111)," *J. Chem. Phys.*, **105** (1996) 1691.
4. K.T. Queeney, C.R. Arumainayagam, A. Balaji*, and C.M. Friend, "Carbon-Carbon Coupling from Formaldehyde Reaction on Mo(110)," *Surface Sci.*, **418** (1998) L31-L38.
5. *Elizabeth Ferrenz, *Andinet Amare, and C. R. Arumainayagam; "An improved method to spot-weld difficult junctions." Submitted *Review of Scientific Instruments* (2000).

Possible REU Projects:

We plan to study the interactions of low-energy electrons with halocarbons using post-irradiation temperature programmed desorption (TPD). We have recently demonstrated that the exposure of multilayers of an adsorbate to low-energy (≤ 55 eV) electrons under ultrahigh vacuum (UHV) conditions ($p \sim 1 \times 10^{-10}$ Torr) followed by temperature programmed desorption is an effective method to investigate a variety of electron-induced reactions including ion-molecule and radical-radical reactions.

Understanding the decomposition of halocarbons by low-energy electrons could provide critical new concepts of importance to the emerging cold plasma technology aimed at on-site, cost-efficient destruction of hazardous halogenated organic compounds. Although relatively high-energy (100 - 300 keV) electrons are utilized to produce the cold plasma, it is the low-energy (≤ 15 eV) secondary electrons that are postulated to initiate the decomposition of the halocarbons. Among the objectives of the proposed research are:

1. Identify all of the electron-induced reaction products of each halomethane. The post-irradiation TPD method is particularly useful in identifying labile products as shown by the first identification of methoxymethanol ($\text{CH}_3\text{OCH}_2\text{OH}$) as a reaction product of electron-induced reactions of methanol (CH_3OH).
2. For each reaction product, the dependence of the yield on electron fluence (electron flux multiplied by exposure time) will be probed. Such studies will yield valuable information on the optimum electron beam dose necessary for the decomposition of halocarbons.
3. The dependence of the reaction cross section on initial electron energy for each reaction pathway will be investigated to obtain additional information regarding the dynamics of electron-induced dissociation of chloromethanes. Such studies will provide insight into the relative roles of electron impact ionization and dissociative electron attachment (DEA) in the decomposition of halogen containing organic molecules.

David R Haines

Associate Professor of Chemistry

Field: Organic Chemistry**Research interests:** Nucleoside analog synthesis and the reaction chemistry of nitrogen heterocycles

A.B.	1976	Earlham College
Ph.D.	1981	University of Illinois

Graduate Advisor: Dr. Nelson Leonard (University of Illinois)**Recent publications (limited to 5) (*indicates undergraduate student co-author):**

1. Tseng, C. K.-H.; Marquez, V. E.; Fuller, R. W.; Goldstein, B. M.; Haines, D. R.; McPherson, H.; Parsons, J. L.; Shannon, W. M.; Arnett, G.; Hollingshead, M.; Driscoll, J. S. "Synthesis of 3-Deazaneplanocin A, a Powerful Inhibitor of S-Adenosyl-homocysteine Hydrolase with Potent and Selective in Vitro and in Vivo Antiviral Activities," *J. Med. Chem.* **1989**, 32, 1442.
2. Haines, D. R.; Fuller, R. W.; Ahmad, S.; Vistica, D. T.; Marquez, V. E. "Selective Cytotoxicity of a System L Specific Amino Acid Nitrogen Mustard," *J. Med. Chem.* **1987**, 30, 542.
3. Haines, D. R.; Tseng, C. K.-H.; Marquez, V. E. "Synthesis and Antiherpetic Activity of a Novel Unsaturated Carboacyclic Nucleoside Analog Series," *J. Med. Chem.* **1987**, 30, 943.
4. Glazer, R. I.; Knode, M. C.; Tseng, C. K.-H.; Haines, D. R.; Marquez, V. E. "3-Deazaneplanocin A: A New Inhibitor of S-Adenosyl-homocysteine Synthesis and Its Effects in Human Colon Carcinoma Cells," *Biochem. Pharmacol.* **1986**, 35, 4523.

Possible REU Projects:

A great many analogs of the natural nucleosides have been synthesized since the importance of nucleosides in the regulation of biological systems was discovered. Synthetic nucleosides have helped to elucidate mechanisms of enzyme action, and have in many instances exhibited useful pharmaceutical properties.

We have been studying several types of adenosine analogs as possible anti-tumor or anti-viral agents. Several of the compounds that we have prepared have proven to be potent antitumor agents, and tests are being conducted at the National Cancer Institute to find their ranges of activities.

Our research involves the design, synthesis, and structure determinations of the compounds being tested. The structure determinations often require advanced NMR techniques for unambiguous proofs and several students have spent a significant amount of their research time perfecting and expanding on these techniques.

Adele J. Wolfson

Professor of Chemistry

Faculty Director of the Science Center

Field: Biochemistry**Research interests:** Proteases and peptidases and their inhibitors; protein structure; physical biochemistry; protein-ligand interactions

A.B.	1971	Brandeis University
Ph.D.	1979	Columbia University
Postdoctoral	1979-80	University of Paris

Graduate Advisor: Seymour Lieberman (Columbia)**Postdoctoral Advisor:** Etienne-Emile Baulieu (University of Paris)**Collaborators other than co-authors:** Nancy Kolodny (Wellesley), Marc Glucksman (Mt.Sinai)**Recent publications (limited to 5) (*indicates undergraduate student co-author):**

1. Wolfson A. J., Branham T.R., *Edgoose J.C., *Hammill A.K., *Lowe K.M., *Spooner A.E., *Lee J., *Kapoor R. and *Shen M.; Kinetics of inhibition of elastase by a chimeric inhibitor containing the reactive site loop from α 1-antitrypsin. *Protein Peptide Lett.* **3**: 293-300 (1996).
2. Wolfson A.J., Shrimpton C.N., Lew R.A. and Smith A.I. Differential activation of Endopeptidase EC 3.4.24.15 towards natural and synthetic substrates by metal ions. *Biochem. Biophys. Res. Comm.* **229**: 341-348 (1996).
3. Wolfson A.J., Hall M.L. and Allen M.M.; Introductory Chemistry and Biology Taught as an Interdisciplinary Mini-Cluster. *J. Chem. Ed.* **75**: 737-739 (1998).
4. Arico-Muendel C.C., Patera A., Pochapsky T.C., Kuti M. and Wolfson A. J.; Solution structure and dynamics of a serpin reactive site loop using Interleukin 1 β as a presentation scaffold. *Protein Engineering* **12**: 189-202 (1999).
5. Smith A. I., Shrimpton C. N., Norman U. M., Clarke I. J., Wolfson A. J. and Lew R. A.; Neuropeptidases regulating gonadal function. *Biochem Soc Transactions* **28**: 430-434 (2000)

Possible REU Projects:

Activation of Endopeptidase 24.15 (thimet oligopeptidase) by metal ions: The goal of these studies is to explore how metal ions increase the rate of hydrolysis of synthetic substrates and the degree of inhibition by inhibitors for this enzyme. We have found that it is activated by calcium and manganese. We will continue to use methods such as kinetics and calorimetry to determine the strength of binding of metal to substrate or to the enzyme-substrate complex, and see if this kind of activation sheds light on other protein-ligand interactions.

Characterization of an enzyme from cyanobacteria: We have identified several proteases that appear in response to nitrogen starvation and refeeding in cyanobacteria (sometimes called blue-green algae). Our goals are to purify and characterize these enzymes, and to determine whether or not they are involved in metabolism of cyanophycin, the unique nitrogen storage molecule in these organisms.

Nancy Harrison Kolodny

Nellie Z. Cohen and Anne Cohen Heller Professor of Chemistry

Field: Physical Chemistry

Research Interests: Applications of magnetic resonance imaging and spectroscopy to problems in biology and medicine; nitrogen metabolism of cyanobacteria; MR imaging of ocular disorders

B.A.	1964	Wellesley College
Ph.D.	1969	Massachusetts Institute of Technology
Postdoctoral	1970-72	Harvard Medical School

Graduate Advisor: Kerry W. Bowers

Postdoctoral Advisor: Paul C. Zamecnik

Collaborators other than co-authors: Adele Wolfson (Wellesley)

Recent publications (limited to 5) (* indicates undergraduate student co-author)

1. Kolodny, N.H., Kohler, S.J., Rettig, E.S.*, Botti, P.A.*, D'Amico, D.J. and Gragoudas, E.S., "A Feasibility Study of ^{23}Na MR Imaging of Human and Rabbit Vitreal Disorders ", *Invest. Ophthalmol. Vis. Sci.* **34**, 1917-1922 (1993).
2. Kolodny, N.H., Freddo, T.F., Lawrence, B.A., Suarez C. and Bartels, S.P., "Contrast-Enhanced MRI Confirmation of an Anterior Protein Pathway in Normal Rabbit Eyes," *Invest. Ophthalmol. Vis. Sci.* **37**, 1602-1607 (1996).
3. Lawrence, B.L., Polse, J.*, DePina, A.*, Allen, M.M. and Kolodny, N.H., " ^{31}P NMR Identification of metabolites and pH determination in the cyanobacterium *Synechocystis* sp. PCC 6308", *Curr. Microbiol.* **34**, 280-283 (1997).
4. Lawrence, B.L., Suarez, C., DePina, A.*, Click, E. *, Kolodny, N.H. and Allen, M.M., "Two Internal pools of soluble polyphosphate in the cyanobacterium *Synechocystis* sp. strain PCC 6308: an *in vivo* ^{31}P NMR spectroscopic study", *Arch. Microbiol.* **169**, 195-200 (1998).
5. Suarez, C, Kohler, S.J., Allen, M.M. and Kolodny, N.H., "NMR study of the metabolic ^{15}N isotopic enrichment of cyanophycin synthesized by the cyanobacterium *Synechocystis* sp. strain PCC6308," *Biochimica et Biophysica Acta* **1426**, 429-438 (1999).

Possible REU Projects:

The goal of these projects is to elucidate the pathways of nitrogen metabolism in cyanobacteria (blue-green algae). Under stressful conditions cyanobacteria store nitrogen in the form of a non-ribosomally synthesized, arginine-aspartate copolymer called cyanophycin granule polypeptide (cyanophycin). ^1H , ^{31}P and ^{15}N NMR spectroscopy of growing cells and extracted cyanophycin are used to examine the response of several strains of wild-type and mutant cyanobacteria to a variety of environmental stresses.

Shane M. Ohline

Assistant Professor of Chemistry

Field: Physical, Biophysical

Research interests: Structure and function of interfaces studied using spectroscopy, atomic force microscopy, and calorimetry.

B.A.	1989	Grinnell College
Ph.D.	1994	UCLA
Postdoctoral	1995	Alexander von Humboldt Fellow: University of Munich
Postdoctoral	1996	University of Toronto

Graduate Advisor: Peter Felker (UCLA)

Postdoctoral Advisors: Wolfgang Zinth (University of Munich) and R.J. Dwayne Miller (Toronto)

Recent publications (limited to 5):

1. Shane M. Ohline, Mary L. Campbell*, Marilyn T. Turnbull and Susan J. Kohler, "Differential Scanning Calorimetric Study of Bilayer Membrane Phase Transitions: A Biophysical Chemistry Experiment." Submitted *J. Chem. Ed.*
2. P.W. Joireman, Shane M. Ohline and P.M. Felker, "Structural Characterization of Aromatic-Aromatic Complexes by Rotational Coherence Spectroscopy." *J. Phys. Chem. A*, **102**, 4481-4494 (1998).
3. P. Hamm, S.M. Ohline and W. Zinth: "Vibrational cooling after ultrafast photoisomerisation of azobenzene measured by femtosecond infrared spectroscopy." *J. Chem. Phys.*, **106**, 519-529 (1997).
4. S.M. Ohline, J. Romascan and P.M. Felker: "Rotational coherence spectroscopy of aromatic-(Ar)_n clusters - geometries of anthracene-(Ar)_n, 9,10-dichloroanthracene(Ar) and tetracene(Ar)." *J. Phys. Chem.* **99**, 7311-7319 (1995).
5. S.M. Ohline, J. Romascan and P. M. Felker: "Time-resolved ionization depletion: A new picosecond method of molecular beam studies." *Chem. Phys. Lett.* **207**, 563-568 (1993).

Possible REU Projects:

Dye aggregation at solid/air interfaces: Aggregation at interfaces leads to unexpected spectroscopic properties of dye molecules. Using UV-Vis spectroscopy, singular value decomposition, and atomic force microscopy, we will analyze the degree of aggregation of dyes at solid/air interfaces. The solids will include flat surfaces, such as glass and gold, and small particles such as semiconductors and other nanoparticles. We will quantify the relative number of dimers to trimers to larger aggregates on these surfaces. We will compare our values with results from solution. The results will aid in the design of materials for energy transfer in solar cells and other devices.

Thermal properties and structure of lipid bilayers: Phospholipid bilayers in the form of multilamellar vesicles have been studied as model systems of cell membranes. We plan to continue studies investigating the structural changes that occur when proteins, antibiotics, and sterols are included in the lipid bilayer. We will use high sensitivity differential scanning calorimetry and Raman spectroscopy to examine the thermodynamic and structural changes. These studies assist in the understanding of cell membrane structure and function.

Julia Hendrix Miwa

Assistant Professor of Chemistry

Field: Organic Chemistry**Research interests:** Peptide conformation; Thioamides and other unnatural peptide backbones; Peptide mimetics and enzyme inhibitors.

B.A.	1985	Haverford College
Ph.D.	1992	Massachusetts Institute of Technology
Postdoctoral	1992-1994	University of California, Berkeley

Graduate Advisor: Peter Lansbury (Massachusetts Institute of Technology)**Postdoctoral Advisor:** Paul Bartlett (University of California, Berkeley)**Collaborators other than co-authors:** Peter S. Kim (Whitehead Institute)**Recent publications (limited to 5) (*indicates undergraduate student co-author):**

1. "A Convergent Synthesis of the Amyloid Protein of Alzheimer's Disease" Hendrix, J. C.; Halverson, K. J.; Lansbury, P. T., Jr. *J. Am. Chem. Soc.* **1993**, *114*, 7930.
2. "Synthesis of a Protected Peptide Corresponding to Residues 1-25 of the β -Amyloid Protein of Alzheimer's Disease" Hendrix, J. C.; Lansbury, P. T., Jr. *J. Org. Chem.* **1992**, *57*, 3421.
3. "Studies Related to a Convergent Fragment-Coupling Approach to Peptide Synthesis Using the Kaiser Oxime Resin" Hendrix, J. C.; Jarrett, J. T.; Anisfeld, S. T.; Lansbury, P. T., Jr. *J. Org. Chem.* **1992**, *57*, 3414.

Possible REU Project:

Thioamide analogs of a beta-hairpin peptide: The goal of these studies is to determine the influence of hydrogen bonding on the stability of the beta sheet secondary structure. We are using a 12 residue peptide that adopts a beta-hairpin conformation in aqueous solution as a model. Substitution of thioamides for selected backbone amide groups allows us to strengthen specific hydrogen bonds and evaluate the impact of the altered hydrogen bonds on the stability of the hairpin conformation. Peptides are prepared via a combination of organic synthesis and solid phase peptide synthesis, and are analyzed by NMR and CD spectroscopy.

Margaret V. Merritt

Professor of Chemistry

Field: Analytical Chemistry**Research Interests:** Reactions at surfaces, bioanalytical chemistry, chemistry of artists' materials.

B.A. 1964 The College of Wooster
Ph.D. 1968 Cornell University (D. Geske, Advisor)

Collaborators other than co-authors: Peter Melling (Remspec Corporation), Robert Pribush (Butler University); Melissa Katz (Wellesley College)

Recent Publications (limited to 5); (Undergraduate student authors indicated with asterisk)

1. Variations in the amino acid composition of cyanophycin from the cyanobacterium *Synechocystis* sp PCC 6308 as a function of cellular growth conditions. Margaret V. Merritt, Silvia S. Sid*, Ludmila Mesh, and Mary M. Allen, 1994. *Arch. Microbiol.*, **162**: 158-166.
2. Enantiomer-Specific Oxygen Exchange Reactions. II. Acid Catalyzed Water Exchange with 1-Phenyl-1-Alkanols. Margaret V. Merritt, Dina B. Anderson*, Kim A. Basu*, I-Wen Chang*, Hee-Joo Cheon*, Nancy E. Mukundan*, Clare A. Flannery*, Alice Y. Kim*, Anjala Vaishampayan*, and Diana A. Yens*, 1994. *J. Am. Chem. Soc.*, **116**: 5551-5559.
3. Micelle-Induced Changes in the Solvation of Carbocations: Effect of SDS Micelles on the Enantiomer-Specific Oxygen Exchange Reaction of 1-Phenyl-1-Ethanol and 1-Phenyl-1-Butanol. Margaret V. Merritt, I-Wen Chang*, Clare A. Flannery*, Show-Jon Hsieh*, Karl Lee*, and Jennifer Yung*, 1995. *J. Am. Chem. Soc.*, **117**: 9791-9799.
4. Margaret V. Merritt, Milan Mrksich, George M. Whitesides. Using self-assembled monolayers to study the interactions of man-made materials with proteins. In: Langer R, ed. *Tissue Engineering*, R. G. Landes Company, Austin, 1997.
5. Carl S. Weisbecker, Margaret V. Merritt, George M. Whitesides. Molecular Self-Assembly of Aliphatic Thiols on Gold Colloids, 1997. *Langmuir* **12**: 3763-3772.

Possible REU Projects:

Reactions at Gold Interfaces. One area of current research is the development of alkanethiol-stabilized gold nanoparticles as model surfaces for probing interfacial effects on the reactions of small molecules and protein-surface interactions. These materials are formed by reduction of AuCl_4^- in the presence of alkanethiols; the resultant products resemble the well-characterized planar self-assembling alkanethiolate-Au monolayers. In contrast to monolayers on planar surfaces, the large surface areas of the gold cluster nanoparticles facilitate the investigation of reactions carried out in their presence. Projects in this area include (1) the synthesis and characterization of alkanethiol-stabilized gold cluster nanostructures presenting ionic functional groups as models for ionic micelles as chiral catalysts and (2) the preparation and characterization of proteins immobilized at colloidal gold and gold nanoparticle surfaces.

Identification of Blue Pigments in Yoruba Art Objects. Microscopy and infrared techniques will be used to identify pigments in selected pieces of wood sculpture from this West African ethnic group. The results will be combined with historical and archaeological data to determine the relative influence of trade and indigenous technology on Yoruba cultural practices in the 19th and early 20th century. Projects in this area will include both lab work at Wellesley and fieldwork in museums with significant Yoruba collections.

Michael J. Hearn
Professor of Chemistry

Field: Organic Chemistry

Research interests: Synthesis and Properties of New Antituberculosis Compounds; Near-Infrared Spectroscopy

B.A.	1971	Rutgers College
Ph.D.	1976	Yale University
Postdoctoral	1976-77	Yale University

Graduate Advisor: Harry H. Wasserman (Yale University)

Collaborators other than co-authors: Michael H. Cynamon, M.D., Professor of Infectious Diseases, Health Sciences Center, State University of New York, Syracuse.

Recent publications (all co-authors were undergraduate research participants):

1. "Preparation and Spectroscopic Properties of 3-Acyl-1,3,4-oxadiazolines," Michael J. Hearn and Phet-Yoon Chanyaputhipong, *Journal of Heterocyclic Chemistry*, **32**, 1647 (1995).
2. "Using Near Infrared Spectroscopy to Monitor the Preparation of Compounds for Screening as Antituberculosis Drugs." Michael J. Hearn, Paul Celi, Phet-Yoon Chanyaputhipong, Wendy Chi, Joo On Kang, Adena Katz, Ruta Shah, Minh Thai and Podaly Ung, *Journal of Near Infrared Spectroscopy* **3** (1) 19-23 (1996).
3. Meeting Report: "Tuberculosis Today. Chemical Perspectives on the Resurgence of the White Plague." *The Nucleus* LXXV (7) 7-11 (1997).
4. "A Convenient Method for the Preparation of Tuberculostatic Diacylhydrazines." Michael J. Hearn, Helen Joo On Kang and Minh Thai, *Bulletin des Societes Chimiques Belges* **106** (2) 109-114 (1997).

Possible REU Projects:

Although the use of traditional mid-range infrared spectroscopy (MIR) has a long and distinguished history for the qualitative determination of organic molecules, progress in the application of near-infrared spectroscopy (NIR) to problems in the chemistry of carbon compounds has been limited. The potential advantages of NIR, which include convenience of sample handling and ease of quantitation, have remained unfulfilled. NIR is indeed the study of overtone and combination bands of vibrations of hydrogenic bonds, but the Herschel (short wavelength) region of the NIR (700-1000 nm) also displays low energy electronic transitions, which could be used in the characterization of highly conjugated p-electron systems. Because of its sensitivity to hydrogen bonding, aggregation, particle size, and charge transfer effects, NIR may have a strong role to play in obtaining a better understanding of interacting molecules in solution. Our present research focuses on the preparation of novel antituberculosis compounds by the methods of synthetic organic chemistry and the application of NIR spectroscopy to their quantitative analysis.

William F. Coleman

Professor of Chemistry

Field: Inorganic Chemistry**Education:**

BS: Eckerd College (1966)

Ph.D.: Indiana University (Bloomington) (1970) (Ward. B Scrap, advisor (deceased))

Postdoctoral: University of Arizona (1970) (Leslie S. Frostier, advisor)

Collaborators other than co-authors: John W. Moore, University of Wisconsin - Madison
Theresa Julia Zielinski, Monmouth University**Recent Publications (limited to 5); (Undergraduate student authors indicated with asterisk):**

1. *Erika Cervasio, *Cynthia Soroos, *Jennifer Williams, and **William F. Coleman**; "Cr(VI)-Cr(III) Energy Transfer in $[\text{Cr}(\text{NH}_3)_6]_2[\text{Cr}_2\text{O}_7]_3$ ", accepted *J. Luminescence* (2000).
2. Coleman, William F., "Metals" in Macmillan Encyclopedia of Chemistry, J&J. Lagowski, ed.: Macmillan Reference, New York, **1997**
3. W.F. Coleman and C.R. Arumainayagam, "Book and Media Reviews: HyperChem 5," *J. Chem. Educ.*, **75** (1998) 416
4. Coleman, William F., "Curve Fitting, An Alternative Approach for Analyzing Kinetic Data in Introductory Chemistry," *J. Chem. Educ.*, **1996**, 238
5. Pavlik, P., Rittenhouse, R., Rose, M and Coleman, W., "Atomic Spectroscopy", *J. Chem. Educ. Software*, Volume VB, **1992**

Possible Student Projects:

1. Energy Transfer Between Cr(VI) and U(VI): We have shown that the efficiency of energy transfer is dependent on both the wavelength and intensity of the incident light. Using techniques of time-resolved laser induced fluorescence we will model the processes responsible for this unusual behavior.
2. Anomalies in the Absorption and Excitation Spectra of Uranyl Complexes in Acidic Solution: We have observed several anomalies including violations of Beer's Law by only certain features in the absorption spectrum. Using computer assisted non-linear curve fitting techniques, together with high resolution absorption spectra and ion chromatography, we will develop models to account for this behavior. We will use lifetime spectroscopy and computer modeling of luminescence decay curves in an effort to understand anomalies in the excitation spectra of these systems.
3. The Development of Spectroscopic Probes of Biological Chromium: Low temperature laser induced emission spectroscopy will be used to characterize the oxidation state and coordination environment of chromium in a number of naturally occurring (e.g. the glucose tolerance factor) and synthetic (e.g. chromium picolinate complexes with small proteins) systems.

Glenn Stark

Associate Professor of Physics & Chair of the Department

Field: Molecular Spectroscopy

Research interests: Oscillator strength measurements of ultraviolet and vacuum ultraviolet molecular transitions of astrophysical interest; high-resolution molecular spectroscopies; atomic cooling and trapping.

A.B.	1976	M.I.T.
Ph.D.	1985	U.C. Berkeley
Postdoctoral	1986-87	Harvard-Smithsonian Center for Astrophysics

Graduate Advisor: Sumner P. Davis (U.C. Berkeley)

Postdoctoral Advisor: William H. Parkinson (Center for Astrophysics)

Collaborators other than co-authors: Robbie Berg & Tom Bauer (Wellesley), Peter L. Smith & K. Yoshino (Center for Astrophysics), K. P. Huber (National Research Council, Canada)

Recent publications (limited to 5)

1. G. Stark and P. L. Smith, *Spectroscopic Techniques: Ultraviolet*, in *Atomic, Molecular, and Optical Physics Reference Book*, edited by G. Drake, American Institute of Physics Press, New York, pp. 487-498 (1996).
2. G. Stark, B. R. Lewis, S. T. Gibson, and J. P. England, *High-resolution oscillator strength measurements for high- v' bands of the $A^1\Pi(v') - X^1\Sigma^+(v''=0)$ system of carbon monoxide*, *Astrophys. J.* 505, 452 (1998).
3. G. Stark, P. L. Smith, J. Rufus, A. P. Thorne, J. C. Pickering, and G. Cox, *High-resolution photoabsorption cross section measurements of SO_2 at 295 K between 198 and 220 nm*, *J. Geophys. Res.* 104, 16585 (1999).
4. G. Stark, K. P. Huber, K. Yoshino, M.-C. Chan, T. Matsui, P. L. Smith, and K. Ito, *Line oscillator strength measurements in the 0-0 band of the $c_4^1\Sigma_u^+ \leftarrow X^1\Sigma_g^+$ transition of N_2* , *Astrophys. J.* 531, 321 (2000).
5. J. R. Gillis, A. Goldman, G. Stark, and C. P. Rinsland, *Line parameters for the $A^2\Sigma^+ - X^2\Pi$ bands of OH*, *J. Quant. Spectrosc. Rad. Trans.*, in press (2000).

Possible REU Projects:

Laser Cooling and Trapping of Atoms: This is a collaborative research effort in the Physics Department to design and construct a cooling and trapping apparatus for rubidium atoms. The laboratory work includes the development of high-resolution diode laser systems, associated electronics, a high-vacuum system, and a magneto-optical trap. The first phase of the project, constructing a tunable and stable diode laser system, was completed this past summer at Wellesley.

Vacuum Ultraviolet Spectroscopy of Astrophysical Molecules: This ongoing project involves the measurement and analysis of high-resolution absorption spectra of molecular nitrogen and sulfur dioxide in the vacuum ultraviolet. Oscillator strengths of individual rotational transitions within the electronic systems of these molecules are extracted from the measurements. The experimental work takes place off-campus; the data reduction and analysis takes place at Wellesley.

Yue Hu

Associate Professor of Physics

Field: Condensed matter physics

Research interests: Colloids and their electrical and rheological properties in electric fields.

B.Sc. 1982 Peking University, China

M.Sc. 1985 Cornell University

Ph.D. 1990 Cornell University

Graduate Advisor: Robert C. Richardson (Cornell, Nobel Prize in Physics, 1996)

Recent publications (limit to 5) (*indicates undergraduate student co-authors):

1. "Observation and simulation of electrohydrodynamic instabilities in aqueous colloidal suspensions", Yue Hu, J. L. Glass*, A. E. Griffith*, and Seth Fraden, *Journal of Chemical Physics*, **100**, 4674 (1994).
2. "Potential energy of a pair of polystyrene spheres in an electric field", San Lin, Seth Fraden, and Yue Hu, *Proceedings of the Electrorheological Materials and Fluids Symposium*, 208th National Meeting of the American Chemical Society, ed. by F. E. Filisko and K. O. Havelka, Plenum Press, New York, p. 359 (1995).
3. "Computer Simulation of Polarization of Mobile Charges on the Surface of a Dielectric Sphere in Transient Electric Fields", Yue Hu and Michelle W. Chen*, *J. Electrostatics*, **43**, 19 (1998).
4. "Effects of an Inner Helmholtz Layer on the Dielectric Dispersion of Colloidal Suspensions", Yue Hu, *Langmuir*, **14**, 271 (1998).
5. "Simulation of Polarization of Surface Charges on a Spherical Particle in Alternating Electric Fields and in a Shearing Flow", Yue Hu, Janet Lee*, and Ting Bao*, *Proceedings of the 6th International Conference on Electrorheological Fluids, Magnetorheological Suspensions and Their Applications*, pp. 123 (1998).

Possible REU Projects:

Computer simulation of electrorheological effects: When electric fields are applied to a suspension of small particles, the viscosity of the suspension can increase by several orders of magnitude. This has important industrial application, but high-quality electrorheological fluids are not available because the mechanism for this effect is not understood at present time. The goal of this project is to conduct computer simulation to test a new model that I have developed. Preliminary computer simulation results are very promising. We will systematically examine the influence of the following system parameters: particle size, dielectric constant and conductivity, frequency of the applied field, and shear rate. We hope to find ways to improve electrorheological fluids.

Robbie Berg
Professor of Physics

Field: Educational Robotics; Laser Spectroscopy

Research interests: Developing new computational tools for use in science education; optical properties of semiconductors; Use of narrow band-width diode lasers to trap and cool rubidium atoms.

A.B.	1978	Princeton University
Ph.D.	1985	University of California, Berkeley

Graduate Advisor: Peter Yu (Berkeley); Ph.D.

Collaborators other than co-authors: Glenn Stark (Wellesley), Ted Ducas (Wellesley); Tom Bauer (Wellesley), Franklyn Turbak (Wellesley)

Recent publications (limited to 5)

1. Mitchel Resnick, Robbie Berg, and Michael Eisenberg, Beyond Black Boxes: Bringing Transparency and Aesthetics Back to Scientific Investigation. *The Journal of the Learning Sciences*, Volume **9**, No. 1, 2000.
2. Mitchel Resnick, Fred Martin, Robbie Berg, Rick Borovoy, Vanessa Colella, Kwin Kramer, & Brian Silverman, Digital Manipulatives: New Toys to Think With. *Proceedings of CHI (Conference on Human Factors in Computing Systems) '98*, ACM Press (Los Angeles, April 1998).
3. Bakhtiar Mikhak, Robbie Berg, Fred Martin, Mitchel Resnick, & Brian Silverman. To Mindstorms and Beyond: Evolution of a Construction Kit for Magical Machines. This is a chapter in the book *Robots for Kids: Exploring New Technologies for Learning Experiences*. (Edited by Allison Druin, published by Morgan Kaufman / Academic Press, San Francisco (2000).
4. Bakhtiar Mikhak, Fred Martin, Robbie Berg, Mitchel Resnick, & Brian Silverman, The Children's Machines: Handheld and Wearable Computers Too. International Symposium on Handheld and Ubiquitous Computing, Karlsruhe, Germany, 1999.
5. Soloway, E., Grant, W., Tinker, R., Roschelle, J., Mills, M., Resnick, M., Berg, R., and Eisenberg, M. Science in the Palms of Their Hands. *Communications of the ACM*, vol. 42, no. 8, pp. 21-26 (1999).

Possible REU Project:

Laser Cooling and Trapping of Rubidium Atoms. We are in the process of implementing a scheme similar to one proposed by Weiman et. al.¹ for cooling (to temperature of a few hundred μ K) and trapping a gas of rubidium atoms using light from a diode laser tuned to the 780 nm transition. We have successfully built the necessary narrow band lasers and during the summer of 2001 we expect to make substantial progress in cooling and trapping the rubidium vapor.

¹ Weiman, et. al., "Laser Cooling and Trapping of Rubidium Atoms", *American Journal of Physics* **63** p. 317 (1995).

SUMMARY PROPOSAL BUDGET YEAR 1

ORGANIZATION Wellesley College				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR				AWARD NO.			
				Proposed	Granted		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-mos.		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1.				0.00	0.00	0.50	\$ 3,000
2.				0.00	0.00	0.00	0
3.							
4.							
5.							
6. (0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. (2) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.50	3,000
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (0) POST DOCTORAL ASSOCIATES				0.00	0.00	0.00	0
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. (0) GRADUATE STUDENTS							0
4. (0) UNDERGRADUATE STUDENTS							0
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. (0) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							3,000
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							852
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							3,852
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL							
1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							0
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ <u>31,000</u>							
2. TRAVEL <u>3,800</u>							
3. SUBSISTENCE <u>9,000</u>							
4. OTHER <u>0</u>							
TOTAL NUMBER OF PARTICIPANTS (10)							
TOTAL PARTICIPANT COSTS							43,800
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							10,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							500
3. CONSULTANT SERVICES							0
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							3,900
TOTAL OTHER DIRECT COSTS							14,400
H. TOTAL DIRECT COSTS (A THROUGH G)							62,052
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)							
TOTAL INDIRECT COSTS (F&A)							0
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							62,052
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 62,052 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI / PD TYPED NAME & SIGNATURE*			DATE		FOR NSF USE ONLY		
					INDIRECT COST RATE VERIFICATION		
ORG. REP. TYPED NAME & SIGNATURE*			DATE		Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET YEAR 2

ORGANIZATION Wellesley College				FOR NSF USE ONLY					
				PROPOSAL NO.	DURATION (months)				
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Chris Arumainayagam				AWARD NO.	Proposed	Granted			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-mos.			Funds Requested By proposer	Funds granted by NSF (if different)	
				CAL	ACAD	SUMR			
1.				0.00	0.00	0.00	\$ 0	\$	
2.				0.00	0.00	0.50	3,000		
3.									
4.									
5.									
6. (0)	OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00	0		
7. (2)	TOTAL SENIOR PERSONNEL (1 - 6)			0.00	0.00	0.50	3,000		
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)									
1. (0)	POST DOCTORAL ASSOCIATES			0.00	0.00	0.00	0		
2. (0)	OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			0.00	0.00	0.00	0		
3. (0)	GRADUATE STUDENTS						0		
4. (0)	UNDERGRADUATE STUDENTS						0		
5. (0)	SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						0		
6. (0)	OTHER						0		
TOTAL SALARIES AND WAGES (A + B)							3,000		
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							852		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							3,852		
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)									
TOTAL EQUIPMENT							0		
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							0		
2. FOREIGN							0		
F. PARTICIPANT SUPPORT COSTS									
1.	STIPENDS	\$	31,000						
2.	TRAVEL		3,800						
3.	SUBSISTENCE		9,000						
4.	OTHER		0						
TOTAL NUMBER OF PARTICIPANTS (10)				TOTAL PARTICIPANT COSTS			43,800		
G. OTHER DIRECT COSTS									
1.	MATERIALS AND SUPPLIES						10,000		
2.	PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						500		
3.	CONSULTANT SERVICES						0		
4.	COMPUTER SERVICES						0		
5.	SUBAWARDS						0		
6.	OTHER						3,900		
TOTAL OTHER DIRECT COSTS							14,400		
H. TOTAL DIRECT COSTS (A THROUGH G)							62,052		
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)									
TOTAL INDIRECT COSTS (F&A)							0		
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							62,052		
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)							0		
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 62,052	\$	
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$					
PI / PD TYPED NAME & SIGNATURE*			DATE	FOR NSF USE ONLY					
				INDIRECT COST RATE VERIFICATION					
ORG. REP. TYPED NAME & SIGNATURE*			DATE	Date Checked	Date Of Rate Sheet	Initials - ORG			

SUMMARY PROPOSAL BUDGET YEAR 3

ORGANIZATION Wellesley College				FOR NSF USE ONLY		
				PROPOSAL NO.	DURATION (months)	
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Chris Arumainayagam				AWARD NO.	Proposed	Granted
					NSF Funded Person-mos.	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				CAL	ACAD	SUMR
1.				0.00	0.00	0.50
2.				0.00	0.00	0.00
3.						
4.						
5.						
6. (0)	OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)			0.00	0.00	0.00
7. (2)	TOTAL SENIOR PERSONNEL (1 - 6)			0.00	0.00	0.50
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (0)	POST DOCTORAL ASSOCIATES			0.00	0.00	0.00
2. (0)	OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			0.00	0.00	0.00
3. (0)	GRADUATE STUDENTS					
4. (0)	UNDERGRADUATE STUDENTS					
5. (0)	SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					
6. (0)	OTHER					
TOTAL SALARIES AND WAGES (A + B)						3,000
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						852
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						3,852
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)						
TOTAL EQUIPMENT						0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						0
2. FOREIGN						0
F. PARTICIPANT SUPPORT COSTS						
1.	STIPENDS	\$	31,000			
2.	TRAVEL		3,800			
3.	SUBSISTENCE		9,000			
4.	OTHER		0			
TOTAL NUMBER OF PARTICIPANTS (10)				TOTAL PARTICIPANT COSTS		43,800
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						10,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						500
3. CONSULTANT SERVICES						0
4. COMPUTER SERVICES						0
5. SUBAWARDS						0
6. OTHER						3,900
TOTAL OTHER DIRECT COSTS						14,400
H. TOTAL DIRECT COSTS (A THROUGH G)						62,052
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) (Rate: , Base:)						
TOTAL INDIRECT COSTS (F&A)						0
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						62,052
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)						0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						\$ 62,052 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$		
PI / PD TYPED NAME & SIGNATURE*			DATE	FOR NSF USE ONLY		
ORG. REP. TYPED NAME & SIGNATURE*			DATE	INDIRECT COST RATE VERIFICATION		
				Date Checked	Date Of Rate Sheet	Initials - ORG

SUMMARY PROPOSAL BUDGET Cumulative

ORGANIZATION Wellesley College				FOR NSF USE ONLY			
				PROPOSAL NO.	DURATION (months)		
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR Chris Arumainayagam				AWARD NO.			
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-mos.		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1.				0.00	0.00	1.00	\$ 6,000
2.				0.00	0.00	0.50	3,000
3.							
4.							
5.							
6. () OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. (2) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	1.50	9,000
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (0) POST DOCTORAL ASSOCIATES				0.00	0.00	0.00	0
2. (0) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. (0) GRADUATE STUDENTS							0
4. (0) UNDERGRADUATE STUDENTS							0
5. (0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. (0) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							9,000
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							2,556
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							11,556
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL							0
1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							0
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____				93,000			
2. TRAVEL _____				11,400			
3. SUBSISTENCE _____				27,000			
4. OTHER _____				0			
TOTAL NUMBER OF PARTICIPANTS (30)							TOTAL PARTICIPANT COSTS 131,400
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							30,000
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							1,500
3. CONSULTANT SERVICES							0
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							11,700
TOTAL OTHER DIRECT COSTS							43,200
H. TOTAL DIRECT COSTS (A THROUGH G)							186,156
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)							0
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							186,156
K. RESIDUAL FUNDS (IF FOR FURTHER SUPPORT OF CURRENT PROJECTS SEE GPG II.D.7.j.)							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 186,156 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI / PD TYPED NAME & SIGNATURE*			DATE	FOR NSF USE ONLY			
ORG. REP. TYPED NAME & SIGNATURE*			DATE	INDIRECT COST RATE VERIFICATION			
				Date Checked	Date Of Rate Sheet	Initials - ORG	

REU Budget Justification

Program Director Salary and Fringe Benefits:

The \$3,000 budgeted will fund a portion of the salary of the Program Director for the administration of the REU program during the summer. The fringe benefits are budgeted at 28.4% of the Program Director's salary. Professors Arumainayagam and Haines will share in the administration of the program over the three years.

Participant Support:

Student Stipends:

The stipends of \$3,100 are commensurate with those offered by other Wellesley College summer research programs. Stipends are requested for 10 students. Because Wellesley College is willing to treat these stipends as scholarships, we are not requesting fringe benefits on these stipends.

Housing:

Wellesley College will provide housing in the college dormitories at cost (10 REU students x \$900 per student) for the ten-week program.

Travel:

In recent years, we have found that most of the non-Wellesley College student participants have been from within the Boston area. For this reason, we are budgeting travel funds, to and from the program, for only two students, at \$400 per student. In recent years, many of our students have presented their research results at National ACS meetings. Because we want to encourage this practice, we have budgeted funds (6 x \$500) to provide partial funding for travel of REU participants to present their results. This is only partial funding of the expected travel expenses, and the College will fund the differential through other grants and internal funds.

Other Direct Costs:

Materials and Supplies, and other Research Expenses:

We have budgeted an amount of \$1,000 per student for the 10 REU students for expenses related to their research.

Publications/Page Charges:

This item will be used for partial payment of journal page charges for manuscripts generated by the research supported by REU site funds. Other College funds will be used to cover additional publication costs.

Other:

This budget line includes funding for a career panel and a graduate school panel (\$1000), publicity and recruitment expenses (\$200), seminars by outside speakers (\$2000), field trips (\$200), and two workshops on scientific writing (\$500).

All students participating in the Wellesley College Department of Chemistry Summer Research Program will participate in the activities being funded by this budget line, regardless of the source of their stipend.

The Career Panel and Graduate School Panel will be held in the early evening, with a catered meal following the panel discussion to foster the continued discussion of the issues that arise during the presentations.

Publicity and Recruitment will support the preparation of brochures describing the Wellesley College REU site program and mailings of information to interested students.

We plan weekly Seminars by Outside Speakers. The funds requested will provide refreshments for the participants and cover meals and other expenses of the speakers.

The cost of Field Trips is limited to the cost of the rental of college owned vans. We plan two Field Trips per year.

The Workshops on Scientific Writing will be run in conjunction with other scientific summer research programs on campus, and the expense of these workshops will be divided between the participating programs.

Indirect Costs:

Wellesley College has agreed to forgo indirect costs for this REU program.

Evaluation and Dissemination:

The costs of evaluating the effectiveness of the program, and of disseminating the results will be paid by the College through ongoing evaluation projects.

CURRENT AND PENDING SUPPORT –Proposal Section G

<u>Name of Principal Investigator/Senior Personnel:</u>	<u>Current Support:</u>	<u>Project Title</u>	<u>Award Amount</u>	<u>Period Covered</u>	<u>Person-Months Committed (per year)</u>			
					<u>Acad Year</u>	<u>Sum-mer</u>	<u>Cal. Year</u>	
Chris Arumainayagam	Current: Henry Dreyfus Teacher Scholar Award	Studies of Radiation Chemistry and Surface Chemistry	\$60,000	1996-2001	-	1		Wellesley
	Current: NSF-REU	Summer Research at Wellesley	\$171,000	1998-2001		0.5		Wellesley
	Pending: NSF-REU	Summer Research at Wellesley	\$186,156	2001-2004		0.5		Wellesley
David Haines	Pending: NSF-REU	Summer Research at Wellesley	\$186,156	2001-2004		0.5		Wellesley
Adele Wolfson	Current: Camille and Henry Dreyfus Scholar/Fellow award	Activation of thimet oligopeptidase by calcium	\$60,000	2000-2002	2	1		Wellesley
	Current: NSF-REU	Summer Research at Wellesley College	\$171,000	1998-2001		0.5	0.5	Wellesley
	Current: NSF-ILI	Establishment of a Thermal Analysis Laboratory	\$134,170 with \$ 62,085 from Wellesley	1998-2000				Wellesley
	Current: NSF-RUI	The synthesis and Degradation of a Unique Bacterial Polymer	\$200,000	1998-2001	2	1	1	Wellesley
	Current: Howard Hughes Medical Institute	Undergraduate Biological Sciences Education Program	\$900,000	2000-2004				Wellesley

Shane Ohline	Current: Research Corporation Cottrell College Science award.	Studies of Molecular Orientation at the Membrane/Air and Membrane/Solution Interface.	\$36,000 (including \$ 4,000 from Wellesley)	1999-2001	1.0		Wellesley
	Current: Camille and Henry Dreyfus Faculty Start-up Grant	Orientalional Structure of and Dynamics at Biomembrane Interfaces Studied by Second Harmonic Generation and Scanning Probe Microscopies	\$12,500	1996-2001	0.5		Wellesley
	Current: NSF-ILI	Establishment of a Thermal Analysis Laboratory	\$134,170 with \$ 62,085 from Wellesley	1998-2000	1		Wellesley
	Current: AAUW American Postdoctoral Fellowship	Molecular Order at the Oil/Water Interface: Vibrational Sum Frequency Spectroscopy of Phospholipids and Proteins	\$37,000 (including \$5,000 from Wellesley)	2000-2001	6		Wellesley and University of Oregon
Yue Hu	Current: US Department of Energy	Two studies of colloidal interactions: Electric polarizability and protein crystallization	\$155,000	1999-2001	1.5	1.5	Brandeis University

Nancy Kolodny	Current: NSF-RUI	The synthesis and Degradation of a Unique Bacterial Polymer	\$200,000	1998-2001	-	1	Wellesley
	Current: NSF-AIRE	Award for the Integration of Research and Education	\$500,000	1998-2001	-	-	Wellesley
Michael Hearn	Current: NIH National Institute of Allergy and Infectious Diseases, Division of AIDS	“New Agents for AIDS-Associated Mycobacterial Infections.”	\$187,000	2000-2002		8	Wellesley
Glenn Stark	Current: NASA Planetary Atmospheres	“Laboratory Measurements of SO ₂ and N ₂ Absorption Spectra”	\$112,900	2000-2002		2	Wellesley
	Current: Brachman-Hoffman Small Grants Program at Wellesley College	“Optical Tweezers and Laser Cooling: Two Techniques for Manipulating Small Particles Using Light”	\$8,000	1999-2000		1	Wellesley
Robert Berg	Current: Intel Corporation	Computer Clubhouse	\$10,000	Fall 2000		1	MIT
	Current: Brachman-Hoffman Small Grants Program at Wellesley College	“Optical Tweezers and Laser Cooling: Two Techniques for Manipulating Small Particles Using Light”	\$8,000	1999-2000		1	Wellesley
	Current: National Institute of Standards and Technology (NIST)	Summer Undergraduate Research Fellowship (SURF) Program	\$20,000	2000			NIST

Facilities, Equipment and Other Resources - Proposal Section H

Major Equipment - Wellesley College Chemistry Department

- Bruker 300MHz and 400MHz NMR spectrometers with broadband probes - the 400MHz system has dual probes, one an inverse probe with z-axis gradients and the other a 20mm wide-bore probe.
- 2 Hewlett-Packard Gas chromatographs with mass selective detectors, both equipped with autosamplers. 1985 acquisition: Model 5995; 1996 acquisition: Model 5890.
- Burleigh Metris-2000 Atomic Force Microscope.
- Waters Liquid Chromatograph equipped with autosampler, variable wavelength UV-vis absorption detector, and conductivity detector for ion chromatography.
- Thermoseparations Spectrophoresis 100 capillary electrophoresis system with variable wavelength UV-vis detector.
- Four FTIR spectrometers (2 Perkin-Elmer 1650, 1 Perkin-Elmer Spectrum One, Nicolet's mid-infrared FTIR (Avatar))
- Four Perkin-Elmer 1310 IR spectrometers
- Numerous vis-UV spectrophotometers including:
 - Cary 500 spectrometer with capabilities in the UV-VIS-NIR regions
 - 4 HP diode array spectrophotometers (automatic sample changer, stopped flow attachment)
 - Cary 14 spectrophotometer
 - IBM 9420 spectrophotometer with reflectance attachment
 - 2 Hitachi spectrophotometers, one with temperature control
 - Perkin-Elmer Lambda 5 spectrophotometer
- SPEX Fluorolog spectrofluorimeter with phosphorescence and lifetime attachments.
- UHV (10^{-11} torr) chamber equipped with a quadrupole mass spectrometer, LEED, and Auger.
- Several gas chromatographs including 4 with FID detectors and capillary capabilities (conductivity and light scattering detectors are also available).
- Several high performance liquid chromatographs including diode array UV-vis detection; conductivity and light scattering detectors are also available.
- BAS 100A electrochemical analyzer; PAR polarographic analyzer
- 2 Perkin-Elmer atomic absorption spectrophotometers, one with a graphite furnace.
- Spinco and Sorvall ultracentrifuges with appropriate rotors; five Sorvall refrigerated centrifuges; Jouan refrigerated low speed centrifuge; several microfuges.
- 2 Philips X-ray generators (Cu and Mo tubes) with computer interfaced powder diffractometer and 2 Weissenberg and precession cameras.
- Millipore 8500 oligonucleotide synthesizer.
- Packard and Beckman liquid scintillation counters; Packard gamma counter.
- LKB enhanced laser densitometer; EC Apparatus integrating densitometer.
- Gel electrophoresis equipment; blotting apparatus; isoelectric focussing apparatus; gel driers
- Room equipped with trans-illuminator and cameras for DNA and protein gel photography
- Autoradiography laboratory and isotope room.
- Environmental chambers including: 15°, 25°, 30° and 37° Harris Environmental Laboratories cold rooms and cold boxes; -20 and -70 freezers; two large incubators.
- Sonics and Materials ultrasonic processor.
- Advanced Chemtech Automated Peptide Synthesizer.
- Microcal VP-DSC Differential Scanning Calorimeter
- Microcal VP-ITC Isothermal Titration Calorimeter

- Laser laboratory including: PAR nitrogen laser and nitrogen pumped dye laser; Lumonics YAG laser; Continuum YAG pumped dye laser; one-meter and several 0.5 meter spectrometers; single photon counting detection; 2 boxcar integrators; lock-in amplifier.
- One SGI Iris Indigo molecular modeling workstations and associated software including the Cambridge Structure Database and the Brookhaven Protein Databank.
- Two SGI O₂ molecular modeling workstation with Spartan, NMR analysis software, and crystallographic software.
- Two Computer laboratories with 25 networked 400 MHz Pentium PC's with HyperChem 6.0, PC Spartan, Excel, EasyPlot, MathCad, Rasmol, Netscape and other Chemistry software.
- An additional 40 high end networked PC's and Macintoshes are available in public computer clusters in the Science Center.