Monthly Meeting
Esselen Award to Ronald Breslow

Andrew H. Weinberg Memorial Lecture
“Systems Biology” by Leroy Hood

Summer Scholar Report
Biocatalytic Resolution of Racemic Cyanohydrins

Phyllis A. Brauner Memorial Lecture Fund
Member News

2002 Draper Prize
Robert Langer. Kenneth J. Germe-shausen Professor of Chemical and Bio-chemical Engineering at M.I.T. The Draper Prize is the most prestigious engineering award, called by some “engineering’s Nobel Prize.”

He is receiving this award in recogni-tion of his work on special polymers and their biomedical applications. Langer also is receiving the 2002 Oth-mer Gold Medal. An account of his research work accompanies the announcement of these awards in C&EN 2002 (Feb. 18), pp. 48ff. Langer was the Esselen Awarded in 1999.

Arthur C. Cope Scholar
James S. Panek of Boston University is one of four national awardees of this prestigious award. He received the award for his outstanding work in syn-thetic organic chemistry. After a Ph.D. from the University of Kansas and 2 years as a NIH Postdoctoral Fellow at Yale, he came to Boston University in 1986, advancing from Assistant Profes-sor to full Professor (1995).

Arthur C. Cope Young Scholar
Matthew D. Shair of Harvard Univer-sity is one of three awardees for 2002. He received a Ph.D. from Yale Univer-sity in 1995, working under S.J. Dan-ishefsky., followed by postdoctoral work at Harvard, which invited him to join its faculty, where he currently holds the rank of Associate Professor. His research area is the construction of com-plex molecules using catalytic reactions and novel synthetic methods.

The Cope Scholar/Young Scholar awards will be made at the Boston National ACS Meeting in August, 2002.

American Chemistry Council 2002 Responsible Care Catalyst Award for Teaching at a 4-Year College/ University
Morton Z. Hoffman, the current NESACS Chair, has been selected as the National Awardee of this award. Corresponding Regional Awards were made and also Awards for teaching in 2-year colleges, High Schools and Pre-Schools. The American Chemistry Council was formerly known as the Manufacturing Chemists Association.

Our congratulations to these outstanding members. ◇
Member News 2

Monthly Meeting 5

Esselen Award to Ronald Breslow: “Chemistry Lessons from Biology and vice versa”

The Andrew H. Weinberg Memorial Lecture 7

Leroy Hood speaks on: “Systems Biology: Integrating Genomics, Proteomics and Computation”

Board of Directors Meeting Reports 8, 9

Annual meeting and regular meeting of January 10, 2002

Book Review 10

“Science, Money and Politics” by Daniel S. Greenberg, reviewed by Marshall E. Deutsch

Phyllis A. Brauner Memorial Lecture Fund 12

ACS Short Course 13

Interpretation of Mass Spectra: May 2, 3

Summer Scholar Report 15

“Green Chemistry Approach to the Biocatalytic Resolution of Racemic Cyanohydrins” by Carmen Amaral and Edward J. Brush

Cover: Ronald Breslow; photo by Peter Cutts, Washington, DC

Deadline: National Meeting Issue: June 28, 2002

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The Nucleus April 2002 3
Ronald Breslow was born in Rahway, New Jersey on March 14, 1931. He received his undergraduate and graduate training at Harvard University, where he received a master’s degree in Medical Science and a Ph.D. in Chemistry. He did his Ph.D. research with Professor R.B. Woodward. He then spent a year in Cambridge, England as a postdoctoral fellow with Lord Todd, and came to Columbia University in 1956 as Instructor in Chemistry. He is now the Samuel Latham Mitchell Professor of Chemistry at Columbia and one of 9 University Professors, and a former Chairman of the Department.

Professor Breslow’s research interests can be described generally as involving the design and synthesis of new molecules with interesting properties, and the study of these properties. Examples include the cyclopropenyl cation, the simplest aromatic system and the first aromatic compound prepared with other than six electrons in a ring. His work establishing the phenomenon of antiaromaticity has also involved the synthesis of novel molecules, as well as their study. Even in work on purely mechanistic questions, such as his discovery of the chemical mechanism used by thiamine (vitamin B-1) in biochemical reactions, the synthesis and study of novel molecules played an important role. Although he continues his interest in unusual conjugated systems, his major emphasis in recent years has been on the synthesis and study of molecules that imitate enzymatic reactions. This work has included the development of remote functionalization reactions and the development of artificial enzymes. Recently he has also developed a new group of cytodifferentiating agents with potential use in cancer chemotherapy. He is the author of about 400 publications.

Professor Breslow is a member of the U.S. National Academy of Sciences, of the American Academy of Arts and Sciences, and of the American Philosophical Society as well as other scientific societies, and is an honorary foreign member of the Indian National Academy of Sciences, of the Korean Chemical Society, of the Royal Society of Chemistry and of the Royal Society of London, both of Great Britain. He has been the Chairman of the Board of Scientific Advisors of the Alfred P. Sloan Foundation, and a member of the Board of Trustees of Rockefeller University. He is on the Editorial Board of a number of scientific journals, and has held over 150 named lectureships and visiting professorships.

His major scientific awards include the American Chemical Society Award in Pure Chemistry (1966), the Fresenius Award of Phi Lambda Upsilon (1966), the Baekeland Medal (1969), the Centenary Medal (1972), the Harrison Howe Award (1974), the Remsen Prize (1977), the Roussel Prize in Steroids (1978), the James Flack Norris Prize in Physical Organic Chemistry of the American Chemical Society (1980), the Richards Medal (1984), the Arthur C. Cope Award (1987), the Kenner Award (1988), the Nichols Medal (1989), the National Academy of Sciences Award in Chemistry (1989), the Allan Day Award (1990), the Paracelsus Award and Medal of the Swiss Chemical Society (1990), and the U. S. National Medal of Science (1991).

He has also received the Mark Van Doren Medal of Columbia University and the Columbia University Great Teacher Award. He was President of the American Chemical Society (1996). He was recently named “One of the Top 75 Contributors to the Chemical Enterprise in the Past 75 Years” by a Chemical and Engineering News poll (1997) and received the Priestley Medal of the American Chemical Society, its highest honor (1999). In 2000 he received the New York City Mayor’s Award in Science.

**New Members**

Includes members relocated to the Northeastern Section

**Invitation to attend a Section meeting**

You are cordially invited to attend one of our upcoming Section meetings as guest of the Section at the Social hour and dinner preceding the meeting.

Please call Marilou Cashman at 800-872-2054, 508-653-6329, or mcash0953@aol.com by noon of the first Thursday of the month, letting her know that you are a new member.

**WANT MORE ARTICLES?**

Membership surveys show that you want more articles in the Nucleus. If you tell our advertisers that you saw their ad in the Nucleus, they will provide more financial support and this will allow us to add articles.
Abstract

Chemistry Lessons from Biology, and vice versa

Chemistry is the Creative Science, inventing new molecules and new reactions. One way in which this invention can be done is by noticing how nature performs chemistry. Chemists can imitate some of the principles of natural chemistry in a field that the speaker has termed Biomimetic Chemistry. However, we take principles from Nature, not blueprints. It has been pointed out that a jumbo jet is not simply a larger version of a pigeon. In this talk the speaker will indicate how he has adopted some of the principles used by enzymes such as the cytochrome P-450s to produce artificial enzymes that perform selective functionalizations at saturated carbons even in the presence of more reactive substrate positions. Geometric control within the catalyst-substrate complex dominates the selectivity, liberating chemistry from the “tyranny” of functional groups.

In this case the information flow is from biology to chemistry, but there are many examples of the reverse process, most obviously in medicinal chemistry. The speaker has been involved in a program over many years, in collaboration with cancer biologists, to develop compounds that induce the differentiation of cancer cells into benign forms. The mechanisms by which they act have been clarified, and in human trials very promising results have been seen. The past, present, and future of this approach to cancer will be described.

Gustavus John Esselen
1888-1952

An extensive biography was published in the April 2000 issue of The NUCLEUS.

Gustavus John Esselen was one of the movers and shakers in the Northeastern Section, having been on numerous committees, was Chairman twice (1922, 1923) and also was a Director of the national ACS. He chaired the national meetings of the ACS held in Boston in 1928 and 1939. He was employed by General Electric Co. in Lynn, then Arthur D. Little, Inc. of Cambridge. In 1921 he founded Gustavus J. Esselen, Inc., which later became the Research Division of the United States Testing Co., Inc. and addressed problems submitted by commercial clients, especially in polymer chemistry and technology. He was greatly interested in furthering the profession of chemistry, and it is in this spirit that the funds donated by the Esselen family to the Northeastern Section were used for establishing the award named in his honor, “...to recognize and reward a chemist whose scientific and technical work has contributed to the public well-being and has thereby communicated positive values of the chemical profession.”

At this year’s 16th anniversary of the award, the recipient Dr. Ronald Breslow amply fulfills these criteria.

A full discussion of the criteria for the award were published in The NUCLEUS, Vol. 75(8), April 1997, p.10

The Public is invited.

Anyone who needs special services or transportation, please call Marilou Cashman. Free Parking in the Broadway St. Garage (3rd level or higher), enter from Cambridge St. via Felton St.

Next Meeting: May 9, 2002, Education Night, Boston University School of Management Building, 595 Commonwealth Ave., Executive Dining Room, 4th Floor. Social Hour and dinner 5:30 pm, evening meeting 7:45 pm. Dr. Carl Selavka of the Mass. State Crime Laboratory to speak.
Call For Papers
Northeast Student Chemistry Research Conference 2002

Open to undergraduates, graduates, and postdoctoral fellows in all areas of chemical research

Saturday, April 27, 2002
Boston University, Science Building

Visit the NESACS YCC website at http://people.bu.edu/nsycc for details.

Abstracts will be accepted on this site. There is no registration fee.

Students are invited to present a poster or a 15 minute oral presentation.

Deadlines:
Oral presentations: April 5, 2002
Poster presentations: April 12, 2002

Undergraduate Research Poster Session

224th National Meeting of the American Chemical Society
Boston, Massachusetts, August 18–22, 2002

The ACS invites undergraduate students to submit abstracts of their research papers for presentation at the Undergraduate Research Poster Session, which will be part of the program for undergraduates at this national meeting.

Abstracts must be submitted electronically:
• Go to the meeting web site:
  html&DOC=meetings%5Cboston2002%5Cindex.html
• Click on “Submitting a Paper”
• Click on “CHED” (Division of Chemical Education)
• Go to “Undergraduate Research Posters”

For further information, contact:
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American Chemical Society
1155 Sixteenth Street, NW
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Tel: (202)872–6166; Fax: (202)833–7732
e–mail: l_garrison@acs.org

Deadline for receipt of abstracts: April 8, 2002

The Andrew H. Weinberg Memorial Lecture

In 1994 Andrew Weinberg was diagnosed with a rare childhood cancer. In spite of aggressive attempts to cure Andrew, he died of cancer shortly before his third birthday. His life and death remains a reminder of the strides that are still needed in the fight against cancer.

Andrew’s father, James S. Weinberg, became acutely aware of the need to develop better, more active, and less toxic chemotherapeutic agents that would help in this battle. With the generous support of family and friends, as well as the Medicinal Chemical Group, the Northeastern Section of the American Chemical Society, and the Dana Farber Cancer Institute, a fund was created in 1994. This fund is dedicated to bringing researchers together from the field of chemotherapy development with those in the medical community.

In 1995, the Andrew H. Weinberg Memorial Lecture was initiated. The goal of the symposium was to bring clinicians and researchers in academia, government and the pharmaceutical industry together to help foster new collaborations. This event highlights achievements and focuses on the development of new strategies in the treatment of cancer patients. This year’s symposium continues that tradition with Dr. Leroy Hood, who will speak on “Computing Life: the Challenges”

The success of the Weinberg Symposium is evidenced by the large and enthusiastic turn out for past speakers.

To continue the important work initiated by the Weinberg family, your help is vital and appreciated.

Contributions can be made to:
The Andrew H. Weinberg Memorial Fund at Dana Farber
c/o Morgan Gaspar, Dana-Farber Cancer Institute,
Division of Development and Jimmy Fund
375 Longwood Ave., Boston, MA 02115-5347

Special gratitude is also extended to:
The members of TEAM ANDREW, The Boston Marathon and Jimmy Fund Walk
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Vertex Pharmaceuticals, Inc.
The Dover Church
Biographical Sketch

Leroy Hood, M.D., Ph.D.

Dr. Hood earned an M.D. from Johns Hopkins University in 1964 and a Ph.D. in biochemistry from the California Institute of Technology in 1968.

His professional career began at Caltech, where he and colleagues pioneered four instruments that constitute the technological foundation for contemporary molecular biology. One of the instruments has revolutionized genomics by allowing the rapid automated sequencing of DNA. Dr. Hood also was one of the first advocates, and is a key player, in the Human Genome Project — the quest to decipher the sequence of human DNA.

In 1992, Dr. Hood moved to the University of Washington to create the cross-disciplinary Department of Molecular Biotechnology. He applied his laboratory’s expertise in DNA mapping to the analysis of human and mouse immune receptors and initiated studies in prostate cancer, autoimmunity, and hematopoietic stem cell development. At the UW, in 1999, Dr. Hood founded the Institute for Systems Biology in Seattle, Washington to pioneer systems approaches to biology and medicine. He is President and Director of this organization and continues with his interest in biology, medicine, technology development, and computational biology.

Dr. Leroy Hood is recognized as one of the world’s leading scientists in molecular biotechnology and genomics. A passionate and dedicated researcher, he holds numerous patents and awards for his scientific breakthroughs. Dr. Hood is a member of the National Academy of Sciences and the American Association of Arts and Sciences.

He also played a pioneering role in deciphering the secrets of antibody diversity.

Dr. Hood has played a role in founding several biotechnology companies, including Amgen, Applied Biosystems, Systemix, Darwin, and Rosetta.

Numerous organizations have honored Dr. Hood with academic and scientific awards. For example, Dr. Hood was given the Lasker Award in 1987 for studies on the mechanism of immune diversity. Dr. Hood also holds honorary degrees from Montana State University, Mt. Sinai School of Medicine of the City University of New York, the University of British Columbia, the University of Southern California, Wesleyan University, Whitman College, Bates College and Johns Hopkins University.

His research focus is to decipher complex biological systems and networks, for they encode some of the most interesting aspects of the biology of higher organisms. In this regard, his laboratory is exploring several complex biological systems and developing tools to decipher these systems. Dr. Hood utilizes genome-wide genetic mapping and the DNA array technologies to stratify prostate and ovarian cancers: that is, dividing them into their various types and using the tools of expressed sequence tag (EST) sequencing and high-speed cell sorting to analyze cancer cells. These studies are moving us toward an exciting systems view of cancer.

Since then, his research has focused on the study of molecular immunology and biotechnology. His interests also include autoimmune diseases, cancer biology and mammalian development. Dr. Hood has published more than 500 peer-reviewed papers and co-authored textbooks in biochemistry, immunology, molecular biology and genetics. He also co-edited Code of Codes, a book discussing scientific, social and ethical issues raised by genetic research.

March Puzzle Solution

The Nucleus April 2002
Board of Directors

Condensed Notes of the Annual Meeting on January 10, 2002

Officers’ Reports:
Chair: T. Frigo thanked the Board members for their support in 2001.
Chair-Elect: Nine meetings were held in 2001 in many areas of interest.
Treasurer: The operating account started 2001 with a balance of $44,446, and had a final balance of $16,559.
Trustees: M. Strem reported that the Section’s investments did well in 2001, showing a gross return of 10.34%. The assets increased from $1,920,000 to $1,945,669, an excellent record.
Auditor: T. Rosner stated that the accounts of the Section were in order.
Archivist: The Section archives remain at the library of Regis College. The Archivist had prepared posters on NESACS History which were shown at two poster sessions at the Chicago National Meeting.

Standing Committees:
Bd. Of Publications: The NUCLEUS budget is in healthy shape.
Editor: Ten issues were published with an average of 22 pages per issue.
Chemistry Education: Four students received Norris/Richards Summer Research Fellowships and have submitted reports on their work for The NUCLEUS. The NE Student Research Conference hosted visiting students from Germany in April. Five students received Grants-in-Aid to present posters at the Spring ACS meeting. Connections to Chemistry was attended by 120 teachers from 79 high schools. Marlita Taylor, a junior at MIT was sponsored by the Section for the ACS Scholars Program. The Undergraduate Research Symposium, co-sponsored by Wheaton College, was attended by 30 students from area colleges and universities.
HS Education Committee: S. Lantos reported that ~140 students took the Ashdown Exam and 20 students took the Chemistry Olympiad exam of whom 3 were invited to participate in the training sessions at the U.S. Air Force Academy for the International Chemistry Olympiad. Having three of our students selected of the total group of 20 at the Air Force Academy speaks well for the quality of teaching in the high schools of our Section. Four grants were made to High School Teachers to attend the NEACT Annual Summer Conference.

Other Committees:
Continuing Education: Two ACS Short Courses were sponsored during 2001: Emulsions and Foams (8 registrants). In the fall, Pharmacology for Chemists was offered, a 3-day course: 58 applications, but only 42 could be accommodated. The net surplus was about $5,000.
Natl. Chemistry Week: Undergraduate Day at Boston University on November 3, 2001 had ~140 students attending the several lectures and workshops.
Chemistry and Art Celebration at the Boston Museum of Science on November 4 drew an audience of about 5,600 to the tours of the museum, demonstrations and two sessions of the demonstration lecture by Prof. Bassam Shakhashiri.
Chemistry and Art Symposium at the Forsyth Institute on November 6 had an audience of about 120.
A Careers in Chemistry Symposium, sponsored by the Student Affiliate Chapter at Suffolk University on November 6 had an attendance of 25 students.
Chemistry and Art Discussions at Emmanuel College on November 7 and 9 had an audience of about 50. On November 10, a Paper Making Workshop at Wheaton College, drew 18 students.

Altogether, Chemistry Week activities involved 151 ACS members, 102 volunteers and an audience of close to 6,000 people.
Condensed from the meeting minutes of Michael Singer. For the complete minutes, see the NESACS website: NESACS.org
Board of Directors

Notes of Meeting of January 10, 2002

NOTE: Board Meetings are held on the monthly meeting day at 4:30 p.m. Section members are invited to attend.

Officers’ Reports:
Chair: 2002 Chair Morton Z. Hoffman greeted old and new members of the Board. He recognized Dr. Timothy Frigo for his service as the NESACS 2001 Chair and presented him with the ACS Past Chair pin.

He pointed out that C&EN of December 17, 2001 summarized National Chemistry Week activities, including those in our Section.

In preparation for the National Meeting in August in Boston, he announced members of the local organizing committee: J. Billo, M. Burgess, P. Gordon, A. Heyn, E. Hopkins, H. Mayne, M. Schwartz, R. Tanner, and A. Tapper. Others may be added, as needed. Our Section is responsible for hospitality, tours and Red Sox tickets. S. Lantos is organizing a high school program to be held jointly with the Division of Chemical Education during the ACS meeting.

The 4th Northeast Student Chemistry Research Conference will be held April 27, 2002.

The February 14 meeting will be held jointly with the YCC and NOBChE. YCC to hold a career development workshop prior to the evening section meeting. ACS scholars and mentors will be invited to the dinner prior to the February Section meeting.

Chair-Elect: J. Neumeyer stated that the September meeting is to be held jointly with the Maine Section at UNH, Durham.

Treasurer: J. Piper presented the December 2001 financial report. The report was ACCEPTED.

Standing Committees:
Bd. Of Publications: F. Gorga presented data from the 2001 reader survey. A summary of the data will be presented at a future meeting.

Editor: The February NUCLEUS will be 20 pages.

Membership: M. Chen reported that one new member will be at the dinner tonight.

Budget: See New Business.

Chemistry Education: R. Tanner announced that a 2002 “Connections to Chemistry” program will be held October 16, 2002 at Burlington H.S.

Local Arrangements: M. Burgess stated that arrangements for tonight’s meeting are in place. The February 14 meeting is to be at the Holiday Inn, Brookline; the March 14 Richards Medal Award Meeting will be at Harvard, the same for the April 18 Esselen Award Meeting, and the May 9 Education Night Meeting will be at BU.

Richards Medal: M. Hoffman stated that the 2002 T.W. Richards Medal will be awarded to Stephen Lippard of M.I.T. at the March 14 meeting.

Esselen Award: J. Koob stated that the...
Board of Directors

Continued from page 9

commitee had met December 18 to select an awardee. The full committee was present, including the external members, one by speakerphone from California. The name of the awardee will be announced at the February Board meeting and in the March NUCLEUS. The Award Meeting will be on April 18 at Harvard. In addition, the committee discussed means of increasing the number of high-quality nominees and making nominators more aware of the award criteria. Necessary budget constraints were also discussed.

Other Committees:
Continuing Education: A. Viola announced that the ACS has agreed to offer the Short Course Interpretation of Mass Spectra in May. Their concern was that a local Short Course might decrease the attendance at the offering of the same course at the August National Meeting in Boston.

Corporate Affiliates: M. Strem stated that the roster will be updated for 2002.

Natl. Chemistry Week: S. Iacobucci stated that there will be a meeting with Museum of Science staff for planning of the 2002 event.

Summerthing: W. Gleekman stated that he is exploring available dates for discounted Red Sox tickets.

Younger Chemists: A. Tapper stated that an organizing meeting is to be held soon to plan 2002 activities.

Medicinal Chemistry: T. Frigo stated that a symposium is being planned for May.

NERM: H. Mayne stated that there will be no 2002 NERM because of the National Meeting being in Boston.

New Business:

Budget Committee: J. Piper presented the 2002 budget which is to be voted at the February Board meeting. The budget shows an expected income of $222,252 and expenses of $248,678. He recommended an aggressive campaign for additional corporate support.

From the minutes of M. Singer.

Book Review

Science, Money and Politics by Daniel S. Greenberg (The University of Chicago Press, 2001) 530pp., ISBN: 0-22630634-8; $35.00 (hardcover)

Reviewed by Marshall E. Deutsch, 41 Concord Road, Sudbury, MA 01776-2328

A good starting point from which to begin the study which is this book’s subject is Vannevar Bush’s 1945 book “Science, The Endless Frontier,” in which he proposed that the federal government assume financial responsibility for the postwar support of science. Indeed, it is generally believed that Bush’s book provided the blueprint for the making of national science policy. However, in this thoroughly researched and entertaining book (because of its irreverent iconoclasm), Daniel Greenberg, documents the intricate politics which led to a final outcome such that “Bush felt he had given birth to an orphan and had little to do with it.” Or, to put it another way, Bush may have turned on the ignition, but he was denied access to the steering wheel.

Further mixing metaphors, this represents only one of many balloons which Greenberg gleefully shoots down. Again and again he demonstrates that we should view with extreme skepticism the pronouncements of official spokesmen concerning federal support of science. For instance, the National Science Foundation warned of a shortfall in Ph.D. production when, in fact, a glut existed, and Greenberg explains why and how this happened. Another example is that at the end of the Cold War, “The predominant collective line, in defiance of fact, [was] that federal support of science wilted ... and its revival [was] impeded by public ignorance.” In fact, “federal support for basic research in total [rose], albeit slowly, since 1989, and federal support for academic basic research actually increased slightly faster-in the post-Cold War period than in 1970-89.” And Greenberg points out the complete lack of correlation.
between the public’s admitted ignorance of science, and governmental support for science. The enormously expensive Superconducting Super Collider (SSC), concerning whose operation and value few of us can claim expertise, received funds far in excess of those awarded projects (e.g., fighting “popular” diseases) whose significance was much clearer to most of us. That is, until vast cost overruns, and a realization by Congress that the promised international collaboration in paying for it had never been a realistic hope, caused it to be finally shot down.

But, you don’t need me to review this book. In an Epilogue, Greenberg makes the following bulleted points, each of which he has thoroughly bolstered with extensive documentation, including many interviews:

“The psyche of science is touched, and scientists are often energized by magical thinking and voodoo misperceptions of plain matters of fact in the political history, financing, and public acceptance of science.”

“Many important institutions of science are bureaucratically calcified, financially insecure, and risk-averse.”

“An infinity of researchable topics renders science insatiable for money and increasingly indiscriminate in ways to get it.”

“Within the metropolis of science, the academic core shuns conventional politics while vigorously employing non-electoral techniques for obtaining government money, the denial of which it attributes to public and political ignorance and hostility.”

The sole exception to the last point was the “large-scale involvement of scientists in national politics [which] took place in the presidential campaign of 1964, under the banner of Scientists and Engineers for Johnson-Humphrey. When the scientists successfully completed their political work in that campaign, many of them feared they had damaged the sanctity of science. Never again in significant numbers did science return to ballot-box politics.” Instead, lobbying is the order of the day, with universities spending large sums on lobbying to obtain vaster sums in the form of earmarked grants, exempt from the sieve of peer review. And, when budgets are being drawn up, our own American Chemical Society enthusiastically participates in lobbying for increased funding for science, both on its own and as a member of the Intersociety Working Group, which is orchestrated by the AAAS. In the chapter on “The Sciences’ Way of Politicking” the ACS comes in for special mention, both for its use of sophisticated email technology for lobbying and for the pay of its Executive Director, John Crum, who has the highest salary listed in the book for such a post, and, I believe the highest salary listed in the book for any post. In 1996, he received a salary of $574,073 plus benefits of $34,900, while in 1997, the figures were

continued on page 17
Dr. Phyllis Ambler Brauner held many positions within the Northeastern Section, as well as chairman of the ACS Public Service Committee. One of the programs she helped to launch was the popular Holiday Lecture, offered as a gift to the people of New England from the Northeastern Section. Now held during National Chemistry Week, the lecture continues to draw enthusiastic audiences of all ages to Dr. Bassam Shakhashiri’s demonstrations. After Dr. Brauner’s death in December, 2000, the lecture was renamed the Phyllis Ambler Brauner Memorial Lecture, and a committee was formed to ensure that it be continued. What follows is some background on Dr. Brauner and the lecture.

In 1992, after she was inducted into the Boston University Graduate School Academy of Distinguished Alumni, Phyllis Brauner reluctantly agreed to be interviewed. In a story in the Middlesex News, she recalled that her interest in chemistry dated back to her Girl Scout days, when she had a wonderful nature teacher.

“I just loved nature,” she said, “and I began to realize at 12 or 13 that the glue that held all this together was chemistry. It was common to all things. It was fascinating to me. It could help mankind and hurt mankind.” The child who was so in awe of nature grew into a woman who wanted to pass on to others, especially young people, her fascination with chemistry. For 34 years, she taught at Simmons College, where she inspired her students not only to love chemistry but also to think about their role in a changing world. One of her former students recalled a story Dr. Brauner told about her two small daughters whispering outside the door as she was trying to write her doctoral dissertation. The student, by then a surgeon, wrote, “That anecdote encapsulated the conflicted concerns and delicate balance which is faced by women hoping to achieve their intellectual potential, become self-supporting, and mothering simultaneously. It was the clearest message I received in college about the reality of a woman’s complex life.”

Dr. Brauner’s life was nothing if not complex. Left a widow after her scientist husband, William Brauner, was killed in a plane crash while on a U.S. government mission, she entered the field when it was still dominated by men. At Purdue University, where she was in graduate school, the joke was the few female students in the class were only interested in getting their MRS degrees.

After William’s death Phyllis moved back to her native Massachusetts, where she and her mother shared a home and child care. At the same time she was teaching full-time at Simmons and attending graduate school at Boston University, where she obtained a Ph.D. in analytical chemistry, working with A. Heyn.

Years later, always interested in travel and other cultures, she took sabbaticals in Switzerland and Sweden, joined a People to People program to Russia and Eastern Europe, took part in the first goodwill trip of the ACS to China, and enthusiastically joined an Earthwatch expedition to Lake Baikal,
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DATES and TIME:  Thursday, May 2, 2002;  8:00 a.m. – 5:00 p.m.
and  Friday, May 3, 2002;  8:30 a.m. – 5:00 p.m.

PLACE:  Snell Library, Room 90, Northeastern University, 360 Huntington Ave., Boston, MA

PROGRAM AGENDA:

Introduction to Chemical Bonding in Organic Molecules as it Pertains to Mass Spectrometry
Naturally Occurring Stable Isotope Abundances and Their Role in Peak Intensity
The Molecular Ion
   Odd-electron ions; the nitrogen rule; logical losses.
Fragmentation as it Relates to Structure, Elemental Composition, and Compound Type.

Mass Spectra of High Molecular Weight Compounds.
MS/MS Mass Spectra – What Are They and How Do We Deal With Them?
Fragmentation of Specific Compound Types – Aliphatic and Aromatic Hydrocarbons, Alcohols, Amines, Acids, Aldehydes, and Ketones.
Library Searches and Mixed Spectral Data
Chemical Ionization and Electron Ionization Spectra Used Together to Determine the Identity and Structure of an Unknown.

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INSTRUCTOR:

O. David Sparkman is an Adjunct Professor of Chemistry at the University of the Pacific in Stockton, Cal., and a consultant to the National Institute of Standards and Technology Mass Spectrometry Data Center. At the University of the Pacific he teaches courses in mass spectrometry and analytical chemistry and manages the mass spectrometry facility. He is on the Editorial Advisory Boards of the Journal of the American Society for Mass Spectrometry and the HD Science GC/MS Update – Part B. He is the author of Mass Spectrometry Desk Reference, and with J. Throck Watson developed the Mass Spectral Interpretation Quick Reference Guide. Professor Sparkman is one of the highest rated instructors in the ACS Short Course program.

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Department of Chemistry
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The Nucleus April 2002 13
Phyllis A. Brauner
Continued from page 12

USSR, and to Rarotonga. Shortly after retiring from Simmons, she taught in Japan and Guam for the University of Maryland before becoming a lecturer at Framingham State College.

Over the years, she devoted many hours to the Northeastern Section, including serving as its first female chairman in 1974. She wore many hats—among them, member of the Board of Directors, Councilor representing NESACS at national ACS meetings, and a member and/or chairman of numerous committees, editor and business manager of The Nucleus, and initiator of the “Summer Thing” annual outing. For her dedication, she received the Henry A. Hill Award for Outstanding Service to the Northeastern Section in 1985.

Especially those activities that encouraged the general public to share her enthusiasm kept her involved with the section. She suggested “ACS Night at POPS,” helped with National Chemistry Day and career days for Boston-area students. She saw the free Holiday Lecture as having the greatest potential for reaching eager young minds. Carolyn Spock, a Simmons College colleague who worked with Dr. Brauner on the lecture from its beginning, remembers that those involved with its creation were aware that children, especially girls, were not being turned on (and in some cases were being turned off) to science in those critical early-childhood years. One of the goals of the lecture was to spark that interest.

The first lecture was scheduled for December 29, 1986 at the Museum of Science and featured Dr. Shakhashiri of the University of Wisconsin and Prof. emer. Hubert Alyea of Princeton. Years later, she liked to recall the dour predictions of a colleague who insisted no one would come. As it turned out, more than 350 people of all ages attended, and 200 more had to be turned away.

She organized similar lectures at Framingham State College during the school year, featuring chemistry educators known for their ability to interact with young people: Hubert Alyea, Jerry Bell, and Dudley Herschbach. The theme of these lectures has always been “Science is Fun,” and Dr. Shakhashiri ensures that it is just that by including demonstrations that smoke, change color, or otherwise amaze the many children in the audience.

These lectures take a tremendous amount of effort to organize. The details to be worked out were endless, especially in the early years: Who would transport and mix the chemicals? What fire laws had to be obeyed? Who would pick up the speaker at the airport and hotel? Fortunately, Dr. Brauner was assisted by Valerie Wilcox and a loyal group of colleagues and able helpers, including staff at the Museum of Science.

In late 2000 she was hospitalized several times but continued to fret over the details of the lecture. On November 5, 2000, the date of the lecture, she was too ill to attend, but was immensely cheered by a call from Dr. Shakhashiri.

The Phyllis A. Brauner Memorial Lecture was one of two Northeastern Section memorials established in her name. (The other is the Phyllis A. Brauner Memorial Book Prize, to be awarded in April.) The committee formed to ensure that it continues is headed by Dr. Doris Lewis and consists of family, colleagues, and Section members. The committee is presently working with the national office of ACS to set up a trust to support the lecture with a goal of raising substantial funds, which may be matched by funds from the ACS Matching Gift Fund Program. Individual or corporate donations of $2,500 or more will be matched by ACS. Donations may be spread over a five-year period.

Committee members are also exploring other funding sources, including foundations.

For information on the ACS Matching Gift Fund Program and other donation opportunities, contact Doris Lewis, 236 Lexington St., Newton, MA 02466; dlewis@cas.suffolk.edu or Susan Brauner, spbrauner@juno.com.
Summer Scholar Report

A Green Chemistry Approach to the Biocatalytic Resolution of Racemic Cyanohydrins

Carmen Amaral* and Edward J. Brush, Department of Chemical Sciences, Bridgewater State College

Introduction. Cyanohydrins offer an enormous synthetic potential as building blocks for synthesizing chiral compounds (1). Cyanohydrins are readily converted into a variety of functional groups that are important precursors in the synthesis of pesticides, pharmaceuticals, agrochemicals and other fine chemicals (2). Therefore the interest in industrial use of these compounds has grown during the last several years.

Investigations on the asymmetric synthesis of cyanohydrins have been going on for almost a century. The first asymmetric synthesis described and the first one catalyzed by an enzyme was the preparation by Rosenthaler in 1908 of (R)-mandelonitrile (MDN) from benzaldehyde and HCN (3). One of the many current approaches for the synthesis of chiral cyanohydrins involves the use of hydroxynitrile lyases (HNLs) to catalyze the stereospecific addition of HCN to the corresponding aldehyde or ketone, Figure 1 (4). This synthetic pathway is not practical due to the high concentration of HCN needed to force the reaction equilibrium to completion. Another limitation of this method is the competing non-enzymatic formation of racemic cyanohydrin that decreases the enantiomeric purity of the product (4). In this process the HNLs are lyophilized and immobilized on a solid support system, and utilized in organic solvents under non-aqueous conditions (2). However, it is difficult for substrates and cofactors to diffuse to the active site of immobilized enzymes resulting in low activity in organic solvents (5). Furthermore, the need for excess HCN and organic solvents in this synthetic approach is inconsistent with the mainstream “Green Chemistry” practices currently supported by academia, industry, and government (6). Cyanide is a health and environmental hazard and the excess use of organic solvents to carry out these reactions also proves to be environmentally detrimental.

The approach being reported in this research involves coupled biocatalysis in a biphasic organic-aqueous reaction system. Biphasic solvent systems offer the possibility to work at high concentrations of poorly water-soluble substrates and/or products (4). Substrate and product inhibition are reduced due to their presence in the organic phase where they are readily soluble and more stable than in an aqueous solution. The interaction between enzyme and substrate has been proposed to occur at the organic-aqueous interface (7), and since the enzymes are not immobilized on a solid support, substrate access to the active site of the enzyme is greatly facilitated.

We have investigated a unique approach using a coupled enzymatic system for the kinetic resolution of racemic cyanohydrins in a biphasic organic-aqueous medium, Figure 2. In this system the HNL mandelonitrile lyase (MNL) catalyzes the dismutation of the cyanohydrin (R)-mandelonitrile (MDN) to benzaldehyde and cyanide, with the (S)-enantiomer left unreacted. The reaction equilibrium is shifted in favor of kinetic resolution by the reduction of benzaldehyde to benzyl alcohol catalyzed by horse liver alcohol dehydrogenase (HLADH) with concomitant oxidation of NADH. Removal of the aldehyde product also prevents the non-enzymatic reaction with cyanide that regenerates the racemic cyanohydrin. In this system (S)-MDN remains in the organic phase where it is stable toward non-enzymatic dismutation. NADH/NAD+ and the enzymes remain in the aqueous phase where their activity can be maximized. The benzyl alcohol product is a potent competitive inhibitor of MNL (8), but it remains predominately in the organic phase where it is effectively isolated from the enzyme. Biocatalysis has been seen as a very efficient alternative in performing highly specific regio- and stereospecific transformations of organic molecules unparalleled by chemical processes (9). The application of biocatalysis in a biphasic system to resolve racemic cyanohydrins may lead to a more environmentally benign and cost effective method of obtaining products of high optical purity.

Evaluation of Kinetic Constants. The first step involved an evaluation of the kinetic constants for the normal MNL reaction as compared to that in the coupled system. The normal MNL assay reaction involves determination of enzymatic activity based on the increase in absorbance at 249nm due to the formation of benzaldehyde from continued on page 16
(R)-mandelonitrile (0.1 M citrate buffer, pH 5.5). Enzymatic activity in the coupled system was determined based on the reduction of benzaldehyde by HLADH with oxidation of NADH to NAD\(^+\), which was monitored at 340nm. Each system was assayed at pH 5.5 for maximum activity of MNL and stability of MDN. The results of these experiments are summarized in Table 1. The kinetic constants determined in each reaction system are nearly identical, suggesting that MNL in the coupled system is as efficient as under the normal reaction conditions. Furthermore, this assay method is suitable for determination of the kinetic constants of a variety of aliphatic and aromatic cyanohydrin substrates for MNL (10).

### Table 1. Evaluation of MNL Kinetic Constants.

<table>
<thead>
<tr>
<th>Assay Method</th>
<th>(K_m) (mM)</th>
<th>(V_{max}) (umole/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal System</td>
<td>0.18</td>
<td>0.12</td>
</tr>
<tr>
<td>Coupled System</td>
<td>0.19</td>
<td>0.08</td>
</tr>
</tbody>
</table>

Efficiency of the Kinetic Resolution.

We next investigated the efficiency of the coupled MNL/HLADH system for the kinetic resolution of racemic MDN. Figure 3 illustrates the progress curve for the consumption of (R)-MDN by MNL under optimum conditions with HLADH (pH 5.5) versus the complete chemical dismutation of MDN at pH 7.

By taking advantage of the direct stoichiometric relationship between benzaldehyde formation from MDN and NADH consumption, we can clearly illustrate the stereospecific dismutation of (R)-MDN into benzaldehyde and HCN. The presence of (S)-MDN in high enantiopurity is suggested by 50% consumption of the total MDN. For comparative purposes we have also presented the progress curve depicting the non-enzymatic dismutation of MDN without MNL. The non-stereospecific chemical reaction is approaching 100% completion, indicating complete dismutation of racemic MDN. This experiment was conducted at pH 7.0 where the non-enzymatic rate of MDN decomposition is increased.

### Kinetic Resolution of Racemic MDN Under Biphasic Conditions.

Once it was determined that MNL does in fact catalyze the stereospecific dismutation of MDN, the effectiveness of the MNL/HLADH coupled system under biphasic reaction conditions was evaluated. The complete biphasic reaction system is illustrated in Figure 2, using equal volumes (10 mL) of 0.1 M citrate buffer, pH 5.5 (MNL, HLADH, 5 mM NADH) in the aqueous phase, and diisopropyl ether (DIPE; 5 mM racemic MDN) as the organic phase. The biphasic reaction mixture was gently stirred to avoid vortex formation, and the DIPE phase was periodically analyzed for MDN, benzyl alcohol, and benzaldehyde by reverse-phase HPLC. The results in Table 2 are nearly identical to those obtained in aqueous buffer alone, and strongly suggest that resolution of racemic MDN occurs efficiently under the biphasic reaction conditions. One of the problems encountered when analyzing the DIPE phase of the biphasic system was that the benzaldehyde was not completely reduced by HLADH/NADH. We have determined that this is not due to HLADH losing activity in the presence of DIPE, but possibly due to mass transfer problems due to a slow stir rate, or too small of a surface area for efficient interaction of the enzyme and substrate at the biphasic reaction interface. Optimization of the biphasic reaction system is in progress.

### Conclusion.
This research has successfully established the feasibility of employing a biphasic aqueous/organic biocatalytic reaction system for the kinetic resolution of racemic mandelonitrile. This approach is consistent with Green Chemistry synthetic practices involving the reduction of toxic substances and use of potentially reusable biocatalysts. We are currently investigating NAD\(^+\)/NADH recycling using 2-propanol. The acetone product should combine with the stoichiometric amounts of cyanide formed during MDN dismutation to produce acetone cyanohydrin. This may allow for...
removal and recycling of cyanide, as acetone cyanohydrin has been utilized as a cyanide donor for the synthesis of racemic cyanohydrins (11).

**Acknowledgements.** I gratefully acknowledge the Northeastern Section of the American Chemical Society for a James Flack Norris and Theodore William Richards Summer 2001 Research Scholarship, and the Department of Chemistry at Bridgewater State College for financial support of this research. I would also like to thank Joel Goldberg and Amir Sapkota for their work in developing the coupled enzyme assay method.

**References**


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**Summer Scholar**

*Continued from page 16*

**From the February Meeting**

*Continued from page 11*

$600,000 and $36,510 respectively. I thought you’d like to know.

Editor’s comment: In order to put Dr. Crum’s salary in the correct perspective, it should be realized that the ACS has an operating budget close to 400M$/year and the Executive Director is the CEO of this corporation. The ACS therefore has to offer its CEO a remuneration compatible with that offered by corporations of similar size. In addition, being a non-profit organization, the ACS cannot offer stock options, which often are a major part of the emoluments at stock-based companies.

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**Book Review**

*Continued from page 11*

Members of the Younger Chemists Group, NOBCChE, and ACS Scholars

1 to r: Dr. Willie E. May, National Institute of Standards and Technology (speaker); Reuben L. Cummings, ACS Scholar, MIT; Dr. Morton Z. Hoffman, NESACS Chair.
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Dr. Vincent P. Stanton, Jr. (Vice President, Variagenics Inc.)
“Genetic Markers Predicting Response to Cancer Chemotherapy”

**CURRENT TOPICS IN MEDICAL CHEMISTRY -- A DISTINGUISHED LECTURE SERIES,**
Boston Univ., 595 Commonwealth Ave., Room 228 Rafik B. Hariri Building, 2:00 pm

Prof. Dr. Geert-Jan Kroes (Univ. of Leiden)
“Vibrational Effects on Dissociative Chemisorption of Hydrogen on Cu(100) and Pt(111)”
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

**April 8**
Prof. Jack Szostak (Harvard Medical School)
“Synthesizing Life - Progress to Date, and the Challenges Ahead”
Boston Univ., 590 Commonwealth Ave., Science Center Auditorium, SCI 107, 4:00 pm

**April 9**
Prof. Lawrence Scott (Boston College)
“Strategies for the Rational Synthesis of Fullerenones and Their Open Geodesic Siblings”
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

**April 16**
Prof. Michael J. Marsella (Univ. of Calif.)
“Classical Annulenes, Non-Classical Applications”
Boston College, Merkert Chemistry Center, Room 130, 2609 Beacon St. 4:00 pm

Prof. Julius Rebek, Jr. (The Scripps Res. Inst. and The Skaggs Inst. for Chemical Biology),
Consensus Pharmaceuticals Lecture,
“Molecular Assembly and Encapsulation”
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

**April 17**
Prof. Cynthia Burrows (Univ. of Utah)
“Chemistry and Biochemistry of Guanine Oxidation in DNA: From Metals to Mutations”
Boston College, Merkert Chemistry Center, Room 130, 2609 Beacon St.
4:00 pm

**April 18**
Prof. Julius Rebek, Jr. (The Scripps Research Institute)
“To Be Announced”
Boston College, Merkert Chemistry Center, Room 127, 2609 Beacon St.
4:00 pm

Prof. Clifford Matthews (Univ. of Illinois at Chicago)
“HCN - a prebiotic polymer”
Northeastern Univ., 129 Hurtig Hall, 4:00 pm

**April 19**
Dr. Dennis Keith (Vice President, Cubist Pharmaceuticals)
“ChemInformatics 3: Converting High-Throughput Screening Hits into Medicinal Chemistry Leads”

**CURRENT TOPICS IN MEDICAL CHEMISTRY -- A DISTINGUISHED LECTURE SERIES,**
Boston Univ., 595 Commonwealth Ave., Room 228 Rafik B. Hariri Building, 2:00 pm

**April 23**
Prof. Kenneth Karlin (Johns Hopkins Univ.)
“Synthetic Modeling of Copper and Heme-Copper Protein Dioxygen Chemistry”
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford, Room 106, 4:30 pm

**April 25**
Prof. Harry B. Gray (Calif. Inst. of Technology and Beckman Institute)
“To Be Announced”
Boston College, Merkert Chemistry Center, Room 127, 2609 Beacon St.
4:00 pm

Prof. Ann Walker (Univ. of Arizona)
“Novel, no-releasing heme proteins from the saliva of blood-sucking insects”
Northeastern Univ., 129 Hurtig Hall, 4:00 pm

**April 26**
Dr. Charles J. Manly (Vice President, Neurogen Corporation)
“Strategies and Technologies in Modern Drug Discovery: Part I - Impact of Integrated High-Throughput Approaches. Part II - Challenges Today and Tomorrow”

**CURRENT TOPICS IN MEDICAL CHEMISTRY -- A DISTINGUISHED LECTURE SERIES,**
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**April 29**
Prof. Tom Lectka (Johns Hopkins Univ.)
“Asymmetric Catalysis with Zwitterionic Enolates: From b-Lactam Synthesis to Enantioselective Halogenation”

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Boston Univ., 595 Commonwealth Ave., Science Center Auditorium, SCI 107, 4:00 pm

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