

THE NUCLEUS

March 2008

Vol. LXXXVI, No. 7

Monthly Meeting

*Richards Medal Award Meeting
at Harvard*

Professor Robert G. Bergman

NCW Report

*National Chemistry Week 2007
Report*

By Christine Jaworek-Lopes

Leslie Orgel

1927-2007

Summer Research Report

By Jiajia Cui and Dean Wilcox



2008 Eastern Analytical Symposium

Creating a Better Tomorrow

November 17 - 20, 2008

Garden State Exhibit Center, Somerset, New Jersey

CALL FOR PAPERS

Deadline – April 15, 2008

The Eastern Analytical Symposium and Exposition is the second largest conference and exposition for laboratory science in the U.S. dedicated to the needs of analytical chemists and those in the allied sciences. We offer high quality cutting-edge technical sessions and state-of-the-art short courses, workshops and seminars. We invite you to be a part of the program by contributing a paper for oral or poster consideration. Please note that all abstracts must be submitted electronically via the EAS web site at www.eas.org. The abstract submission deadline is April 15.

To submit a contributed paper for the 2008 EAS Technical Program, please submit abstracts through our web site at www.eas.org, between March 1 and April 15, and follow the instructions for abstract submission. *Invited speakers must not submit abstracts to EAS until requested.*

Please carefully review the following information:

- All contributed abstracts must be submitted through our web site at www.eas.org between March 1 and April 15, 2008. No faxed, e-mailed, or mailed abstracts will be accepted.
- Please note that no one author may submit and present more than two posters.
- All abstracts will be acknowledged via e-mail.
- The title of the presentation and the list of authors that you submit are final, and may not be changed.
- The abstract that you submit will be considered to be your final abstract that will be printed in the abstract book for the 2008 Eastern Analytical Symposium.
- Presenting authors of contributed submissions will be notified in June 2008 of the status of the abstract and its session assignment.

If you have questions concerning the submission of abstracts, please contact us at:

EAS Hotline	301-682-3701
EAS Faxline	301-668-4312
EAS E-mail	askEAS@aol.com

Eastern Analytical Symposium & Exposition, Inc.
P.O. Box 370, Walkersville, MD 21793

WWW.EAS.ORG

The Northeastern Section of the American Chemical Society, Inc.

Office: Marilou Cashman, 23 Cottage St., Natick, MA 01360. 1-800-872-2054 (Voice or FAX) or 508-653-6329.

e-mail: mcash0953(at)aol.com

Any Section business may be conducted via the business office above.

NESACS Homepage:

http://www.NESACS.org

David Cunningham, Webmaster

ACS Hotline, Washington, D.C.:

1-800-227-5558

Officers 2008

Chair:

Marietta Schwartz

Chemistry Department, UMASS-Boston

Boston, MA 02125

617-287-6146; marietta.schwartz(at)umb.edu

Chair-Elect:

Dr. E. Joseph Billo

13 Shattuck Street

Natick, MA 01760

508-653-3074, joseph.billo(at)verizon.net

Immediate Past Chair:

Mukund Chorghade

14 Carlson Circle, Natick, MA 01360

508-651-7809 and 308-3891

Chorghade(at)comcast.net

Secretary:

Michael Singer

Sigma-Aldrich

3 Strathmore Rd., Natick, MA 01360

508-651-8151X291; msinger(at)sial.com

Treasurer:

James Piper

19 Mill Rd., Harvard, MA 01451

978-456-3155, piper28(at)attglobal.net

Auditor:

Anthony Rosner

Archivist:

Myron S. Simon

20 Somerset Rd.

Newton, MA 02465; 617-332-5273

Romysimon(at)mindspring.com

Trustees:

Joseph A. Lima, Esther A. H. Hopkins,

Michael E. Strem

Councilors

Term Ends 12/31/2008

Doris I. Lewis

Morton Z. Hoffman

Christine Jaworek-Lopes

Mary Burgess

Donald O. Rickter

Term Ends 12/31/2009

Catherine Costello

Patricia Mabrouk

Michaeline F. Chen

Dorothy J. Phillips

Amy Tapper

Term Ends 12/31/2010

Thomas R. Gilbert

Pamela Nagafuji

Robert Lichter

Michael Singer

Alternate Councilors

Patrick M. Gordon

Michael P. Filosa

Lawrence Scott

Liming Shao

S.B. Rajur

Julia H. Miwa

Alfred Viola

Jerry P. Jasinski

Eva B. Binnun

Barney Grubbs

Timothy B. Frigo

Mark Froimowitz

David Cunningham

Erik Rozners

All Chairs of standing Committees, the editor of THE NUCLEUS, and the Trustees of Section Funds are members of the Board of Directors. Any Councilor of the American Chemical Society residing within the section area is an ex officio member of the Board of Directors.



Contents

Announcements 4

Norris and Richards Undergraduate Research Scholarships

Call for papers: Northeast Student Chemistry Research Conference

Monthly Meeting 5

2008 ACS Richards Medal Award Meeting

Awarded to Professor Robert G. Bergman, University of California, Berkeley

National Chemistry Week 2007 Report 6

By Christine Jaworek-Lopes

Leslie Orgel 1927-2007 8

Renowned Chemical Evolution Scientist Dies

5th Annual YCC Career Fair 9

Northeast Student Chemistry Career Fair at Brookline Holiday Inn

Summer Research Report 10

Nickel Binding Properties of the C-terminal Histidine-rich Sequence of the Metallochaperone UreE from Klebsiella aerogenes

By Jiajia Cui and Dean E. Wilcox, Department of Chemistry, Dartmouth College, Hanover, NH

March Historical Events in Chemistry 14

By Professor Leopold May, Catholic University of America

Call for Nominations 15

2008 ACS Northeast Region Awards

Cover: *Professor Robert G. Bergman, University of California at Berkeley, 2008 Richards Award Winner (Photo courtesy of Professor Bergman)*

Deadlines: *May 2008 Issue: March 11, 2008*

Summer 2008 Issue: June 16, 2008

THE NUCLEUS

The Nucleus is published monthly, except June and August by the Northeastern Section of the American Chemical Society, Inc. Forms close for advertising on the 1st of the month of the preceding issue. Text must be received by the editor six weeks before the date of issue.

Editor:

Michael P. Filosa, Ph.D., ZINK Imaging, Inc., 16 Crosby Drive, Building 4G, Bedford, MA 01730 Email: Michael.filosa(at)zink.com; Tel: 508-843-9070

Associate Editors:

Myron S. Simon, 20 Somerset Rd., W. Newton, MA 02465, Tel: 617-332-5273
Sheila E Rodman, Konarka Technologies Inc., 116 John St. Suite 12, Lowell, MA 01852 email: srodman(at)konarka.com tel 978-569-1414

Board of Publications:

Vivian K. Walworth (Chair), Mary Mahaney, David Cunningham

Business Manager:

Karen Piper, 19 Mill Rd., Harvard, MA 01451, Tel: 978-456-8622

Advertising Manager:

Vincent J. Gale, P.O. Box 1150, Marshfield, MA 02050, Tel: 781-837-0424; FAX: 781-837-1453

Contributing Editors:

Morton Hoffman, Feature Editor; Dennis Sardella, Book Reviews

Calendar Coordinator:

Sheila Rodman, email: srodman(at)konarka.com

Photographers:

Morton Z. Hoffman and James Phillips

Proofreaders:

Donald O. Rickter, Myron S. Simon, Vivian K. Walworth, E. Joseph Billo

Webmaster:

David Cunningham, webmaster(at)nesacs.org

Copyright 2008, Northeastern Section of the American Chemical Society, Inc.

The James Flack Norris and Theodore William Richards Undergraduate Summer Research Scholarships

The Northeastern Section of the American Chemical Society (NESACS) established the James Flack Norris and Theodore William Richards Undergraduate Summer Scholarships to honor the memories of Professors Norris and Richards by promoting research interactions between undergraduate students and faculty.

Research awards of \$3250 will be given for the summer of 2008. The student stipend is \$2750 for a minimum commitment of ten weeks of full-time research work. The remaining \$500 of the award can be spent on supplies, travel, and other items relevant to the student project.

Institutions whose student/faculty team receives a Norris/Richards Undergraduate Summer Research Scholarship are expected to contribute toward the support of the faculty members and to waive any student fees for summer research. Academic credit may be granted to the students at the discretion of the institutions.

Award winners are required to submit a report (~5-7 double-spaced pages including figures, tables, and bibliography) of their summer projects to the NESACS Education Committee by November 3, 2008 for publication in *The Nucleus*. They are also required to participate in the Northeast Student Chemistry Research Conference (NSCRC) in April 2009.

Call for Papers



Northeast Student Chemistry Research Conference 2008

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

Saturday, April 19th, 2008

MIT

The Ray and Maria Stata Center

Visit the NESACS YCC website for more details at www.nsycc.org.

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 presentation: April 8th, 2008

Poster presentations: April 10th, 2008 ◇

Eligibility: Applications will be accepted from student/faculty teams at colleges and universities within the Northeastern Section. The undergraduate student must be a chemistry, biochemistry, chemical engineering, or molecular biology major in good standing, and have completed at least two full years of college-level chemistry by summer, 2008.

Application: Application forms are available on the NESACS web site at <http://www.nesacs.org>. Completed applications are to be submitted no later than April 4, 2008 to the Chair of the Selection Committee:

Professor Edwin Jahngen
University of Massachusetts Lowell
Chemistry Department,
Room 520, Olney Hall
1 University Avenue
Lowell, MA 01854-5047

Notification: Applicants will be notified of the results by e-mail on April 23, 2008 with written confirmation to follow. ◇

Corporate Patrons (\$2000+)

Abbott Laboratories
Lyophilization Service of New England
Merck
National ACS
Novartis
Pfizer
Sepracor
Strem Chemicals
Vertex Pharmaceuticals

Patrons (\$1000-\$1999)

Astra-Zeneca R&D Boston
IRIX Pharmaceuticals
Millenium Pharmaceuticals
Shasun Pharmaceuticals
ZINK Imaging
Ziopharm Oncology, Inc.

Donors (\$300-\$999)

Cambridge Major Laboratories
Occidental Petroleum
Organix
PCI Synthesis
Royal Society of Chemistry
Sero Research Institute
Wyeth Pharmaceuticals

New Members

Invitation to attend a meeting

You are cordially invited to attend one of our upcoming Section meetings as a 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: [Mcash\(at\)aol.com](mailto:Mcash(at)aol.com) by noon of the first Thursday of the month, letting her know that you are a new member. ◇

**Looking for seminars
in the Boston area?**

**Check out the
NESACS Calendar**

www.nesacs.org/seminars

Monthly Meeting

The 886th Meeting of the Northeastern Section of the American Chemical Society

2008 ACS Richards Medal Award Meeting

Thursday – March 13, 2008

Harvard Faculty Club,

20 Quincy St., Cambridge, MA.

5:30 pm Social Hour

6:15 pm Dinner

8:15 pm **Richards Award Ceremony**

Mallinckrodt Building, Pfizer Lecture Hall - MB23,
12 Oxford Street, Cambridge, MA.

Professor Marietta Schwartz, NESACS Chair, Presiding

“Theodore William Richards”, Professor Gary R. Weisman, Chair,
Richards Medal Committee

Introduction of 2008 Medalist by Professor Peter Vollhardt, University of California, Berkeley

2008 Richards Medalist - Prof. Robert G. Bergman, Gerald E. K. Branch Distinguished Professor, University of California, Berkeley, *“Selective Organic and Organometallic Transformations Mediated by Molecular and Supramolecular Environments.”*

Dinner reservations should be made no later than noon, Thursday, March 6, 2006. Please call or fax Marilou Cashman at 800-872-2054 or e-mail at Mcash0953(at)aol.com. Please specify vegetarian. Reservations not cancelled at least 24 hours in advance must be paid. Members, \$30; Non-members, \$35; Retirees, \$20; Students, \$10.

THE PUBLIC IS INVITED

Anyone who needs special services or transportation, please call Marilou Cashman a few days in advance so that suitable arrangements can be made.

Free parking in the Broadway St. Garage (3rd level or higher), enter from Cambridge Street via Felton, St.

Next Meeting: Esselen Award Meeting, April 17, 2008, Harvard University. Reception and dinner: 5:30 pm, Harvard Faculty Club; Award Meeting: 8:15 pm, Pfizer Lecture Hall, Mallinckrodt Chemistry Building, 12 Oxford Street, Cambridge. Dr. John A. Katzenellenbogen, Swanlund Professor of Chemistry, University of Illinois Urbana-Champaign: “Estrogens and Estrogen Receptors as a Nexus of Chemistry and Biology in Health and Disease” ◇

Biography

Robert G. Bergman was born in Chicago, Illinois in 1942. After completing his undergraduate studies in chemistry at Carleton College in 1963, he received his Ph.D. at the University of Wisconsin in 1966 under the direction of Jerome A. Berson. Bergman spent 1966-67 as a NATO Fellow in Ronald Breslow's laboratories at Columbia, and following that went to the California Institute of Technology as a Noyes Research Instructor. He was promoted to assistant professor in 1969, associate professor in 1971, and full professor in 1973. He accepted an appointment as Professor of Chemistry at the University of California, Berkeley in 1977 and was appointed Gerald E. K. Branch Distinguished Professor at Berkeley in 2002.

Bergman was trained as an organic chemist and spent the first part of his independent career at Caltech investigating the mechanisms of organic reactions. He also developed methods for the generation and study of unusually reactive molecules, such as 1,3-diradicals and vinyl cations. In 1972 he discovered the thermal cyclization of *cis*-1,5-hexadiyne-3-enes to 1,4-dehydrobenzene diradicals. In the 1980's this transformation of enediyne was identified as a crucial DNA-cleaving reaction in several antibiotics that bind to nucleic acids, and the enediyne reaction is now often referred to as the “Bergman cyclization”. In the mid-1970's Bergman's research broadened to include organometallic chemistry. Since moving to Berkeley he has made contributions to the synthesis and chemistry of several types of organotransition metal complexes and to improving our understanding of the mechanisms of their reactions. In this area he has focused on migratory insertion and oxidative addition reactions, the chem-

continued on page 16

bond activation and pericyclic reactions. The lecture will include a focus on the study of reaction mechanisms to provide a rational approach to reaction optimization. ◇

Abstract

Selective Organic and Organometallic Transformations Mediated by Molecular and Supramolecular Environments

This lecture will discuss several approaches to the development of selective organic and organometallic reactions. Examples will be drawn from our group's efforts to use molecular and/or supramolecular environments to control the selectivity of organic and organometallic reactions such as hydrolyses, carbon-hydrogen

National Chemistry Week 2007 Report

The Northeastern Section Celebrates The Many Faces of Chemistry

By Christine Jaworek-Lopes

In preparation for National Chemistry Week 2007, a volunteer preparation day was held at Emmanuel College on Saturday, October 13, 2007. More than 50 individuals attended this event, which allowed volunteers to practice the hands-on activities and demonstrations in advance of the October celebration. A member of the Boston Children's Museum staff was on hand to choose which activities worked best for her audience.

On Sunday, October 21, 2007, the Northeastern Section of the American Chemical Society sponsored a National Chemistry Week 2007 Kick-Off Event at Museum of Science-Boston (MoS). More than 50 volunteers (from ACS, Boston Latin School, the Brauner Committee, Emmanuel College, Malden High School, Merck Research Laboratories – Boston, Stonehill College, Suffolk University, Tufts University) ensured that the more than 1000

visitors to the daylong event enjoyed a number of hands-on activities.

Hands-on activities included: isolating iron from Total® cereal, making play putty, studying the chemistry of different types of nails, making UV detector bracelets, making marker butterflies, assessing sugar content in cereals and beverages, and learning how mood lipsticks work.

Among the highlights of the day were the two lecture demonstrations, as part of the Phyllis A. Brauner Memorial lectures, presented by Dr. Bassam Shkhashiri, Professor of Chemistry at the University of Wisconsin-Madison. These captivating lectures were enjoyed by children and adults alike. Approximately 300 individuals attended these lectures which were free with admission to the MoS. In addition, Dr. Shkhashiri was presented with a Salute to Excellence Award for his continued involvement

with the NESACS NCW events.

On October 22, 2007, a diverse audience of 225 area high school students participated in a daylong program at the Museum of Science-Boston high-lighting the variety of careers impacted by chemistry. This program was funded by receipt of a Local Section Innovative Grant, local section funds, and a donation from Merck Research Laboratory – Boston.

The day commenced with the students participating in an interactive lecture-demonstration given by Dr. Bassam Shkhashiri. The students then had the opportunity to meet and talk at informal conversation stations with scientists from a variety of organizations. Each scientist brought a hands-on activity or demonstration to encourage conversation. The scientists that participated in this event were:

- Marta Biarnes – a former cosmetic chemist from L'Oreal USA, now a member of the MoS staff
- Jennifer Chute – Criminalist, Boston Police Department Crime Lab
- Raksmev Derival – Program Manager, Beyond Benign
- Pamela Hatchfield – Head of Objects Conservation, Museum of Fine Arts, Boston
- Peter Jepson – Materials Scientist, H.C. Starck
- Christian Krahforst – Staff Scientist, Massachusetts Bay's National Estuary Program
- Mimi Leveque – Art Conservator, Peabody Essex Museum
- Jacqueline Massua – Forensic Laboratory Technician, Boston Police Department Crime Lab
- James Waters – Technical Support, Waters Corporation
- Bassam Shkhashiri – Professor of Chemistry, University of Wisconsin-Madison

The students also had the opportunity to participate in two hands-on activi-

IQsynthesis
Custom Molecules for Life
Formerly Gateway Technologies

Custom Synthesis Services
IQsynthesis, formerly Gateway Chemical Technology, provides customized chemical synthesis at milligram to kilogram quantities.

- Active Pharmaceutical Ingredients
- Analytical Reference Standards
- Precursors and Intermediates
- Degradants and Metabolites
- Agrochemicals
- Bio-organic Molecules
- Chiral Synthesis
- Combinational Platforms
- Process Development

IQsynthesis
11810 Borman Drive
St. Louis, MO 63146
314-991-1857
1-800-506-9892
www.iqsynthesis.com
info@iqsynthesis.com

INNOVATION | QUALITY

Chemistry Week

Continued from page 6

ties related to nutrition and tour the MoS. Finally, students had the option of interviewing a scientist and submitting the interview to the NCW committee. The winning essay was submitted by Sean Kinnane.

In addition, an NCW event was held at the Boston Children's Museum on Saturday, October 27, 2007. Approximately 1300 individuals participated in NCW hands-on activities and demonstrations. A particular favorite at the Boston Children's Museum was making marker butterflies. More than 40 volunteers from Boston Latin School, Bridgewater State College, Emmanuel College, Gordon College, Merck Research Laboratories- Boston, Simmons College, Suffolk University, and Tufts University were available to assist visitors throughout the day.

Children grades K-12 were able to participate in the national poster competition. Seventeen posters were submitted for the NCW poster competition. These posters were judged by the scientists who participated in the Monday program. The winners from the NESACS were: K-2: Adam Canfield and Jordyn Cooper (joint entry from the Young Scientists Club, Littleton MA); grades 9-12: Marina Kem from Malden High School. Children grades K-12 had the option of participating in a puzzle contest. The puzzle was designed by Dr. Christopher Morse. Upon solving the criss-cross puzzle, the participants learned they needed to write an essay of fewer than two hundred words, about a Nobel prize winning chemist. The winning essay was submitted by Jeffrey Yu.

NESACS received a \$3000 Local Section Innovative Grant to defray the cost of the Monday program. Special thanks to all of our volunteers, Boston Children's Museum, Lynn Baum, Alissa Daniels, Museum of Science Boston, Northeastern Section of the American Chemical Society, David Sittenfeld, Dr. Bassam Shakhshiri, Mariko Taniguchi, and the Phyllis A.

Brauner Memorial Lecture Committee.

The theme for NCW 2008 is "Having a Ball with Chemistry" to be celebrated from October 19-25, 2008.

Winning Entry: Interviewing a Scientist

Christian Krahforst /Chemist

By Sean Kinnane

I am taking a class in environmental science presently and I thought it might be fun to interview the chemist most closely related to that field, and Mr. Krahforst was just the person that I needed to see.

Mr. Krahforst had a lot of interesting things to say and show. One very interesting thing that he had at his table was a tool called a sonde. This tool is used to measure the temperature of the water, its conditions, including the oxygen and chlorophyll levels, the water's conductivity, and the amount of light the water has. Once they do all of this they try to answer their biggest question and how to fix their biggest problem, the nitrogen level. The nitrogen is what is causing all of the algae to spread out over the water. The more nitrogen that there is the more algae

that grows and when the algae grows to be enough to cover all the water it blocks the sun from coming in. When there is no sun that means that the animals and plants that live there can't survive. The nitrogen acts somewhat as a shield to the water, but not in a good way.

Now that all of that is clear, we go back to the sonde process. Now that you know what they use the sonde for, let's go through the process of how they take the information that is given to them from the instrument. The information tells you what is in the water and whether it is bad or good. When scientists know the types of chemicals or types of algae in the water, they can find or create their own chemicals to help get whatever is bad out of the water so that the plants and animals that are having trouble living down there have the ability to have a chance to survive.

Well, if you're wondering where all that nitrogen comes from, here are just a few examples. It comes from places such as storm drains, lawn fertilizers, and pesticides that find their

Continued on page 16

We Focus on Doing Chemistry!

- FDA Inspected
- cGMP Synthesis
- Controlled Substances
- Custom Synthesis
- Small Lots Manufacturing
- Polymer Chemistry
- Process Development

Chemo Dynamics, LP

Contact: S. N. Bharathi, Ph.D.
3 Crossman Road South
Sayreville, NJ 08872
Phone: (732)721-4700
Fax: (731)721-6835
www.chemodynamics.com
E-Mail: info@chemodynamics.com

Salk Chemical Evolution Scientist Leslie Orgel: 1927–2007

Leslie Orgel was well known to NESACS. He was featured in the January 2003 *Nucleus* as the speaker at the Monthly Meeting. In addition, his son Robert, is married to the daughter of former NESACS Chair, John Neumeyer.

The following was released by the Salk Institute on October 30, 2007.

LA JOLLA, CA — Salk scientist Leslie Orgel, Ph.D., who dedicated much of his career to the study of how life began on Earth roughly 4 billion years ago, died on October 27 from pancreatic cancer. He was 80 years old.

Orgel, a professor and head of the Chemical Evolution Laboratory, aimed not only to discover the chemical reactions that led to the first life forms on the primitive Earth, but also to solve the mystery of how, during this prebiological time, a replicative molecule

arose that could pass on life's genetic blueprint to future generations.

He was among the first scientists, in the 1960's, to suggest that RNA, rather than DNA, was that early replicative molecule. He suspected that an even simpler genetic precursor to RNA itself must have existed.

The notion of an "RNA world," as RNA-based life is often called, was coincidentally shared by the scientist who helped discover the structure of DNA – Orgel's Salk colleague and friend, the late Francis Crick.

In acknowledging that common assumptions – such as the belief that DNA is more important than RNA – are often based on lack of evidence, Crick once jokingly credited Orgel with Orgel's Second Rule: "Evolution is cleverer than you are." This statement is now broadly used today as a general rejoinder to arguments made from ignorance.

Born in 1927, in London, England, Leslie Eleazer Orgel earned a bachelor's degree (1949) and his doctorate (1951) in chemistry from Oxford University, and accepted research fellowships at California Institute of Technology and the University of Chicago in 1954 and 1955, respectively. Orgel then returned to Britain and served as assistant director of research at Cambridge's Theoretical Chemistry Department. There he helped develop ligand field theory, which describes chemical bonding in metals. Orgel published *An Introduction to Transition-Metal Chemistry: The Ligand Field Theory* in 1961.

Orgel became a fellow at the Salk Institute in 1964 and became interested in what distinguishes living organic things from non-living things. He found it intriguing that the proteins found in all of Earth's life forms are made from one set of 20 standard amino acids and that their genetic information is stored in nucleic acids – DNA and RNA – that use the same genetic code. Moreover, RNA uses that information to produce proteins, and proteins, in turn, are needed to help duplicate DNA. But there is a central paradox Orgel and others pointed out: there can be no proteins without DNA, and there can be no DNA without proteins.

Orgel suggested a way out of this chicken-and-egg conundrum, as did Crick and American microbiologist Carol Woese, each of whom published their ideas independently. They speculated that both DNA and proteins could be descendants of RNA. Being more complex and stable, DNA could then have taken over RNA's role as the guardian of heredity, while RNA took on a more supporting role.

Proposing that RNA might have evolved in a way that is consistent with Darwinian selection, Orgel published his thoughts in the 1973 book *The Origins of Life: Molecules and Natural Selection*.



Eastern Scientific

301 Winter Street
Hanover MA 02339

781-826-3456

Vacuum Pump Problems?

Eastern Scientific specializes in the repair and precision rebuilding of all makes of mechanical vacuum pumps.

Free pick-up & delivery
Restrictions apply



Leslie Orgel

Continued from page 8

But more than a decade later, when evidence for an RNA world came with the discovery of an RNA enzyme (ribozymes) that catalyze biochemical reactions, Orgel expressed new doubts. Attempts to form RNA under laboratory conditions that mimic the primordial Earth had been only marginally successful, largely because ribose (a component of the RNA backbone) is a sugar that Orgel said may not have been stable enough to survive the low oxygen and high radiation conditions of the early Earth.

Orgel suggested that RNA probably took over from some more primitive precursor. Accordingly, he and his group at Salk studied alternative genetic backbones that may have preceded nucleic acids. They found that a compound known as peptide nucleic acid (PNA), which is much simpler than RNA, can be copied in the test tube. Their work demonstrated that the evolution of a more complex, self-replicating molecule from a simpler precursor is at least possible.

Orgel's origin-of-life work also had practical applications. During studies in the Chemical Evolution Laboratory, he and his colleagues came across a straightforward way to synthesize cytosine arabinoside (Ara C), a compound that is one of today's most commonly used anti-cancer agents.

Orgel also enjoyed purely theoretical investigations, and mused about how a universal genetic code could have evolved. In 1973, Orgel and Crick put forward the notion that "directed panspermia" – the seeding of life on other worlds by a guiding intelligence – could solve the mystery. In an article in the journal *Icarus*, they said that while it is possible that life reached Earth in this way, the scientific evidence for this is so inadequate that no one can say anything about the probability. Crick expanded these ideas in his book "*Life Itself: Its Origins and Nature*."

Because of his long association with NASA, Orgel would have been one of the first to know if other planets had been so seeded. He was one of five

principal investigators of the NASA-sponsored research and training program in exobiology. He also participated in NASA's Viking Mars Lander Program as a member of the Molecular Analysis Team that designed the gas chromatography mass spectrometer instrument.

In 1998, he chaired the Task Group on Sample Return from Small Solar Systems Bodies, and served on NASA's astrobiology oversight committee since 1999. Orgel was also part of a strategic planning group for the SETI Institute's Center for the Study of Life in the Universe. In addition to his work at Salk, Orgel was also an adjunct professor in the Department of Chemistry and Biochemistry at UCSD.

Fifth Annual Northeast Student Chemistry Career Fair

Thursday, April 24, 2008

3PM – 7PM

Brookline Holiday Inn

1200 Beacon Street, Brookline, MA

Register to participate:

ACS Career Services workshops on resume writing and interviewing skills will be performed on-site. Have your resume reviewed.

Job Fair – Meet with representatives from companies in the Northeast about employment opportunities. Hand deliver your resume to company scientists and HR representatives.

Last Year

Over 110 resume submissions
12 companies recruiting new hires

Come, network with your future colleagues
Corporate sponsorship inquiries: 617-304-6474, Lee Johnson.

FREE ONLINE REGISTRATION

(Returnable Deposit): *Please register at the Northeastern Section Younger Chemists Committee website: www.nsycc.org*

Participating companies and all details will be listed.

Orgel's contributions have been recognized throughout his career. In Britain, he was awarded the Harrison Prize in 1957 for his work in inorganic chemistry, was elected a Fellow of the Royal Society in 1962. In the United States, he received a Guggenheim Fellowship in 1971, the Evans Award from Ohio State University in 1975, and the H.C. Urey Medal from the International Society for the Study of the Origin of Life in 1993. He was elected a member of the National Academy of Sciences in 1990.

Leslie Orgel is survived by his wife, Alice Orgel, M.D., Ph.D., a pediatric allergist, now retired, his two sons Richard and Robert, his daughter Vivian, and their grandchildren. ◇

Summer Research Report

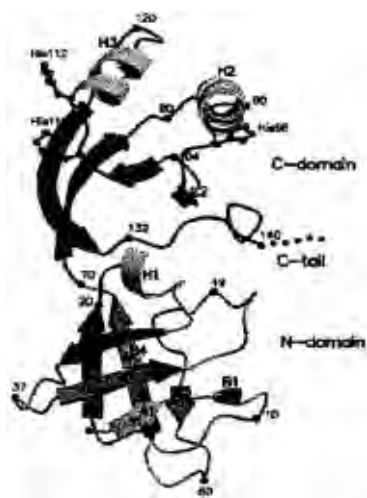
Nickel Binding Properties of the C-terminal Histidine-rich Sequence of the Metallochaperone UreE from Klebsiella aerogenes

Jiajia Cui and Dean E. Wilcox Department of Chemistry, Dartmouth College, Hanover, NH 03755

Introduction

Urease is a nickel-containing enzyme found in plants and certain microorganisms, where it catalyzes the hydrolysis of urea to ammonia and carbon dioxide. This enzyme is important in biochemical nitrogen cycles and the uptake of urea fertilizer, and has been implicated as a bacterial virulence factor in various human and animal diseases (1). The bacterial urease possesses three structural subunits, designated *UreA*, *UreB*, *UreC*, and contains a bi-nickel active site buried in the *UreC* subunit (2). Assembly of the functional urease metallocenter, however, requires the participation of four accessory proteins, designated *UreD*, *UreE*, *UreF*, and *UreG* (Figure 1) (3). Deletion of the genes for these proteins does not affect urease subunit biosynthesis, and studies have shown that *UreD*, *UreF*, and *UreG* stabilize the urease apo (metal-free) protein (4) for nickel insertion by *UreE*, which is the metallochaperone donor of nickel ions to the *UreC* subunit (5).

Figure 1: Crystal structure of the metal free *K. aerogenes UreE* monomer (8).



The *UreE* from *Klebsiella aerogenes* (*KaUreE*) functions as an apparent dimer ($M_r = 35,000$) that binds 5-6 Ni^{2+} ions per dimer with an experimental K_d value of approximately $10 \mu\text{M}$, as measured with equilibrium dialysis (5). X-ray absorption and other spectroscopic studies have shown that the Ni^{2+} ions coordinate to 3-5 histidine residues in a pseudo-octahedral geometry (5, 6). Mutagenesis studies (7) and X-ray crystallography (8) of *KaUreE* (Figure 2) have implicated several nickel binding sites, including His-96 at the dimer interface, His-110 and His-112 at the periphery of the two subunits, and the histidine-rich carboxyl terminus, which has the sequence HGHHHAHHD-HHAHSH.

A number of organisms, however, have a *UreE* metal-

lochaperone that lacks the histidine-rich carboxyl terminus. The best-studied example is *Bacillus pasteurii UreE*, which has a His-Gln-His carboxyl terminus and binds two nickel ions per dimer (9). Studies of a truncated form of *KaUreE*, H144**UreE*, that lacks the 15 carboxy-terminal residues indicate that it binds two Ni^{2+} ions and retains ~75% of the specific urease-activating activity of wild type *KaUreE* (10). This indicates that the 10 C-terminal His residues are not essential for the delivery of nickel ions to urease. Consequently, the histidine-rich carboxyl terminus of *KaUreE* must play another role in urease activation, possibly temporary metal storage for *UreE*.

Few studies have investigated the thermodynamics of metal ions binding to proteins, which is important for understanding the delivery of metal ions by metallochaperones. A recent calorimetric study of metals binding to the truncated H144**UreE* confirmed the binding stoichiometry of two Ni^{2+} per dimer and reported a condition independent binding constant of 6.3×10^8 (11). Additional measurements on the wild type *KaUreE* protein showed that the C-terminal tail of the *KaUreE* dimer is able to bind 3-4 nickel ions and allowed the thermodynamics of this binding to be estimated (11). To further understand the biological role of this histidine-rich carboxy-terminal sequence, which is found in many, but not all, *UreE* proteins, a peptide corresponding to these residues was studied.

Isothermal titration calorimetry (ITC), which directly measures the heat generated or consumed in binding reactions, was used to determine the thermodynamics of nickel binding to the *KaUreE* C-terminal peptide. The instrument consists of sample and reference cells that are connected by a thermocouple, and heat that is associated with the titration in the sample cell is determined by detecting and correcting for any temperature difference between the two cells. The experimental parameters, n (stoichiometry), DH_{ITC} , and K_{ITC} , are determined by fitting the ITC data to an appropriate binding model. Further analysis then leads to the condition-independent thermodynamics of the binding reaction.

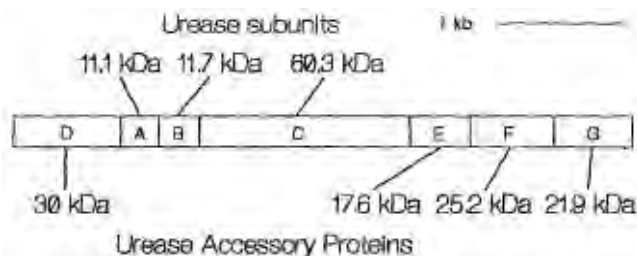


Figure 2: *K. aerogenes* urease gene cluster, which consists of three structural genes (*UreA*, *UreB*, *UreC*) and four accessory genes (*UreD*, *UreE*, *UreF*, *UreG*) (5).

Experimental

NiCl₂ was the highest purity chloride salt received from either Fisher or Sigma. Tris (2-amino-2-[hydroxymethyl]-1,3-propanediol, 99% pure) was obtained from Fisher. Tes (2-[tris(hydroxymethyl)methylamino]-1-ethanesulfonic acid, 99% pure) and EDTA (ethylenediaminetetraacetic acid, 99% pure) were obtained from Sigma. The N-acetylated 15 residue *UreE* carboxy-terminal peptide (~85% pure) was obtained from Bio Synthesis Inc., and further purified using reverse phase HPLC (~95% pure).

ITC experiments were carried out at 25°C with a MicroCal MCS titration calorimeter. Solutions were buffered with either 100 mM Tris or 50 mM Tes at pH 7.45. Ionic strength was adjusted to 0.1 M using NaCl. Metal analysis by ICP-MS and EDTA titrations was used to determine the concentration of the metal solutions. The concentration of *UreE* peptide solutions was determined by the peptide mass and verified by ITC measurements with Ni²⁺ solutions of known concentration. The ITC data were obtained for Ni²⁺ titrations into the *KaUreE* peptide in Tris or Tes buffered solutions and analogous titrations of the peptide into Ni²⁺ solutions. Four or five data sets were collected for each type of titration and the average best-fit ITC values are reported.

Analysis

The enthalpies and binding constants obtained from ITC measurements are net values for all reactions in the sample cell upon addition of titrant. Therefore, care must be taken to separate the enthalpy of metal-peptide binding from the enthalpies of metal-buffer interaction, proton displacement and subsequent buffer protonation, and other coupled equilibria. Hess's law (Equation 1), where M, L, and B correspond to metal, ligand, and buffer, respectively, can be used to extract the desired ΔH_{ML} from other known enthalpy contributions.

$$\Delta H_{ITC} = \Delta H_{ML} - n_{H^+}(\Delta H_{HL} + \Delta H_{HL_2}) - \Delta H_{MB} + n_{H^+} \Delta H_{HB}$$

Equation 1.

Protons are often displaced when metal ions bind to peptides or proteins. In order to calculate the number of displaced protons in a given reaction, ITC data are collected in at least two different buffers at the same pH. Equation 1 can be rearranged to give equation 2.

$$\Delta H_{ITC} + \Delta H_{MB} = n_{H^+} \Delta H_{HB} + [\Delta H_{ML} - n_{H^+}(\Delta H_{HL} + \Delta H_{HL_2})]$$

Equation 2.

Plotting $\Delta H_{ITC} + \Delta H_{MB}$ versus ΔH_{HB} for different buffers gives a linear relationship with slope.

Finally, given ΔH_{MB} and, condition-independent values for the desired K_{ML} and ΔH_{ML} can be calculated from equations 3 and 4, respectively (12).

Results

Experimental ITC measurements of the *KaUreE* carboxy-terminal peptide (Figure 3 and 4) indicate that it binds ~1 Ni²⁺ ion. Analysis of the experimental enthalpy for titra-

$$K_{ML} = K_{ITC} (1 + K_M [H^+] + \beta_{2,H,L} [H^+]^2) (1 + K_{MB} [B])$$

$$\beta_{2,H,L} = K_M K_{HL}$$

Equation 3.

$$\Delta H_{ML} = \Delta H_{ITC} + (r+s)\Delta H_{ML} + s\Delta H_{HL} - n_{H^+} \Delta H_{MB} + a\Delta H_{MB}$$

$$r = \frac{K_M [H^+]}{1 + K_M [H^+] + \beta_{2,H,L} [H^+]^2}$$

$$s = \frac{\beta_{2,H,L} [H^+]^2}{1 + K_M [H^+] + \beta_{2,H,L} [H^+]^2}$$

$$a = \frac{K_{MB} [B]}{1 + K_{MB} [B]}$$

Equation 4.

tions in Tris and Tes buffers indicate that 0.94 protons are displaced when Ni²⁺ binds to the peptide at pH 7.45.

The analysis to determine the condition-independent thermodynamics requires certain values. The value of ΔH_{MB} for Tris and Tes was determined from the enthalpy of Ni²⁺ titrations of EDTA in these buffers and comparison to the known enthalpy of Ni²⁺ binding to EDTA. The value for K_{HL} was approximated from the results of Grosseohme, *et al*, who measured the four His pK_a values of the histidine-rich peptide, PHGHGHGHGP, and found them to be 3.44, 5.32, 6.65, and 7.43 (13). The *KaUreE* peptide contains 10 histidine residues, whose pK_a values may be spread over a similar range. Thus, a pK_a of 7.45 was used for the proton displaced upon Ni²⁺ binding to the *KaUreE* peptide. A better estimate of this pK_a value could be obtained from an analysis of a pH titration of the peptide. Finally, values for *r*, *s*,

Continued on page 12

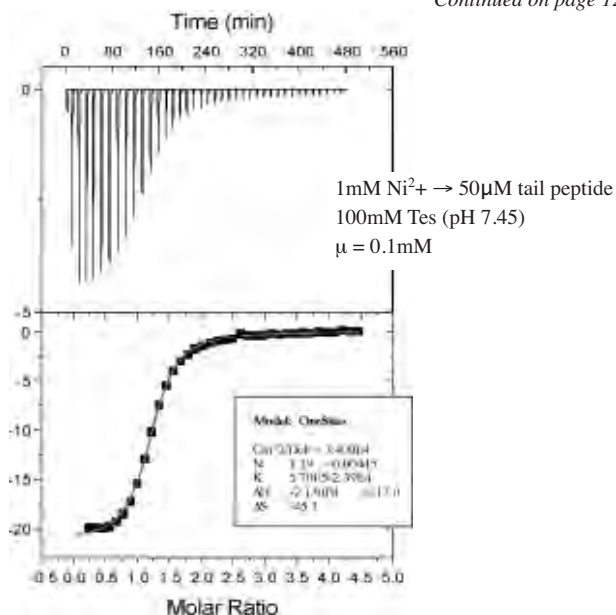


Figure 3: ITC data for 1mM nickel titration into 50mM histidine-rich carboxyl terminal peptide in 100mM Tris pH 7.45.

Summer Scholar

Continued from page 11

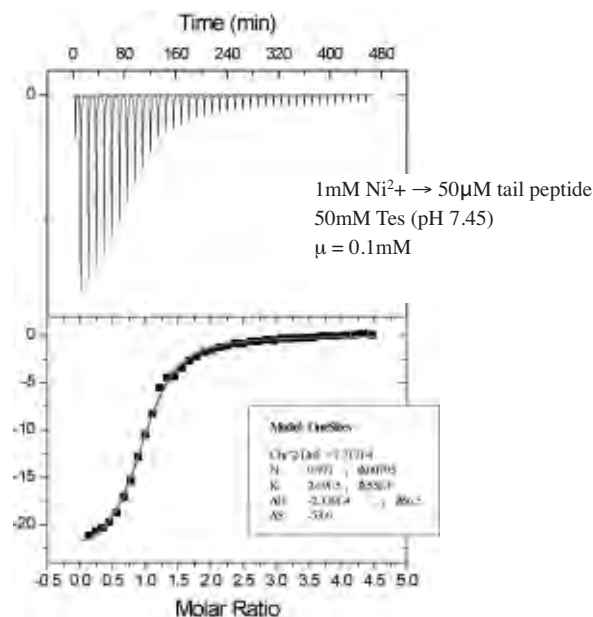


Figure 4: ITC data for 1mM nickel titration into 50mM histidine-rich carboxyl terminal peptide in 50mM Tes pH 7.45.

and a in equation 4 were calculated to be 0.667, 0, and 0.886, respectively, for the experimental conditions of pH 7.45 and 100 mM Tris buffer. The average best-fit experimental values and the corresponding condition-independent thermodynamic values for Ni^{2+} binding to the peptide are summarized in Table 1.

Buffer	n	K_{ITC}	ΔH_{ITC} (kcal/mol)	K	ΔH° (kcal/mol)
Tris	1.2	4.5×10^7	-21.7	1.2×10^7	-22.6
Tes	1.0	2.2×10^7	-23.2		

Table 1: Calorimetric values for Ni^{2+} binding to the C-terminal *KaUreE* peptide in Tris or Tes buffers at pH 7.45, and the corresponding condition-independent values for the data in Tris buffer.

Discussion

To further understand the role of the cluster of histidine residues at the carboxyl terminus of *UreE* from some species, but not others, the Ni^{2+} -binding properties of a peptide corresponding to this sequence from *Klebsiella aerogenes* have been measured with ITC. Analysis of the best-fit experimental values gives the buffer- and pH-independent thermodynamics of this binding. These values for Ni^{2+} binding to the peptide are compared in Table 2 with analogous values estimated for this sequence when it is part of the native *KaUreE* protein (11) and values determined for a peptide that corresponds to a His-rich sequence in the iron-transport protein IRT1, PHGHGHGHGP (13).

ITC data for Ni^{2+} titrations of this His-rich peptide indicate that one nickel ion binds to the peptide, displacing approximately one proton from the histidine residues at pH 7.45. Compared to the peptide sequence in the native protein dimer, which binds 3.3 Ni^{2+} ions, the isolated peptide binds 2.0-2.4 Ni^{2+} ions per dimer. Thus, more Ni^{2+} ions bind to these histidine residues in the native *KaUreE* protein dimer, where X-ray crystallography of H144**UreE* indicates that the two C-terminal sequences are held in close proximity. This is consistent with the storage, or queuing, of additional Ni^{2+} ions by these residues of this metallochaperone protein.

The affinity of this peptide for Ni^{2+} was found to be identical to that estimated for the sequence in the whole protein, with condition-independent log K values of 7.07 and 6.98 (11), respectively, corresponding to ΔG° values of -9.6 kcal/mol for the isolated peptide and -9.5 kcal/mol for the sequence in the protein. A similar, but slightly lower, Ni^{2+} affinity (log $K = 6.47$) was found for another His-rich peptide (Table 2), indicating that several histidine residues create a relatively stable protein binding site for Ni^{2+} ions. The Ni^{2+} affinity of the C-terminal sequence is 1-2 orders of magnitude lower than *UreE* affinity for the two Ni^{2+} ions that it transfers to apourease, further supporting a storage or queuing role for this sequence.

These calorimetric measurements have allowed the enthalpy and the entropy of Ni^{2+} binding to be quantified. The value of ΔH° for Ni^{2+} binding to the isolated peptide (-22.6 kcal/mol) is significantly more negative than ΔH° for the same sequence in the native protein (~ -5 kcal/mol). However, a similarly large negative enthalpy for Ni^{2+} binding to another His-rich peptide (Table 2) suggests that molecular interactions in the dimeric *KaUreE* protein modulate the enthalpy of Ni^{2+} binding. On the other hand, the entropy of binding (ΔS°) of the isolated peptide (-43 cal/mol K) is quite unfavorable, in contrast to the positive value of ΔS° for the sequence in the native dimeric protein (+15 cal/mol K). As found with the enthalpy, the ΔS° value for Ni^{2+} binding to another His-rich peptide (Table 2) is more similar to that of the *KaUreE* peptide than the same sequence in the protein. Thus, a more favorable enthalpy and a very disfavorable entropy may be hallmarks of metal ions binding to isolated peptides. These data also indicate

Ligand	n	K	ΔG° (kcal/mol)	ΔH° (kcal/mol)	ΔS° (cal/mol K)
<i>KaUreE</i> peptide	1.2	1.2×10^7	-9.6	-22.6	-43
<i>KaUreE</i> tail	1.7	9.5×10^6	-9.5	-5	15
IRT1 peptide	1.0	3.0×10^6	-8.8	-15.9	-24

Table 2: Thermodynamic values for Ni^{2+} binding to the *KaUreE* C-terminal peptide, the native *KaUreE* C-terminal tail sequence (11) and the peptide corresponding to the His-rich sequence from IRT1, PHGHGHGHGP (13).

Summer Scholar

Continued from page 12

that this is another example of a phenomenon known as enthalpy-entropy compensation, where a very different combination of enthalpic and entropic contributions to binding leads to a similar overall change in free energy and affinity.

New insight about the thermodynamics of Ni²⁺ binding to the histidine-rich carboxy-terminal sequence of the *Klebsiella aerogenes* metallochaperone *UreE* has been obtained in this study of an isolated peptide corresponding to this sequence. Differences in the Ni²⁺ binding stoichiometry and thermodynamics between the peptide and the sequence in *KaUreE* may originate from interaction between pairs of these sequences in the dimeric protein. Thus, future studies will investigate N-terminal tethered pairs of these peptides to better mimic the dimeric protein context for their Ni²⁺ binding properties.

References

1. R. P. Hausinger and P. A. Karplus (2001) Urease, in *Handbook of Metalloproteins* (A. Messerschmidt, R. Huber, T. Poulos, K. Weighardt, Eds) Wiley, Chichester, pp. 866-879.
2. E. Jabri, M. B. Carr, R. P. Hausinger, P. A. Karplus (1995) The Crystal Structure of Urease from *Klebsiella aerogenes*, *Science* 268: 998-1004.
3. M. H. Lee, S.B. Mulrooney, M. J. Renner, Y. Markowicz, R. P. Hausinger (1992) *Klebsiella aerogenes* Urease Gene Cluster: Sequence of *ureD* and Demonstration that Four Accessory Genes (*ureD*, *ureE*, *ureF*, and *ureG*) Are Involved in Nickel Metallocenter Biosynthesis, *J. Bacteriol.* 174: 4324-4330.
4. I. S. Park and R. P. Hausinger (1995) Evidence for the Presence of Urease Apoprotein Complexes Containing UreD, UreF and UreG in Cells that are Competent for in vivo Enzyme Activation, *J. Bacteriol.* 177: 1947-1951.
5. M. H. Lee, H. S. Pankratz, S. Wang, R. A. Scott, M. G. Finnegan, M. K. Johnson, J. A. Ippolito, D. W. Christianson, R. P. Hausinger (1993) Purification and Characterization of *Klebsiella aerogenes* UreE Protein: a Nickel-binding Protein that Functions in Urease Metallocenter Assembly, *Protein Sci.* 2: 1042-1052.
6. G. J. Colpas, T. G. Brayman, J. McCracken, M. A. Pressler, G. T. Babcock, L. J. Ming, C. M. Colangelo, R. A. Scott, R. P. Hausinger (1998) Spectroscopic Characterization of Metal Binding by *Klebsiella aerogenes* UreE Urease Accessory Protein, *J. Biol. Inorg. Chem.* 3: 150-160.
7. G. J. Colpas, T. G. Brayman, L. J. Ming, R. P. Hausinger (1999) Identification of Metal-binding Residues in the *Klebsiella aerogenes* Urease Nickel Metallochaperone, UreE, *Biochemistry* 38: 4078-4088.
8. H. K. Song, S. B. Mulrooney, R. B. Hubert, R. P. Hausinger (2001) Crystal Structure of *Klebsiella aerogenes* UreE, a Nickel-binding Metallochaperone for Urease Activation, *J. Biol. Chem.* 276: 49359-49364.
9. S. Ciurli, N. Safarov, S. Miletti, A. Dikiy, S. K. Christensen, K. Kornetzky, D. A. Bryant, I. Vandenberghe, B. Devreese, B. Samyn, H. Remaut and J. Van Beeumen (2002) Molecular Characterization of *Bacillus pasteurii* UreE, a Metal-binding Chaperone for the Assembly of the Urease Active Site, *J. Biol. Inorg. Chem.* 7: 623-631.
10. T. G. Brayman and R. P. Hausinger (1996) Purification, Characterization and Functional Analysis of a Truncated *Klebsiella aerogenes* UreE Urease Accessory Protein Lacking the Histidine-rich Carboxyl Terminus, *J. Bacteriol.* 178: 5410-5416.
11. N. E. Grossoehme, S. B. Mulrooney, R. P. Hausinger, D. E. Wilcox (2007) Thermodynamics of Ni²⁺, Cu²⁺ and Zn²⁺ binding to the urease metallochaperone UreE, *Biochemistry* 46: 10506-10516.
12. N. E. Grossoehme (2007), Dartmouth College, Ph.D. Thesis.
13. N. E. Grossoehme, S. Akilesh, M. L. Guerinot, D. E. Wilcox (2006) Metal Binding Thermodynamics of the Histidine-rich Sequence from the Iron Transport Protein IRT1 from *Arabidopsis thaliana*, *Inorg. Chem.* 45: 8500-8598. ◇

**A good vacuum system
needs a great vacuum trap:**

Posi-Trap positive flow
vacuum inlet traps!

- No "blow-by" . . . **ever!**
- Filter elements matched to **your** application.
- **Easy** cleaning and changing.

When you want the best, you want MV Products.

MV PRODUCTS A Division of Mass-Vac, Inc.
247 Rangeway Road • PO Box 359 • North Billerica, MA 01862
978 667 2393 Fax 978 671 0014 sales@massvac.com www.massvac.com

March Historical Events In Chemistry

by Leopold May

The Catholic University of America, Washington, DC

March 1, 1771

John McLean, first professor of chemistry, at Princeton, established the first laboratory of chemistry on this day in North America.

March 3, 1709

Andreas S. Marggraf, who was born on this date, isolated zinc from calamine. He distinguished between potash and soda by flame test, found alumina in clay, and discovered beet sugar in beetroot.

March 5, 1817

The inventor of the first colorimeter, Jules Duboscq, was born on this day. The Duboscq Colorimeter was used for visual colorimetric quantitative analysis and pH measurements.

March 7, 1839

Ludvig Mond, who discovered Mond producer gas and nickel carbonyl, was born on this date. He and John Brunner founded a company that later became Imperial Chemical Industries (ICI).

March 10, 1851

William McMurtie, who was born on this day, did research on methods for converting sewage to fertilizer. He served as president of the American Chemical Society.

March 12, 1824

Gustav R. Kirchhoff, who invented the spectroscope with Robert Bunsen in 1859, was born on this date. He and Robert Bunsen discovered cesium in 1860, and rubidium in 1861. He discovered that substances which emit radiation absorb the same type of radiation when cool (Kirchhoff's Law).

March 14, 1854

One hundred years ago, Paul Ehrlich and Ilya Ilyich Mechnikov shared the Nobel Prize in Medicine with in recognition of their work on immunity. Ehrlich was a researcher in immunity & chemotherapy and discovered Salvarsan (No. 606) & neosalvarsan. He improved laboratory staining methods and was born on this day.

March 16, 1666

Johann Conrad Barchusen, who was born on this date, was a chemical lecturer at Utrecht University. He did chemical analysis using fire and interpreted alchemical transmutation as metallic substitution reactions.

March 18, 1900

Laurien B. Hitchcock, an expert in chemistry of the environment, was born on this date.

March 19, 1883

One hundred and twenty-five years ago, Walter N. Haworth was born on this date. He synthesized ascorbic acid (Vitamin C) in 1933 and did research on sugars and dextran as blood plasma substitute. In 1937, he shared the Nobel Prize in Chemistry with Paul Karrer for vitamin synthesis.

March 20, 1908

One hundred years ago, Bausch & Lomb was incorporated as Bausch & Lomb Co., on this day.

March 21, 1817

George W. Rains, who was a chemistry teacher and Confederate Army chemist, was born on this date.

March 23, 1867

Charles L. Parsons, who was born on this date, obtained the federal charter for the ACS. He helped establish the Petroleum Research Fund and did research on beryllium.

March 26, 1838

A. Crum Brown, who devised modern structural formulae in 1864, was born on this date. He formulated rules for substitution in benzene derivatives named after him and did research in the theory of isomerism and organic compounds of sulfur.

March 27, 1847

Otto Wallach, a researcher on essential oils & terpenes, was born on this date. In 1910, he received the Nobel Prize in Chemistry in recognition of his services to organic chemistry and the chemical industry by his pioneering work in the field of alicyclic compounds.

March 29, 1883

One hundred and fifty years ago, Donald D. Van Slyke was born on this day. He was a pioneer in clinical chemistry. ◇

What's Yours?

DMPK Scientist,
LC/MS Product Specialist,
Mass Spec Operator,
Staff Investigator,
Process Chemist,
QA Manager,
Synthetic Chemist,
Lab Instructor

Many local employers post positions
on the NESACS job board.

Find yours at
www.nesacs.org/jobs

The NESACS website

Updated frequently · Late-breaking news · position postings
Back issues of the Nucleus archived · Career-related Links · Awards and Scholarships

[WWW.NESACS.ORG](http://www.nesacs.org)



CALL FOR NOMINATIONS FOR THE 2008 NORTHEAST REGION AWARDS

NeRACS



Northeast Region of the American Chemical Society, Inc.

Dr. Julianne Smist, Chair

Mr. D. Richard Cobb, Vice Chair

Dr. Christopher Masi, Secretary

Dr. Wayne Jones, Treasurer

THE ACS DIVISION OF CHEMICAL EDUCATION NORTHEAST REGION AWARD FOR EXCELLENCE IN HIGH SCHOOL TEACHING

Purpose: To recognize, encourage, and stimulate outstanding teachers of high school chemistry in the Northeast Region.

Eligibility: The nominee must be actively engaged in the teaching of chemistry or a chemical science in a high school (grades 9-12) on at least a half-time basis.

THE NORTHEAST REGIONAL AWARD FOR EXCELLENCE IN VOLUNTEER SERVICES

Purpose: To recognize the volunteer efforts of individuals who have served the American Chemical Society by contributing significantly to the goals and objectives of the Society through their Regional Activities.

Purpose: The nominee must be a member of the ACS, residing in a Local Section within the Northeast Region, who has made significant contributions to the Section and Region of the ACS.

STANLEY C. ISRAEL REGIONAL AWARD

Purpose: Its purpose is to recognize individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the region.

Purpose: Individuals nominated for the award may come from any professional setting: academia, industry, government, or other independent facility. Nominees may also be organizations, including ACS local sections and divisions. The awardees will have increased the participation and leadership of persons from diverse or underrepresented minority group(s), persons with disabilities, or women.

Deadline: The deadline for all of these awards is March 31, 2008.

For More Information: Contact D. Richard Cobb at <d.richard.cobb@kodak.com>

Nominating Forms: Available on the NESACS website <www.nesacs.org>

Presentation of the Awards: At the 2008 Northeast Regional Meeting (NERM) in Burlington, Vermont, June 29–July 2.

Chemistry Week

Continued from page 7

way to our water sources. Once the nitrogen finds its way to the water, the damage can begin.

It was enjoyable and informative to speak with Mr. Krahforst. I am hopeful that I can use the knowledge gained as I continue my Environmental Science class. Of all the things he said, this particular sentence has stayed with me from our conversation and it is the following quote:

“As stewards of the environment, we must leave something healthy for the future.”

Thank you Mr. Krahforst!!!

Winning Puzzle Contest Essay

Nobel Prize-Winning Chemist Kary Mullis

By Jeffrey Yu

Kary Mullis was born on December 28, 1944 in Lenoir, North Carolina. He attended high school in South Carolina where he grew up, and then moved on to the Georgia Institute of Technology in Atlanta where he acquired a Bachelor of Science Degree in Chemistry. Seven years later he earned a Ph.D. from the University of California, Berkeley in Biochemistry.

Kary Mullis is accredited along with Michael Smith of Canada for developing the Polymerase Chain Reaction (PCR) technique. The procedure is significant because through PCR, segments of DNA are able to be amplified. Replicating DNA is a tool that can be used when there is not enough DNA available to be analyzed and tested. It helps during medical diagnosis to identify bacteria and viruses that cause infections; it can also be used in genetic testing too. In genetic testing, PCR amplifies a certain gene which is then sequenced so that mutations can be seen. By catching mutations early on, the disease risk in patients can be determined and lives can be saved. Mullis' PCR technique has advanced the field of Medicine and allowed further discoveries to be unearthed. His research has improved the quality of life of many. ◇

Biography

Continued from page 5

istry of new dinuclear complexes, the investigation of organometallic compounds having metal-oxygen and -nitrogen bonds (as part of this work he uncovered one of the earliest examples of early-transition metal alkyne and allene hydroamination processes), and the reactions of organotransition metal enolates. He is probably best known for his discovery of the first soluble organometallic complexes that undergo intermolecular insertion of transition metals into the carbon-hydrogen bonds of alkanes and the use of liquefied noble gas solvents in the study of these reactions, and most recently he has been involved in the application of C-H activation reactions to problems in organic synthesis.

Bergman has been the recipient of numerous awards: an Alfred P. Sloan Fellowship (1969), a Camille and Henry Dreyfus Foundation Teacher-Scholar Award (1970), the Caltech Student Government Award for Excellence in Teaching (1978), the ACS Award in Organometallic Chemistry (1986), an ACS Arthur C. Cope Scholar Award (1987), the E.O. Lawrence Award in Chemistry (U.S. Department of Energy, 1994), the ACS Arthur C. Cope Award (1996), the Edward Leete Award for Teaching and Research in Organic Chemistry (2001), the UC Berkeley Department of Chemistry Teaching Award (2002), the ACS James Flack Norris Award in Physical Organic Chemistry (2003), and an Award for Excellence in Technology Transfer from the Lawrence Berkeley National Laboratory (2005). Bergman is an elected member of the National Academy of Sciences and the American Academy of Arts and Sciences (both in 1984). In 2007 he was chosen by the National Academy of Sciences to receive the NAS Award in Chemical Sciences. He has served as a member of several editorial advisory boards including those of the *Journal of Organic Chemistry*, *Organometallics*, *Chemical Reviews*, the *International Journal of Chemical Kinetics*, the *Journal of the American Chemical*

November Meeting Photos

by Robert Lichter



A collection of Norris Award Recipients at the November Meeting. (l-r) A. Truman Schwartz (1997), Mary Virginia Orna (1996), Michael P. Doyle (1995), Diane Bunce (2007), John W. Moore (1991), and Morton Z. Hoffman (2005).



New NESACS members at the Norris Award Dinner



Myke Simon, NESACS Archivist and Vivian Walworth, Board of Publications

Society, and *Organic Letters*. At Berkeley he has served as Vice-chair of the Department of Chemistry (1985-87) and three times as Assistant Dean of the College of Chemistry. He has also been elected to serve on the Executive Committees of both the Organic Division (1981-84) and the Inorganic Division (1984) of the ACS, the latter as chairman of the Organometallic Subdivision. ◇

BUSINESS DIRECTORY

Calendar

Mar 27 *Continued from page 20*

Prof. Martin Gruebele (University of Illinois at Urbana-Champaign)
"Vibrational Energy Flow and Mode Selectivity: What Happens as Molecules Get Larger"
Boston College, Merkert Chemistry Center,
Room 130
4:00 pm

Harry L. Anderson (University of Oxford)
Merck-Karl Pfister Lectures in Organic Chemistry
TBA
MIT, Room 6-120
4:00p-6:00 pm

Mar 28

Harry L. Anderson (University of Oxford)
Merck-Karl Pfister Lectures in Organic Chemistry
TBA
MIT, Room 6-120
4:00 pm

Mar 31

Prof. Jeffrey A. Cina (University of Oregon)
TBA
Boston Univ., Life Science and Engineering
Building Auditorium (B01)
4:00 pm

Notices for The Nucleus Calendar of Seminars should be sent to:

Sheila E Rodman
250 Kennedy Drive
Unit #403, Malden, MA 02148.
E-MAIL: serodman(at)hotmail.com

VOLUNTEERS

**Reporters needed
to cover ACSNES
monthly meeting
lectures**

Phone for more details
Myke S. Simon
Nucleus Associate Editor
Tel: 617-332-5273

Q. Exactly, how many awards and
scholarships does NESACS sponsor?

A) One b) Two c) Many

www.nesacs.org/awards

SERVICES



**PCI
Synthesis Inc.**

Serving the greater Boston/
Cambridge area and beyond.

**Your local source for cGMP
manufacturing and
custom synthesis.**

PCI Synthesis has an experienced
team of professionals whose
goal is to ensure 100% on time
delivery and marketplace
success for our customers.

It never hurts to make that call.....
so call us now!

PCI Synthesis

B&D	Headquarters:
88 Jackson Rd.	9 Opportunity Way
Devens, MA 01434	Newburyport, MA 01950
PH: 978-772-3111	PH: 978-462-5555
Fax: 978-862-0036	Fax: 978-465-2057

e-mail: info@pcisynthesis.com
http://www.pcisynthesis.com

SERVICES

NMR Service **500MHz**

***Mass**

***Elemental Analysis**

NuMega Resonance Labs

Tel: (858) 793-6057

NMR - IR/FTIR - UV/VIS/FL
Sampling supplies & accessories

See our full catalogs / current pricing at
www.newera-spectro.com

CAGE Code: 44ME9
DUNS: 556785657

NEWERA
New Era Enterprises, Inc.
1-800-821-4667
cs@newera-spectro.com

TELL OUR ADVERTISERS

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

[THE FUTURE OF LIQUID
CHROMATOGRAPHY
IS ACQUITY UPLC]



Waters ACQUITY UltraPerformance LC® (UPLC®)
provides more information, increases laboratory
throughput, and can enhance your lab's existing
MS technologies.

Learn more about the UPLC advantage at:
www.waters.com/uplc

©2007 Waters Corporation, Milford, MA 01850
Waters, ACQUITY, and UPLC are trademarks of Waters Corporation.

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™



Bruker Daltonics

Hit the Target!

... with sub-ppm confidence on
the Bruker micrOTOF-Q™ for
empirical formula determination

www.bdal.com • (978) 663-3660

think forward

ESI-Qq-TOF MS

BUSINESS DIRECTORY

SERVICES

STATISTICAL QC: Onsite inspection looming?
Failed your inorganic PT?
Dealing with deficiencies?
We can help!

Laboratory Compliance Services, Inc.
978-235-2075 labcompliance@verizon.net

Front Run OrganX, inc.

Custom Synthesis & Process Chemistry

WHEN QUALITY MATTERS

High Purity, Scalable Solutions
to Challenging Organic Synthesis

Starting Materials to Pre-clinical
Single to Multi-Step mg to Kgm

98% min. purity

Phone 978-356-7133 Fax 978-356-7449

Email Frontrun@Sprynet.com
www.FrontRunOrg.com

Preclinic DMPK

LCMS, MSn, Mass analysis with
ESI/APCI/Maldi-TOF/NanoSpray

www.HT-LABS.com

info@HT-Labs.com (858)677-9432

Achieve Your Goals in Organic Chemistry

We deliver *On time, On cost,*
and *On target.*

For Excellence in Organic Chemistry

Come to Organix Inc. for:

- Contract research and development
- Custom synthesis (milligram to kilogram) in all areas of organic and medicinal chemistry
- ¹H NMR and ¹³C NMR Spectra
- Structural Interpretation
- LC/MS Services

ORGANIX
Inc.

Phone: (781) 932.4142

Fax: (781) 933.6695

Email: organix@organixinc.com

www.organixinc.com

SERVICES


Scientific glassblowers
serving
New England
for over 40 years

Solving your Pyrex or Quartz
glassware needs from custom
fabrication to repairs

www.finkenbeiner.com

SCHWARZKOPF Microanalytical Laboratory

Elemental & Trace Analysis
Organics, Inorganics
Organometallics
Metals by AA & Graphic Furnace
Functional Grps. - Mol. Wt.
Calorimetry
Total S. F. Halogens TOX
Coneg Testing Custom Analysis
56-19 37th Ave. Woodside, N.Y. 11377
(718) 429-6248
schwarzkopfmicro@aol.com

SERVICES


micron inc.
Analytical Services
Complete Materials Characterization
Morphology Chemistry Structure

3815 LANCASTER PIKE, WILMINGTON DE. 19805
PHONE 302 - 998 - 1184, FAX 302 - 998 - 1836

MICRONANALYTICAL@COMPUSERVE.COM
WWW.MICRONANALYTICAL.COM

**LABORATORY
EQUIPMENT**

Bought • Sold • Exchanged
MARCH SPECIAL

Antek 9000 Series HPLC-CLND
Chemiluminescent nitrogen specific
HPLC detector with furnace and
Vacubrand vacuum pump.

Call for details
American Instrument Exchange, Inc.
1023 Western Ave., Haverhill, MA 01832
TEL: 978-521-2221 FAX: 978-521-8822
www.americaninstrument.com
E-Mail: info@americaninstrument.com

Rapid Results • Quality • Accuracy • Competitive Pricing



Robertson Microlit Laboratories

- Elemental CHN, S, X, Analysis - *same day service!*
- Metals by ICP-OES, ICP-MS, A/A
- FTIR, UV/VIS Spectroscopy
- Ion Chromatography
- Bioavailability
- Polarimetry
- DSC
- KF Aquametry, Titrimetry

P. O. Box 927 • 29 Samson Avenue • Madison, NJ 07940

Tel: (973) 966-6668 • Fax (973) 966-0136

www.robertson-microlit.com • email: results@robertsonmicrolit.com

FDA Inspected



DuPont Analytical Solutions

From rapid, routine testing to complex problem-solving. One
of the world's largest, and most diverse analytical laboratories,
with the experience to solve your analytical challenges in :

Electronic Materials • Personal Care • Catalysis • Coatings, Pigments, and Adhesives
Specialty Chemicals • Films and Packaging • Pharmaceuticals • Plastics • Fibers • Textiles

DuPont Analytical Solutions
P.O. Box 80302
Wilmington, DE 19880-0302
Phone: (302) 695-1018

e-mail: DASolutions@usa.dupont.com
web: <http://analyticalsolutions.dupont.com>
FAX: (302) 695-1717

Contact us for all your analytical needs.



BUSINESS DIRECTORY

SERVICES



- CHN • O • S
- Halogens • Bomb Oxidation
- Metals • ICP • ICP/MS • AAS
- Anions • Ion Chromatography
- Dry Box • Air Sensitive Samples
- Fuel Testing • BTU • Prox • Ultimate • Sulfur • Ash Analysis
- Inquire about other capabilities



Desert Analytics
3860 S. Palo Verde, Suite 303
Tucson, AZ 85714 - 520.623.3381
thelab@desertanalytics.com
We accept VISA, MC & AMEX

WWW.DESERTANALYTICS.COM

SERVICES

Chemical Analysis Services



- Materials Identification
- Deformulation
- Polymer Analysis & Testing
- Failure Analysis
- Consulting Services

800.659.7659
www.chemir.com

Arendt & Assoc. IP Group
Registered Patent Attorneys

- Global Patent Protection
- Licensing
- Controlling Patent Costs

(978)897-8400 or (978)807-5278
111 at Interlakes 495, Southborough, MA
jarendt@arendtpatentlaw.com

Elemental Analysis

HUFFMAN
LABORATORIES, INC.
Quality Analytical Services Since 1936

CHNOS ash
ICP • AA • ICP/MS
TOC • TOX • BTU
Problem Solving

Phone (303) 278-4455
FAX (303) 278-7012
chemistry@huffmanlabs.com
www.huffmanlabs.com

CAREER SERVICES

PROMOTE YOUR PRODUCTS AND SERVICES • ADVERTISE IN THE NUCLEUS

The Nucleus readership is greater Massachusetts's largest source for chemical and biochemical buyers. *The Nucleus* reaches more than 7,000 readers each month. It has been estimated that these buyers annually purchase more than \$3,500,000 of:

- EQUIPMENT
- SUPPLIES
- CONSULTING SERVICES

Placing an advertisement in *The Nucleus* is the lowest cost method of reaching this select audience.

For further information and other options for promoting your company's products and services visit:
www.mboservices.net



PolyOrg, Inc.
Chemical Solutions for the Life Science Industry

- Custom Organic Synthesis
- Process Development
- Contract R & D
- Pharmaceutical Intermediates
- Medicinal Chemistry Support
- Biotechnology Specialty Reagents
- Solid Support Reactions
- Process Validation
- Gram to Multi-Kilogram Synthesis



PolyOrg Inc.
10 Powers Street, Leominster, MA 01453
Phone: 978-466-7978 1-866-Poly-002
Fax: 978-466-8084 info@polyorginc.com
www.polyorginc.com

NESACS VOLUNTEERING

We need several volunteers to help with Nucleus activities

No experience needed

Just a willingness to learn and a sense of humor

For further information contact
Vivian Walworth
Phone-978-369-3735
Fax-978-369-7306
Email vwalworth@comcast.net

Index of Advertisers

Am. Instrument Exchange.....	18
Arendt & Associates IP Group.....	19
Bruker Daltonics, Inc.	17
Chemir Analytical Services.....	19
Chemo Dynamics LP	7
Desert Analytics Laboratory	19
DuPont Analytical Solutions	18
Eastern Analytical Symposium.	2
Eastern Scientific Co.....	8
G. Finkenbeiner, Inc.....	18
Front Run OrganX, Inc.	18
HT Laboratories, Inc.	18
Huffman Laboratories, Inc.....	19
IQSynthesis	6
Laboratory Compliance Services ..	18
Mass-Vac, Inc.	13
Micron Inc.	18
New Era Enterprises, Inc.....	17
NuMega Resonance Labs.....	17
Organix, Inc.....	18
PCI Synthesis	17
PolyOrg Inc.	19
Robertson Microlit Labs.	18
Schwarzkopf Microanalytical	18
Waters Corporation	17

19 Mill Road
Harvard, MA 01451

THE NUCLEUS

NONPROFIT ORG.
U.S. POSTAGE PAID
NORTHEASTERN
SECTION
AMERICAN CHEMICAL
SOCIETY

Calendar

Check the NESACS Homepage
for late additions:
<http://www.NESACS.org>

Note also the Chemistry Department web
pages for travel directions and updates.

These include:

<http://chemserv.bc.edu/seminar.html>

<http://www.bu.edu/chemistry/events/>

<http://www.chem.brandeis.edu/colloquium.shtml>

<http://www-chem.harvard.edu/events/>

<http://web.mit.edu/chemistry/>

www.chem.neu.edu/web/calendar/index.html

<http://chem.tufts.edu/seminars.html> [CHEM.]

<http://ase.tufts.edu/chemical/seminar.htm>

[CHEM. ENGG.]

<http://www.chem.umb.edu/>

www.umassd.edu/cas/chemistry/seminars.cfm

www.uml.edu/Dept/Chemistry/speakers.html

<http://www.unh.edu/chemistry/seminars.html>

Mar 3

Professor David Cane (Brown University)

'Polyketide Antibiotic

Biosynthesis: Mechanistic and Structural Basis
of the Programming of Multistep Biosynthetic
Pathways'

Boston Univ., Life Science and Engineering

Building Auditorium (B01)

4:00 pm

Christina D. Smolke (California Institute of
Technology)

TBA

Harvard Univ., Pfizer Lecture Hall

4:15 pm

Mar 4

Dr. John L. Marshall (Zink Imaging, Inc.)

'Zero Ink - Amorphochromic Dyes and Thermal
Printing'

Univ. New Hampshire, Iddles Room L103

11:10 am

Prof. Robert Madix (Stanford University)

'Structure Sensitivity of Styrene Epoxidation on
Silver: Mechanistic Origins'

Tufts University, Pearson Chemistry Building,
Room P-106

4:30 pm

Prof. Eli Pollak (Weizmann Institute of Science)

'The Semiclassical Route to Quantum Dynamics
of Systems with many Degrees of Freedom'

MIT, Room 4-237

4:00 pm

Mar 5

Dr. David E. Budil (Northeastern University)

'Spin Labeling Studies of Ligand-dependent
Structural Changes in the Estrogen Receptor'

UMass Dartmouth, Building Group II,
Room 115

4:00 pm

Mar 10

Mohammad Movassaghi (Massachusetts

Institute of Technology)

Boehringer-Ingelheim Symposium

TBA

Harvard Univ., Pfizer Lecture Hall

3:30 pm

Mar 11

Prof. Yoshihisa Kobayashi (University of

California, San Diego)

'Heterocycles in Natural Product Synthesis'

Boston College, Merkert Chemistry Center,
Room 130

4:00 pm

Dr. Fran Ligler (Naval Research Labs)

'The Array Biosensor and Beyond'

Tufts University, Pearson Chemistry Building,
Room P-106

4:30 pm

Mar 12

Dr. Heather Carlson (University of Michigan)

TBA

Northeastern Univ., 129 Hurtig Hall

12 noon

Dr. Jason Sello (Brown University)

TBA

UMass Dartmouth, Building Group II,
Room 115

4:00 pm

Daniel Dubois (Pacific Northwest National Lab)

TBA

MIT, Room 6-120

4:00 pm

4:00 pm

Mar 13

Prof. Mark Johnson (Yale University)

TBA

Univ. New Hampshire, Iddles Room L103

11:10 am

Mar 17

Prof. Robin Kinnel (Hamilton College)

'Adventures and Lessons from Three Decades of
Natural Products — Some Finished and
Unfinished Business'

Boston College, Merkert Chemistry Center,
Room 130

4:00 pm

4:00 pm

Dr. John R. Engen (Northeastern Univ.)

TBA

Brandeis Univ., Gerstenzang 122

3:45 pm

Prof. Ann Valentine (Yale University)

'Bioinorganic Chemistry of Titanium in
Medicine and the Environment'

Boston Univ., Life Science and Engineering
Building Auditorium (B01)

4:00 pm

Mar 19

Dr. Marina Petrukhina (University at Albany)

'Fullerene Fragments: Molecular Geometry,
Solid State Packing, and Reactivity'

Northeastern Univ., 129 Hurtig Hall

12 noon

Mar 20

Jon S. Thorson (University of Wisconsin)

TBA

Bristol-Myers Squibb Lectures in Organic

Synthesis: Jon Thorson, University of Wisconsin

MIT, Room 6-120

4:00 pm

Prof. Shaul Mukamel (U. of California-Irvine)

'Probing Electron and Nuclear Correlations by
Coherent Multidimensional Optical
Spectroscopy from NMR to X-rays'

MIT, Room 6-321

5:00 pm

Mar 24

BUWIC Colloquium

Dr. Jennifer Hollingsworth (Los Alamos

National Laboratory)

TBA

Boston Univ., Life Science and Engineering

Building Auditorium (B01)

4:00 PM

Mar 25

Prof. Christopher Cheatum (University of Iowa)

'Watching the Protein Mambo: Fast Enzyme
Dynamics'

Tufts University, Pearson Chemistry Building,
Room P-106

4:30 pm

4:30 pm

Kathryn Steen (Drexel University)

'Patriotism and Patents: The U.S. Synthetic
Organic Chemicals Industry in World War I and
the 1920s'

Univ. New Hampshire, Iddles Room L103

11:10 am

Prof. Chaitan Kosla (Stanford University)

'New Insights into Macrolide Biosynthesis'

Boston College, Merkert Chemistry Center,
Room 130

4:00 pm

4:00 pm

4:00 pm

Dr. Richard Vachet (University of

Massachusetts, Amherst)

'High Throughput Analysis of Proteins Using

Multiplexed Tandem Mass Spectrometry'

New England Society for Applied Spectroscopy

Meeting

Hampton Inn, Natick MA

7:30 pm — Dinner @6:30 contact Mark Druy

[druy\(at\)psicorp.com](mailto:druy(at)psicorp.com)

Mar 26

Dr. Carol Korzeniewski (Texas Tech University)

TBA

Northeastern Univ., 129 Hurtig Hall

12 noon

Peidong Yang (University of California,

Berkeley)

TBA

Harvard Univ. Pfizer Lecture Hall

4:00 pm

Mar 27

Dr. Fred Walder

TBA

UMass Dartmouth, Building Group II,
Room 115

4:00 pm

4:00 pm

Prof. Martin Gruebele (University of Illinois at

Urbana-Champaign)

Continued on page 17