

# THE NUCLEUS

February 2002

Vol. LXXX, No. 6

## Monthly Meeting

*Willie E. May speaks about NIST programs in chemical metrology*

## Book Review

*"The Thirteenth Element"*  
by John Emsley

## Summer Scholar Report

*Modeling of Blood-Brain Barrier Permeability for Drugs*

## Board of Directors

*Notes of the Meeting of November 8, 2001*



**Eastern Analytical Symposium**

**Full page Ad Appears here**

**Ad # EAST 698N**

**Strip Film Neg supplied**

**The Northeastern Section of the American Chemical Society, Inc.**

Office: Marilou Cashman, 23 Cottage St., Natick, MA 01760. 1-800-872-2054 (Voice or FAX) or 508-653-6329.

e-mail: mcash0953@aol.com

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

NESACS Homepage:

<http://www.NESACS.org>

Frank R. Gorga, Webmaster

Washington, D.C. ACS Hotline:

1-800-227-5558

**Officers 2002**

*Chair:*

Morton Z. Hoffman

Chemistry Department, Boston University

Boston, MA 02215-2507;

617-353-2494 hoffman@chem.bu.edu

*Chair-Elect:*

John L. Neumeyer

1 Holiday Rd.

Wayland, MA 01778;

617-855-3388 neumeyer@mclean.harvard.edu

*Immediate Past Chair:*

Timothy B. Frigo

Advanced Magnetics, Inc.

61 Mooney St., Cambridge, MA 02138

617-497-2070x3007 tfrigo@hotmail.com

*Secretary:*

Michael Singer

Sigma RBI

1 Strathmore Rd.

Natick, MA 01760-2447

508-651-8151x291

msinger@sial.com

*Treasurer:*

James Piper

Simmons College, 300 The Fenway

Boston, MA 02115,

617-521-2722 piper@simmons.edu

*Auditor:*

Anthony Rosner

*Archivist:*

Myron Simon

20 Somerset Rd.

Newton, MA 02465; 617-332-5273

romysimon@mindspring.com

*Trustees:*

Michael E. Strem, Joseph A. Lima,

Esther A.H. Hopkins

**Councilors:**

*Term Ends 12/31/2002*

Mary T. Burgess

Michaeline F. Chen

Doris I. Lewis

Julia H. Miwa

*Term Ends 12/31/2003*

Catherine E. Costello

William Klemperer

Dorothy J. Phillips

Barbara G. Wood

*Term Ends 12/31/2004*

Thomas R. Gilbert

Patricia H. Hamm

Michael J. Hearn

Arlene W. Light

**Alternate Councilors:**

*Term Ends 12/31/2002*

Michael J. Dube

Jean Fuller-Stanley

Patrick M. Gordon

John L. Neumeyer

*Term Ends 12/31/2003*

Wallace J. Gleekman

Arno H.A. Heyn

Howard R. Mayne

Alfred Viola

*Term Ends 12/31/2004*

Timothy B. Frigo

Morton Z. Hoffman

Truman S. Light

Donald O. Rickter

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

**NESACS Committee Chairs for 2002** \_\_\_\_\_ **4**

**Monthly Meeting** \_\_\_\_\_ **5**

*Joint Meeting with YCC and NOBCCHE. Willie E. May from the National Institute of Standards and Technology speaks on its programs in chemical metrology*

**NOBCCHE** \_\_\_\_\_ **7**

*The National Organization for the Professional Advancement of Black Chemists and Chemical Engineers*

**Book Review** \_\_\_\_\_ **7**

*"The Thirteenth Element" by John Emsley, reviewed by Dennis Sardella*

**Board of Directors** \_\_\_\_\_ **9**

*Notes of the Meeting of November 8, 2001*

**Summer Scholar Report** \_\_\_\_\_ **11**

*"Modeling of Blood-Brain Barrier Permeability for Drug and Drug-Like Compounds" by Kimberly Rose and Lowell H. Hall*

**Applications Invited** \_\_\_\_\_ **16**

*James F. Norris and T.W. Richards Undergraduate Summer Research Scholarships for 2002*

**Puzzle Column** \_\_\_\_\_ **17**

**Cover:** *Dr. Willie E. May (NIST)*

**Deadlines:** *April 2002 issue: February 21, 2002*

*May 2002 issue: March 14, 2002*

## THE NUCLEUS

*The Nucleus is distributed to the members of the Northeastern Section of the American Chemical Society, to the secretaries of the Local Sections, and to editors of all local A.C.S. Section publications. 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:*

Arno Heyn, 21 Alexander Rd., Newton, MA 02461,

Tel: 617-969-5712, FAX: 617-527-2032; e-mail: arnoheyn@juno.com

*Associate Editor:*

Myron S. Simon, 20 Somerset Rd., W. Newton, MA 02465, Tel: 617-332-5273

*Board of Publications:*

Patrick M. Gordon (Chair), Frank R. Gorga, Marietta H. Schwartz, E. Joseph Billo (Consultant)

*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: 781-837-8792

*Contributing Editors:*

Mukund Chorghade, Patricia Hamm, Features; Edward Atkinson, History of Chemistry; Maryann Solstad, Health; Dennis Sardella, Book Reviews; Marietta H. Schwartz, Software Reviews; E. Joseph Billo, Puzzles.

*Calendar Coordinator:*

Donald O. Rickter, e-mail: 72133.3015@compuserve.com

*Proofreaders:*

E. Joseph Billo, Donald O. Rickter, M.S. Simon

*Webpage:*

Webmaster: Frank R. Gorga, fgorga@bridgew.edu

Asst. Webmasters: Terry Brush, tbrush@mediaone.net

Kurt Heinselman, heinslmm@earthlink.net

Copyright 2002, Northeastern Section of the American Chemical Society, Inc.

# Committee Chairs for 2002

<b>Awards</b>	Michael Dube
<b>Brauner Award</b>	Doris Lewis
<b>Bd. of Publications</b>	Patrick Gordon
<b>Budget</b>	James Piper
<b>Business Liaison</b>	Michael Strem
<b>Chem. Health &amp; Safety</b>	Mary Ann Solstad
<b>Chemical Education</b>	Ruth Tanner
<b>Constitution and Bylaws</b>	Catherine Costello
<b>Continuing Education</b>	Alfred Viola
<b>Education Task Force</b>	James Golen
<b>Esselen Award</b>	Judith Koob
<b>Government Relations</b>	Michael Hearn
<b>Local Arrangements</b>	Mary Burgess
<b>Medicinal Chemistry</b>	Ernie Groman
<b>Membership</b>	Michaeline Chen
<b>National Chemistry Week</b>	Sara Iacobucci
<b>National Meeting</b>	Morton Hoffman
<b>Nomination</b>	Tim Frigo
<b>Norris Award</b>	Patricia Samuel
<b>Professional Services</b>	Patricia Hamm
<b>Programming</b>	John Neumeyer
<b>Project SEED</b>	Patricia Mabrouk
<b>Public Relations</b>	Mukund Chorghade
<b>Public Service</b>	James Golen
<b>Richards Medal</b>	Patricia Mabrouk
<b>Senior Chemists</b>	Charles Bardsley
<b>Speakers' Bureau</b>	Susan Chiri-Buta
<b>Summerthing</b>	Wallace Gleekman
<b>Webmaster</b>	Frank Gorga
<b>Younger Chemists</b>	Amy Tapper ◇

# YCC Career Event

February 14, 2002,  
3:30-5:30 pm

Holiday Inn, Brookline, MA  
1200 Beacon St.

Younger Chemists are invited to attend this Career Clinic to learn about possible careers in chemistry. The FREE event will be held before the monthly meeting of the Northeastern Section, ACS. Contact Marilou Cashman at mcash0953@aol.com or at 800-872-2054 if you wish to stay for dinner and the evening lecture. For students the dinner price is only \$ 8.00!

**3:30-4:00** *Résumé Writing.* Dr. Mukund Chorghade, Geltex Pharmaceuticals

**4:00-4:20** *Industry.* Mark Behnke, Genetics Institute/Wyeth-Ayerst Research

**4:20-4:40** *Patent Law.* Dr. Jesse Fecker, Hamilton, Brook, Smith & Reynolds

**4:40-5:00** *Industry.* Dr. Angeles Dios, Geltex Pharmaceuticals

**5:00-5:20** *Academia.* Prof. Cheryl Schnitzer, Stonehill College ◇

## Corporate Patrons

Alfa Aesar, a Johnson Matthey Company  
Hoechst Marion Roussel Co.  
Pharm-Eco Laboratories, Inc.  
Physical Sciences, Inc.  
Polaroid Corporation  
Strem Chemicals, Inc.

## Corporate Sponsors

Aerodyne Research, Inc.  
AstraZeneca R&D  
Borregaard Synthesis, Inc.  
Bristol-Myers Squibb  
Cambridge Isotope Labs  
Consulting Resources Corporation  
Dike, Bronstein, Roberts & Cushman, LLP  
Houghton Chemical Corp.  
JEOL, USA, Inc.  
MassTrace, Inc.  
New England Biolabs  
Organix, Inc.  
Pfizer, Inc.  
Research Biochemicals Int'l  
Zymark Corporation

# Directions

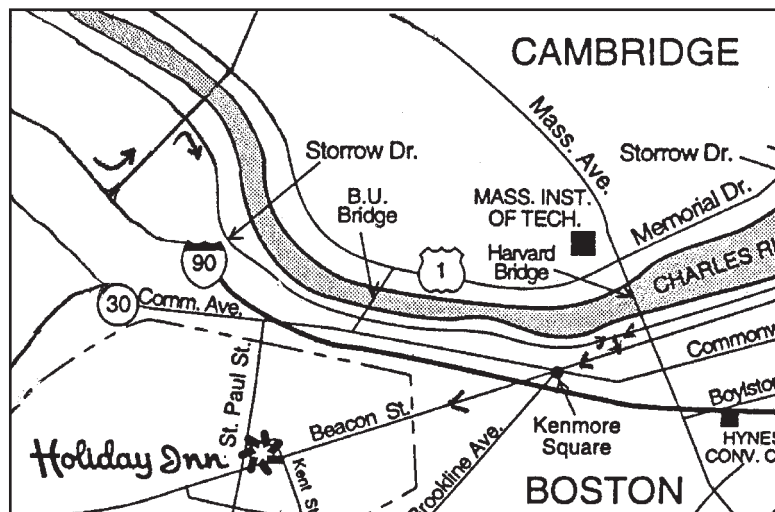
**From the West:** Take the Mass. Turnpike (I-90) to Exit 18. Exit left, follow signs to Cambridge. At the second set of lights turn right into Storrow Drive. Exit at the Kenmore Square Exit. Follow \* below.

**From the South or North:** Take Rte. I-93 to Boston. Exit into Storrow Drive at Exit 26. Continue on Storrow Drive to the Kenmore Exit. Follow \* below.

## \*From the Kenmore Exit off Storrow Drive:

At the first set of lights turn right into Beacon Street. In Kenmore Square stay in the center lane and take the center road, which is Beacon St. The Holiday Inn is about 0.6 Mi. on the right at St. Paul St. Enter the driveway into the garage at the in-town end of the building. Bring parking ticket to dinner desk for validation. Parking at meters on Beacon Street may also be available, should the garage be full (no meter charge after 6:00 pm).

**By Public Transportation:** Take (or change at Park St. to) the Green Line, "C" train. Exit at the St. Paul St. stop (3rd. stop after Kenmore) across from the Holiday Inn ◇



# Monthly Meeting

*The 831<sup>st</sup> Meeting of the Northeastern Section of the American Chemical Society, held jointly with the Younger Chemists Committee and the National Organization for the Professional Advancement of Black Chemists and Engineers*

Thursday, February 14, 2002 at the Holiday Inn,  
1200 Beacon St., Brookline, MA

**5:30 pm** Social Hour; a table of Career Services Literature and Aids will be available

**6:30 pm** Dinner

**7:45 pm** Evening Meeting, Dr. Morton Z. Hoffman, Chair, presiding

Dr. Willie E. May, Analytical Chemistry Division, Chemical Science and Technology Laboratory, National Institute of Standards and Technology: *NIST Program in Chemical Metrology and its Impact on U.S. Industrial Competitiveness, Trade, and Quality of Life*

*In honor of the day, you are invited to bring your special Valentine to the dinner as guest of the Section.*

Dinner reservations should be made no later than noon, February 7, 2002. Please call or fax Marilou Cashman at (800) 872-2054 or e-mail at [MCash0953@aol.com](mailto:MCash0953@aol.com). Reservations not cancelled at least 24 hours in advance must be paid. Members, \$25.00; Non-members, \$28.00; Retirees, \$15.00; Students, \$ 8.00.

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 underground Hotel garage, enter from westbound Beacon St. Obtain voucher at dinner desk.

**Next Meeting: Richards Medal Award to Prof. Stephen J. Lippard (M.I.T.)**  
*“Three Avenues in Bioinorganic Chemistry: Cisplatin, Methane Monooxygenase, and Metalloneurochemistry*

\$6M supports programs of other Federal and State Government Agencies and/or American Industry on a cost reimbursable basis.

The Division serves as the Nation's reference laboratory for chemical measurements and standards. The core competencies reside in five Groups: Spectrochemical Methods, Organic Analytical Methods, Gas Metrology and Classical Methods, Molecular Spectrometry and Microfluidic Methods, and Nuclear Analytical Methods.

Dr. May's personal research activities were focussed in the area of trace organic analytical chemistry, with special emphasis on the development of liquid chromatographic methods for the determination of individual organic species in complex mixtures (i.e., extracts of environmental, food, and clinical samples) and the development of liquid chromatographic methods for the determination of physico-chemical properties such as aqueous solubilities, octanol/water partition coefficients, and vapor pressures of organic compounds. This work is described in more than 100 peer-reviewed publications. He has presented more than 150 invited lectures during his 30-year professional career at U.S. industrial sites, Colleges/Universities and Technical Meetings throughout the world.

Dr. May has several leadership responsibilities in addition to those at NIST. Currently he is Chair, Organic Analysis Working Group, Consultative Committee on the Quantity of Material, International Committee for Weights and Measures; Chair, Technical Committee, North American Metrology Cooperation; and Chair, Chemical Metrology Working Group, Interamerican System for Metrology. In the past he has served as President and Executive Board Member for the International Society for Polycyclic Aromatic Compounds; Chair, Physical Sciences Panel, Ford Foundation Pre-doctoral Fellowship Evaluation Board; Chair, Chemistry Panel, Texas Higher Education Coordinating Board; Chair, Chemical Metrology Subpanel, Institute for National Measurement Stan-

*continued on page 6*

## Biography

**Willie E. May** received the B.S. degree in chemistry from Knoxville College, Knoxville, TN in 1968 and a Ph.D. in analytical chemistry from the University of Maryland at College Park, MD in 1977. He was employed at the Oak Ridge Gaseous Diffusion Plant from 1968-1971. He joined the National Bureau of Standards, as a Research Chemist, in 1971. He became Group Leader for Liquid Chromatography, Organic Analytical Research Division 1976 and became Chief of the Division in 1983. In 1994,

Dr. May became Chief of the Analytical Chemistry Division (a combination of the Organic Analytical and Inorganic Analytical Chemistry Divisions).

The Analytical Chemistry Division is one of five Divisions in the Chemical Science and Technology Laboratory, National Institute of Standards and Technology. Dr. May is responsible for policy development, planning, priority setting, fiscal allocation, staffing, and management of the day-to-day operations of the Division's approximately 100 scientists, technicians and administrative/ clerical support staff. The Division has an annual budget of about \$15M of which about

## Biography

Continued from page 5

dards, Canadian National Research Council; and Chair, Committee on Minority Affairs, American Chemical Society.

Honors and Awards presented to Dr. May include: Department of Commerce Bronze, Silver and Gold Medals; National Institute of Standards and Technology Equal Employment Opportunity Award (1982 and 1993); Arthur S. Flemming Award for Outstanding Individual Performance in the Federal Government before the age of 40; Presidential Award for Senior Executive Service to the Federal Government; the NOBCCHE Percy L. Julian Award for Outstanding Research in Organic Analytical Chemistry; and the 2001 Distinguished Service in the Advancement of Analytical Chemistry Award given by the Analytical Division of the American Chemical Society.

Dr. May is married (Jeannie Tramble) and the proud father of Jeanniece Michele and Eric Jermaine May. ◇

## Abstract

### *NIST Program in Chemical Metrology and its Impact on U.S. Industrial Competitiveness, Trade and Quality of Life*

From its very inception, the United States established the authority of Congress to "... fix the standard of weights and measures..." (Constitution of the United States, Article 1, § 8). The national importance of measurement science and measurement standards in the U.S. and a commitment to a strong Federal role was again recognized in the early 20th century with the establishment of the National Bureau of Standards (NBS) in 1901.

This well-defined role for NBS was re-articulated and expanded when the Bureau was renamed the National Institute of Standards and Technology (NIST) in the Omnibus Trade and Competitiveness Act of 1988. NIST was asked to:

*"... augment its unique ability to enhance the competitiveness of American industry while maintaining its traditional func-*

*tion as lead national laboratory for providing the measurement, calibrations, and quality assurance techniques which underpin U.S. commerce, technological progress, improved product reliability and manufacturing processes and public safety;"*

Although physical quantities such as length, mass, temperature, time, etc. are the first to come to mind when one thinks about NIST and measurement standards, chemical measurement research and standards have been a major activity since the establishment of NBS. Because the analytical chemistry function at NIST has a different objective than similarly named functions in industry or academia, it is carried out at NIST in a somewhat different manner.

This talk will describe how NIST's research and service programs in Analytical Chemistry are structured to provide the reference base and underpinning for chemical measurements made throughout the U.S. and on a *de facto* basis – through much of world. Examples will be given regarding the economic and social impact of research and measurement service activities in the areas of:

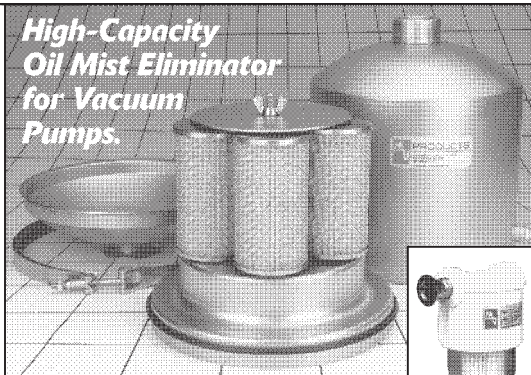
- Healthcare
- Food and Nutrition
- the Environment
- Forensics
- Pricing and Trade of Commodities
- Advanced Materials Characterization ◇

### Do Away with Vacuum Pump Oil Mist

#### with MV Oil Mist Eliminators

- Removes oil mist from vacuum pump exhaust
- Coalescing filters drain oil into a reservoir for easy recovery
- Protects clean rooms from pump vapors
- Keeps oil residue from sticking to furniture, walls and floors

High-Capacity Oil Mist Eliminator for Vacuum Pumps.



MV VISI-MIST Oil Mist Eliminator for Smaller Pumps

Vacuum pump oil mist contaminates the surrounding air, settles on surfaces and you breathe it. Eliminate this problem by installing MV oil mist eliminators on your vacuum pumps. The coalescing filter elements remove oil mist at 0.1 micron with an efficiency of 99.999%. Contact MV Products for the oil mist eliminators best suited for your requirements.



PRODUCTS

A Division of Mass-Vac, Inc.

247 Rangeway Road • PO Box 359 • North Billerica, MA 01862

978-667-2393

FAX 978-671-0014

E-MAIL sales@massvac.com

WEB www.massvac.com

Have you looked at the NESACS website?

**WWW.NESACS.org**

# NOBCChE

*The National Organization for the Professional Advancement of Black Chemists and Chemical Engineers*

(Pronounced "No be shay",  
[www.nobcche.org](http://www.nobcche.org))

NOBCChE, which was established in 1975, is committed to the discovery, transmittal, and application of knowledge in the fields of science and engineering. The mission of NOBCChE therefore is to build an eminent community of scientists and engineers by increasing the number of minorities in these fields. NOBCChE will achieve its mission through diverse programs designed to foster professional development and encourage students to pursue careers in science and technical fields. To this end, NOBCChE will establish educational partnerships with school districts, municipalities, businesses, industries, other institutions and organizations in the public and private sectors.

Awards are presented to recognize achievements by outstanding minority scientists, engineers and science teachers who have made significant contributions in their fields. These are very prestigious awards and are judged carefully by peers as well as by the Awards Committee.

The Organization's first national meeting was held in March 1974 in New Orleans and has continued to be a strong program throughout the years. The national meeting provides a rare opportunity for Afro-American chemists and chemical engineers to discuss issues of significance to their careers, to present technical papers, to formulate priorities and topics for future Meetings.

Dorothy J. Phillips ♦

## BOOST NUCLEUS RATINGS

Tell Nucleus advertisers you saw their ad in the Nucleus, when you call or write them. It boosts our ratings with them and helps to reduce our expenses.

# Book Review

*The Thirteenth Element: The Sordid Tale of Murder, Fire and Phosphorus,*

by John Emsley (John Wiley & Sons, 2000) 327 pp., ISBN 0.471 39455-6; \$24.95 (hardcover)

Reviewed by Dennis J. Sardella  
Department of Chemistry Boston College, Chestnut Hill, MA. 02467

"The Thirteenth Element", by John Emsley, traces the history of phosphorus from its discovery to its importance in the present day. The book is billed as the first biography of an element, although I would almost be tempted to describe it as something between a portrait and a police "rap sheet".

The story begins in the latter part of the seventeenth century with an account of the discovery of elemental phosphorus by the alchemist Hennig Brandt. Seeking the philosopher's stone, the legendary substance reputed to be able to convert base metals into gold, Brandt pyrolyzed the residue of large volumes of urine, obtaining the first impure sample of the element. Fascinated by its luminescence, Brandt spent several years vainly attempting to use it to transmute elements. Eventually, he settled into a less dramatic, albeit somewhat more lucrative, career as a supplier of phosphorus to others, who took the element "on the road" as a scientific curiosity, performing demonstrations at the courts of European princes, and for groups of scientists willing to pay for the privilege of witnessing its eerie glow and ability to combust spontaneously. During the twilight period when alchemy was gradually transforming into chemistry, the unique behavior of phosphorus brought it to the attention of serious scientists, who seem to have expected it to have almost magical powers. The story of Robert Boyle's fascination with phosphorus is intriguing and illustrative of the times, encompassing extensive scientific study of its properties, attempts to use it to transmute base metals into gold, and what can only be described as the type of antics that would get a freshman chemistry student thrown out of lab.

"His [Boyle's] favorite trick was to dip his finger in the liquid phosphorus and draw lines on linen or on the hands of guests, both men and women, noting how a little phosphorus went a long way, and that those hands he touched could then touch others and pass the luminosity on."

By the time Boyle got around to phosphorus, however, it was already on the medical map, a subject taken up by Emsley in chapter 3. Paracelsus' conviction that all disease had a chemical basis had prepared the ground for the use of chemicals as medications, and the seemingly magical properties of elemental phosphorus naturally led to its use as a tincture to treat a wide variety of conditions. Oddly, despite the twin impediments of its ineffectiveness and its toxicity, its use persisted even into the very early twentieth century, and one wonders what collateral damage its prescription might have entailed. (One rather amusing sidelight: a nineteenth century source refers delicately to its ability to produce "venereal excitation", conjuring up a picture of phosphorus as a kind of potential Victorian Viagra.)

By far, though, the most widespread use of phosphorus was in the production of lucifers and strike-anywhere matches, and Emsley devotes several chapters to the development, growth, and social impact of the match industry, including the dreadful plague of "phossy jaw" that afflicted its workers. This material is really social history, and provided me with more information about the match industry than I really wanted to know.

The catalog of grim stories continues in the next chapter, with an account in gory detail (in both the literal and

*Ucontinued on page 9*

# smallTalk2002

**The Microfluidics, Microarrays and BioMEMS Conference**  
**July 28-31, 2002, Sheraton San Diego Hotel, San Diego, CA**  
**Abstract Deadline March 15, 2002**

## Technical Topics

- Microarrays
- Microreactors
- Combinatorial Chemistry
- Genomics
- BioMEMS
- Biomaterials
- Proteomics
- Microfluidics
- Drug Discovery Chemistry
- Clinical Applications
- Molecular Diagnostics
- Point-of-Care Systems
- Separation Systems
- Modeling
- Standards
- Information Management
- Detection Technologies
- Microfabrication Technologies
- Hyphenated Microtechnologies
- Macro/Micro and Micro/Macro Interfaces
- Materials
- Informatics
- Data Visualization
- Unique Micro Phenomena
- Nanotechnology

## Short Courses

- Microfluidics
- Microarrays
- Microtechnology
- Mass spectroscopy

**Visit our Website and follow  
the smallTalk link to:  
Submit an abstract  
Register**

**Apply for an Academic Grant  
Become an Exhibitor or Sponsor**

**Or contact the ALA Office:  
smallTalk2002**

1201 Don Diego Avenue  
Santa Fe, NM 87505  
Tel: (505) 988-5326  
Fax: (505) 989-1073

email: [office@labautomation.org](mailto:office@labautomation.org)  
website: <http://labautomation.org>

... smallTalk 2002 Sponsors ...



Chemistry  
IN BRITAIN

AMGEN

OMNI  
OMIX  
Omnimix.com

LAP  
ON A  
CHIP



Association for Laboratory Automation



## Book Review

Continued from page 7

metaphorical senses) of the development of phosphorus incendiary bombs in the war. Here again, the chapter read much longer than it was. Was a day-by-day account of the firebombing of Hamburg really necessary?

Succeeding chapters recount the use of phosphorus in nerve gases and insecticides, and as a readily available, cheap, and apparently common poison (in the latter instance, in perhaps somewhat more detail than was warranted). Quite a few murder cases were outlined, most of which seemed rather repetitive without affording much new insight.

Chapter 10 affords a brief respite, with the story of the growth of the phosphorus industry, but is quickly succeeded by a survey in chapter 11 of environmental disasters involving phosphorus.

Chapter 12 finally brings some welcome relief from the rather long and dreary tale of illness, death and destruction by introducing phosphorus' ubiquitous role in the biosphere, principally in the forms of adenosine diphosphate and adenosine triphosphate. Justus Von Liebig's research in agricultural chemistry led him to formulate the Law of the Minimum, essentially an application of the limiting reagent principle, a theme continued as Emsley outlines the positive role of phosphorus, and I found myself wishing this portion of the book were longer.

In the book's final chapter, Emsley veers toward the border of the gothic, focusing on the topic of spontaneous human combustion, a subject that I have hitherto tended to associate more with supermarket tabloid headlines and horror films than with serious science. Nonetheless, he recounts several instances throughout history (including some supposed eyewitness reports) in which humans have allegedly spontaneously burst into flame and been virtually entirely consumed.

Seeing possible significance in the common observation that flames seem often to initially erupt from the chest cavity, Emsley hypothesizes that one conceivable mechanism might be the

generation of the pyrophoric gas diphosphine ( $P_2H_4$ ) in the stomach or intestines and its subsequent contact with oxygen, either internally, or through body openings. Since it is unclear whether there is any evidence for the metabolic production of diphosphine, this hypothesis, while interesting and perhaps entertaining, seems speculative at best.

The book underwent a name change at some point on its transatlantic journey, from "The Shocking History of Phosphorus", a title both less mysterious than "The Thirteenth Element", and more subtle than its subtitle "The Sordid Tale of Murder, Fire and Phosphorus." In fact, Emsley's Acknowledgements and his Introduction still refer to it by the British title, a small slip that should have been caught for the sake of consistency.

Like all of Emsley's books, The "Thirteenth Element" is entertaining and informative, although since the chemistry of phosphorus is relatively limited, there is little in the way of variety that Emsley is able to offer, and he thus places much more emphasis on the misuses of phosphorus, Mr. Hyde

## New Members

### Invitation to attend a 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](mailto:mcash0953@aol.com) by noon of the first Thursday of the month, letting her know that you are a new member. ◇

after all, being rather more interesting than Dr. Jekyll. However, I am reminded of having once heard someone comment of "Paradise Lost" that Milton did such a masterful job of depicting the evil persona of Satan, that God rather paled by comparison, and while it is entertaining and informative, I am a bit concerned that the long litany of perfidy and harm in "The Thirteenth Element" might only serve more to reinforce a non-scientist's preconceptions about chemicals than to create a positive impression of their importance. ◇

*Where speed and accuracy are elemental*



**Robertson Microlit  
Laboratories, Inc.**

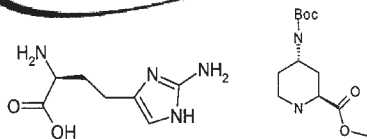
P.O. Box 927, 29 Samson Ave., Madison, NJ 07940

Phone (973) 966-6668 • Fax (973) 966-0136

[RobertsonMicrolit@worldnet.att.net](mailto:RobertsonMicrolit@worldnet.att.net)

[www.robertson-microlit.com](http://www.robertson-microlit.com)

- **Elemental Analysis**  
CHNSX  
Metals
- **Spectroscopy**  
MS  
FT-IR  
UV/VIS
- **Polarimetry**  
Specific Rotation
- **Trace Elements**  
ICP/AA  
Ion Chromatography
- **Bioavailability**  
pKa  
Log D (pH7.4), Log P, Log Pi  
Solubility
- **HPLC**  
Method Validation  
Method Development



106 South Street Hopkinton, MA 01748  
Phone: 1-888-777-4622/1-508-544-8265  
Fax: 1-888-777-3624/1-508-544-8259  
email: [rsp@amino-acids.com](mailto:rsp@amino-acids.com)  
<http://www.amino-acids.com>

The Amino Acid Company - Tailoring Amino Acid Analogues for Medicinal Chemistry

Log-In at [www.amino-acids.com](http://www.amino-acids.com) to access our Structural Index, Pipeline Products, and Capabilities.

**Come and see us at:**

- ACS National Meeting in Orlando, April 8-10, 2002
- ACS National Meeting in Boston, August 19-21, 2002
- 27th European Peptide Symposium in Sorrento, Italy, Aug 31st -September 6th, 2002

Visit our **NEW** web site to view our index, market selection analogues, and capabilities

***Our laboratory is expanding and Chemist employment positions are available***

## Eastern Scientific

1/2 page Ad Appears here

Ad # EAST 584N

Strip Repro supplied

# ACS News

## *NIST Designated as a National Historic Landmark*

Celebrating the National Institute of Standards and Technology's 100th anniversary, the American Chemical Society designated NIST as a National Historic Chemical Landmark on December 5. NIST formerly the National Bureau of Standards, was founded in 1901 to develop measurements and standards that strengthen the economy and improve quality of life. Throughout its history, the Institute has been a reliable source of assistance to industry, science, and government. NIST laboratories and other programs provide critical measurements, technology support, and start-up funding that benefit factories, communication networks, laboratories, educational organizations and other aspects of the new economy.

"Few Americans appreciate all the many ways the National Institute of Standards and Technology has made our lives richer, easier, and safer—from preserving national treasures such as the Declaration of Independence, to developing air traffic control systems that enable pilots to land planes in poor visibility, to setting national standards for radiation doses used in medical diagnosis and cancer therapy,"

stated ACS Board Chair Nina E. McClelland during the ceremony at NIST's campus in Gaithersburg, Maryland.

ACS established its landmarks program to honor and preserve milestones in the history of chemistry and to heighten public awareness of the key role chemistry plays in our daily lives. More than 35 places, discoveries and devices have achieved landmark status since the program's inception in 1992.

To learn more about NIST's chemical landmark designation go to <http://www.chemistry.org/landmarks>.

*From the December 2001 ACS "Capitol Connection."* ◇

# Summer Scholar Report

## *Modeling of Blood-Brain Barrier Permeability for Drug and Drug-Like Compounds*

Kimberly Rose<sup>#</sup> and Lowell H. Hall<sup>\*</sup>  
Department of Chemistry, Eastern Nazarene College  
Quincy, MA

### Introduction

A significant challenge in contemporary drug-design is proper targeting of the molecule to the appropriate tissues. One particularly crucial area is penetration of the blood-brain barrier (BB). Whether a molecule has the potential to penetrate the BB arises from non-covalent interactions, due to the structural and electronic features of the molecule. Small polar molecules and lipophilic drugs are known to cross the barrier. Larger polar molecules and lipid-insoluble organic molecules, including plasma proteins, do not penetrate well. The partitioning of a compound across the BB is measured experimentally as the ratio of the concentration of the compound in the brain to that in the blood:  $BB = \frac{[brain]}{[blood]}$ .

Given the cost of time and fiscal resources to accurately measure blood-brain barrier partitioning, the ability to model this property accurately is valued. Use of such a

model as a predictive scheme should be rapid, reliable, easy-to-use, and lend itself to interpretation of the structural features that influence BB partitioning.

A hypothesized relation exists between local hydrophobicity, molecular size, lipophilicity and molecular flexibility<sup>1</sup> to BB partitioning, but no mathematical relationship has been given. Attempts to delineate the relationship have resulted in models based on various 3D methods. In this present investigation, only topological structure descriptors are employed to create the mathematical model that relates structure to BB penetration. The topological method applied to the BB partitioning data leads to a model that is statistically equivalent or somewhat better than models reported in the literature<sup>2,3</sup>. Further, the method based on topological structure representation is considerably less time-consuming and less expensive to apply. Finally, interpretation of significant structural features is obtained by analysis of each of the structure descriptors in the model.

Topological methods have been explored for the last 20 years<sup>4-6</sup>, resulting in a variety of structurally descriptive indices (electrotopological state indices<sup>4</sup>, molecular connectivity chi indices, and kappa shape indices). These topological indices are relevant for describing facets of structure that influence non-covalent intermolecular interactions. These interactions are largely due to the distribution of the electrons on the surface of the molecule. This distribution comes from the physical arrangements of atoms (connectivity and

<sup>#</sup> 2001 Norris/Richards Summer Scholar

<sup>\*</sup> e-mail: hall@enc.edu

*continued on page 12*

## Two Day Training Course in Heterocyclic Chemistry

May 20 and 21st, 2002 at the Bayside Expo Center in Boston

The 2-day training course in heterocyclic chemistry includes:

Twelve hours of lectures by Professors

Albert Padwa (Emory Univ.) and Will Pearson (Univ. of Michigan)

750 pages of notes complete with up-to-date reference citations

Lunch plus morning and afternoon snacks for both days

Reservations must be received no later than **April 15, 2002**

*FOR MORE INFORMATION, PRICING and COURSE CATALOG*

**Check out our home page on the www at URL**

**[<http://euch6f.chem.emory.edu/heterocourse.html>]**

## Summer Scholar

Continued from page 11

shape) but is most elegantly described by the electrotopological indices, because these indices encode both the electronic and topological character molecule.

In the electrotopological approach to structure representation (E-State), basic structure information is developed for each atom (such as  $>N-$ ,  $=O$ ,  $-Cl$ ) and each hydride group (such as  $-CH_3$ ,  $-NH_2$ ,  $-OH$ ) in the molecule. The E-State index for an atom in a molecule,  $S(i)$ , is composed of an intrinsic state,  $I_i$ , derived from a measure of valence state electronegativity and a measure of the local topology, plus the sum of perturbations,  $\Delta I_{ij}$ , from other atoms. The E-State value for atom  $i$  in a molecule is computed as follows:  $S(i) = I_i + \sum_j \Delta I_{ij}$  (sum over all other atoms  $j$ ).

Through the E-state formalism, a value is created for each atom that describes the electron accessibility at a particular atom site in the molecule due to the electronic and topological nature of the entire molecule<sup>4</sup>. The E-State value  $S(i)$  is computed for each atom in the molecule and is called the *atom-level E-State value*. Variations of this definition include the *atom-type E-state*, a sum of the E-states for each type of atom in a molecule, and *hydrogen E-states*<sup>5</sup>. Due to the heterogeneity of the BB data set, only atom-type E-State and hydrogen E-states are used along with chi and kappa indices.

In this investigation, we developed a model for blood-

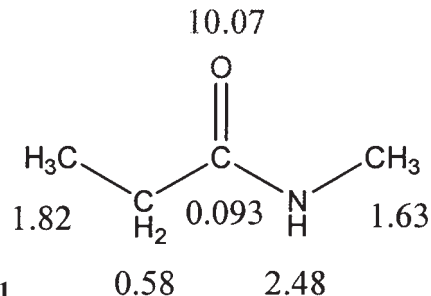


Figure 1

N-methylpropylamide with the calculated E-state values encoding electron accessibility for each atom.

-Oxygen has the highest value, as expected for an atom with the greatest electronegativity. This accessibility is due both to the topology of the molecule and electron distribution of two lone pairs and a pi bond within the carbonyl group arrangement.

-From similar reasoning, the carbonyl carbon has the lowest value. This is due to its sheltered location within the molecule and the presence of two nearby electronegative groups (O and N).

-The two methyl groups on the end of the atoms both have low values due to low electronegativity. However, the values for the groups are different due to the differing environments. The lower value occurs on the methyl next to the electronegative nitrogen.

brain barrier partitioning and demonstrated its validity by prediction of external test sets. The whole data set consists of 106 observations on neutral compounds ranging from  $CH_4$  and benzene to acetylsalicylic acid and caffeine to vera-

Lab support

1/2 page Ad Appears here

Ad # 446N

Strip Neg Supplied

pamil and indomethacin. The logBB values range over three and one half orders of magnitude of BB from -2.15 to +1.44; the molecular weight ranges from 16.0 to 613.8.

## Methods

**Data Entry.** While a variety of blood-brain barrier partitioning data obtained through various protocols is available, we limited the data to *in vivo* measurements obtained from rats. The data and molecular structures were taken from eleven sources<sup>2,3</sup>. The resulting data set contains 106 compounds with the corresponding BB values. These BB values were converted to the logarithm basis. Compounds were entered as structure drawings with ChemDraw<sup>7</sup> and structure data saved as MDL mol files. All structure indices used in this investigation were computed from Molconn-Z, ver 3.50<sup>8</sup>.

For QSAR analysis, we selected atom-type E-State and hydrogen E-State indices, along with molecular connectivity chi and difference chi indices, and with kappa shape indices.

**Statistical Analysis.** The data matrix was submitted for statistical analysis using the SAS system<sup>9</sup>. The RSQUARE selection method in proc REG was used to examine every QSAR equation from one to five variables, listing the top 10 most statistically significant. The most important variables, because they appear the most often, are E-State indices that emphasizes hydrogen bond donating ability,  $HS^T(\text{HBd})$ , along with certain non-polar structure features,  $HS^T(\text{arom})$ , and skeletal architecture, in the difference chi index,  $d^2\chi^v$ .

At this point in the model development, we introduced squares of the prominent variables to simulate a possible non-linear relation between structure and logBB. Significant improvement was obtained in the regressions. Only the squares of the  $HS^T(\text{arom})$  and  $d^2\chi^v$  variables were statistically significant. Based on these preliminary investigations, three structure descriptors were selected for further modeling and validation:  $HS^T(\text{HBd})$ ,  $[HS^T(\text{arom})]^2$ , and  $[d^2\chi^v]^2$ .

**Development of Final Model.** Based on the preliminary analysis and on validation studies, the three selected structure descriptors were considered good choices for this data set. To create a final model that could be used for prediction of compounds not in the current data set, we established a model for the whole set of 106 compounds and carefully examined the residuals. In order to optimize predictive ability, we decided to remove observations with large residuals, that is, residuals greater than 2.5 standard deviations. We found four observations with residuals greater than  $\pm 1.2$  and deleted them. The  $q^2$  value, based on the leave-one-out (LOO) method, improved from 0.52 to 0.62 upon removal of the four observations. The final model is shown in equation 1.

**Validation Studies.** Four standard approaches to validation of the model were adopted for this data set: creation of an external validation test set (20% of data set), cross-validation by the leave-group-out method<sup>10</sup>, prediction of an entirely different (+/-) data set, and extension of the model to a large database of drug and drug-like compounds. The results of these validation studies supported the predictive ability of the model.

## Results and Discussion

### The QSAR Model

The model based on three variables yielded statistical information as follows: eq. 1

$$\log\text{BB} = -0.202(\pm 0.026) HS^T(\text{HBd}) + 0.00627(\pm 0.00095) [HS^T(\text{arom})]^2 - 0.105(\pm 0.016) [d^2\chi^v]^2 - 0.425(\pm 0.069)$$

$$r^2 = 0.66, s = 0.45, F = 62.4, n = 102, q^2 = 0.62, s_{\text{press}} = 0.48$$

Quantities in parentheses are the standard deviations of the coefficients. The statistical quantities  $q^2$  ( $= r^2_{\text{press}}$ ) and  $s_{\text{press}}$  are based on the leave-one-out (LOO) method. A plot of the calculated logBB versus observed logBB values (Fig. 2) revealed a linear trend. An examination of the plot of residuals versus observed logBB revealed no trends and appears to be randomly distributed.

The statistical criteria for selection of the QSAR model for the logBB data are based on the following:  $r^2$  and  $q^2$  for the final model ( $n=102$ ); the mean absolute error (MAE) for the test set ( $n=20$ ); and the MAE for the cross-validation

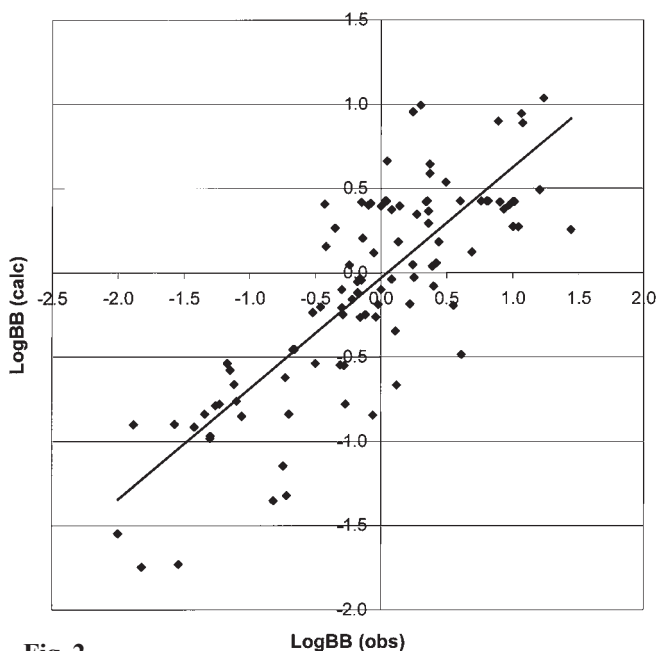


Fig. 2

(five-fold cross-validation). The MAE value was considered the most important statistic because an equation should not be considered a QSAR model unless it has demonstrated predictive value.

**Interpretation of the Model.** The three-variable model (eq. 1) adequately represents the logBB data for both training and test sets. Each of the variables is a descriptor of an aspect of molecular structure and will be discussed to indicate the specific structure information encoded. Let us consider three representative molecules from the data set in Table 1.

The  $HS^T(\text{HBd})$  term describes the hydrogen-bond donor ability of a molecule. The hydrogen E-state values of

*continued on page 14*

## Summer Scholar

Continued from page 13

all electron-donating groups (-OH, -NH<sub>2</sub>, and -NH-) are combined. Molecules with stronger hydrogen-bond donor abilities have high values for the HS<sup>T</sup>(HBd) index. Being rather hydrophilic, such molecules normally do not penetrate the BB well. For example, note that salicylic acid has a large HS<sup>T</sup>(HBd) value and it does not penetrate, as would be expected for a topical therapeutic agent.

The [HS<sup>T</sup>(arom)]<sup>2</sup> term describes the hydrogen E-state of all aromatic hydrogens. These hydrogens are related to a measure of the non-polar aromaticity and lipophilicity of a molecule. The more aromaticity a compound has, the higher its [HS<sup>T</sup>(arom)]<sup>2</sup>. Lipophilic compounds tend to cross the BB, as seen in the example of promazine, an antipsychotic CNS drug.

The third term, [d<sup>2</sup>χ<sup>v</sup>]<sup>2</sup>, is a measure of the skeletal branching and general polarity within the molecule. This index provides more fine-tuned structure information about the nonpolar aromatic groups and electronegative groups. Molecules with less branching tend to penetrate the barrier more easily. Caffeine is only marginally penetrating due to its branching and polarity.

In summary, the model given as eq. 1 indicates that

Compound and Use	Structure	LogBB	Calc Log	Res	HS <sup>T</sup> (HBd)	HS <sup>T</sup> (arom) <sup>2</sup>	(d <sup>2</sup> χ <sup>v</sup> ) <sup>2</sup>
promazine (84) antipsychotic penetrates well		1.230	1.036	0.194	0.000	102.26	0.280
caffeine (72) CNS stimulant penetrates marginally		-0.055	0.119	-0.174	0.000	0.000	2.919
salicylic acid (99) keratolytic does not penetrate		-1.100	-0.761	-0.339	5.297	26.207	2.678

**Table 1-** Representative molecules from the 106 compound data set. These compounds were chosen as examples of well-predicted molecules that either easily penetrate the BB (promazine), do not penetrate (salicylic acid), or marginally penetrate (caffeine).

blood-barrier penetration is favored for compounds with aromatic CH groups, less skeletal branching, and no hydrogen bond donor groups. The model permits the direct estimation of logBB for organic structures and blends together the structure information of the three structure descriptors in eq. 1.

At the conclusion of this analysis, a 3-variable model is produced to describe the relationship between molecular structures and blood-brain barrier partitioning. This model is found to successfully predict a molecule's BB penetration behavior and provides easily interpretable results. These

**Kelly Scientific Resources**

**1/2 page Ad Appears here**

**Ad # KELL 674N**

**Strip Repro supplied**

results are obtained quickly (4,000-5,000 compounds/minute) and in a cost-effective manner. In addition, the excellent outcome was obtained independent of information from 3D geometry based considerations.

**Note:** During the research project, models were also developed for toxicity of chlorophenols to various organisms and for fish toxicity of anilines, alkyl- and chlorophenols, and nitro- and halo-aromatics.

**Acknowledgements:** K. Rose acknowledges the support of the Northeastern Section, ACS, through a Norris/Richards Summer Research Fellowship. The author also wishes to express her thanks for the support and advice by Prof. Lowell H. Hall.

#### References

- 1 Crivori, P.; Cruciani, G.; Carrupt, P.; Testa, B. Predicting Blood-Brain Barrier Permeation from Three-Dimensional Molecular Structure, *J. Med. Chem.* **2000**, *43*, 2204-2216.
- 2 Luco, J. Prediction of the Blood-Brain Distribution of a Large Set of Drugs from Structurally Derived Descriptors Using Partial Least-Squares (PLS) Modeling. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 396-404.
- 3 Keserü, G.; Molnár, L. High-Throughput Prediction of Blood-Brain Partitioning: A Thermodynamic Approach, *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 120-128, and sources within.
- 4 Kier, L.B.; Hall, L.H. *Molecular Structure Description: The Electrotopological State*, Academic Press, San Diego, CA, 1999
- 5 Hall, L.H.; Kier, L.B. Electrotopological state indices for atom types: A novel combination of electronic, topological and valence state information, *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 1039-1045.
- 6 Hall, L.H.; Kier, L.B. Molecular Connectivity Chi Indices for Database Analysis and Structure-Property Modeling, in *Topological Indices and Related Descriptors in QSAR and QSPR*, Devillers, James; Balaban, Alexandru T., Eds., Gordon and Breach, Reading, UK, 307-360, 1999
- 7 ChemDraw, ver 4.5, CambridgeSoft, Cambridge, MA.
- 8 Molconn-Z, ver 3.50, available from: Hall Associates Consulting, Quincy, MA; EduSoft, LC, Ashland, VA; SciVision, Inc., Burlington, MA.
- 9 SAS, ver 8.0, SAS Institute, Cary, NC 27513
- 10 Maw, H.H.; Hall, L.H. E-State Modeling of Corticosteroids Binding Affinity Validation of Model For Small Data Set, *J. Chem. Inf. Comput. Sci.* **2001**, *41*, 1248-1254 ◇

# Board of Directors

## Notes of Meeting of November 8, 2001

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

#### Officers' Reports:

**Chair:** (Holiday Lecture), Bassam Shakhshiri was awarded an Honorary Lifetime Membership in the Northeastern Section.

The Division of Chemical Technicians is seeking new members and asks for the support of Local Sections in this effort.

**Chair-Elect:** M. Hoffman stated that a mini-grant proposal has been submitted to the ACS Office of Diversity for support of the February 2002 joint meeting of NESACS and YCC with NOBCCChE.

**Treasurer:** J. Piper, via written report, presented the status of the NESACS cash flow for October 2001. the Board APPROVED the report.

#### Standing Committees:

**Bd. Of Publications:** P. Gordon reported that the Committee had approved a 2002 budget request.

He stated that the Bd. of Pubs. requested that M. Schwartz remain on the committee as the appointee for 2002, and that P. Gordon assume the chair of the Board of Publications.

**Editor:** A. Heyn stated that the December 2001 issue will be 20 pages.

**Membership:** M. Chen reported that letters of welcome were sent to 450 new members in September. 5 new members attended the October Section Meeting. Three new members expected for tonight's meeting.

**Nominating:** Nominees for the Nominating Committee to be elected by the Board were presented by Tim Frigo. The Board elected M. Hearn and J. Billo as the Board representatives on the Committee.

**Chemistry Education:** M. Hoffman reported for R. Tanner that the Undergraduate Day was a big success and was very well attended.

Applications for the YCC visit to Germany in March 2002 are due by December 31, 2001. An ACS mini-grant has been awarded by the ACS to NEACS for supporting *Connections to Chemistry*

R. Tanner stated that this program was oversubscribed: 150 High School Teachers applied for 110 places.

Only six applications have been received for Grants-in-aid for attending the Orlando meeting. The BU Undergraduate Day had 125 participants from 16 colleges and universities.

**Constitution and Bylaws:** C. Costello stated that the C&B changes which had been approved at the October Board meeting have been submitted to the ACS C&B Committee for a preliminary review.

**Esselen Award:** J. Koob submitted a written report, stating that the process has moved into the selection stage from the four nominations which have been received. Selection of an awardee will be made in early January. The Committee is seeking ways to reduce the cost of the award event which went over budget last year.

#### Other Committees:

**Continuing Education:** A. Viola was happy to report that the fall Short Course produced a positive balance of about \$5,000. For 2002, because of Boston being the site of the Fall meeting, a short course will be impractical.

**Government Affairs:** M. Hearn reported that a new initiative is being planned for the spring of 2002, including outreach to new Congressmen from Massachusetts.

**Natl. Chemistry Week:** S. Iacobucci reported that the Science Museum was very happy about the good response to the November 3 program and the cooperation by members of NESACS with the arrangements. Four schools sent volunteers. The Forsyth event on November 6 also was very well attended. This has been the biggest NESACS NCW program to date.

**Younger Chemists:** A. Tapper stated that the group is looking for people to assume leadership positions.

**New Business:** M. Hoffman expressed his thanks for condolences sent him on the death of his mother. ◇

# Applications Invited

## *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 2002. 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 bibliog-

raphy) of their summer projects to the NESACS Education Committee by November 8, 2002 for publication in *The Nucleus*. They are also required to participate in the Northeast Student Chemistry Research Conference (NSCRC) in April 2003.

**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, 2002.

**Application:** Application forms are available on the NESACS web site at <http://www.nesacs.org>. Completed applications are to be submitted no later than March 22, 2002 to the Chair of the Selection Committee:

*Professor Edwin Jahngen,  
University of Massachusetts Lowell  
Chemistry Department, Room 520  
265 Riverside Street, Olney Hall  
Lowell, MA 01854-5047*

**Notification:** Applicants will be notified of the results by e-mail on April 26, 2002. Written confirmation will follow.



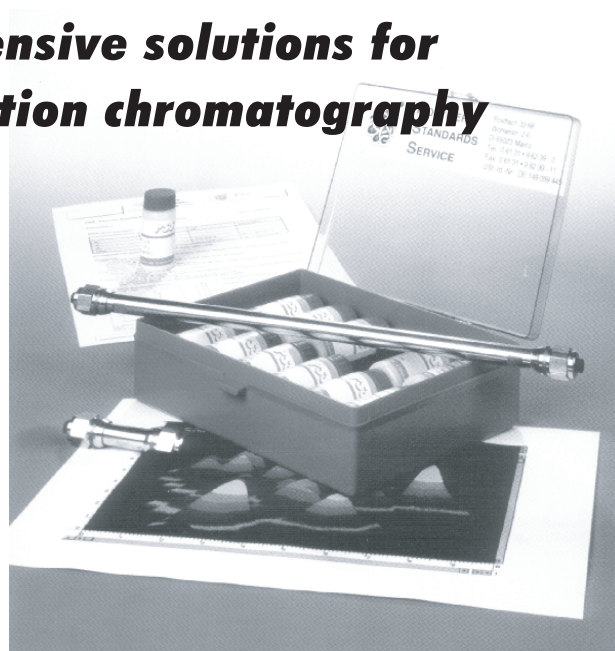
# PSS

## Polymer Standards Service

### **comprehensive solutions for gel permeation chromatography**

Certified Calibration standards  
Validation Kits  
Universal and specialty columns  
WINPC/POROCHECK software  
Sample testing services  
Instrumentation

Professional expertise  
ISO 9001 reliability



10111 Colesville Road, Ste 123, Silver Spring, MD 20901

Toll Free 888-477-7872 Fax 301-681-2709 e-mail [mgray@polymer.de](mailto:mgray@polymer.de) <http://www.polymer.de>



# Puzzle Column

By permission, from the INDICATOR of the North Jersey/New York Sections, March 2001

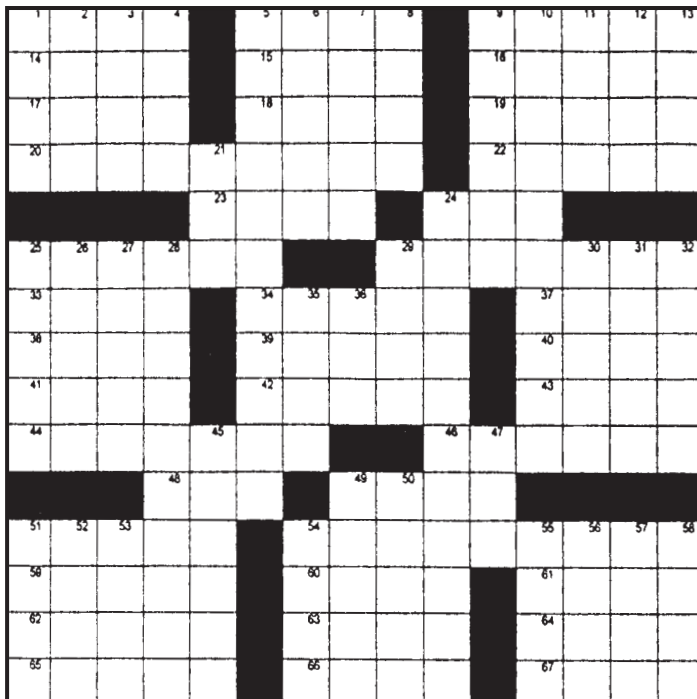
Gasoline by Colleen M. Parriott

## Across

1. Self-luminous heavenly body
5. Prepare flour
9. Squirrel food
14. Crippled
15. Unicorn fish
16. Fiber from nettle
17. Very dry
18. Stocking problems
19. Persona \_\_\_\_\_
20. In making gasoline, these are removed from petroleum for use in candles
22. German submarine
23. Tastes a taco
24. Peleg's son
25. Unit for angular velocity
29. 42 gallon units of petroleum
33. \_\_\_\_\_, \_\_\_\_\_ and away
34. Shy
37. Biblical kingdom
38. South American native
39. Criminal cover-up
40. Albacore or Bluefin
41. \_\_\_\_\_ do-good
42. Antibiotic acids produced by basidiomycetes
43. Central Europe river
44. O-rings, such as for gasoline tanks
46. Take into police custody
48. Afternoons/evenings
49. Heap
51. Violin family member
54. Ratio that needs careful adjustment to maximize performance in gasoline engines
59. Concerning
60. Mark for life
61. \_\_\_\_\_ boy!
62. Sudden voltage increase
63. Small amount
64. Without: French
65. Lock of hair
66. Staircase section
67. This and \_\_\_\_\_

## Down

1. Hit
2. Gone With the Wind plantation
3. Islamic chieftain
4. Scarlet letter
5. Compounds in gasoline that help keep an engine clean
6. Eskimo
7. Natives of Helsinki
8. Hardy heroine
9. One who disagrees
10. Internal combustion engine device for mixing vaporized gasoline with air
11. Hawaiian thrush
12. Educating \_\_\_\_\_ (Michael Cain film)



- |   |                          |                              |
|---|--------------------------|------------------------------|
| 13. Without solvent                         | 29. Lady: India          | 50. Very angry               |
| 21. Admission charge                        | 30. Evade                | 51. Set of actors            |
| 24. What an antiknock agent acts as         | 31. Bowling alleys       | 52. Ivory: Latin             |
| 25. Feeling sorrow over                     | 32. Intelligent          | 53. Folk story               |
| 26. Sleep disturbance                       | 35. Laomedon's father    | 54. Words in a used car ad   |
| 27. Dictators                               | 36. Central              | 55. Rapid                    |
| 28. Devices in cylinders to ignite gasoline | 45. Behaves theatrically | 56. The Beehive State        |
|   | 47. _____ Speedwagon     | 57. Active volcano in Sicily |
|   | 49. Embroidery loop      | 58. Final ◇                  |

## Chemo Dynamics LP

1/3 page Ad Appears here

Ad # CHEM 681N

Strip Neg Supplied

# BUSINESS DIRECTORY

## SERVICES

### SCHWARZKOPF Microanalytical Laboratory

Elemental & Trace Analysis  
Organics, Inorganics  
Organometalics  
Metals by AA & Graphite 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

### LABORATORY EQUIPMENT

Bought • Sold • Exchanged

#### FEBRUARY SPECIAL

Kelvinator flammable storage and  
explosion proof refrigerators  
and freezers.

*In like new condition.*

American Instrument Exchange, Inc.  
1023 Western Ave., Haverhill MA 01832  
TEL: 978-521-2221 FAX: 978-521-8822  
www.americaninstrument.com

### HT Labs

#### Mass Spec Analysis

ESI, APCI, MALDI, LCMS (24hrs turnaround time)

#### Elemental Analysis, CHN

#### Custom Synthesis

Phone: 858.677.9432 Fax: 858.677.0240  
Info@HT-Labs.com www.HT-Labs.com

### NMR ANALYSIS

270 - 360 - 400 MHz • 1D/2D  
Liquids/Solids • GLP/GMP Compliance  
SPECTRAL DATA SERVICES, INC.  
818 Pioneer • Champaign, IL 61820  
(217) 352-7084 • Fax (217) 352-9748  
http://www.sdsnmr.com sdsnmr@sdsnmr.com

### ORGANIX

#### CONTRACT RESEARCH

#### CUSTOM SYNTHESIS

Milligram to kilogram scale  
in all areas of Organic Chemistry

240 Salem Street, Woburn MA 01801  
Phone: 781-932-4142 Fax: 781-933-6695  
Web: www.organixinc.com

Have you looked at the  
NESACS website?  
**WWW.NESACS.ORG**

## SERVICES

### DESERT ANALYTICS LABORATORY

- CHNOSP Halogens
- Metals by AA/ICP
- Ion Chromatography
- Trace Analysis
- Coal/Petroleum

≡ Fast, Reliable Service ≡

No Charge for Phone/Fax Results

P.O. Box 41838 245 S. Plumer, #24  
Tucson, AZ 85717 Tucson, AZ 85719  
Fax 520-623-9218 Phone 520-623-3381

Web: [desertanalytics.com](http://desertanalytics.com)

E-mail: [thelab@desertanalytics.com](mailto:thelab@desertanalytics.com)

ANALYSIS FOR THE CHEMICAL ELEMENTS

## A CALL FOR NUCLEUS VOLUNTEERS

Help publish the *Nucleus*  
You can do so in a variety of ways

#### Writers

Roving Reporters in the academic or  
corporate communities

#### Proofers

Editors and editorial assistants

You can help make the *Nucleus* more  
useful to our members. We adjust  
our schedule to yours, and you serve  
with your peers in the process.

Phone for more details  
Arno Heyn  
*Nucleus* Editor  
Tel: 617-969-5712

## SERVICES

### QTI

 QUANTITATIVE TECHNOLOGIES INC.  
*The Proven Leader in...*

### Elemental Analysis

- ✓ CHNSX  
-24 HR. RESULTS
- ✓ TRACE LEVEL ANALYSIS
- ✓ WET CHEMISTRY
- ✓ AA, GFAA, ICP
- ✓ HPLC, GC

### Pharmaceutical Support

- ✓ METHOD DEVELOPMENT
- ✓ DISSOLUTION
- ✓ STABILITY

Salem Industrial Park, #5 • Route 22 East  
Whitehouse, NJ 08839-0470

To check out more about QTI, call

**908-534-4445**

e-mail - [info@qtionline.com](mailto:info@qtionline.com) [www.QTIonline.com](http://www.QTIonline.com)

### PRIME

Prime Organics Inc.

### SURE, WE CAN MAKE THAT!

Custom synthesis  
Contract R&D  
Manufacturing

- Milligram to multi-kilogram synthesis
- Multi-step synthesis
- Process R&D
- Combinatorial Chemistry
- Building Blocks
- Libraries
- Medicinal Intermediates
- Impurity Synthesis
- Heterocycles
- Nucleosides/RNA
- Taxanes
- And much more. Just ask!

450 Chelmsford St.  
Lowell, MA 01851  
Phone: 978-970-1074  
Fax: 978-934-0731  
[info@primeorg.com](mailto:info@primeorg.com)  
[www.primeorg.com](http://www.primeorg.com)

# BUSINESS DIRECTORY

## SERVICES

### Yasui Seiki Co., (USA)

#### Coating Test Laboratory

- ◆ Battery Electrode and Primer
- ◆ Pattern or 'Patch' Coating
- ◆ Display Coatings 0.1 to 1  $\mu$
- ◆ Photo / Photo-Resist 0.1 to 9  $\mu$
- ◆ 1 micron UV Hardcoats

Featuring *Precise* Yasui Seiki Machines  
Tel 812.331.0700 ◆ Fax 812.331.2800  
www.yasui.com ◆ yasui@ix.netcom.com

### CNH Technologies, Inc.

Contract Organic Synthesis - R & D - mg-kg  
*On Time & On Spec*

10A Henshaw St. Ph: 781 367-4047  
Woburn, MA 01801 Fax: 781 933-1839  
e-mail: services@cnhtechnologies.com

### \*NMR Service 500MHz

### \*MASS \*Elemental Analysis

Fast Turnaround / Accurate results

**NuMega Resonance Labs.**  
(858) 793-6057 Fax (858) 793-2607

### PROTECT

Your Expensive Lab Work With Research  
and Development Record Books

#### STOCK RECORD BOOKS

B50D --- Fifty pages and fifty duplicates  
1/4 inch sqs. on right pages

B100P --- 100 - 1/4 inch sqs. on right pages  
100 - 10 sqs. per inch on left pages.

B200P --- 208 1/4 inch sqs. on right and left pages  
B200PH - 208 horizontally lines right and left pages.

Books have instruction and TOC's. Page size 11 x 8 1/2.  
Hard extension brown cloth covers. Pages open flat.

\$14.50 EACH, FOB Chicago  
CUSTOM MADE BOOKS TO ORDER

Scientific Bindery Productions  
60 E. 13th Street Chicago, IL 60605  
Phone: 312-939-3449 Fax: 312-939-3787  
www.scientificbindery88yrs.com



### 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

## CAREER OPPS

### VOLUNTEERS

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

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

### Chemical Analysis Services

- ▲ Materials ID/Deformulation
- ▲ Competitive Product Analysis
- ▲ Defects/Failure Analysis
- ▲ Polymer Analysis & Testing



**Chemir / Polytech**  
Laboratories, Inc.

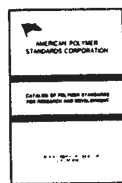
(800) 659-7659

chemir.com

2672 Metro Blvd.  
Maryland Heights  
Missouri 63043

FREE

### Polymer Standards Catalog



AMERICAN POLYMER  
STANDARDS CORPORATION  
P. O. Box 901, Mentor, Ohio 44061-0901  
Phone: 440-255-2211 Fax: 440-255-8397

### BOOST NUCLEUS RATINGS

Tell Nucleus advertisers you saw their ad in  
the Nucleus, when you call or write them.  
It boosts our ratings with them and  
helps to reduce our expenses.

### Front Run OrganX, inc.

Custom/Contract Synth.-Process R&D  
Scaffolds B-Blocks Pre-Clinical  
Simple.....Complex

FrontRun@sprynet.com Ph 978-356-7133  
17 Hayward St., Ipswich, Ma. 01938 Fax-7449

## CAREER OPPS

### RECRUITING ?

The Nucleus readership is New England's largest source for chemical and bio-chemical personnel.

The Nucleus reaches more than 15,000 readers each month. These professionals perform in the following areas:

INDUSTRY	Management & R&D	67%
ACADEME	Faculty & Admin	14%
STUDENTS	Grad & post-docs	10%
CONSULTING & CLINICAL LABS		5%
GOVERNMENT		4%

One company recruiting through  
The Nucleus said ----

We received more *qualified resumes*  
from our ad in *The Nucleus* than we did  
from our newspaper ad.

Contact Customer Service for info at:

Phone - 781-837-0424 or  
email vincgale@tiac.net

### Index of Advertisers

Am. Instrument Exchange.....	18
Am. Polymer Standards Corp.....	19
Association for Lab Automation ....	8
Chemir/Polytech Laboratories.....	19
Chemo Dynamics LP .....	17
CNH Technologies, Inc. ....	19
Desert Analytics Laboratory.....	18
Eastern Analytical Symposium .....	2
Eastern Scientific Co.....	10
Front Run Organx.....	19
Heterodata, Inc. ....	11
HT Laboratories, Inc. ....	18
Kelly Scientific Resources .....	14
Lab Support .....	12
Mass-Vac, Inc. ....	6
Micron Inc. ....	19
NuMega Resonance Labs .....	19
Organix, Inc.....	18
Polymer Standards Services .....	16
Prime Organics .....	18
Quantitative Technologies, Inc. ....	18
Robertson Microlit Labs, Inc. ....	9
RSP Amino Acid Analogues, Inc. ....	10
Schwarzkopf Microanalytical.....	18
Scientific Bindery.....	19
Spectral Data Services, Inc.....	18
Yasui Seiki Co. ....	19

19 Mill Road  
Harvard, MA 01451

# THE NUCLEUS

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

## Calendar

### For additional information, call:

Am. Assoc. Clinical Chemists - (617) 732-6987,  
pager 11161  
Boston College - (617) 552-2605  
Boston University - (617) 353-4277  
Brandeis University - (781) 736-2500  
Dartmouth College - (603) 646-2501  
Harvard University - (617) 495-4198  
Mass. Inst. Technology - (617) 253-1803  
Northeastern University - (617) 373-2822  
Tufts Univ. - (617) 627-2634  
UMass Boston - (617) 287-6130  
UMass Dartmouth - (508) 999-8232  
UMass Lowell - (978) 934-3675  
Univ. of New Hampshire - (603) 862-1550  
Worcester Polytechnic Institute - (508) 831-5250

**Check the NESACS Homepage for late  
additions:**

<http://www.NESACS.org>

Note also the MIT Chemistry Department  
Webpage calendar: <http://web.mit.edu/chemistry/www/temp/seminars/pchemseminars.html>  
and the Harvard Chemistry web site for updates:  
[http://www-chem.harvard.edu/events/Physical\\_Seminars.html](http://www-chem.harvard.edu/events/Physical_Seminars.html)  
(which includes the Harvard/MIT joint seminars)

### February 4

Prof. George Whitesides (Harvard Univ.)  
“Unconventional Nanofabrication. Using soft-lithographic tools to make patterned nanostructures”  
Boston Univ., 590 Commonwealth Ave., Science Center Auditorium, SCI 107, 4:00 pm

### February 6

Dr. Chris Chang (Nocera Group)  
TBA [Inorganic Chemistry Seminar]  
MIT, Room 6-120, 4 pm

### February 7

Prof. Paul Alivisato (UC Berkeley)  
Harvard Univ., MB-23 Pfizer Lecture Hall, 4:15 pm

### February 11

Prof. Mike Maroney (Univ. of Massachusetts)  
“Structure and Function in Metallobiochemistry: A Nickel Tour.”  
Boston Univ., 590 Commonwealth Ave., Science Center Auditorium, SCI 107, 4:00 pm

### February 12

Prof. Marisa Kozlowski (Univ. of Pennsylvania)  
TBA  
Boston College, Merkert Chemistry Center,  
Room 130, 2609 Beacon St.  
4:00 pm

Prof. Andrew Marcus (Univ. of Oregon)  
TBA [Physical Chemistry Seminar]  
MIT, Rm. 2-105, 4 pm

Prof. Andrei Tokmakoff (Mass. Institute of Technology)  
“Molecular Structure and Dynamics in Solution Observed Through Two-Dimensional Infrared Spectroscopy”  
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford,  
Room 106, 4:30 pm

### February 13

Prof. Tom Tullius (Boston Univ.)  
TBA  
Boston College, Merkert Chemistry Center,  
Room 130, 2609 Beacon St.  
4:00 pm

Prof. Jeffrey S. Moore (Univ. of Illinois)  
TBA [Karl Pfister Lectures in Organic Chemistry]  
MIT, Room 6-120, 4 pm

### February 14

Prof. Hagan Baley (Texas A&M Univ., Dept. Medical Biochem. & Genetics)  
Harvard Univ., MB-23 Pfizer Lecture Hall,  
4:15 pm

Prof. Jeffrey S. Moore (Univ. of Illinois)  
TBA [Karl Pfister Lectures in Organic Chemistry]  
MIT, Room 6-120, 4 pm

Prof. George Kebalka (Univ. of Tenn, Knoxville)  
“Organic Synthesis Using Organometallic Reagents in the Absence of Organic Solvents: Green Chemistry”  
Northeastern Univ., 129 Hurtig Hall, 4:00 pm

### February 18

Prof. Michael Gelb (Univ. of Washington)  
“Interfacial Enzymology and Cell Biology of the Mammalian Phospholipase A2 Family”  
MIT, Room 6-120, 4 pm

### February 19

Prof. Martin Gruebele (Univ. of Illinois)  
TBA [Physical Chemistry Seminar]  
MIT, Rm. 2-105, 4 pm

Prof. Seiichi Matsuda (Rice Univ.)  
“Tinkering with Terpene Biosynthesis”  
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford,  
Room 106, 4:30 pm

### February 20

Prof. Guillermo Bazan (Univ. of California)  
TBA [Harvard/MIT Inorganic Chemistry Seminar @ MIT]  
MIT, Room 6-120, 4 pm

### February 21

Prof. David Bruns (Univ. of Virginia)  
“Evidence-Based Laboratory Medicine”  
American Association for Clinical Chemistry,  
DoubleTree Guest Suites Hotel, Waltham at 128;  
Social, 6 pm; dinner, 7 pm; lecture, 8 pm

Dr. Mukund Chorghade (Geltex Pharmaceuticals, Inc.)  
“Progress of a Drug from Conception to Commercialization”  
Tufts Univ., Chemistry Seminar Hosted by the ACS Student Affiliate Chapter at Tufts,  
Pearson Chem. Building, room 106, 4:30 pm

### February 25

Prof. Wes Sundquist (Univ. of Utah)  
Boston Univ., 590 Commonwealth Ave., Science Center Auditorium, SCI 107, 4:00 pm

### February 26

Prof. Tom Wandless (Stanford Univ.)  
TBA  
Boston College, Merkert Chemistry Center,  
Room 130, 2609 Beacon St.  
4:00 pm  
Prof. Steve Bradforth (Univ. of Southern California)  
“The Mechanisms for Electron Photoejection in Liquid Water”  
MIT, Rm. 2-105, 4 pm  
Prof. John T. Groves (Princeton Univ.)  
TBA  
Tufts Univ., Pearson Chem. Building, 62 Talbot Ave., Medford,  
Room 106, 4:30 pm

Prof. John MacDonald (Worcester Polytechnic Institute)  
“Supramolecular Synthesis of Organic and Organometallic Crystalline Materials”  
Univ. of New Hampshire, Durham, Iddles Auditorium L103, 11:00 am

### February 28

Prof. Jonathan L. Sessler (Univ. of Texas)  
TBA [Seminar in Organic Chemistry]  
MIT, Room 6-120, 4 pm

### Notices for the Nucleus Calendar should be sent to:

Dr. Donald O. Rickter, 88 Hemlock St.,  
Arlington, MA 02474-2157  
e-mail: 72133.3015@compuserve.com