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NORTHEASTERN SECTION • AMERICAN CHEMICAL SOCIETY
NESACS

THE NUCLEUS

May 1999 *Vol. LXXVII, No. 9*

Monthly Meeting

Education Night:
Prof. Eric Martz Speaks on Molecular Modeling

NESACS Election

Candidates' Bios and Statements

Book Review

The Molecular Modeling Workbook
By Warren J. Hehre et al.

Summer Scholar Report

On Target-Specific Nucleic Acid Ligands By Matthew D. Simon and Clemens Richert

The Northeastern Section of the American Chemical Society, Inc.

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Any Section business may be conducted via the business office above.
New NESACS Homepage: http://people.ne.mediaone.net/obermayer/nesacs
Washington, D.C. ACS Hotline: 1-800-227-5558

Contents

Deadlines: *Summer Issue: June 11, 1999*
September Issue: July 16, 1999

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.

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Council Meeting

Anaheim, CA, March 24, 1999

Report on the Meeting and the Doings of Your Representatives

The Northeastern Section was represented by ten Councilors/Alternate Councilors at the Anaheim ACS National Meeting.

As usual, the representatives gathered shortly after 7 a.m. for a complimentary continental breakfast, followed by trumpet calls at 8:00 a.m. to convene the Council Meeting.

The first item of business was the introduction of the slate of four nominees for President-Elect for 2000, from which the Council had to select two candidates, which will be on the ballot for election by the members of the ACS in the fall, together with any possible petition candidates. These four were introduced to at the meeting and were allotted 5 minutes each to present their views. The four nominees were:

F. Peter Boer (Tiger Scientific Co., FL)

James A. Bristol (Parke Davis Pharmaceutical Res. Div., Ann Arbor, MI)

Attila E. Pavlath (USDA, Albany, CA)

Alan Schriesheim (Argonne Natl. Lab., Argonne, IL)

The Council selected the last two to be the candidates for President-Elect, one to be elected in the fall by the members.

As usual, there were reports of the officers of the ACS and reports on interim actions.

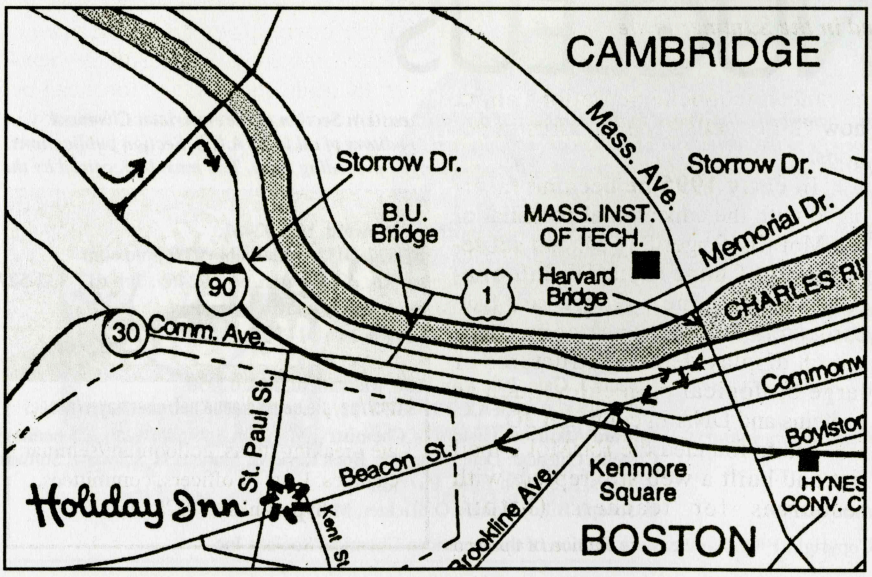
The Chairs of the several committees presented their reports. The action items were as follows:

The Committee on Committees recommended that the Committee Professional Training be continued for another five-year period (all "other" committees must be reviewed every 5 years), and the Council voted, with no dissent, to continue this committee, as recommended.

Also under the aegis of the Committee on Committees, a petition to amend Bylaw III, Sec. 3,d,(1)(c), to amend the duties of the Committee on Divisional Activities by including under its duties recommendations for combination or dissolving Divisions. (This followed similar wording added to the duties of the Local Section Affairs Committee in 1998, for recommending the dissolving or combing of Local Sections.)

The Council voted unanimously to approve the petition. The amendment is to take effect after approval by the Board of Directors.

continued on page 6



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 unto Storrow Drive. Exit at the Kenmore Square Exit. Follow * below.

From the South or North: Take Rte. I-93 to Boston. Exit unto 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 onto 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. 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 807th Meeting of the Northeastern Section of the American Chemical Society

Education Night

Thursday, May 13, 1999

Holiday Inn, 1200 Beacon St., Brookline, Mass.

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. Donald O. Rickter, Chair, presiding

Address: *Exploration of Macromolecular Structure with 3D Visualization Freeware for Personal Computers*
Prof. Eric Martz, Dept. of Microbiology, Univ. of Massachusetts, Amherst

Presentation of Awards
- Philip L. Levins Memorial Prize
- James Flack Norris/Theodore William Richards Undergraduate Research Fellowships
- Undergraduate Grants-in-Aid
- Undergraduate Research Symposium
- 1998 Project SEED students
- Excellence in Teaching at the Secondary School Level
- Induction of New Members into *Aula Laudis*
- Avery A. Ashdown Chemistry Examination; Simmons College Prize

Dinner reservations should be made no later than May 6, noon. Please call or fax Marilou Cashman at 800-872-2054. Reservations not canceled 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 Marilo Cashman a few days in advance so that suitable arrangements can be made.

Free Parking: Basement level; enter from westbound Beacon St. (space limited — if full, park on the street at meters – free after 6 pm.)

Watch for Summerthing, to be announced in the Summer Issue

Biography

Eric Martz is Professor of Immunology in the Department of Microbiology at the University of Massachusetts, Amherst. He has recently switched the focus of his work to educational molecular visualization. For some 20 years he did research on cell interactions and immunology, during which he defined the early steps in the interactions of cytotoxic T lymphocyte "killer cells" with target cells. He was co-discoverer of an important leukocyte integrin adhesion molecule (LFA-1), and advanced iconoclastic notions about how "killer cells" control virus infections.

In early 1995 he became fascinated with the educational potential of RasMol (by Roger Sayle), and subsequently of Chime (by MDL Information Systems, Inc.). These are free programs for personal computers which display detailed structures of large biological molecules, such as proteins and DNA in color and 3D.

Martz founded the RasMol e-mail list and built a web site replete with resources for teachers (http://

continued on page 6

Abstract

Genomics and advances in protein structure science are yielding an exponentially growing amount of information about 3D structures of macromolecules. These structures are increasingly important in research on protein function, drug design, and biotechnology. Thus it is ever more crucial that students, educators, and scientists in many different specialties be able to access easily and understand 3D macromolecular structures. Free software well adapted to 3D visualization of large molecules (up to 25,000 atoms or so) on personal computers began to be available in the early 1990's (Kinemages and RasMol). More recently, the Netscape plugin Chime, a free derivative of RasMol developed by MDL Information Systems, Inc., has extended these capabilities dramatically. Already available, built with Chime, are a viewer able to show any published 3D structure immediately from the web; numerous interactive educational tutorials; movies showing the relation between two different conformations of a protein by morphing, and tools which make it easy to visualize specific aspects of structure. Examples of such tools include one for finding the non-covalent bonds between a protein and its ligand, and another for showing the vibrations of a small molecule which correspond to a peak in an infrared spectrum. The resulting viewers, tutorials, movies, and tools can be used from the web on either Windows or Macintosh personal computers. ◇

Visit
the NESACS Website:

http://people.ne.mediaone.net/obermayer/nesacs

Late breaking items, colloquium/seminar changes. Lists of officers, committees, hyperlinks to ACS, etc.

Microsoft Excel® for Scientists and Engineers

A Two-Day Hands-On Short Course

Instructor: Prof. E. Joseph Billo, Boston College

Thursday, May 13 - Friday, May 14, 1999

8:00 AM - 4:00 PM

Computer Career Institute, 4 California Avenue, Framingham MA

Program:

Shortcuts and tips to format, edit, and print spreadsheets.
How to customize menus and toolbars for scientific computing.
How to produce professional quality spreadsheets and charts.
How to link documents, how to import data into Excel, and how to set up Excel to perform iterative calculations automatically.
How to use Excel's built-in mathematical functions to perform multiple linear regression analysis, matrix mathematics, numerical differentiation and integration, solutions of systems of linear equations, and more.
How to use the Solver, Excel's powerful optimization package, to perform nonlinear least squares curve fitting.
How to create simple macros to automate routine spreadsheet tasks.
How to write advanced macros to carry out complex, repetitive calculations automatically.

Prof. Billo is the author of *Excel for Chemists: A Comprehensive Guide*, John Wiley and Sons, 1997, 480 pp. He has taught this course to over 500 scientists at locations including Amoco, Biogen, Chevron, Eastman Kodak, Genzyme, National Cancer Institute, Naval Research Laboratory, Procter & Gamble, Shell and Texaco. This is the same course that has been offered at ACS National Meetings for $925.

This is not a course for beginners. You must have some familiarity with Excel in order to benefit from this course.

Pre-registration required. Registration is limited to 24 attendees.

Each participant will have his/her own PC workstation.

Registration Fee (add $50 to receive a copy of *Excel for Chemists*):

	On or before Apr. 30	After Apr. 30
A. C. S Members	$375.00	$425.00
Non - A. C. S Members	$475.00	$525.00

For further information: (617) 552-3619 or joseph.billo@bc.edu

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Registration form for **MICROSOFT EXCEL FOR SCIENTISTS**

☐ Check to order a copy of *Excel for Chemists* (add $50 to registration fee)

Name _____ ☐ ACS Member

Mailing Address _____ Tel.: _____

_____ Total enclosed:

_____ $_____

Mail with remittance to: Dr. E. J. Billo, 13 Shattuck Street, Natick MA 01760
(Please make check payable to E. J. Billo)

Biography

continued from page 5

www.umass.edu/microbio/rasmol During its 3.5 years of existence this web site has been visited by over 300,000 people from over 100 countries. Martz pioneered educational RasMol "movie" scripting, and subsequently developed novel educational resources with Chime. These include illustrations for lectures as well as sites for interactive self-paced student exploration, such as a site on DNA structure, the "Protein Morpher", and the "Noncovalent Bond Finder". These have been downloaded over 10,000 times by educators and are used in hundreds of high schools and colleges worldwide.

Martz also designed "PDB Lite", a web search interface with a built-in molecule viewer at the international Protein Data Bank, Brookhaven National Laboratory, which is used over a thousand times a day. With a grant from the Division of Undergraduate Education of the National Science Foundation Martz has given workshops to enable college faculty to incorporate molecular visualization into their teaching. "As the offspring of artist-parents, I have always longed to create beauty as well as truth", says Martz. "RasMol and Chime enable me to do both." ◇

Council Report

continued from page 4

The Committee on Nominations and Elections reported that there is an imbalance in the number of members in some of the Regions, which exceeds the 10% imbalance allowed in the documents of the Society. This will make a realignment of Regions necessary, to be presented at the fall meeting in New Orleans. The Regions are of importance in that six of the Directors on the ACS Board of Directors represent one of the six Regions, respectively and are elected by the Councilors in that Region.

Each spring the Society Committee on Budget and Finance has to present a recommendation for the next year's member dues. According to the

Trustees Report for 1998

Condensed from the original report

The members of Board of Trustees for 1998 have been Dr. Esther A.H. Hopkins, Dr. Michael Strem, and Mr. Joseph Lima.

The overall value of the assets in the endowment and income Trust Accounts amounted to $ 1,889,371 on December 31, 1998, an increase of approx. 7% for 1998.

Market Value of Trust Funds

December 31, 1998

	1997 Total	Securities	Money Funds	Total
Richards Medal	$ 71,510	$ 52,497	$ 3,924	$ 56,421
Norris Award	31,804	19,719	6,600	26,319
Publications	21,485	14,127	529	14,656
Permanent	53,984	37,673	10,382	48,055
Hill Awards	2,111	2,219	2,219	
Total Inc. Accts.	180,874	124,016	23,654	147,670
Consolidated	1,231,259	1,297,867	60,136	1,358,003
Esselen Award	335,190	364,686	2,208	366,894
Levins Prize	17,518	14,098	2,706	16,804
Total	***1,784,841***	**1,800,667**	**88,704**	**1,889,371** ◇

Council Report

continued from page 6

formula, based on the previous year's dues and the "dues escalator", calculated from the Cost of Services Index, the dues for 2000 would be $3 higher than the 1999 dues, i.e. $108 for full-dues paying members. The Council has the option of accepting this figure, or the current dues, or any whole-dollar amount in-between. Often this is a very contentious issue, but this time the B&F recommendation was accepted with only a small scattering of "no" votes, amounting to about 10%. Of the NESACS representatives, Michael Hearn voted "NO" on the dues increase.

The Chair of the Committee on Economic and Professional Affairs reported that at the Employment Clearing House, the employers reported 1500 positions looking for employees, while 1100 candidates had registered, a very favorable ratio for chemist-employees.

The Chair of the Committee on Local Section Affairs reported the unusual event, that all 188 Local Sections had turned in their 1998 reports.

The Committee on Meetings and Expositions gave a lengthy report on the finances of national meetings in support of the request to raise registration fees for future meetings. Most national meetings cost more than the funds collected from registration fees and other meeting income. For 1999 the projected shortfall amounts to about $40 per registrant. (The 1998 Boston meeting, by contrast, generated a surplus of about $6 per registrant because of excellent attendance – 13,941, about 4,000 higher than most other meetings).

No action had to be taken on this issue at this time.

This Committee also asked for approval of Salt Lake City for the site for the Spring 2009 meeting, which was approved unanimously.

The Committee on Membership Affairs reported on a promising start of the "2000" Membership Campaign.

A petition to amend Bylaw I, Sec. 4 was presented for action. This petition will remove the requirement of a reinstatement fee for former members whose membership has lapsed, or who have resigned previously. This petition was approved unanimously.

The Committee on Constitution and Bylaws reported that four petitions for amending the Bylaws had been received and will be up for action at the fall meeting, unless withdrawn by the petitioners.

Your representatives attended committee meetings of the committees to which they are assigned: Catherine Costello attended the International Activities and Constitution and Bylaws Committee, Thomas Gilbert the Meetings and Expositions Committee – he is chair of the subcommittee on site selec-

continued on page 21

Northeastern Section

Election of Candidates for 2000

In the interest of providing maximum information and expression of opinion by the candidates for election in 1999, the Nominating Committee has prepared this section of the NUCLEUS for mailing concurrently with the ballots. All candidates were asked to submit biographical material and, with the exception of committee member nominees, position statements. To attain uniformity of format, the biographical data have been rearranged, and, where the text exceeded the allotted space, abbreviated. The statements have been reproduced without change. An official ballot, along with a ballot envelope and return envelope have been provided. The election and balloting are being carried out in conformance with Article VIII of the Constitution of the Northeastern Section. The order of candidates for each office has been determined by lot. Comments regarding the election may be addressed to the Nominating Committee Chair, Dr. Michael J. Hearn (address on p.3)

BALLOT DIRECTIONS: Vote for the candidate(s) of your choice, insert your ballot into the ballot envelope. (Neither the ballot nor ballot envelope may have any writing or identification). Insert the sealed ballot envelope into the return envelope and sign your name on the return envelope only, affix postage and mail.

The ballot must be received by June 1, 1999. ◇

Chair-Elect

(Three-year sequence: Chair-Elect, Chair, Past Chair)
One to be elected

Mukund S. Chorghade

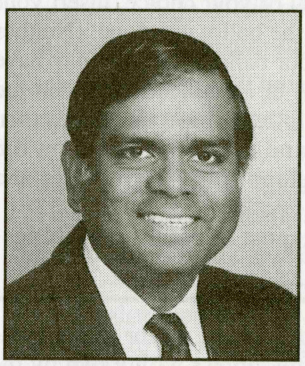
Education: B.Sc. 1971, M.Sc. 1973 (1st Class Honors) Univ. of Poona, India; Ph.D. (Organic Chemistry), 1982, Georgetown University.

Professional Experience: Research Fellow, National Chemical Laboratory (1981-82); Postdoctoral Res. Assoc., Univ. of Virginia (1982-84); Postdoctoral Research Fellow, Harvard University (1984-85); Sr. Res. Chemist (1985-89), Project Leader (1989-90), Dow Chemical Co.; Res. Scientist/Asst. Director, College de France, Paris and Universite Louis Pasteur (1990-91); Project Mgr., Abbott Laboratories, Pharmaceutical Research (1992-95); Sr. Director, Chemical Sciences Research & Development, CytoMed, Inc. (1997-98); President, CP Consulting, Inc. (1995- present); Consultant, LeukoSite, Inc. (1999-present). Visiting Scholar, Univ. of British Columbia, Univ. of Chicago, Northwestern Univ. and others.

ACS Service: Member since 1982. Chairman, Brazoport Section (1990); Organic Division, member; Chairman, Symposium on Industrial Chem., Great Lakes Regional Meeting, May 1997.

NESACS Service: Public Services Committee, Chair; Professional Services Committee, member;

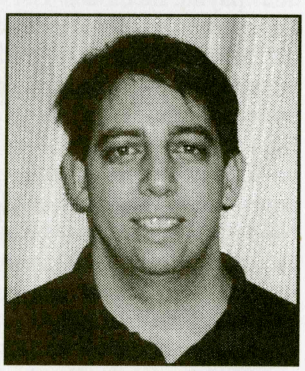
Memberships, Honors: IUPAC; Royal Society of Chemistry (Elected Fellow); New York Acad. Of Sciences; Am. Institute of Chemists (Elected Fellow); AAAS; Sigma Xi; Indian Society of Bio-Organic Chemists; IUPAC Commission on Biotechnology, Medicinal Chemistry, New Technologies and Special Topics, Assoc. member; 20th IUPAC Conference on the Chemistry of Natural Products, Chicago, 1996: Chair, Scientific Programs Comm.; on Advisory Bd. for *Organic Process Research and Development*; Reviewer of manuscripts for numerous leading professional journals. Awarded "Diamond Jubilee Fellowship", Univ. Dept. of Chemical Technology, Mumbia, India; Awarded "B.D. Tilak Distinguished Visiting Fellowship", Univ. of Bombay, India. Listed in *American Men and Women of Science, Who's Who in Science and Engineering.* Actively involved with Indian Cultural Coordination Committee, Washington, DC. Leadership roles in several community groups.



Statement: It is a singular honor and privilege to have been nominated to the position of Chair-Elect for the Northeastern Section. The breadth, depth and sophistication of the talent and creativity of the individuals in the section is truly outstanding. We have eminent researchers representing the strategic triad of academia, government and industry from all subdisciplines of chemistry.

It will be my endeavor to (1) Foster greater interaction between the ACS and the other professional bodies catering to the cause of chemistry - the American Institute of Chemists and the International Union of Pure and Applied Chemistry come readily to mind. A one-day joint meeting featuring several prominent scientists can be envisioned. This could provide a useful forum for productive exchange of ideas. (2) Organize a speakers bureau to provide guest lectures to school, universities and civic and community groups. The topics can encompass issues of topical interest, e.g., chemical safety, environmental and the contributions made by chemists/chemistry to the benefit of society at large. (3) Expand the activities of the Professional Training/Education Committee. Regular workshops will be used to educate students at local colleges/universities about the diverse opportunities in chemistry, resume writing, interviewing skills/techniques and related topics. (4) Organize a symposium on the progress of a drug from conception to commercialization. This will build a much needed bridge between the medicinal and process chemistry groups and is expected to attract several scientists in the area. (5) Organize a few lunch time lectures to attract researchers who, because of their busy schedules, are not able to attend the evening lectures. (6) Increase participation of members in the section activities and increase the membership of the ACS and the section. This will also allow greater opportunities for networking among chemists. (7) Increase participation of the section in the international activities of the ACS.

Timothy B. Frigo



Education: B.A. (chem.) Lawrence University, Appleton, WI (1982); Ph.D. (org. chem.), Univ. of Wisconsin (1988)

Professional Experience: Post-doctoral at MIT and BU Medical Ctr.; currently: Advanced Magnetics, Inc., Cambridge, MA.

NESACS Service: Secretary and Program Chair, Medicinal Chem. Group (1997-98); currently: Chair, Medicinal Chem. Group.

Statement: The solid tradition of the NESACS continues to meet up with the changing science and society as we approach the new millennium. I believe the past and current chair and committee members have done an excellent job of meeting this challenge by fulfilling their role of serving the chemical community through their efforts in the many edu-

cational and social programs they have overseen. I would gladly accept this opportunity to serve as chairman in 2001, to explore these challenges, and meet new ones. As chair of the NESACS, I would be committed to serving the office in the fullest capacity by striving to continue the high degree of excellence they have achieved, and by looking for other areas in which I may serve.

Secretary:

(Two year term, one to be elected)

Sonja Fetela

Education: B.S., Industrial Chemistry

Professional Experience: Inks Chemist, Mearl Corp.; Currently: Laboratory/Project Management, Polyonics, Inc., Westmoreland, NH from 5 months after the start of the company to present, involved in the manufacture of printable label stock for circuit boards and static dissipative coatings and inks.

NESACS Service: Career Employment Services Committee, currently Secretary of NESACS.

Statement: I am seeking for another term to try to improve my skills in the area of being a secretary so that it may benefit the organization to a higher level. Having some difficulty in the past year, I have not been able to attend a few meetings and my note taking skills could use some improvement. I have however managed to comply with the full attendance of Councilors/Alternates at many meetings.

With a growing company, and learning more about responsibility, I would like to seek another term as Secretary to extend the knowledge I have gained from my learning.

Michael Singer

Education: B.S., State Univ. of New York at Stony Brook (1986); M.S.; Chemistry, Brandeis Univ. (1988); Ph.D., Brandeis Univ. (1993).

Professional Experience: Post-doctoral Res. Assoc., Organix, Inc., Woburn, MA (1991-94); Senior Scientist (1994-96), Group Leader, Automated Combinatorial Synthesis, ArQule, Inc., Medford, MA (1996-present)

ACS Service: Councilor, Northeastern Sect. (1996-)

NESACS Service: Bd. Of Directors (1993-); Bd. Of Publications (1998-); Medicin. Chem. Group: Member (1991-); Treasurer (1992-93); Program Chair (1994); Chair (1995-96).

Statement: The Northeastern Section of the American Chemical Society is a section with a deep sense of heritage and tradition. During my involvement over the last 6 years on the Board of Directors of the NESACS I have had the opportunity to participate in the heritage and the traditions of the section. The role of Secretary of the NESACS is charged with documenting the activities of the Section as we look forward to new challenges while maintaining a link to our heritage and tradition. The biggest skill that I bring to position is a commitment to details. I believe that few things are as important to a large section such as ours, as the accurate and timely dissemination of information to the membership. One of my goals, if elected, is to work with the Nucleus Staff and the Section Webmaster to publish the minutes and activities of the section in a more timely fashion to the entire membership.

As with any volunteer organization, the organization is only as strong as the membership and those members that actively participate in the planning and execution of the various events. During my last 6 years on the Board, and 8 years on the Medicinal Chemistry Group, I have been an active and enthusiastic participant. With your support, I will bring my experience and enthusiasm to the position of Secretary of the NESACS.

Trustee

(Three-year term, one to be elected)

Truman S. Light

Education: Harvard University, S.B. (1944); University of Minnesota, M.S. (1949); University of Rome (Italy), Doctor of Chemistry (1961).

Professional Experience: Boston College, Assistant Professor (1949-1959); Avco R&D, Sr. Scientist (1959-64); The Foxboro Co., Principal Research Scientist (1964-88); Consultant (1988-present); Consultant in Analytical Chemistry and Instrumentation (1988-); Adjunct Professor, Chemical Instrumentation, Boston College (1987, and 1999), Suffolk University (1992), Aquinas College, Newton (1994-5).

ACS Service:

Councilor (1976-1995); Committee memberships: Local Section Affairs, Constitution and Bylaws, Membership Affairs, Employment Services Advisory Board, Copyrights.

NESACS Service: Chairman (1978); Councilor (1976-1995); Alternate Councilor (1996-present); Member and Chairman of various Committees: Student Affiliate; Constitution and Bylaws; Esselen Award; Professional Services, Employment Services.

Memberships, Honors: National Science Foundation Science Faculty Fellowship, 1959-61 (Rome), Henry Hill Award for Outstanding Service to the Northeastern Section (with Arlene Light), 1993; Waters Symposium Award (Ion Selective Electrodes), Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, (1996).

Statement: I am a candidate for Trustee, because I believe I have achieved the maturity needed for financial guardianship of the NESACS by virtue of many years of Local and National ACS experience and managing my own financial survival after 10 years of retirement.

Michael E. Strem

Education: A.B., Brown Univ. (1958); M.S. (1961); Ph.D., Univ. of Pittsburgh (1964).

Professional Experience: Strem Chemicals, Inc., President (1964- present).

ACS Service: Member, Bd. of Directors elected from Region I (1998-2000); Comm. on Committees (1993-97); Society Comm. on Budget and Finance (Associate, 1994-present); service on numerous other committees 1987-1992. Division of Small Businesses, Councilor (1986-96), Chairman (1982-83, 1985)

NESACS Service: Chairman-Elect (1988); Chairman (1989); Bd. Of Publications, Chairman (1991, 1994); Chairman, Nominating Committee (1990-92); Northeast Regional Meeting, Exhibits Chairman (1993)

Memberships, Honors: Member: Royal Soc. Of Chemistry, Gesellschaft Deutscher Chemiker, Societé Francaise de Chimie; Materials Research Soc. Henry A. Hill Award for Distinguished Service to the Northeastern Section (1995).

Statement: Many years of experience have taught me much about the finances of the Northeastern Section. I am aware of the fiscally conservative attitudes prevalent within our membership and will act accordingly if you elect me as Trustee. I promise also to work actively with the officers and board members in fiscal matters to support them in reaching the goals they have set for the Section. I feel that being president of a corporation for over 30 years has provided me with the skills to managed the Section's funds properly, and I look forward to your support.

Councilor/Alternate Councilor

(Three-year terms; four Councilors and four Alternate Councilors to be elected)

Mary M. Burgess

Education: B.S., Simmons College

ACS Service: I have been a member of the Committee on Professional Relations and Liaison to the Women's Chemist Committee. I have also been a member of the Local Sections Activities Committee. Councilor (Northeastern Section) (1987-95; 1997-99); Hospitality Chair for Northeastern Regional Meeting (NERM), 1978; National ACS Meeting in Boston, 1990; Northeastern Regional Meeting (NERM23) Boston, 1993; National ACS Meeting, Boston, 1998.

NESACS Service: As a member of the Northeastern Section during my entire career, I have participated as Hospitality Chairperson for many years. Programs related to Education and Professional Relations included the development of the Student Awards Program and the Henry Hill Award. I have also been a member of the Pops Programs and Summerthing Programs.

Statement: I have been active in both local and national affairs. I will continue to encourage participation in the involvement of members of the section, especially to encourage new and younger members to participate in the programs. I will be proud to continue to represent our section as Councilor of the Northeastern Section. I ask for your continued support and ask you to vote for me for Councilor of the Section.

Michaeline F. Chen

Education: B.A., Clarke College; M.S., Boston College

Professional Experience: US Army Research Laboratory (1985-97) Ceramic Research Branch, the Armor/Structural Ceramics Team. Chemist in advanced materials research, synthesis, processing, surface science and materials characterization.

ACS Service: Member since 1976. Councilor, Northeastern Section (1988-present); Public Relations Comm. (1987-88); Economic Status Comm., Associate (1988), Member (1989-93); Economic and Professional Affairs Comm. (1994); International Activities Comm. (1995-); Comm. on Admissions (1998-).

NESACS Service: Board of Directors (1984-present); Professional Relations Comm. (1988-); Public Relations Chair (1988); National Meeting and Centennial Committees (1998); Nominating Comm. (1988, 1995); Summerthing/Fallfest Comm. member and/or chair (1982-92); National Meeting Planning Comm. –Public Relations Chairperson (1990); Hospitality Committee Chair (1984-87), incl. Boston 1986 IUPAC Meeting.

Memberships, Honors: Henry A. Hill Award for Outstanding Service to the Northeastern Section (1997).

Statement: I shall continue to broaden our Northeastern Section's influence on National ACS policy decisions; increase interactions between our Section and the National Society; promote new and interesting programs, and increase the involvement of the membership in its activities. I would sincerely appreciate your support and your vote so that I may continue to serve you as a councilor.

Michael J. Dube

Education: Ph.D., Organic Chemistry, Brown University, 1993; B.S., *cum laude*, Chemistry, Southeastern Massachusetts University, 1987;

Professional Experience: Assistant Professor, Wellesley College (1993-1996); Visiting Lecturer, University Massachusetts at Dartmouth (1996-1998); Adjunct Professor, University of Massachusetts at Dartmouth (1998-present); Laboratory Manager, Nye Lubricants Inc., (1998-present).

ACS Service: Councilor (1998); Alternate Councilor (1996-1997) .

NESACS Service: Chairman, Awards Committee (1998-present); Chairman, James Flack Norris Speakers Bureau (1994-present).

Statement: I seek to serve the NESACS as Councilor and represent our section at the ACS national level. As anyone who has been a Councilor can attest, it takes time to build relationships that will promote service on ACS national committees. If elected, I intend to continue building the relationships necessary to represent our interests at ACS meetings. My prior service within NESACS and my professional experience will allow me to accurately and faithfully represent the needs and concerns of NESACS.

Jean A. Fuller-Stanley

Education: B.Sc., honors in chemistry, University of London, England (1976); Ph.D. in organic chemistry, Univ. of Nebraska-Lincoln (1984).

Professional Experience: Associate Professor of Chemistry at Wellesley College where she has been since 1984. Primary teaching responsibilities in organic and introductory chemistry. Since 1994 she has been the Director of Wellesley College's Minority Mentorship in Science program. Her research interest is in the area of physical organic chemistry with particular emphasis on the use of NMR spectroscopic techniques to elucidate structural phenomena. Since being at Wellesley College she has supervised many undergraduates in research both during the academic year and summer. She and her students have presented their work at National and Regional ACS meetings regularly.

ACS Service: Member since 1984.

Memberships, Honors: She has been a member of the Council on Undergraduate Research (CUR) since joining the Wellesley faculty. She was elected CUR councilor, 1994-1997 and is currently serving out a second term 1997-2000.

Statement: This Fall, 1998 I attended a "Mentoring for Success" workshop conducted by the Minority Affairs Office of ACS. My primary reason for attending that workshop is the same reason I have for wanting to be elected Councilor/ Alternate Councilor. The goals of the "Peer Mentoring" program that I would like to help establish at the NE Section is to make ALL who attend meetings feel that they are an integral part of this section. I must confess that I have attended very few of the Local Section monthly meetings. However, the few I attended, I found quite unwelcoming. If elected I would work to increase participation of dormant and new members and create an environment that is *deliberately welcoming*. One example of a *deliberately welcoming* environment is to have '*hospitality buddies*'. This group of trained volunteers would be strategically placed during NE section meetings so as to involve as many people as possible in conversations. I will work with the local section to provide regular workshops on such things as "the nuts and bolts of networking", strengths and weaknesses of Industrial *vs.* Academia work environment". These are just a few examples of the kinds of service the NE Section could provide that might appeal to a broader spectrum of members. I believe that the NE Section can provide its members with many opportunities to acquire the social skills needed for advancement in the field.

Patrick M. Gordon

Education: B.S., University of Guyana (1977); M.S., University of New South Wales, Australia (1982); Ph.D. University of Manitoba, Canada (1987)

Professional Experience: Post Doctoral Associate, Kansas State University (1987-1988); Organix Inc., Woburn, MA (1988-1991); Scientist, Polaroid Corporation (1991 to present).

ACS Service: Alternate Councilor (1994-96 and 1997 - 99).

NESACS Service: Centennial Committee, Co-chair (1998).

Statement: I have been privileged to serve the Northeastern Section of the American Chemical Society since 1990 as a result of my involvement with the Medicinal Chemistry Group. Most recently, it was an honor to be asked to co-chair, with Dorothy Phillips, the Centennial Committee during the Section's Centennial Celebration in 1998. Thanks to all who helped us in that effort.

It is my hope that I can, together with other Section Leaders, provide the necessary support and guidance to steer the Section on the right course for the next 100 years. I would appreciate your vote of confidence.

Doris I. Lewis

Education: Duke University, B.S. (1965), Tufts University, Ph.D. (1972)

Professional Experience: Suffolk University 1975-present (Chemistry Department Chair, 1995-present); Newton College of the Sacred Heart 1970-75.

ACS Service: Councilor, 1994-98; Alternate Councilor, 1991-93; Associate, ACS Council Committee on Local Section Activities, 1997; ACS National Science Funding Network 1991-present.

NESACS Service: Chair-elect, 1999; Board of Publications 1995-97; chair, 1997-8; Task Force to start up Section Web Page, 1996; National Meeting Committee 1990,1998; Student Affiliate Coordinator 1978-90; Continuing Education Committee, 1979-81

Statement: Since I already have experience as a councilor, I would like to take this opportunity to share the philosophy with which I have tried to serve this section. First, I have tried to represent our many constituencies fairly. Industrial and academic chemists, those employed or seeking employment, younger chemists or retired chemists, high

school chemistry teachers, and the chemists of the future, our student affiliates and graduate students, all should be served by the Society and considered in its policies. I have taken seriously my role in representing the many and varied members of this section while considering as well the needs of the larger organization. The councilor serves as something as a bridge between the national organization and the individual member. I have done my best in that role, and have also done what I could to make the gap between the national organization and the member less wide, for I am one of those who believe that gap to be greater than it ought to be.

I believe the local section to be potentially the most important unit of the ACS in delivering member services. As a member of the Board of Directors of the Section I have been involved in Local Section activities, and supported the efforts of the national office in that regard. The American Chemical Society is at a watershed point, as the publications functions that have served as a major source of prestige and financial support are undergoing major changes. I would be honored to be your representative in Council during this important period. I would appreciate your vote for Councilor for the Northeastern Section, and I would further ask if I am elected that you share with me your views and concerns so that I can serve you and the Section better.

Truman S. Light

*(see bio and statement under **Trustee**)*

Julia H. Miwa

Education: B.A. Chemistry, Haverford College (1985), High Honors, Phi Beta Kappa. Ph.D. Massachusetts Institute of Technology (1992).

Professional Experience: Teaneck High School: Chemistry and Physics Teacher (1985-87). University of California at Berkeley: NIH Postdoctoral Fellow (1992-94), Lecturer in Organic Chemistry (1993). Wellesley College: Assistant Professor of Chemistry (1994-present). Whitehead Institute for Biomedical Research: Visiting Scientist (1998-99).

ACS Service: Member since 1987; member of divisions ORG, CHED.

Memberships, Honors: Camille and Henry Dreyfus Foundation Faculty Startup Grant for Undergraduate Institutions (1994). Wellesley College Pinanski Prize for Excellence in Teaching (1997).

M.I.T. Chemistry Outreach Program (1990-92). Invited speaker: M.I.T. Women in Chemistry Symposium (1994). Invited speaker: M.I.T. Careers in Chemistry at Predominantly Undergraduate Institutions (1998). Invited speaker: IAAY Boston Area College Colloquium (1996-98). Wellesley (Town of) Science Education Committee.

Statement: After years of participation in local and national ACS meetings as presenter or attendee, this is my first foray into governance. The Northeastern Section comprises a large and diverse group of chemists, from industry and a wide variety of academic institutions. I would like to represent our section, and in particular the interests of young (untenured) faculty, women, and liberal arts college faculty at the ACS National

Meetings. I hope to bring enthusiasm and fresh ideas in the areas of chemical education and career services for recent Ph.D.'s. Locally, I would like to help in efforts to increase the participation in section activities by reaching out to the many new faculty members who enter our area each year. Throughout my career, I have participated in many activities designed to increase the public's understanding of and appreciation for chemistry. Fuller participation in the ACS is a natural way to further these goals, as well.

John L. Neumeyer

Education: B.S., Columbia Univ. (1952); Ph.D. in Medicinal Chemistry, Univ. of Wisconsin (1961).

Professional Experience: Research Chemist, Ethicon (Division of Johnson & Johnson) (1952-57); Sr. Research Chemist, FMC Corp., (1961-63); Staff Scientist, Arthur D. Little, Inc. (1963-69); Professor of Medicinal Chemistry and Chemistry, Northeastern Univ. (1969-91); Visiting Professor of Chemistry, University of Konstanz, Germany (1975-76); Visiting Scientist, McLean Hospital, Harvard Medical School (1985-86); Scientific Director, Chairman and Co-founder, Research Biochemicals (1980-96); Director, Medicinal Chemistry Program, McLean Hospital Alcohol and Drug Abuse Research Center, Harvard Medical School (1996-present); Visiting Professor, University of Groningen, Holland (1997).

ACS Service: Division of Medicinal Chemistry, Councilor, Executive Comm. (1971-81) Vice Chairman (1981) Chairman (1982) Councilor (1983-87); Councilor (Northeastern Section) (1988-95); Alternate Councilor (Northeastern Section) (1995-present). ACS Board of Publications (1990-93).

NESACS Service: Founder and Chairman, Medicinal Chemistry Group (1964-65); Trustee (1989-93); Board of Publications (1976-78, 1985-87), Chairman (1977, 1986)

Memberships, Honors: Board of Editors, *J. of Medicinal Chem.,* Member (1974-95); Henry A. Hill Award for Outstanding Service to the Northeastern Section (1998).

Statement: Having served the American Chemical Society in a variety of positions both nationally and locally over the past 35 years, I am very much aware of the problems and concerns of its members. If elected, I shall continue to devote my energies and experience to furthering the objectives of the Society and its members. In particular, I shall

work towards recruiting young and energetic new members to actively participate in the governance of the Northeastern Section.

Director-At-Large

(two to be elected)

David R. Haines

Education: B.A., Earlham College (1976); Ph.D., org. chemistry, Univ. of Illinois (1981) with Prof. Nelson J. Leonard.

Professional Experience: Chemistry Dept., Wellesley College: Asst. Professor (1981-1987); Assoc. Prof. (1987-present); IPA Visiting Scholar, National Cancer Institute, Bethesda, MD (1985-86) in the Laboratory of Medicinal Chemistry with Drs. John Driscoll and Victor Marquez on Neplanocin A analogs.

NESACS Service: James Flack Norris Award Committee, Chair 1991. Contributing Editor, *The NUCLEUS* (1983-85)

James A. Kaufman

Education: B.S., Tufts University (1965); Ph.D., Worcester Polytechnic Inst. (1971);

Professional Experience: Post-Doctoral Fellow, W.P.I. Chemical Engineering Department, 1971-73. Worcester Polytechnic Inst., Instructor (1966-69); Holy Cross College, Res. Assoc. (1970-71); Dow Chemical, Sr. Res. Chemist (1973-77); Curry College, Assoc. Prof. (1977-82), Professor (1982-), Director Health, Safety & Environmental Affairs (1991-93); Laboratory Safety Consultant (1980-); Founder/President The Laboratory Safety Workshop (1981-).

ACS Service: Member, Council Comm. on Chemical Safety (1979-88); Div. of Chemical Health and Safety (1975-), Editor of Div. newsletter, 1 year; Membership comm., 6 years, Chmn. (1986); Developed letter on lab safety from ACS President to college/university presidents, and on national awards for college/university lab safety programs; Organized and Chaired Several DCHAS Symposia; ACS Tour Speaker (1991-).

NESACS Service: Director-at-Large (1997-); Councilor (1982-87); Alternate Councilor (1981); Auditor (1981); Health and Safety Comm. (1978-), Chmn. (1978-91, 1996); Editor, Nucleus safety column, 2 years; Chmn., Safety Symposium for NERM-8; Safety Symposia for Mass Safety Council Annual Mtg. (1978, 1981); Moderator, Hazardous Waste Symp., Simmons College (1984); Nominating committee (1985, 1994-5); Workplace Chemicals Conference (May 1986); Helped to develop and organized Academic Lab Safety Council (1989); Participated in symposia on lecture demonstrations, home chemical safety, and lab safety; Chairman-Elect (1993; Chairman (1994); Past-Chairman (1995). Lab Safety training seminars for students (1997-).

Mary Ann Solstad

Professional Experience: Chemist/industrial hygienist. Analytical chemist who segued into the second career about 20 years ago. Currently: Health and Safety Evaluations.

ACS Service: Section Councilor and alternate ~dozen years (Northeastern Section); Past Chair of DivCHAS, where worked up through the ranks from founding of the Division.

NESACS Service: Writer of safety column for Nucleus for like period. Chair, NEACS Speaker's Bureau for 13 years.

Richards Medal Committee

(Four year term, two to be elected)

David Ray Burgess

(no statement received)

David M. Lemal

(no statement received)

Mary A. Mahaney

Education: B.A. Emmanuel College (1971); M.S. Northeastern University (1973); Dr.rer.nat. University of Constance, Germany (1977); M.B.A. Worcester Polytechnic Institute (1996)

Professional Experience: Polaroid Corporation (1982 - 1998); University of Zurich, Switzerland (1979 - 1981); University of Constance, Germany (1977 - 1979)

ACS Service: Member since 1977

NESACS Service: Continuing Education Committee (1998 -)

Vahé M. Marganian

Professional Experience: Professor and former Chair, Chemistry Department (1968-present). Sabbatical appointments in Inorganic Chemistry at the Universities of Edinburgh, Oxford, Boston College.

NESACS Service: Coordinator of Student Affiliate Chapters; hosted two NESACS monthly meetings on the Bridgewater campus.

Memberships, Honors: Awarded Fulbright Senior Lectureship for the Fall 1999 term in Environmental Chemistry, Erevan, Armenia.

Esselen Award Committee

(Four-year term, two to be elected)

Henry Brown

Education: A.B., Univ. of Michigan (1941); M.D., Univ. of Pennsylvania; Graduate work in Surgery, Univ. of Pennsylvania,

Professional Experience: Senior Medical Officer on an aircraft carrier; Nutrition Facility, Naval Research Institute, Bethesda, MD; Runyon Cancer Fellowship, University of Cambridge, England with Dr. F. Sanger, sequencing amino acids of insulin, the first protein to be sequenced. Department of Surgery at the Univ. of Wisconsin at Madison, WI for 10 years. On the surgical faculty, Harvard Medical School for the past 36 years. There, at MIT and the Shriners' Burn Institute, wrote books and numerous book chapters and peer reviewed papers on chemical and metabolic aspects of liver failure, particularly ammonium and protein chemistry and metabolism and wound healing. Presently he is in the Division of Plastic Surgery, Brigham and Womens' Hospital, teaches gross anatomy and tutors Harvard Medical School Freshmen. For 11 years had a collaborative research and student exchange program with the Dept. of Anatomy, University of Paris.

ACS Service: Long-standing member.

NESACS Service: Active meeting participant for many years.

Arno H.A. Heyn

Education: B.S., Ph.D., Univ. of Michigan (analyt. chemistry).

Professional Experience: Boston University (Instructor to Professor, 1947-84); Prof. emer. (1984); visiting scienist appointments at Brookhaven Laboratory (summers 1954-56); Eidgen. Techn. Hochschule (Zurich, 1965); Kernforschungzentrum Karlsruhe (1973, 1980, summers 1981, 1982, 1986).

ACS Service: 50-year member; Councilor (1967-1997); Elected ACS Committees: Comm. On Committees (1992-94); Council Policy Comm.. (1986-91; vice-chairman 1987-88). Council Committees: Local Section Activities (Associate, 8/1996-1997). Const. And Bylaws (1980-85; chairman 1983-85); Membership Affairs (1968-72, 1973-79; Secretary 1970-72, 1973-79). Canvassing Committee for ACS Inorg. Chemistry Award (approx. 1985)

NESACS Service: Currently: Editor of The Nucleus (7/1989-present); Const. And Bylaws Comm.; Awards Committee (chair 1996-1997); Nominating Committee several times, last: 1996; Chairman sequence (1967-69); Treasurer (1959-62); member and chairman of numerous committees in the past.

Memberships, Awards: Henry A. Hill Award for Outstanding Service to the Northeastern Section, 1986. AAAS (Fellow); Am. Assn. of Univ. Professors, member since about 1948, Treasurer of Boston Univ. Chapter (approx.1978-81).

Judith L. Koob

Education: A.B. *cum laude*, Smith College (1961); M.S. in Chemistry, Univ. of Illinois, Urbana, IL (1967)

Professional Experience: For 17 years, at Thiokol, Morton-Thiokol, now Morton International, Inc. as an analytical chemist; Research Assistant for 5 years, Univ. of Illinois under Prof. Herbert Carter until 1967.

ACS Service: Member, 1961-~1970 and 1981-present.

NESACS Service: Attended local meetings occasionally, but am interested in becoming more active in NESACS.

Memberships, Honors: Society for Applied Spectroscopy; Eastern Analytical Symposium (Board member)

I have two grown daughters, one a biochemist, the other a chemist.

Lloyd D. Taylor

Professional Experience: Thirty-five years of chemical research, retired in 1993 as Senior Research and Engineering Fellow and corporate officer at the Polaroid Corporation. Currently President of Chemsociates, Inc., a consulting firm for polymer, organic and photographic chemistry. Research interests in polymer and organic chemistry and the chemistry of instant photography; synthesis of novel polymers and monomers; temperature dependence of complex chemical systems; mass transfer with chemical reactions; critical phenomena in polymer solutions; blocking groups for the release of a reagent from a substrate, catalyzed by heat, light, alkali, or silver ion; molecular recognition and self-assembly. 103 US patents and 45 publications.

NESACS Service: Chairman sequence (1986-88).

Nominating Committee

(One-year term, two to be elected)

Kathleen S. Gallagher

Education: A.B., Syracuse Univ. (1965); M.A.(analyt. chemistry), Boston Univ. (1969).

Professional Experience: High School Chemistry teacher in Mass. (1967-77); Instrumentation Center, Univ. of New Hampshire, Manager of the NMR facility and instrumentation specialist (1978-present); Visiting Research Scientist, Laboratory of Chemistry, National Heart, Lung, and Blood Institute, Natl. Institute of Health (1985-87), investigating the conformation of several peptides in the laboratory of James A. Ferretti.

NESACS Activities: ACS Public School outreach programs

Memberships, Honors: Active in the New England Assn. of Chemistry Teachers; Sigma Xi, Iota Sigma Xi, American Women in Science, member of the Newburyport Choral Society.

Jerry P. Jasinski

Education: B.A., Chemistry, (1964); MA. M.S.T., Chemistry, University of New Hampshire, Durham, N.H., M.N.S., Natural Science, Worcester Polytechnic Institute, Worcester, MA(1968); Ph.D.,Chemistry, University of Wyoming, Laramie, Wyoming.(Smith L. Holt) (1974).

Professional Experience: Teacher, Chemistry/Physics, Secondary schools in New York, New Hampshire, Vermont (1964-70); Summer Visiting NATO Research Fellow, University of Copenhagen (Prof. Carl Ballhausen) (1972); AWU Research Fellow, Los Alamos Scientific Laboratory (1973); Post-Doctoral Research Associate, Univ. of Virginia (Paul N. Schatz, 1974); Teacher, Chemistry/Physics, Springfield High School, Springfield, VT (1975-78); Keene State College, Keene, NH: Asst. Prof (Chemistry) (1978-83); Assoc. Prof. (1983-89); Professor (1989-present). Author and co-author of 66 research papers, many with undergraduate co-authors; Director of the New England Molecular Structure Center in the Chemistry Dept., Keene State College (1990-present)

Memberships, Honors: American Institute of Chemists; New England Institute of Chemists: Treasurer, (1988-present); Board of Directors, AIC (1999-); American Crystallographic Soc.; Council for Undergrad. Research; New England Assoc. of Chemistry Teachers.

Cynthia B. McGowan

(no statement received)

Marilyn B. Turnbull

Education: BA Wellesley College (1969);
MS, University of California at Berkeley (1970).

Professional Experience: Sr. Instructor in Chemistry Laboratory, Wellesley College (1980-present); Sr. Research Chemist, Dow Chemical Co. (1972-1980).

Currently reside in Wayland with husband and three children. ◇

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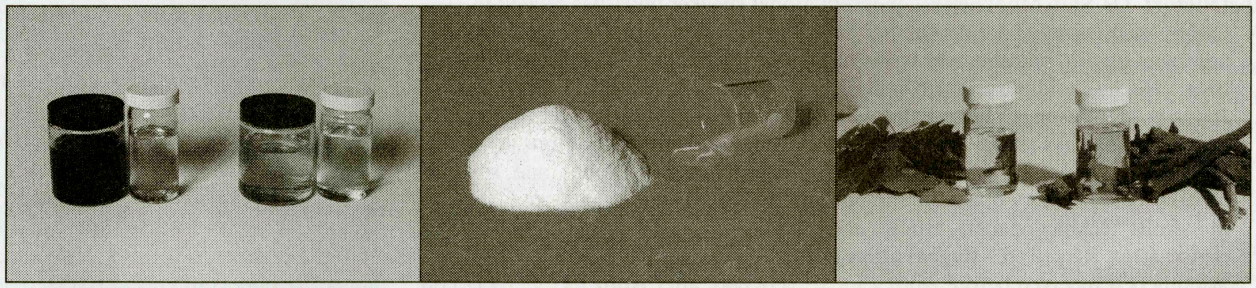

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ACS SHORT COURSE

Methods Development, Validation Procedures, and Conformity Assessment in the Analytical Laboratory

A Two-Day Short Course Sponsored by the Northeastern Section, ACS, Committee on Continuing Education

Save more than $500 over the registration fee charged for this course when it is offered at ACS National Meetings.

National ACS is making top-rated ACS Short Courses available to local sections at tuition fees greatly reduced from the normal $845. The NESACS Committee on Continuing Education is pleased to present this freshly updated course.

DATES and TIME: Monday, May 10, 1999, 8:00 a.m. - 5:30 p.m.
and Tuesday, May 11, 1999, 8:30 a.m. - 5:30 p.m.

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

PROGRAM AGENDA: **Fundamental**: Quality, Quality Control, and Quality Assurance

Method Validation: Guidelines Derived from GLP, AOAC, ISO 9000, and ICH

Method Development and Optimization by Example and Case Histories: How to systematically develop and optimize an assay for a trace component in a very complex sample matrix

Method Development and Optimization in HPLC as an Example of Current Analytical Technique: Aspects of HPLC that need to be developed and optimized - and how; Peak purity, spectral match, peak tailing, and other considerations in HPLC

Methods Optimization Considerations in Spectroscopic (UV-VIS, AA) and Classical Techniques

Statistical Treatment of Analytical Data - Mean, Mode, Standard Deviation, Control Charts, etc.

Statistical Process Control (SPC) Applications for Process Improvement and Process Optimization

International Harmonization Efforts and Their Relevance to Current Analytical Issues and Trends

Instructor: Dr. Shib Mookherjea, an international speaker on issues related to quality assurance and validation, has extensive experience in R&D, quality assurance, and quality management in major pharmaceutical and chemical industries. He has held positions in analytical research, QA, and R&D support at Johnson & Johnson, Colgate-Palmolive, and BASF Corporation over the past 25 years. He also has several years of experience in academic institutions and government agencies. He has participated in numerous task forces and subcommittees on laboratory quality assurance and ISO 9000 and has authored numerous technical papers, articles and reports.

Pre-registration Required - Registration Fees:

ACS Members if received before April 23 .....$325.00; after April 23 .....$375.00
non-ACS Members if received before April 23 .....$425.00; after April 23 .....$475.00

There will be a limited number of scholarships for unemployed ACS Members on a space-available basis.

Parking Fee $6.00/day **University cafeterias will be available for lunches.**

For further information contact: Prof. Alfred Viola - (617) 373 2809

Registration form for Short Course: Methods Development, Validation Procedures, and Conformity Assessment in the Analytical Laboratory

Name: _____ Affiliation: _____

Mailing _____ Telephone: _____

Address _____

Mail with remittance to :
(Please make checks payable to NESACS)

Prof. Alfred Viola, Chair
NESACS Committee on Cont. Ed.
Department of Chemistry
Northeastern University
Boston, MA 02115

Medicinal Chemistry Group

Symposium on Kinase Inhibitors

Thursday, May 6, 1999

Massachusetts Institute of Technology, Faculty Club
50 Memorial Drive, Cambridge

3:30 Coffee

4:00 Dr. Tom Sawyer, Director of Drug Discovery, Ariad Pharmaceuticals, Cambridge, MA. : *TBA*

5:00 Dr. Joseph Nunes, Medicinal Chemistry, Kinetix Pharmaceuticals, Inc., Medford, MA: *"Kinase Array Assay Screening for Lead Discovery and Optimization"*

6:00 Social Hour (Wine, Cheese)

6:30 Dinner

7:30 Dr. Cho Tang, Senior Director of Chemistry, Sugen, Inc., San Francisco, CA: *"Synthesis of Selective Kinase Inhibitors"*

Dinner reservations should be made no later than Monday, May 3, 1999, noon. Please call or fax Marilou Cashman at 800-872-2054 (voice or fax). Reservations not canceled at least 24 hours in advance must be paid. Members: $20.00, Non-members: $25.00; Students: $10.00

APRIL PUZZLE SOLUTION

1 P	2 A	S	3 S	4 E	5 R	6 I	7 N	8 I	
9 A	R		10 E	N	A	M	I	N	11 E
12 S	Y	N		13 E	N		T		N
14 T	N				15 E	A	R		V
16 E	E	17 L			Y		18 E	19 N	E
U		20 D	21 E	22 F		23 E	N	O	L
R		24 A	N	T	I		E		O
	25 R		D			26 A		27 S	P
28 A	U	X	O	C	H	R	O	M	E

Book Review

The Molecular Modeling Workbook for ORGANIC CHEMISTRY, by Warren J. Hehre, Alan J. Shusterman, and Janet E. Nelson; Wavefunction. Inc., 1998, 307 pp, $29.95 softcover: ISBN 1-390661-06-6

Reviewed by Marietta H. Schwartz, Department of Chemistry, University of Massachusetts Boston

The use of molecular modeling in the chemistry curriculum. particularly in the undergraduate organic chemistry sequence has become more and more prevalent over the past few years. A number of manuals/handbooks/workbooks have been published which tend to be, understandably, program-specific and, in one case at least, textbook-specific, as well. The prices for these books range from $8 to $30, and all contain an amount of information and exercises that correlates fairly well with the thickness of the book. Two examples are: (a) *Molecular Modeling Using ChemOffice Ltd*, bv David M. Collard and Howard M. Deutsch; Jones & Bartlett Publishers, 1998, 56 pp., softcover; and (b) *Using ChemOffice with Brown: Organic Chemistrv*, bv L. Kraig Steffen; Saunders College Publishing, 1996, 110pp., softcover.

One of the more detailed and problem-oriented texts, and, not surprisingly, one of the more expensive ones, is *The Molecular Modeling Workbook*, published by Wavefunction, Inc., makers of the Spartan™ family of molecular modeling software, including PC Spartan and MacSpartan, among others; see their web site at http:// www. wavefun.com for more information on software products.

One major selling point is the fact that the software is included. It runs on a PC or a Mac, I ran the program on a PC using Win98 with no difficulty. There are plenty of exercises in the workbook, spanning a wide range of difficulties, as well as a series of introductory, essays that are very informative.

The software isn't Spartan itself, which retails for an academic price of between $300 and $700 depending on the version desired. Instead, it's something called SpartanView, which is essentially an extremely, pared-down version of Spartan with the creative end excised. The students work with pre-drawn structures and cannot do much in the way of exploring "outside the box". It is possible to create additional exercises for the students, and instructions for doing this are included in the book, but this requires the instructor to have access to a fully operational version of Spartan.

After skimming the table of contents and reading the introductory essays *To the Student* and *To the Teacher*, the next thing the user encounters is *How to Use SpartanView*, a tutorial that puts the program through its paces. Here we run into problem #1: starting the program!

While more and more of our students are increasingly computer literate, in my opinion a good software program should never assume anything beyond basic ability with a mouse and understanding of the commonly used computer terms such as "click", "double-click", and "click and drag". *How to Use SpartanView* leaps right into a discussion of the various menus, beginning with the File menu, without ever mentioning how to start the program. One needs to start *Wfview.exe* (it came up as *SpartanView* on a Mac) on the CD by whatever method is most convenient. Once you get past that hurdle, the rest of the tutorial goes by without incident and does indeed provide a thorough exploration of the capabilities of *SpartanView*, beginning with the basics: selecting, rotating, and translating molecules, and proceeding to more complex features such as phase-transfer catalysis and magnetic anisotropy. One of my favorites is the ability to show predicted vibrational frequencies — the on-screen molecule will even vibrate of otherwise waggle about the appropriate bonds when a specific frequency is chosen, which could be very useful in illustrating the concept of molecular vibrations. A variety of surface displays including HOMO, LUMO, and electrostatic potential maps are also present. Not every surface is available for every molecule, but the displays are very informative.

A nifty feature is the ability of the program to show structures in true 3D by the use of red and blue stereo glasses which are provided with the workbook.

After the tutorial comes a series of essays on how to use the program to solve problems. These essays *How to Use Energies to Calculate Thermodynamic and Kinetic Data, Molecular Orbitals; Quantum Mechanics in Pictures*; *Electron Densities and the Sizes and Shapes of Molecules*; and *Electrostatic Potential Maps and Molecular Charge Distributions* are well-written summaries that do a good job of explaining how to interpret the various pieces of information that SpartanView provides.

The final section, and, indeed, the bulk of the book, consists of the exercises themselves. There are 21 chapters, beginning with Lewis structures and resonance theory and working through various functional groups, electrophilic and nucleophilic aromatic substitution, free radicals, polymers, and spectroscopy, to name a few of the topics covered. There are more than 200 problems spread out over these 21 chapters, giving students a wealth of opportunity for learning. The solutions are not given in the workbook, but are instead available an a separate CD-ROM. Each exercise is contained on one page, and includes background material, experimental observations, and a list of questions to be answered. For instance, one problem is entitled, *Resonance Structures. The Sum of the Parts*. A short paragraph on resonance is presented, and then the student is asked to look at benzene, ethane, and

continued on page20

Book Review

continued from page 19

ethylene, measure the carbon-carbon bond distances in all three, and then compare the results. The question is presented: are the six bonds in benzene all the same distance, or are they different? And how do they compare to the bonds in ethane and ethylene? A second analysis, using the formate anion, formaldehyde, and methanol looks at carbon-oxygen bonds. These two examples do a good job of illustrating the case where two or more resonance structures are equivalent. The carbon-oxygen bond case is then extended to the phenoxide ion, which has non-equivalent resonance structures, and finally, another set of molecules is used to illustrate resonance involving nitrogen-nitrogen bonds.

The computer is not the only tool used in this workbook. In many of the problems the student is asked to draw pictures on his/her own. For instance, in the problem discussed above, the student draws the various resonance contributors and decides whether or not they are equivalent. Many of the questions posed in the problems require more than a simple numerical answer, such as a bond length or energy; instead, the student must interpret the data (as described in the introductory essays) in order to answer the question. Looking at an intermediate-level question, *Steric Control of Ring Conformation I*, which compares axial and equatorial methyl groups in chair cyclohexane, students not only obtain the energies of the two conformations, but must then identify the preferred conformer and say something about the differences in the two energies and the possible causes of those differences.

At the more difficult end of the spectrum, modeling is used to probe the McLafferty Rearrangement in mass spectrometry and to look at, substituent effects on ^{13}C NMR chemical shifts. These sorts of problems really bring home the electronic basis for many spectroscopic effects and make it easier to understand why molecules

Book Review

continued from page 20

behave the way they do.

To summarize, this workbook is jam-packed with material. There is something for every student, from the very beginnings of organic chemistry, (e.g., Lewis structures, resonance delocalization) to an analysis of the effects of conformation on the rate of a Diels-Alder reaction, complete with a plot of energy versus dihedral angle. The requirement of one page per problem makes the background material necessarily sketchy in places. However, the book is not intended as a stand-alone organic text, but rather as a valuable tool for understanding the electronic nature of organic chemistry and the importance of structure, stability, and reactivity. The authors succeed admirably in their presentation. ◇

Council Report

continued from page 7

tion and in that capacity attended a Task Force meeting in Washington in February. Michael Hearn attended the Committee on Public Policy, Arno Heyn (as guest) attended the C&B meetings. Dorothy Phillips attended the Membership Affairs Committee meeting and, as liaison, the Divisional Activities Committee. Don Rickter attended activities having to do with Chemistry information, OLGA, and Minority Affairs. As Chair of the Section, he presented the ACS Norris Award in Physical Organic Chemistry, which is sponsored by NESACS, to Barry Carpenter at the Awards Meeting, which the NESACS representatives attended in honor of the award recipients. Don Rickter also attended Robert Langer's address at the meeting in honor of his receiving the ACS Award in Polymer Chemistry. (Langer was our speaker at the February monthly NESACS meeting, and was the award recipient of the Gustavus J. Esselen Award at our April 8, 1999 meeting.)

Reported by A. Heyn ◇

Puzzle Column

From the Puzzle Editor: Most scientists love a puzzle. In addition to the monthly crossword puzzle that appears in The Nucleus, I will be presenting, on a semi-regular basis, puzzles that I have come across that I think will appeal to the readers of The Nucleus.

Joe Billo

ANAGRAMS

I received the following exceptionally clever anagrams by means of the Internet. Someone out there either has 'way too much time to waste or is deadly at Scrabble. The last one is too perfect to believe.

Each phrase can be rearranged (with no letters left over, and using each letter only once) into a word or phrase that is its "definition".

Dirty room

A rope ends it

Here come dots

Cash lost in 'em

Is no amity

Large picture halls, I bet

I'm a dot in place

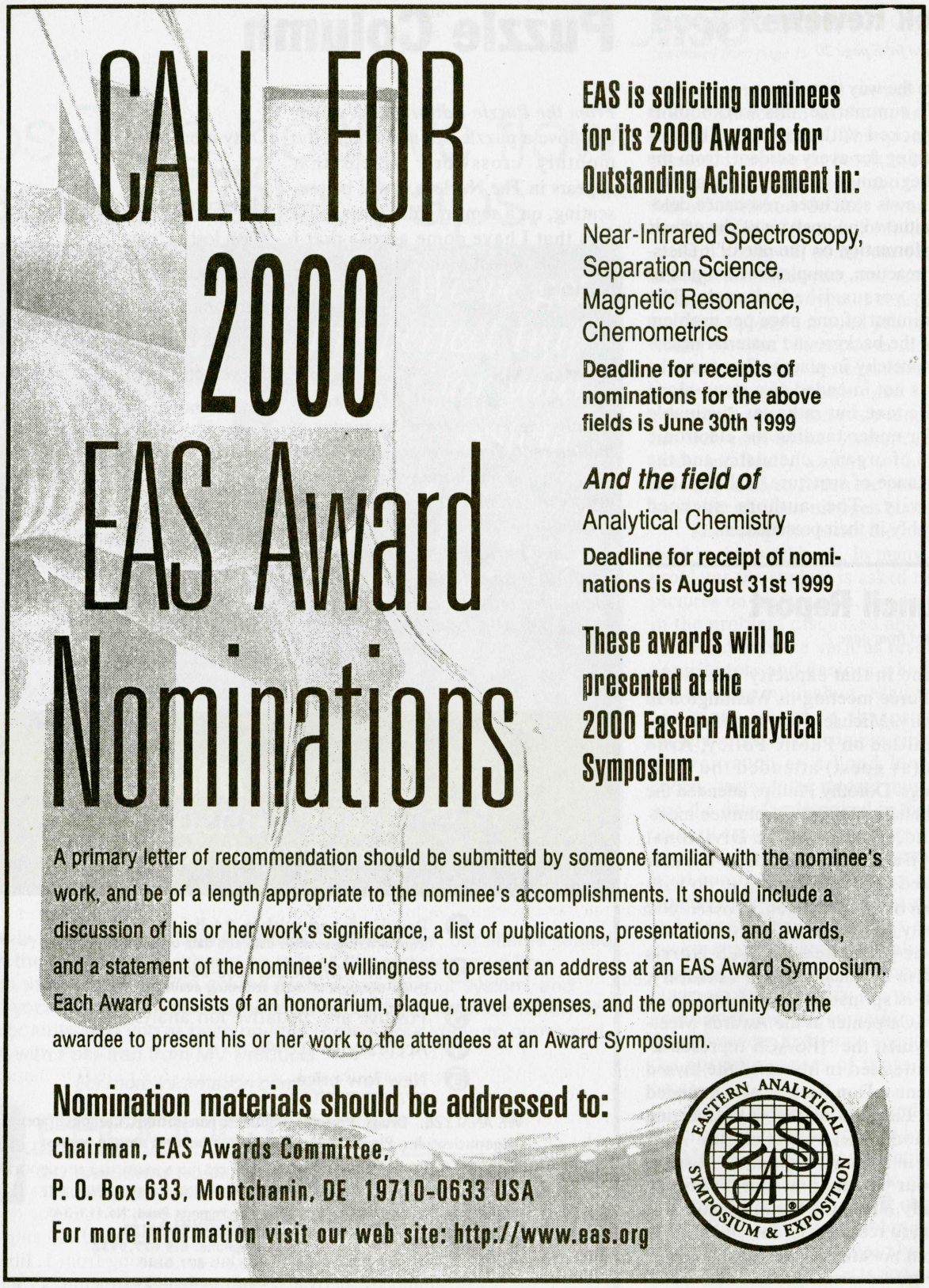
Eleven plus two

Accord not in it

And the grand finale:

In one of the Bard's best-thought-of tragedies, our insistent hero, Hamlet, queries on two fronts about how life turns rotten.

Answers next issue.



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A primary letter of recommendation should be submitted by someone familiar with the nominee's work, and be of a length appropriate to the nominee's accomplishments. It should include a discussion of his or her work's significance, a list of publications, presentations, and awards, and a statement of the nominee's willingness to present an address at an EAS Award Symposium. Each Award consists of an honorarium, plaque, travel expenses, and the opportunity for the awardee to present his or her work to the attendees at an Award Symposium.

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Summer Scholar Report

Sythesis and Selection of Aminoacyl- and Dipeptidyl-Tetraphenylporphyrins: Toward Target-Specific Nucleic-Acid Ligands

By Matthew D. Simon* and Clemens Richert
Tufts University, November 1998

Abstract: Small combinatorial libraries of p-substituted tetraphenylporphyrins were prepared in solution-phase couplings between *N*α-Boc-amino acid building blocks and 5,10,15,20-tetrakis(*p*-aminophenyl)porphyrin. *In vitro* selection assays were established, in which the depletion of those porphyrins that bind to DNA on controlled pore glass is detected in MALDI-TOF mass spectra of the incubation medium. A UV-vis titration of 5,10,15,20-tetrakis (*L*-arginyl-*L*- aspartylaminophenyl)-porphyrin with the loop-forming oligonucleotide 5'-(GCGAAGC-3' yielded an apparent dissociation constant of ≤ 3 nM.

Introduction: Porphyrins are 18π-macrocycles with important biological functions, such as light harvesting, oxygen transport, and catalysis. They are also large, lipophilic scaffolds with a chromophore that allows facile and sensitive detection of binding events. Tetraphenyl- and tetrapyridylporphyrins are readily prepared and a number of their derivatives have been shown to bind to nucleic acids.[1] The size and lipophilicity of the tetraphenylporphyrin scaffolds suggests that it may be particularly suitable for binding larger hydrophobic patches of folded nucleic acid structures. This was recently confirmed for G-tetrades, potential targets for telomerase inhibition.[2] We became interested in exploring the binding of tetraphenylporphyrins to loop and bulge structures. These contain a cleft with exposed nucleobases and occur frequently in folded DNA and RNA, including the genome of the HIV virus. In order to study interactions on a broad structural basis, we decided to develop a combinatorial synthesis of aminoacyl and peptidyl substituted tetraphenylporphyrin libraries and a methodology for subjecting these libraries to spectrometrically monitored selection experiments (SMOSE).[3]

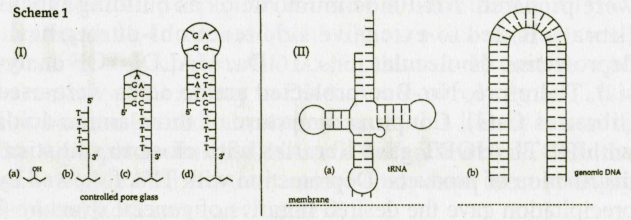
Results and Discussion: The first binding experiments were performed with a library of lipophilic tetraphenylporphyrins (**A**, Table 1), whose synthesis has recently been established in these laboratories.[4] This was formulated in DOPC liposomes,[3] and partitioning from the membrane phase to presumed lipophilic sites of two DNA loops was assayed. For this, three oligonucleotides[5] permanently attached to controlled pore glass (CPG) were synthesized (**I** in Scheme 1), using a modification [6] of the procedure reported by Southern and collaborators.[7] Even after incubating library **A** for 24 h, no binding to any of the DNA-bearing glass beads was observed.

This prompted us to explore tetraphenylporphyrins with more polar substituents. For this, a synthesis of small chemical libraries of derivatives of tetrakis(*p*-aminophenyl)porphyrin (**1**) was established (Scheme 2). Porphyrin synthesis started from pyrrole and *p*-nitrobenzaldehyde, whose Rothemund cyclization, followed by air oxidation and Sn(II) reduction was performed under literature conditions.[8] Tetraaminoporphyrin **1** was then coupled to a mixture of two aromatic carboxylic acids, one a quinolone antibiotic with known DNA-binding potential (oxolinic acid), and the other a methoxybenzofuran derivative. A mixture of coupling agents commonly employed in peptide synthesis (HBTU. HOB T) proved efficient enough to acylate the aromatic amines of **1**. According to MALDI-TOF mass spectra, the resulting library of *p*-substituted tetraphenylporphyrins was biased towards the furan-substituted components and had unexpected properties, in that it did not get efficiently incorporated in DOPC liposomes, and the incorporated portion did not bind to immobilized oligonucleotides **Ib-Id.**

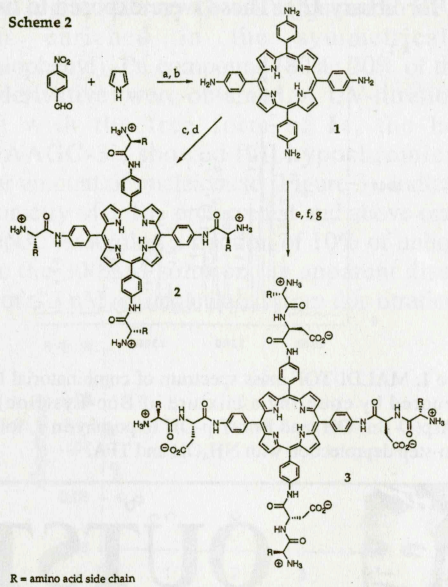
Extension of the substituent pool to amino acids yielded ionic compounds with a greater likelihood of being soluble without liposome formulation. Starting from **1**, libraries of aminoacyl-derivatives of the general structure **2** (Scheme 2)

continued on page 24

Scheme 1



Scheme 2



R = amino acid side chain

Reagents: (a) AcOH, Ac_2O; (b) $SnCl_2$, HCl; (c) Boc-Aa-OH, HBTU, HOBT, Hünig's base; (d) TFA; (e) Boc-Asp(OBn)-OH, HBTU, HOBT, Hünig's base; (f) NH_4OH; (g) TFA. Aa = amino acid residue

* 1998 Norris/Richards Summer Scholar

Summer Scholar Report

continued from page 23

were prepared. *N*α-Fmoc-amino acids as building blocks (library **B**) led to extensive side reactions during basic deprotection (molecular ions -16 Da, MALDI-TOF analysis). Therefore, Nα-Boc-protected amino acids were used (libraries **C-G**). Coupling a mixture of three amino acids with HBTU/HOBT gave libraries with close to statistical distribution of products. Deprotection with TFA followed by precipitation gave the desired libraries of general structure **2** (Figure 1 for library **C**). These were exposed to two different nucleic acid targets in solution: a mixture of commercially available tRNAs and genomic double-stranded DNA from calf thymus. After incubation, the unbound porphyrin species were assayed by subjecting the mixture to spin-filtration with membranes (**II**, Scheme 1). Initially, anion-exchange membranes were used that retain the nucleic acids but bind the cationic porphyrins to a lesser extent than other membranes. While binding was detected, MALDI-spectra of the filtrates showed essentially unchanged porphyrin distributions for a tryptophan/lysine/aspartic acid library exposed to the loop-containing tRNAs or the genomic DNA. This was attributed to a competition between the cationic exchange membrane and the cationic porphyrins, in which the cooperativity expected for resins prevented the desired selection. A number of non-ionic membranes were therefore screened, but in all cases unspecific binding of the porphyrin species to those membranes was observed.

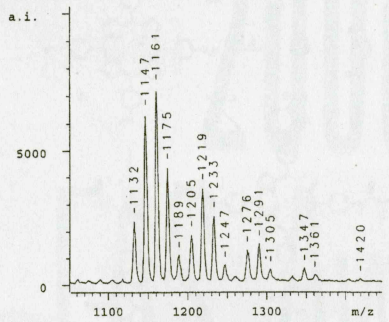


Figure 1. MALDI-TOF mass spectrum of combinatorial library **C** prepared by coupling a mixture of Boc-Lys(Boc)-OH, Boc-Asp(*O*-Bn)-OH, and Boc-Trp-OH to porphyrin **1**, followed by two-step deprotection with NH_4OH and TFA.

Tetrakis(dipeptidylaminophenyl)porphyrins of general structure **3** (Scheme 2) were prepared next. These contain aspartic acid residues as the proximal substituents and different residues as the distal substituents and can therefore be expected to be more soluble in water and less prone to show unspecific adsorption on anionic and hydrophobic surfaces. This required synthesis of **2**, where R is the benzyl ester of the aspartic acid side chain, its coupling to Boc-protected amino acids and a two-step deprotection. The first deprotec-

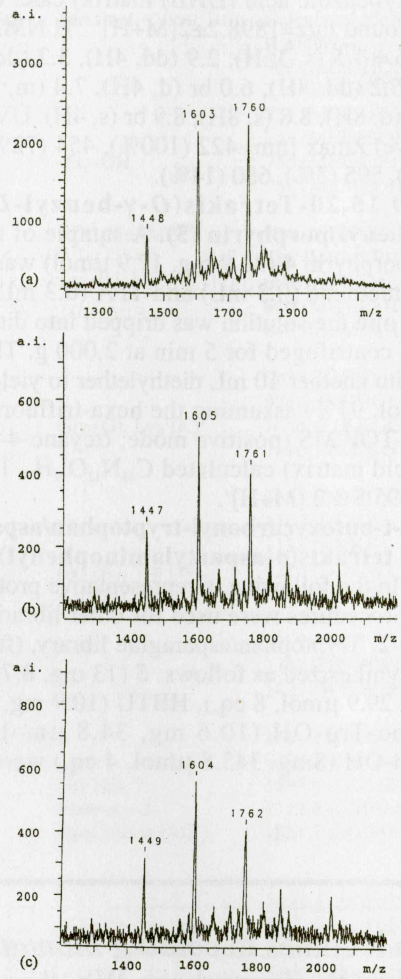


Figure 2. MALDI-TOF mass spectra of solutions of arginyl-library **G** incubated with: (a) DNA-free CPG **Ia**, (b) CPG bearing dodecamer GCGAAGCTTTTT **Ic**, and (c) CPG bearing the nonadecamer CTAGCGGAGGCTAGTTTTT **Id**. Note that the highest molecular weight component, the tetraarginyl porphyrin, is depleted from the solution in (b) and (c). Spectra were acquired under conditions previously shown to allow quantitative detection of porphyrin acids.[3]

tion step was hydrolysis of the benzyl esters with saturated aqueous ammonia (ammonium hydroxide), and the second removal of the N-terminal Boc groups with TFA. Performing the Boc-deprotection last was convenient, as it gives only volatile protecting group fragments (isobutene and CO_2). Crude libraries of satisfactory composition were obtained with this procedure, according to MALDI-TOF mass spectra.

Four libraries of general structure **3** with two different distal substituents were prepared (Table 1). Libraries with glycine/7-methoxy-2-benzofuran carboxylic acid (**D**) and tryptophan/asparagine substituents (**F**) were poorly soluble in buffered aqueous media. A mixture of tryptophanyl and aspartic acid residues (library **E**) gave more soluble material, which also bound to tRNA and genomic DNA, albeit with little selectivity between the individual components. A small library generated by partial derivatization of **2** with arginine substituents (**G**) gave more gratifying results, in that the total porphyrin binding to immobilized DNA sequences **Ia-Id** differed, with almost twice as much total porphyrin on cpg for **Id** (95 %) than on **Ib** and **Ic**, and essentially no binding to DNA-free control cpg **Ia** (1%). Further, the individual components of this library bound to the solid-phase-linked DNA to a different extent, with the most highly charged tetraarginyl compound most strongly depleted from solution (Figure 2).

When arginyl-library **G** was subjected to RP_{18} HPLC, fractions enriched in the symmetrical (Arg-Asp-aminophenyl)$_4$-Pn compound (80%; 20% of the trisubstituted derivative) were obtained. A UV-titration of this material with the free form of **Ic**, the heptamer 5'-GCGAAGC-3', showed full hypochromicity at an equimolar amount of nucleic acid (Figure 3), indicating that a stoichiometry of 1:1 is preferred at and above one equivalent of DNA. Assuming a fraction of 10% of unbound porphyrin in the 200 nM solution, an apparent dissociation constant of ≤ 3 nM was calculated from this titration.[9]

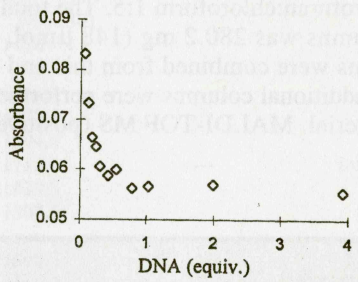


Figure 3. Results of a UV-vis titration experiment with 5,10,15,20-tetrakis(*L*-arginyl-*L*- aspartylaminophenyl)porphyrin, the highest affinity compound found in the assays documented in Figure 2, and DNA heptamer GCGAAGC. UV absorbance at 441 nm was monitored in 150 mM NH_4OAc solution, pH 6.0 with 2% DMSO.

In conclusion, these results show that small chemical libraries of peptidyl-tetraphenylporphyrins can be prepared and subjected to mass spectrometrically monitored selections for DNA-binding. A number of technological difficulties, as well as solubility phenomena were observed that are reminiscent of effects typically observed with misfolded polypeptides, highlighting the increasing protein-like properties of these molecular hybrids. As expected based on electrostatic considerations, cationic porphyrins bind more tightly than their strongly lipophilic, net-neutral or anionic counterparts. Combining cationic arginyl- with anionic aspartyl-residues (that are more typical for non-nucleic acid binding porphyrin cofactors) does not appear to override the attraction between the guanidinium-bearing moieties and the DNA.

Experimental Part:

5,10,15,20-Tetrakis(*Nα-t*-butyloxycarbonyl-*O* γ-benzyl-*L*-aspartylaminophenyl)porphyrin (4).

continued on page 26

Summer Scholar Report

continued from page 25

Tetrakis(*p*-aminotetraphenyl)porphyrin **1** (200 mg, 296 μmol) was combined with *N*Boc-*L*-Asp(*O*-Bn)-OH (766 mg, 2.37 mmol, 8 eq.), hydroxybenzotriazole (HOBt) (363 mg, 2.37 mmol, 8 eq.) and 2-(1H-benzotriazole 1-yl)-1,1,3,3,-tetramethyluronium hexafluorophosphate (HBTU) (899 mg, 2.37 mmol, 8 eq.). The powder was dried for 1.5 h at 0.1 torr. DMF (7.5 mL) was added, creating a dark red solution, to which ethyl diisopropylamine (0.81 mL) was added. The reaction was allowed to proceed for 1 h before quenching with acetic acid (50 μL). The reaction solution was transferred to a separatory funnel using ethyl acetate (50 mL). The organic phase was washed three times with a total of 250 mL of water and dried using rotary evaporation before being precipitated with hexane. The precipitated material was purified on a silica column using chloroform:ethyl acetate 3:1 with 0.5% water. The pure fractions were combined, dried and reprecipitated from chloroform/hexane to yield 140 mg of **4**. The impure fractions were combined and purified on another silica column using tetrahydrofuran:chloroform 1:5. The total yield from these two columns was 280.2 mg (148 μmol, 50%). The impure fractions were combined from this and subsequent reactions and additional columns were performed to isolate more pure material. MALDI-TOF MS (positive mode; 2,5 dihydroxybenzoic acid (DHB) matrix) calc. $C_{108}N_{12}O_{20}H_{110}$ 1897.1, found m/z=1898.2±2[M+H]$^+$. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 1.5 (s, 36H), 2.9 (dd, 4H), 3.2 (dd, 4H), 4.8 br (s, 4H), 5.2 (dd, 8H), 6.0 br (d, 4H), 7.4 (m, 20H), 7.9 (d, 8H), 8.2 (d, 8H), 8.8 (s, 8H), 8.9 br (s, 4H). UV-vis (CH_2CI_2, qualitative) λmax [nm] 422 (100%), 454 (72%), 517 (6%), 554 (4%), 595 (3%), 680 (14%).

5,10,15,20-Tetrakis(*O*-γ-benzyl-*L*-aspartylaminophenyl)porphyrin (5). A sample of the protected aspartylporphyrin **4** (33.9 mg, 17.9 μmol) was dissolved in dichloromethane (0.3 mL) and TFA (0.3 mL) was added. After 20 min the solution was dripped into diethylether (10 mL) and centrifuged for 5 min at 2,000 g. The pellet was rinsed with another 10 mL diethylether to yield **5** (37.7 mg, 17.3 μmol, 97%) assuming the hexa-trifluoroacetate salt. MALDI-TOF MS (positive mode; αcyano-4- hydroxycinnamic acid matrix) calculated $C_{88}N_{12}O_{12}H_{78}$ 1495.7, found m/z = 1495.5 ± 2 [M+H]$^+$.

***N* α-t-butoxycarbonyl-tryptophan/asparagine-substituted tetrakis(*p*-aspartylaminophenyl)- porphyrin library**. In the following, a representative protocol is given. Similar procedures were used for other libraries of general structure **2**. Tryptophan/asparagine library, (fully protected **F**) was synthesized as follows: **5** (13 mg, 8.7μmol), HOBt (4.4 mg, 29.9 μmol, 8 eq.), HBTU (10.9 mg, 28.9 μmol, 8 eq.), Boc-Trp-OH (10.6 mg, 34.8 μmol, 4 eq.) and Boc-Asn-OH (8mg, 343.8 μmol, 4 eq.) were dried at 0.1

Table I

Library	Scaffold	Terminal	Calculated Masses Residue(s)	Observed m/z $[M+H]^+$	Selection Assay	Binding
			702 (EtEtOHOH)	703.9		
			714 (EtEtEtOH)	716.0		
			731 (MEEtOHOH)	734.3		
			744 (MEEtEtOH)	746.6		
A	TPP[a]	-Et, -OH	756 (MEEtEtEt)	758.5	**I (a-d)**	None
			762 (MEMEOHOH)	764.4	Liposomes	Observed
		-CO_2Me (ME)[b]	774 (MEMEEtOH)	776.4		
			786 (MEMEEtEt)	788.5		
			804(MEMEMEOH)	806.4		
			816 (MEMEMEEt)	818.5		
			846 (MEMEMEME)	848.5		
			903 (GGGG)	888.5, 903.6		Strong Binding to
			974.1 (KGGG)	959.6, 974.6		All CPG,
B	**1**	Gly (G), Lys (K)	1045..2 (KKGG) 1	030.7, 1045.7	**I (a-d)**	including
			1116.1 (KKKG)	1116.9		**Ia**
			1135 (DDDD), 1148 (DDDK)	1132, 1147		
			1162 (DDKK), 1175 (DKKK)	1161, 1175		Binding,
			1188 (KKKK), 1205 (DDDW)	1189, 1205		
C	**1**	Lys (K), Trp (W),	1220 (DDKW), 1232 (DKKW)	1219, 1233	**II (a)**	No
		Asp (D)	1248 (KKKW), 1278 (DDWW)	1247, 1276		Selectivity
			1290 (DKWW), 1303 (KKWW)	1291, 1305		
			1348 (DWWW), 1362 (KWWW)	1347, 1361		
			1421 (WWWW)	1420		
			1363.3 (GGGG)	1361.4		
			1480.4 (GGGMB)	1478.4		
		Gly (G), 7-	1595.5 (GGMBMB)	1594.4		
D	**2**	Methoxy-2-	1714.6 (GMBMBMB)	1712.6	—	Insoluble
		Benzofuran (MB)	1831.7 (MBMBMBMB)	1829.8		
				1307.5		
			1595.5 (DDDD)	1590.3		Binding,
E	**2**	Asp (D), Trp (W)	1660.6 (DDDW)	1661.2	**II (b)**	No
			1737.7 (DDWW)	1733.1		Selectivity
			1808.9 (DWWW)	1805.0		
			1587.5 (NNNN)	1588.5		
			1660.6 (NNNW)	1660.7		Low
F	**2**	Asn (N), Trp (W)	1733.7 (NNWW)	1732.9		Solubility
			1806.8 (NWWW)	1788.7, 1806.0 —		
			1879.9 (WWWW)	1860.7, 1876.9		
			1447.5 (RR) 1448.0 See			
G	**2**	Arg (R), -H	1603.7 (RRR)	1604.6	**I (a-d)**	Figures 2/3
			1759.9 (RRRR)	1760.2		

(a) *p*-substituted 5,10,15,20-tetraphenylporphyrin. (b) see ref. 4 for preparation of lipophilic porphyrin libraries.

torr for 1 h. DMF was added until complete dissolution (250 µL), and then ethyl diisopropylamine (24 µL, 139.2 µmol, 16 eq.) was added. The reaction was allowed to proceed for 1 h. Dichloromethane (30 mL) was added and the solution was washed with deionized water (60 mL), then a saturated sodium bicarbonate solution (60 mL) and finally a saturated sodium chloride solution (60 mL), followed by rotary evaporation. The dry material was dissolved in dichloromethane (2 mL) and precipitated with hexane (5 mL). The precipitate was washed with water (10 mL) and diethylether (5 mL). For MALDI-TOF analysis, 0. 1 mg of the crude library was dissolved in tetrahydrofuran (100 µL). Dowex 50W cation exchange beads (1 mg, ammonium form) were added. The solution (1 µL) was applied to a MALDI-TOF target, along with a 1 µL aliquot of acetonitrile saturated with DHB. Calc. for $(Boc\text{-}Asn)_4$-**2** $C_{124}N_{20}O_{28}H_{130}$ 2349.5 found 2353.0 $[M+H]^+$, calc. for $(BocAsn)_3/(Boc\text{-}Trp)_2$-**2** $C_{131}N_{20}O_{27}H_{136}$ 2423.6 found 2424.1 $[M+H]^+$, calc. for $(Boc\text{-}Asn)_2/(Boc\text{-}Trp)_2$-**2** $C_{138}N_{20}O_{26}H_{141}$ 2496.8 found 2496.3 $[M+H]^+$, calc. for $(Boc\text{-}Asn)/(Boc\text{-}Trp)_3$-**2** $C_{145}N_{20}O_{25}H_{146}$ 2569.9 found 2568.5

continued on page28

Summer Scholar

continued from page 27

$[M+H]^+$, calc. for $(Boc\text{-}Trp)_4$-**2** $C_{152}N_{20}O_{24}H_{151}$ 2643.0, found 2639.8 $[M+H]^+$.

***N* α-*t*-butoxycarbonyl-tryptophan/asparagine-substituted tetrakis(*p*-aspartylaminophenyl) -porphyrin library.** 5 mg of the protected library described above were dissolved in tetrahydrofuran (200μL) and concentrated ammonia (0.5 mL) was added, leading to two phases. Methanol (50 μL) was added until one phase was formed. The solution was heated to 40° C for 30 min. The volatile components were evaporated using a gentle stream of argon. The remaining material was dried at 0.2 torr over night.

Tryptophan/asparagine-substituted-tetrakis(*p*-aspartylaminophenyl) -porphyrin library (F).

The *N*-Boc protected library was dissolved in trifluoroacetic acid (0.5 mL) and allowed to react for 15 min before being dripped into diethylether (10 mL). The light green precipitate was centrifuged at 2,000 g for 5 min, and the resulting pellet was washed with another 10 mL of diethylether. MALDI-TOF analysis of this library used a 30% acetonitrile/water solution containing 0.1% TFA and α-cyano-4hydroxy-cinnamic acid as matrix. Calc. for $(Asn)_4$-**2**, $C_{76}N_{20}O_{20}H_{74}$ 1588.5 found 1588.5 $[M+H]^+$, calc. for Asn_3/Trp-**2** $C_{83}N_{20}O_{19}H_{179}$ 1661.7 found 1660.7 $[M+H]^+$, calc. for Asn_2/Trp_2-**2** $C_{90}N_{20}O_{18}H_{84}$ 1734.7 found 1732.9 $[M+H]^+$, calc. for Asn/Trp_3-**2** $C_{97}N_{20}O_{17}H_{89}$ 1807.8 found 1806.0 $[M+H]^+$ and 1788.7 $[M+H\text{-}17]^+$, calc for Trp_4-**2** $C_{104}N_{20}O_{16}H_{94}$ 1880.9, found 1876.9 $[M+H]^+$ and 1860.7 $[M+H\text{-}16]^+$.

Selection system I. 2 mg of each CPG (**Ia-d**) were weighed into separate 0.6 mL polyethylene reaction vessels. To each of these vessels a solution containing library **G** (40 μL, 8.82 μM total porphyrin, 150 mM NH_4OAc. 1 mM cholic acid, 2% DMSO) was added. The solution was vortexed briefly, centrifuged for a few seconds and mixed for, 45 min. A 20 μL sample of the supernatant was removed for UV-vis analysis and another 10 μL were removed for MALDI-TOF analysis. Both aliquots were dried for 3 h at 0. 1 torr before analysis.

Selection system II. Solutions containing nucleic acid targets (**IIa** or **b**) were added to a porphyrin library (150 mM NH_4OAc, 2% DMSO) in nucleobase:porphyrin ratios ranging from 1:1 to 10,000:1. These solutions were mixed for 15 min and centrifuged through Millipore DEAE anion-exchange spin columns. The eluted material was dried at 0.1 torr and analyzed using MALDI-TOF MS.

Acknowledgments: The authors wish to thank C. Bleczinski, D. Daniels and C. Tetzlaff for DNA syntheses and D. Sarracino for performing a UV titration. This work was made possible by a James Flack Norris/Theodore William Richards Summer Research Scholarship to M.D.S.

References and Notes:

1 Selected references: (a) Fiel, R.J., *et al. Nucleic Acids Res.* **1979**, *6*, 3093-3118. (b) Pasternack, R.F., *et al. Biochemistry* **1983**, *22*, 2406-2414. (c) Jain, R.K., *et al. Chem. Commun.* **1998**, 423-424.

2 (a) Fedoroff, O.Y., *et al. Biochemistry* **1998**, *37*, 12367-12374, (b) Wheelhouse, R.T., *et al. J. Am. Chem. Soc.* **1998**, *120*, 3261-3262.

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7 (a) Southern, E.M., *et al. Nucleic Acids Res.* **1994**, *22*, 1368-1373. (b) Maskos, U.; Southern, E.M. *Nucleic Acids Res.* **1992**, *20*, 1679-1684.

8 (a) Bettelheim, A., *et al. Inorg. Chem.* **1987**, *26*, 1009. (b) B. C. Bookser; T. C. Bruice *J. Am. Chem.. Soc.*, **1991**, *113*, 4208.

9 For a discussion of aggregation phenomena observed for less polar porphyrins and polymeric DNA see: Pasternack, R.F., *et al. J. Am. Chem. Soc.* **1998**, *120*, 5873-5878 and references therein. ◇

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continued from page 32

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Prof. Claudia Abeijon
"Biosynthesis of Cell Wall b(1_6) Glycan in Yeast"
Boston Glycobiology Discussion Group
Mass Inst. of Technology
Faculty Club, at 6:30 PM
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Apr. 19

Prof. Michael Fayer (Stanford Univ.)
"Protein Dynamics of Myoglobin: Ultrafast Infrared Vibrational Echo Experiments"
Boston College
Merkert Chem. Ctr., Rm. 127, at 4 PM

Prof. Shu Kobayashi (Univ. Tokyo)
"New Dimensions of Organic Synthesis Toward the 21st Century"
Harvard Univ.
Pfizer Lecture Hall, at 4:15 PM

Apr. 20

Prof. Gregory Verdine (Harvard Univ.)
"The Secret Life of the Genome: Enzymatic Processing of DNA"
Tufts University
Pearson Hall, Room 106, at 4:30 PM

Prof. James Pavlik (Worcester Polytechnic Inst.)
"Photochemistry of Thiazoles and Isothiazoles"
UMass Boston, Harbor Campus
Science Bldg, 1st Fl, Rm. 089, at 4:30 PM

Prof. Ira Krull
"Improved CIEF and CZE Analysis for Peptides and proteins Using Alternative Tagging Methods"
CESONE Night on Biotech CE
Beckman-Coulter Instruments Facility - Cafeteria
401 Edgewater place, Wakefield, MA at 5:30 PM
Reserv. < Apr. 16: Al Nitowski (203-573-3495, albie@aol.com)

Apr. 22

Dr. Michelle Palmer
"Chemiluminescence in High Throughput Screening"
Northeast AACC Meeting
Jimmy Fund Auditorium, Dana Farber Cancer Inst., at 5 PM
Contact: Dr. D. Drum
dedrum@bics.bwh.harvard.edu

Apr. 26

Prof. John Dawson (Univ. So. Carolina)
"Spectroscopic and Mechanistic Studies of Cytochrome P450, Nitric Oxide Synthase and Related Heme Systems"
Boston University
Science Ctr. Auditorium, at 4 PM

Apr. 27

Prof. Chad Mirkin (Northwestern Univ.)
"The Programmed Assembly of Nanoscale Building Blocks into Functional Materials"
Tufts University
Pearson Hall, Room 106, at 4:30 PM

Apr. 27/8

Technical and Management Topics in Clinical Laboratory Science
Northeast Conference and Exhibition
Holiday Inn, Boxborough, MA, 8 AM- 8 PM
Contact: Dr. D. Drum
dedrum@bics.bwh.harvard.edu

Apr. 29

Dr. Michael Eck (Dana Farber Cancer Inst./HMS)
Title TBA
Mass. Inst. of Technology
Room 6-120, at 4 PM

May 3

1st Joint Mini-Symposium of Advances in Separation Science and Mass Spectrometry
Prof. Fred Regnier (Purdue Univ.)
"Developments in Microfabricated Chips for High Efficiency Separations"
Prof. Paul Vouros
"Capillary LC/MS and CE/MS for Analyzing DNA Adducts"
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Northeastern Univ.
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May 3/4

1999 Max Tishler Symposium
Prof. Peter Dervan (Cal. Inst. Technol.)
Title TBA
Harvard Univ.
Pfizer Lecture Hall, at 4:15 PM

May 5

Prof. John Osborn (Univ. Strasbourg, France)
Title TBA
Mass. Inst. of Technology
Room 6-120, at 4 PM

Prof. Annette Herscovics
"Class I Processing Mannosidases"
Boston Glycobiology Discussion Group
Mass Inst. of Technology
Faculty Club, at 6:30 PM
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Prof. George Whitesides (Harvard Univ.)
"Unconventional Microfabrication"
Northeastern Univ.
Egan Bldg., Raytheon Amphitheater at 4 PM

May 6

Prof. George Whitesides (Harvard Univ.)
"Using Capillary Electrophoresis to Study Electrostatic Effects in Biochemistry"
Northeastern Univ.
129 Hurtig, at 4 PM

Prof. Robert Silbey (Mass. Inst. of Technology)
Title TBA
Univ. Mass, Lowell
Olney Hall, OH-428, at 3:30 PM

May 7

Research Symposium on Advances in Organic Synthesis
Prof. Marc Snapper (Boston College)
Prof. Rick Danheiser (MIT)
Prof. Stephen F. Martin (Univ. Texas, Austin)
Mass. Inst. of Technology
Room 6-120, at 4 PM

May 10

Prof. Yoshihiko Ito (Kyoto Univ.)
Title TBA
Harvard Univ.
Pfizer Lecture Hall, at 4:15 PM

May 12

Prof. James McCusker (Univ. CA, Berkeley)
"Electronic Structure Effects on the Photo-Induced Dynamics of Transition Metal Complexes"
Mass. Inst. of Technology
Room 6-120, at 4 PM

May 13

Robert Pfeifer (Waters Corp.)
"Analytical Chemistry in Industry - Balancing Good Science with Good Business"
Northeastern Univ.
129 Hurtig, at 4 PM

May 20

Prof. Fritz Vögtle (Univ. Bonn, Germany)
Title TBA
Mass. Inst. of Technology
Room 6-120, at 4 PM

Prof. D. L. Sparks (Northeastern Univ.)
"Synthesis of Novel Probes for the Estrogen Receptor Hormone Binding Domain"
Northeastern Univ.
129 Hurtig, at 4 PM

May 27

Prof. Robert Hanson (Univ. Delaware)
"Metal Sorption Rates and Mechanisms at the Mineral-Water Interface"
Northeastern Univ.
129 Hurtig, at 4 PM

June 3

Symposium: Molecular Diagnostics
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continued on page 29