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MARYLAND SECTION
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NUMBER 9



THE MARYLAND CHEMIST OF THE YEAR



American Chemical Society

CERTIFICATE OF EXCELLENCE

IN THE MEDIUM-LARGE CATEGORY IN 1994
MARYLAND

In Recognition of Outstanding Service to its Members and for Meritorious Contributions to the Chemical Profession and Public Understanding of the Fundamental Importance of Chemistry

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THE CHESAPEAKE CHEMIST STAFF

Raymond C. Petersen.....Editor
9329 Joey Drive
Ellicott City, MD 21042
(410) 465-8520

Bruce L. Solnick....Business Manager
P. O. Box 2355, Lab. Adm.
Baltimore, MD 21203
225-6209

SECTION OFFICERS

Shekar Munavalli.....Chairman
700 Paige Circle
Bel Air, MD 21014
(410) 838-7565 (H)
(410) 671-2819 (W)

Shirish Shah.....Chairman-elect
College of Notre Dame
4701 North Charles Street
Baltimore, MD 21210
(410) 532-5712

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202 Wight Avenue
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771-7471

Jan Kolakowski.....Treasurer
2610 Stanley Drive
Baldwin, MD 21013
(410) 836-6712

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(410) 617-2563

Charles Rowell....U.S. Naval Academy
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Baltimore, MD 21237
(410) 780-6613

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RICHARD H. SMITH, JR.

Richard H. Smith, Jr. received a BS in chemistry from Washington College in 1966 and a Ph.D. in organic chemistry from the University of Virginia in 1970. Following a year of post doctoral studies with Dr. Paul Gassman at the Ohio State University, he joined the faculty of Western Maryland College in 1971, where he has held the rank of Professor since 1985. He was a 1993 recipient of a Camille and Henry Dreyfus Scholar-Fellow grant. In that same year he received an NSF-ILI grant to support the incorporation of molecular modeling across all four years of the chemistry curriculum. In 1990 he developed and continues to teach a course in the history of scientific thought. This course is based on a compilation of excerpts from forty landmark publications and is open to science and non-science majors. From 1979 to the present he has been a Visiting Scientist at the National Cancer Institute's Frederick Cancer Research and Development Center (FCRDC). His primary area of research expertise is in the areas of physical organic and computational chemistry. His research on the chemistry of triazenes as it relates to the development of new anti-tumor drugs has involved over thirty student collaborators and has resulted in twenty-five journal articles, the majority coauthored by students. In addition to support from FCRDC, this project has been funded by grants from PRF, the Research Corporation, and, for nine consecutive years, the NSF-RUI program. In 1993 a second student-faculty project was undertaken, the design of new non-nucleoside inhibitors of the enzyme HIV-1 reverse transcriptase. Both projects involve complementary kinetic and computational experiments.

COMPUTATIONAL AND KINETIC INVESTIGATIONS OF NONNUCLEOSIDE INHIBITORS OF HIV-1 REVERSE TRANSCRIPTASE

HIV-1 RT is an enzyme critical to the replication of the AIDS virus in humans and thus is an attractive target for drug development. As a class, nonnucleoside inhibitors of RT, while structurally very divergent, have in general been shown to bind in a similar fashion to a common site in the protein. This binding site, which is not present in the uncomplexed enzyme, is proximal to, but different from, the site of polymerase activity. Thus, the observed noncompetitive inhibition is believed to be a consequence of an allosteric effect.

A model consisting of 155 amino acid residues surrounding the inhibitor binding site has been constructed based on crystallographic data from several RT/inhibitor complexes. Modeling studies consisted of molecular mechanics minimizations to relax residual strains followed by detailed analysis of the magnitude and source of the binding energy between the inhibitor and the protein. Surprising results include the fact that, although drug activity does correlate with overall calculated binding energy, neither of these parameters is reliably predicted by the drug-protein interaction energy alone. Further, it appears that predictions based on a "generic" site are not feasible. These findings are most likely a direct result of the unusual flexibility of the RT protein. The results of this study have proven useful in the design of new, more potent inhibitors of HIV-1 RT.

MARYLAND SECTION FUTURE MEETINGS

DATE	PLACE	SPEAKER	SUBJECT
February 14	Goucher	John Daly	Biologically Active Alkaloids from Poison
March 13	McCormick	David McGurvey	Malaria, Current Research
April 17	Western Maryland	Jeffrey Smart	History of Chemical Warfare up to and Including the Civil War
May 15	Johns Hopkins	Awardee	Renssen Award

THE MARYLAND CHEMIST AWARD

DATE & PLACE:

Wednesday, December 13, 1995
University of Maryland
Baltimore County
Faculty/Staff Dining Area

SCHEDULE:

- 5:30 Ramachandra S. Hosmane
UMBC
"Hemoglobin-based Oxygen Carriers and Aberrant Nucleosides and Nucleotides Containing 'Fat' and 'Slim' Base-analogs"
- 6:15 Social Hour
- 7:00 Dinner
- 8:00 THE MARYLAND CHEMIST AWARD ADDRESS

Richard H. Smith, Jr.
Western Maryland College
"Computational and Kinetic Investigations of Nonnucleoside Inhibitors of HIV-1 Reverse Transcriptase"

Dinner price is \$16.00 per person, but spouses and retired chemists may attend for \$14.00; students may attend for \$8.00.

It is not necessary to be a member of the American Chemical Society to attend. You may attend the lectures without attending the dinner.

Dinner reservations should be made by mailing checks, payable to Maryland Section of ACS, to

Dr. Shirish Shah
College of Notre Dame
4701 North Charles Street
Baltimore, MD 21210

by December 6. Late reservations may be made by calling

(410) 532-5712

by December 8; answering machine is available at this number.



RAMACHANDRA S. HOSMANE

AUDIO TRAINING KITS

The Maryland Section has a small selection of ACS audio training kits for loan. These are high quality kits on the following topics:

Statistics for Chemists
Infrared Spectroscopy
Scientific German
C-13 NMR Spectroscopy

Each can be borrowed for up to one month for a small handling charge to pay for postage and insurance.

Other topics may be added in the future, depending on demand.

Contact Dr. Shirish Shah at the College of Notre Dame, phone (410) 532-5712.

MARYLAND CHEMIST AWARD

The Maryland Chemist Award was established in 1962 to recognize and to honor, each year, a member of the Maryland Section for outstanding achievement in the field of chemistry. The achievement, as originally stated, may be in pure or applied chemistry, chemical engineering, or chemical education. Some recipients have distinguished themselves in management.

The Executive Committee of the Section has clarified the original definition of the award as follows:

Recipients of the Maryland Chemist Award must have been members of the Section for a minimum of five years and have made outstanding contributions to chemistry as defined in Article II of the Constitution of the Society (Chemistry is defined in broad terms). The work on which the award is based should have been performed in Maryland. Recommendations of the Maryland Chemist Awards Committee must be approved by the Executive Committee.

Previous recipients have been:

1962 E. Emmet Reid	1979 Emil H. White
1963 W. Mansfield Clark	1980 M. Gali Sanchez
1964 Alsoph H. Corwin	1981 Paul O. P. Ts'o
1965 John C. Krantz, Jr.	1982 Joseph L. Katz
1966 Belle O. Talbot	1983 Shih-Yi Wang
1967 Walter S. Koski	1984 Nicholas Zenker
1968 George L. Bruade	1985 John Lambooy
1969 Leslie Hellerman	1986 David F. Roswell
1970 Paul H. Emmett	1987 Gary H. Posner
1971 Giles B. Cooke	1988 Edward J. Poziomek
1972 Arnold M. Seligman	1989 Catherine Clarke Fenselau
1973 Lester P. Kuhn	1990 Alex Nickon
1974 Joyce J. Kaufman	1991 Cecil H. Robinson
1975 Benjamin Witten	1992 Craig A. Townsend
1976 Richard L. Hall	1993 Ernest F. Silversmith
1977 Henry C. Freimuth	1994 Yale H. Caplan
1978 Gunther L. Eichhorn	



THE JOHNS HOPKINS UNIVERSITY
1995 FALL CHEMISTRY COLLOQUIUM SCHEDULE
Remsen 233, Tuesdays, 4:15 p.m.

For more information, contact Rosalie Elder (410) 516-7432

December 5	Dr. Christopher Bryant Armour Pharmaceutical Co.	"Development of Plasma Butyryl- cholinesterase for the Treat- ment of Cocaine Overdose"
December 12	Professor David Schwartz New York University	"New Physical Approaches to Genome Analysis"

RAMACHANDRA S. HOSMANE

Ramachandra S. Hosmane was born in the state of Karnataka in India, and received B.Sc. & M.Sc. from Karnataka University in India. He received his MS and Ph.D. in Chemistry from the University of South Florida.

Professor Hosmane has held faculty positions in chemistry at UMBC since 1982. He has received numerous research grants from private sources as well as state and federal agencies. He has published over 72 journal articles. In this current year he has already published seven articles.

He has been very active in professional activities, memberships, and departmental and campus activities, at UMBC.

HEMOGLOBIN-BASED OXYGEN CARRIERS AND ABERRANT NUCLEOSIDES AND NUCLEOTIDES CONTAINING 'FAT' and 'SLIM' BASE-ANALOGS

The need for an alternative oxygen carrier in place of blood is critical. While the use of cell-free human hemoglobin instead of whole blood would be ideal, there are two major problems that need to be overcome. The cell-free hemoglobin does not stay long in the circulatory system, and is easily eliminated by the kidneys. Secondly, the oxygen affinity of hemoglobin outside of red blood cells is so high that it does not adequately transport oxygen from lungs to tissues. The cross-linked hemoglobin is anticipated to eliminate both of these problems. Our research is directed at design and synthesis of novel polyfunctional organic reagents to cross-link hemoglobin. New findings on this subject will be presented.

Ring-enlarged ['fat'] and ring-contracted ['slim'] analogs of natural nucleosides and nucleotides hold promise as substrates or inhibitors of purine and pyrimidine metabolizing enzyme systems as well as of enzymes requiring nucleotide cofactors. Replacement of natural bases with fatter or slimmer bases brings into play various stereochemical and conformational constraints that cause distortion of nucleic acid double helices, eventually leading to chain termination. This would potentially result in the inhibition of viral or tumor growth. Our recent results lend support for these considerations.

BECTON DICKINSON RECOGNIZES DHANESAR

Dr. Subhash Dhanesar, a research chemist with Becton Dickinson Microbiological Systems, Cockeysville, Maryland has received a Community Service Award for his outstanding contributions to the Abell Foundation Ingenuity Program and Baltimore Educational System. The Abell Foundation's efforts focus on the inner city program designed to develop math and science skills of middle school students. He is also associated with the Maryland Section of the American Chemical Society where he is involved with Science Teacher Development and National Chemistry Week programs. The Becton Dickinson award of \$3500 will go to Abell Foundation, Maryland Section of the American Chemical Society, Morgan State University and Baltimore Science Fair. The Becton Dickinson Company, Franklin Lakes, NJ, has over 18,000 employees worldwide.

E-MAIL ADDRESSES

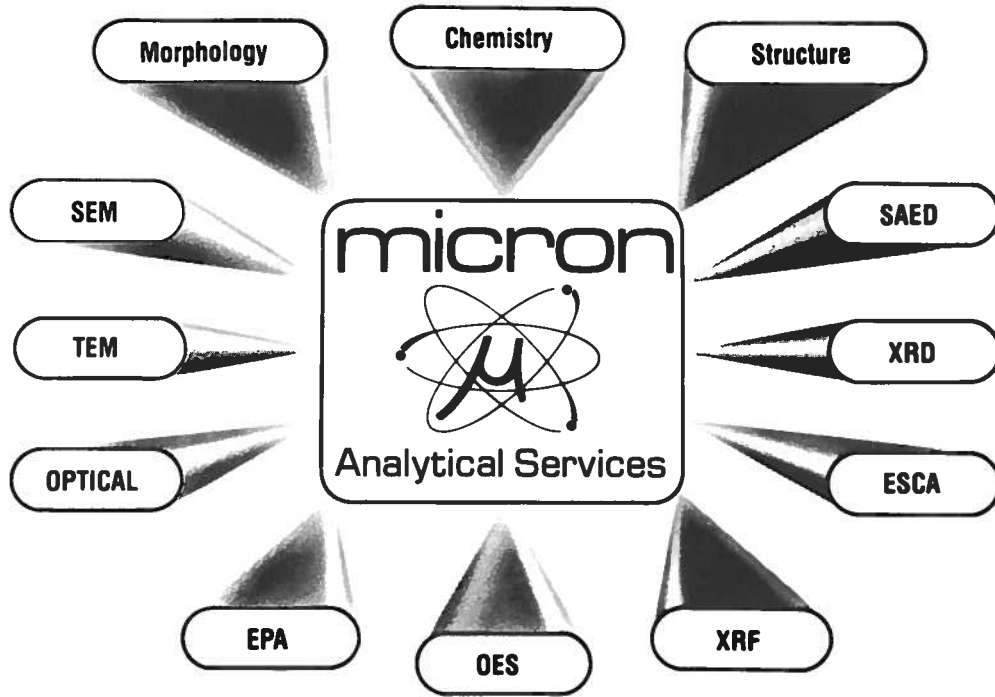
Members who wish to have their E-mail addresses registered with the Section should contact Diane Schmidt at the address given below. We may find this system useful for notification about events and Society matters. For the initial contact, please use the following scheme: line 1 - E-mail address; line 2 - name; and line 3 - any other note.

Contact: DM1@VM.CFSAN.FDA.GOV on Internet or DM1@BFD on Bitnet.

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