

# The TarHelium

Volume 31, Number 4

April, 2001



STATE OF THE SECTION

- Sancar Named NC Distinguished Lecturer
- New Science and Mathematics Building at Meredith
- Welcome New NC-ACS Members
- 115<sup>th</sup> Local Section Conference
- 18<sup>th</sup> Annual TCDG Symposium and Instrument Exhibit
- Seniors Chemist Committee Formed
- 2004 SERMACS Organizational Meeting



## Professor Sancar Named 2001 NC Distinguished Lecturer

**A**ziz Sancar, the Sarah Graham Kenan Professor of Biochemistry and Biophysics at the University of North Carolina, Chapel Hill, has been named the 2001 NC Distinguished Lecturer. Professor Sancar's research interests lie at the interface of chemistry and molecular biology.

Professor Sancar came to North Carolina in 1982 and has published over 200 journal articles in the field of DNA repair. Professor Sancar will deliver his lecture during the 115<sup>th</sup> Local Section Conference held on April 21<sup>st</sup> in Dabney Hall, Room 124 on the North Carolina State University Campus (see following pages for complete program).

All four issues of the TarHelium will accept advertising. The cost is \$25 per column-inch based on a 3.5 inch width; two-inch minimum. There is a 10% discount for advertising in three or more issues in a publication year which runs bimonthly from September through April.

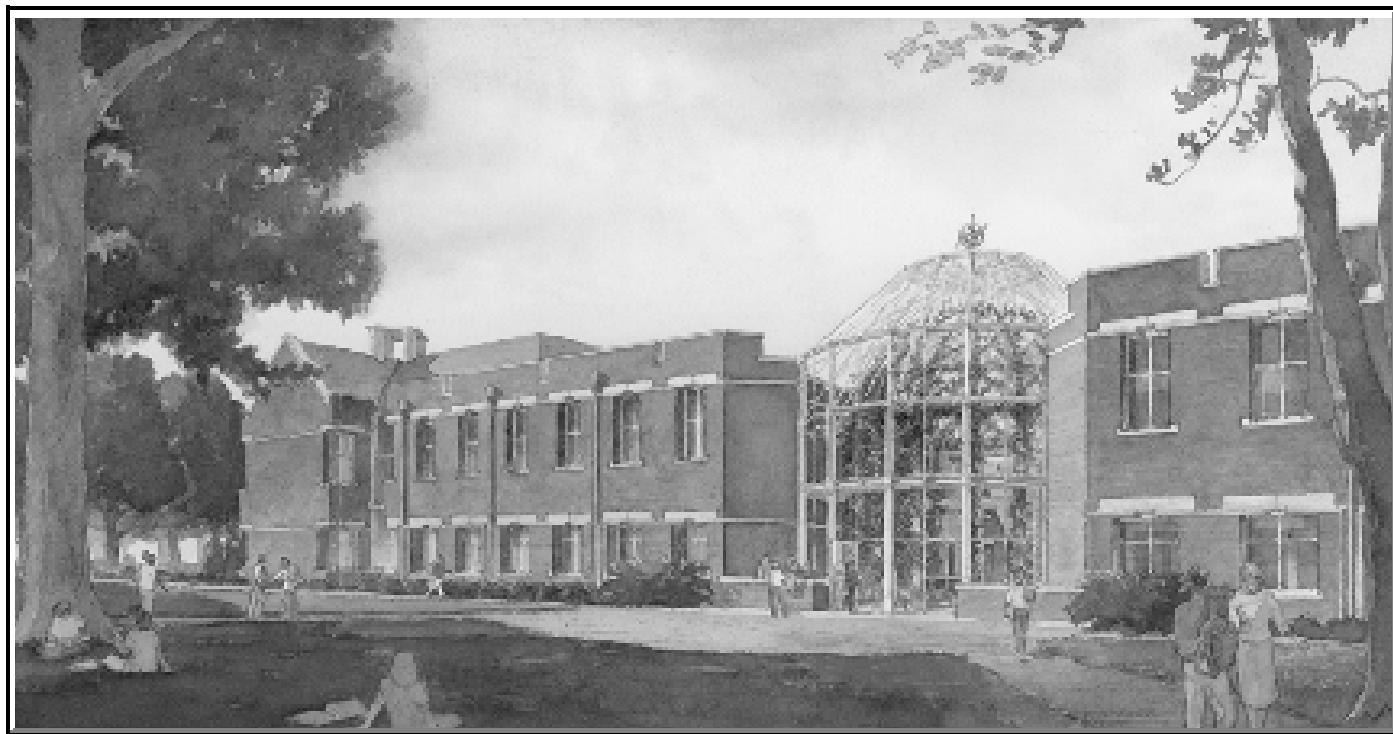


Donations to the NC Section of the ACS help sustain Local Section activities. All contributions are tax deductible and greatly appreciated.

Contact the editor, Brad Sturgeon at [sturgeon@ncssm.edu](mailto:sturgeon@ncssm.edu)

## INSIDE THIS ISSUE

|  |    |
|--|----|
| Professor Sancar Named Distinguished Lecturer              | 1  |
| Meredith Trustees Approve Science and Mathematics Building | 2  |
| Advertisers  | 3  |
| Welcome New NC-ACS Members                                 | 4  |
| 115 <sup>th</sup> Local Sectional Conference Program       | 5  |
| 2004 SERMACS Organizational Meeting                        | 9  |
| Job Vacancies  | 10 |



BJLAS Architecture

## Meredith Trustees Approve Design of a New Science and Mathematics Building

The Meredith College Board of Trustees approved the final design of an 80,000-square-foot science/mathematics building during the February 23 meeting of the full 40-member board. The state-of-the-art facility, recommended in Meredith's strategic plan, is a key element of the College's initiative to prepare women for science- and math-related careers—two traditionally male-dominated fields. "This new facility will support our students to become leaders in a society that is increasingly based in science and technology," said Meredith College President Maureen Hartford. Meredith officials will break ground on the facility, the College's first new classroom building since 1993, during a 2:30 p.m. ceremony on April 9, 2001. Completion of the science/mathematics building is expected in January 2003. The facility will be constructed on the south side of the Meredith campus, and will necessitate the relocation of the Mae Grimmer Alumnae House this summer. The new building will face the Shearon Harris Building, forming a quad between Harris and the Cate Center. The building will house the biology and health sciences, the chemistry and physical science, and the mathematics and computer science departments.

Currently, the science departments are located in Hunter Hall and the math department is located in Harris Building. The new facility will consolidate these three departments,

freeing space in Hunter and Harris for other academic uses. The new facility will include:

- specialized laboratories for genetics/evolution, cell biology/biochemistry, micro/molecular biology, anatomy and physiology, ecology, organic chemistry, inorganic chemistry, earth science, physics, computer science, and others;
- a roof-top telescope platform for astronomy observations;
- an open courtyard in the center of the building for outdoor lectures;
- community spaces to foster collaborative learning among students and faculty; and
- a student/faculty research laboratory for each full-time faculty member in the sciences.

Meredith has contracted with BJLAS Architecture for the building's design and with Rodgers Construction for the construction of the building. Both are women-owned firms. With an enrollment of over 2,600 students, Meredith College is the largest women's college in the Southeast.

*Submitted by:  
Kristi Eaves-McLennan  
Assistant Director of Communications  
Meredith College*

# Advertisements



**Integrated Software Solutions...  
Easier Done than Said**


Do you find yourself juggling data, methods, references and hypotheses? Spectroscopic tools from Advanced Chemistry Development integrate three main areas: spectral processing, databases, and prediction. ACD processing software allows you to associate chemical structures with spectra. ACD/SpecManager allows you to create databases for NMR, MS, UV-Vis, and IR data searchable by chemical structure, substructure, and other parameters. ACD/NMR Predictors predict  $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^{13}\text{C}$ , and  $^1\text{H}$  spectra and allow you to increase prediction accuracy by using your own experimental data. Look-up databases of assigned  $^1\text{H}$  and  $^{13}\text{C}$  spectra contain over 100,000 chemical structures each.

Chromatographic tools from Advanced Chemistry Development are also adept at juggling processing, databases and prediction. ACD/ChromManager processes experimental data, and includes the ability to assign chemical structures as well as a sophisticated deconvolution routine. Write your chromatograms to a fully searchable database. Or, transfer your data to our prediction engine for method optimization in ACD/LC Simulator. Chemical structure knowledge can be integrated with experimental data, thereby cutting method development time considerably, and it's all easier done than said.



**Advanced  
Chemistry  
Development**


90 Adelaide St. W. Suite 702  
Toronto, ON M5H 3V9 Canada  
Tel: (416) 368-3435  
Fax: (416) 368-5596  
Toll Free: 1-800-304-3988  
info@acdlabs.com  
www.acdlabs.com




For all your analysis needs . . .

Agilent Technologies has a solution!

- Capillary Electrophoresis
- Biochemical Analysis
- Sample Preparation
- Liquid Chromatography
- Gas Chromatography
- LC/MS & LC/MS/MS
- GC/MS
- UV-Vis Spectroscopy
- Columns & Supplies
- User Training
- Data Systems
- Instrument Repair
- ICP/MS



For more information, call:  
For more information call 1-800-227-9770, or  
visit our web site at [www.agilent.com/chem](http://www.agilent.com/chem)



**Agilent Technologies**  
Innovating the HP Way

**novocontrol** →

NOVOCONTROL, the world leader in Broadband Dielectric Spectroscopy, offers advanced turnkey instrumentation for dielectric and impedance spectroscopy with precise temperature control.

With our instruments we cover a broad frequency range from 3  $\mu\text{Hz}$  to 1.8 GHz and a temperature range from  $-160^\circ\text{C}$  to  $+500^\circ\text{C}$ .

For more information please contact:

NOVOCONTROL America, Inc.  
Dr. Joachim Vinson  
phone: 1-877-639-9323 (toll free)  
fax: 1-919-639-7523  
e-mail: [vinson@ntwrks.com](mailto:vinson@ntwrks.com)  
<http://www.novocontrol.com>

## Welcome to Our Newest NC-ACS Members

Amanda G. Alford  
Eric J. Allain  
Shawn Paul Allwein  
Michelle .E Arnold  
Isaac Ashie  
A. Ayesb  
Manny Bacolod  
Michael D. Baker  
Juan C. Bastidas  
Ronald Baynes  
Mark J. Bednarcik  
Shikha Bhatnagar  
Pamela Schultz Birak  
Luther Bradford Black  
Barbara Blair  
Arthur C Bond  
Pam Bowden  
G. D. Bowers  
Mark Bowers  
Daniel M. Bowles  
Paula M. Briggs  
John M. Brittingham  
Andrew Brogan  
Andrew Brogan  
Douglas C. Brower  
Chaozhong Cai  
Marlene Carol Capraro  
Dominick Cerminaro  
Harinath Chakrapani  
Michael D. Chu  
Donna Marie Coleman  
S. Robert Collins  
Stephen Lawrence Craig  
Grace M. Credo  
Christine N. Dalton  
Shelley Danek  
Ryan M. Danell  
Roderick G. Davis  
Cynthia R. De Haas  
Victor R. Dejesus  
Rodolfo O. Domingo  
Anthony Kwabla Dotse  
Marc Doyle  
Robert F. Dream  
Kenyon McLane Evans  
Brian Edward Fee  
Lanette Renee FeeTodd Fields  
Anne Finefrock  
Dennis Kiyoshi Fujii  
Nathan O. Fuller  
Amy E. Garrett  
Willard Max Gentry  
Marisha L Godek  
Varvara P. Grichko  
Rich Guerra  
Julia C. Guo  
Michael Heien  
Christopher Herhenkels

Thomas Hessellund  
Anne-Cecile Hiebel  
Ian Hirst  
William Phillip Hodges  
Hans P. Huiuzenga  
Mohammed Jaoui  
Wendy Jones  
Jamande Jones  
Biren K. Joshi  
Joseph Mark Jump  
Jason Scott Keiper  
Valerie R. Kempf  
Moussa Khobzaoui  
Deborah W. Kittrell  
J. M. Knight  
Douglas Kojetin  
Vasu Kokkuvayil  
Jochen Kupper  
Rick D. Lafleur  
Jennifer L Lefler  
Yanxin Li  
Yue Li  
Timothy P. Malone  
Elizabeth L. Malson  
Shelia Jane Maness  
Kenneth G. Manton  
Marshall Martin  
Cynthia K. Matherly  
Anshu B. Mathur  
J. McClain  
Mark McCormick  
Jayesh M Mehta  
Gulzhan Menzeleeva  
Mark A. Miller  
James W. L. Monkman  
Beverly Mowrey  
Denise F. Muck  
Dr. Kannan Muthukumaran  
Brooke Ncghee  
Mary E. Newton  
Christopher K. Njue  
E. J. Noga  
Dimpal Patel  
Daniel E. Patterson  
David E. Paulsen  
Jennifer Perry  
Keith Petschke  
Wayne Harold Pitcher  
Erica E. Poe  
Ashley P. Porter  
Dawn C. Pramuk  
David L. Price  
Omar A Quintero  
Patrick Rainey  
Mark J. Rashkin  
Andrew D. Reinhardt  
Steven M. Reister

Marjorie S. Remick  
Christie C. Rich  
Thomas P. Robinson  
Oliver A. Roholt  
Eric D. Roush  
Janelle Y. Saulter  
Barbara S. Shane  
Hong Shen  
Frenchie Simpson  
David J. Slade  
Leslie S. Sloan  
Grace R. Smalley  
Caroline Q .Smith ONeill  
Nathan Somasund  
Lillian Stanajevic  
Julie Ann Stenken  
Zendre L. Strother Brown  
Terri Sumner

Ling Tan  
Choon Teo  
Marc Alan Ter Horst  
Bryan Thompson  
Billy Gene Tweedy  
Paul F. Uliana  
Emily M Walker  
Jing Wan  
Ke Wang  
David J. Slade  
Debra Weigl  
W. T. Wrighten  
Nathan J. Wymer  
Chungeng Xia  
Wayne C. Yount  
Yun Zhang  
Yun Fan Zou  
Yunfan Zou

# WANTED

A position is open for National Chemistry Week Organizer for the North Carolina chapter of the ACS in the Triangle. This is an opportunity to design and plan outreach programs for the chemical sciences. During the National ACS's designated week in November (Nov. 4-11, 2001) the section holds events to celebrate the science of chemistry and the role of chemists in our society. Past programs have consisted of hands-on demonstrations of chemistry concepts in multiple locations in the Triangle. The budget for last year's programs was around \$2500.

The National ACS provides some supplies and handouts for NCW as well as an informative website at <http://www.acs.org/ncw>. Recently, National has started promoting adherence to a theme for NCW to help sections generate ideas for programs. Past themes include polymers and kitchen chemistry. This year's theme, "Chemistry in Art", has great potential for some creative ideas.

If you are interested in this position, please send an email to Maury Balik, chair of the NC-ACS section ([balik@ncsu.edu](mailto:balik@ncsu.edu)).

Submitted by  
Bill Switzer  
[bill\\_switzer@ncsu.edu](mailto:bill_switzer@ncsu.edu)



115th North Carolina-ACS Sectional Conference  
 Saturday, April 21, 2001  
 Dabney Hall  
 North Carolina State University

## TECHNICAL PROGRAM

**Note:** Posters will be displayed from 8:30-12:00 noon.  
 Presenters will be available for discussion at the times below.

### General Session

Awards, NC Distinguished Lecture . . . 12:10 pm - 1:10 pm  
 Lunch . . . . . 1:15 pm

### Analytical Chemistry (ANYL)

Oral Presentations . . . . . 8:40 am - 12:00 pm  
 Poster Presentations . . . . . 10:00 am - 11:00 am

### Biological Chemistry (BIOL)

Oral Presentations . . . . . 10:40 am - 12:00 pm  
 Poster Presentations . . . . . 9:00 am - 10:00 am

### Inorganic (INOR) & Organic Chemistry (ORGN)

Oral Presentations . . . . . 10:20 am - 12:00 pm  
 Poster Presentations . . . . . 8:45 am - 9:45 am

### Chemical Education

Oral Presentations . . . . . 8:40 am - 10:00 am

### Nuclear Magnetic Resonance Spectroscopy (NMR)

Oral Presentations . . . . . 8:20 am - 12:00 pm  
 Poster Presentations . . . . . 9:40 am - 10:40 am

### Physical Chemistry (PHYS)

Poster Presentations . . . . . 11:00 am - 12:00 pm

### Polymer Chemistry (POLY)

Oral Presentations . . . . . 10:20 am - 12:00 pm  
 Poster Presentations . . . . . 8:40 am - 9:40 am

## ACKNOWLEDGEMENTS

The NC-ACS Local Section gratefully acknowledges the Chemistry Department at NCSU for hosting this event, and Dr. William L. Switzer of the NCSU Chemistry Department for coordinating the use of the NCSU facilities. Many thanks to the projectionists and other assistants from NCSU. CIIT Centers for Health Research is acknowledged for developing and printing the program and related materials.

## VIDEO PRESENTATION

The program includes a videotape presentation entitled:

### *"North Carolina's Research Triangle Park: An Investment in the Future"*

This video was produced by PBS and aired by WUNC-TV. It details the development of the Research Triangle Park and it cites the involvement of several members of the NC-ACS local section. It will be shown continuously in the first floor Dabney-Cox Lounge area.

### **Senior Chemists Committee Launches Today! Dabney Hall, Room 623**

The NC-ACS executive committee has approved funding for the creation of the Senior Chemists Committee whose purpose is to address areas of special interest to our senior chemists in the section. A targeted mailing was made to over 560 members of the section inviting them to attend the kick-off meeting of the committee and elect new officers. We anticipate about 10 members who will actually celebrate their 50th year membership anniversaries and be recognized with plaques during today's award ceremony. The organizing committee has recommended discussions on "life after retirement", consulting clearing houses, liability and term insurance plans, charitable giving, and other topics along with social meetings to enjoy baseball, barbecues, and other recreational outings (golf).

### GENERAL SESSION

DABNEY HALL Room 124

12:10 pm - 1:10 pm

1:15 pm: Buffet lunch served on First Floor

Maury Balik (NCSU), NC-ACS Chair, presiding

- Presentation of the 2001 Marcus E. Hobbs award.
- Recognition of the 50-year ACS members.
- Recognition of the 2001 Barbara Whittaker Award.
- Presentation of the Undergraduate Scholarship Award
- Presentation of the 2001 NC-ACS Distinguished Lecture Award to:

**Dr. Aziz Sancar**

**Department of Biochemistry and Biophysics  
 University of North Carolina at Chapel Hill**

For questions about the program please contact:  
 Dr. Susan Sumner, Program Chair  
 CIIT Centers for Health Research  
 Six Davis Drive, Research Triangle Park, NC.  
 Phone: 919-558-1343; E-mail, sumner@ciit.org

**ANALYTICAL CHEMISTRY (ANYL)**

Dabney Hall, Room 330

8:40 am - 12:00 pm

8:40, 01-ANYL. Application of a New Tandem Ionization Source for Direct Mass Spectrometric Analysis of Semi-volatiles. **Christine N. Dalton**<sup>1</sup>, Zhengqi Ye<sup>2</sup>, Howard Weinberg<sup>2</sup>, and Gary L. Glush<sup>1</sup>. <sup>1</sup>Dept. of Chemistry, <sup>2</sup>Dept. of Environ. Sci. and Eng., UNC-CH.

9:00, 02-ANYL. Conventional CID vs. IRMPD for the Analysis of Polymers in a Quadrupole Ion Trap. **Sara C. McGrath** and Gary L. Glush. Department of Chemistry. UNC-CH.

9:20, 03-ANYL. Using a DNA Aptamer as a Novel Stationary Phase in Capillary Electrochromatographic Separations of Isomeric Dipeptides. **Joseph A. M. Charles** and Linda B. McGown. Department of Chemistry, Duke University.

9:40, 04-ANYL. Determination of the Polarity of Small Unilamellar Vesicles Using A Homologous Series of Pi\* Indicators. **Jennifer M. Carrozzino**<sup>1</sup>, Robin Helburn<sup>2</sup>, and Morteza G. Khaledi<sup>1</sup>. <sup>1</sup>Department of Chemistry, NCSU, <sup>2</sup>Research Triangle Institute.

10:00 **BREAK/Poster Session (40 min)**. Dabney Hall, 1st Floor

10:40, 05-ANYL. Determination of Liposome-Water Partition Coefficients using Electrokinetic Chromatography (LEKC). **Scott T. Burns** and Morteza G. Khaledi. Department of Chemistry, NCSU.

11:00, 06-ANYL. Retention Behavior of Solutes and Linear Solvation Free Energy Relationship in Vesicular Electrokinetic Chromatography. **Hai H. Bui** and Morteza G. Khaledi. Department of Chemistry, NCSU.

11:20, 07-ANYL. Cooperative Hydrogen Bonding in CO<sub>2</sub>-Specific Interactions. **Raveendran Poovathinthodiyil** and Scott L. Wallen. Department of Chemistry, UNC-CH.

11:40, 08-ANYL. Model for Two-step Quasi-Reversible Surface Reaction. **John J. O'Dea**. Department of Chemistry, NCSU.

**ANALYTICAL & MATERIAL CHEM. POSTER SESSION**

- Dabney Hall, First Floor

8:30 am - 12:00 pm (posted times)

10:00 am - 11:00 am (discussion times)

09-ANYL. Quality Assessment of Frying Oil by Quantitative Proton and Carbon-13 NMR Spectra. **Ming Li**, Kevin M. Keener, and Brian E. Farkas. Department of Food Science, NCSU.

01-MAT. Chemical Modification of Carbon Nanotubes. Bin Cheng and Edward T. Samulski. Department of Chemistry, UNC-CH.

**BIOLOGICAL CHEMISTRY (BIOL)**

Dabney Hall, Room 331 10:40 - 12:00 pm

Michael C. Fitzgerald (Duke University), presiding

10:40, 01-BIOL. The Energetic Contribution of a Backbone-Backbone Hydrogen-Bond to the Thermodynamic Stability of Arc Repressor. **Thomas E. Wales** and Michael C. Fitzgerald. Department of Chemistry, Duke University.

11:00, 02-BIOL. The Role of Backbone-Backbone Hydrogen Bonds in the Folding and Stability of a Homo-Hexameric Enzyme. **Peter Silinski**, M. J. Allingham, and Michael C. Fitzgerald. Department of Chemistry, Duke University.

11:40, 04-BIOL. High Sensitivity Measurements of Protein Stability by H/D Exchange and Matrix-Assisted Laser Desorption/Ionization (MALDI) Mass Spectrometry. **Kendall D. Powell** and Michael C. Fitzgerald. Department of Chemistry, Duke University.

**BIOLOGICAL CHEM. POSTER SESSION**

Dabney Hall, First Floor

8:30 am - 12:00 pm (posted times)

9:00 am - 10:00 am (discussion times)

05-BIOL. Using NMR in Toxicology Studies. **Timothy R. Fennell**, Carla C. Williams, and Susan C. J. Sumner. CIIT Centers for Health Research.

06-BIOL. Rapid Analysis of Hemoglobin Adducts by Liquid Chromatography-Mass Spectrometry. **Rodney W. Snyder**, W. Krol, S. C. J. Sumner, and T.R. Fennell. CIIT Centers for Health Research.

**INORGANIC AND ORGANIC CHEMISTRY (INOR/ORG)**

Cox Hall, Room 200 10:20 am - 12:00 pm

Shawn C. Sendlinger (NCCU), presiding

10:20, 01-INOR. Bulk Liquid Membrane Transport of Iron (III)-Hydroxamate Complexes by Carriers Utilizing First Coordination Sphere Recognition. **Joseph I. Wirgau** and Alvin L. Crumbliss. Dept. of Chemistry, Duke University.

10:40, 02-INOR. Siderophore Molecular Recognition: Crystal Structure of Ferrioxamine B and Ionophore-Siderophore Host-Guest Complexation. **Suraj Dhungana**<sup>1</sup>, P. S. White<sup>2</sup>, S. M. Trzaska<sup>1</sup>, and Alvin L. Crumbliss<sup>1</sup>. Department of Chemistry, <sup>1</sup>Duke University, <sup>2</sup>UNC-CH.

11:00, 03-INOR. Step-Scan FTIR Time-Resolved Spectroscopy of Copper (I) Complexes of 2,9-Substituted 1,10-Phenanthroline Ligands. **Yu Lu**, M. S. Hutson, M. W. Grinstaff, and R. A. Palmer. Department of Chemistry, Duke University.

11:20, 04-INOR. Development of an Iron Chelating Hydrogel. **Megan M. Flaherty** and Alvin L. Crumbliss. Department of Chemistry, Duke University.

11:40, 01-ORG. Development of Stereoselective Intramolecular Hydride Transfer Reactions: Insight into the Catalytic, Asymmetric Aldol-Tishchenko Reaction. **Steven P. Miller**, Cheryl M. Mascarenhas, and James P. Morken. Department of Chemistry, UNC-CH.



**INORGANIC CHEM. POSTER SESSION**

Dabney Hall, First Floor

8:30 am - 12:00 pm (posted times)

8:45 am - 9:45 am (discussion times)

**05-INOR.** Probing the Origin of Selective Rebinding in Molecularly Imprinted Polymers. **Melanie A. Pribisko**, N. M. Brunkan, and M. R. Gagne. Dept. of Chemistry, UNC-CH.

**06-INOR.** New Synthetic Routes to Tungsten-Bromide Compounds. **Amin Bhuiyan**<sup>1</sup>, Shawn C. Sendlinger<sup>1</sup>, Willie R. Hargrove<sup>1</sup>, Peter S. White<sup>2</sup>. Department of Chemistry, <sup>1</sup>NCCU, <sup>2</sup>UNC-CH.

**ORGANIC CHEMISTRY POSTER SESSION**

Dabney Hall, First Floor

8:30 am - 12:00 pm (posted times)

8:45 am - 9:45 am (discussion times)

**02-ORGN.** Toward a More Efficient Macroporous Polymer Immobilized Catalyst System. **Shannon L. Vinson** and Michael R. Gagne. Department of Chemistry, UNC-CH.

**03-ORGN.** Progress Towards the Chemical Synthesis of Macrophage Migration Inhibitory Factor (MIF). **Laura E. Weeshoff**, T. E. Whales, and M. C. Fitzgerald. Department of Chemistry, Duke University.

**04-ORGN.** Peptide Growth Utilizing Novel Linkers as Self-Assembled Monolayers on Polycrystalline Gold. Kevin W. Kittredge<sup>1</sup>, M. A. Minton<sup>2</sup>, James K. Whitesell<sup>1</sup>, and Mary Anne Fox<sup>1</sup>. <sup>1</sup>Department of Chemistry, NCSU, <sup>2</sup>New Mexico Highlands University.

**CHEMICAL EDUCATION (CHEM EDU)**

Dabney Hall, Room 331

8:40 am - 10:00 am

**Maria Oliver-Hoyo (NCSU), presiding**

**8:40, 01-CHEM EDU.** Concept Advancement through Chemistry Lab-Lecture (cAcL2): Inception, Growth, and Expectation. **DeeDee A. Allen** and Maria T. Oliver-Hoyo. Department of Chemistry, NCSU.

**9:00, 02-CHEM EDU.** Engaging Student Attention and Participation in Large Chemistry Classes. **Kay A. Sandberg**. Department of Chemistry, NCSU.

**9:20, 03-CHEM EDU.** Solid Phase Organic Chemistry and Combinatorial Chemistry: An Undergraduate Laboratory Preparation of Oligopeptides. **J. Hodge Markgraf**<sup>1</sup>, George A. Truran<sup>2</sup>, Karelle S. Aiken<sup>3</sup>, Thomas R. Fleming<sup>3</sup>, and Peter J. Web3. <sup>1</sup>Dept. of Chemistry, Duke University, <sup>2</sup>University of Connecticut, <sup>3</sup>Williams College.

**9:40, 04-CHEM EDU.** Using WebAssign, an On-line Quizzing Package, for Submitting Paperless Lab Reports. **William L. Switzer**, Department of Chemistry, NCSU.

**NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY (NMR)**

Cox Hall, Room 214

8:20 am - 12:00 pm

**Scott L. Wallen (UNC-CH), presiding**

**8:20, 01-NMR.** NMR Quantum Computation. **E. O. Stejskal**<sup>1</sup>, David Collins<sup>2</sup>, K. W. Kim<sup>2</sup>, W. C. Holton<sup>2</sup>, and H. Sierzputowska-Gracz<sup>3</sup>. <sup>1</sup>Dept. of Chem., <sup>2</sup>Dept. of Electrical & Chem. Eng., and <sup>3</sup>Dept. of Biochem NCSU.

**8:40, 02-NMR.** Approaches and Applications of High-Pressure NMR. **Laura K. Schoenbachler**, Scott L. Wallen, and P. Raveendren. Department of Chemistry, UNC-CH.

**9:00, 03-NMR.** The Solvation Structure of a Reversed-Phase Liquid Chromatographic (RPLC) System. **Erica D. Dawson** and Scott L. Wallen. Department of Chemistry, UNC-CH.

**9:20, 04-NMR.** NMR Spectroscopy and Imaging Applications to Tissue Engineering. **Jeffrey M. Macdonald**. Department of Physiology, UNC-CH.

**9:40, 05-NMR.** The Analysis of Pharmaceutical Molecules in Chiral Liquid Crystals. **Thomas M. O'Connell**. GlaxoSmithKline.

**10:00 BREAK/Poster Session (20 min).** Dabney Hall, 1<sup>st</sup> Floor

**Sharon Campbell (UNC-CH), presiding**

**10:20, 06-NMR.** Temperature Dependence of Dynamics in a Calmodulin Complex: Viewing the Glass Transition with Solution NMR. **Andrew L Lee**. School of Pharmacy, UNC-CH.

**10:40, 07-NMR.** NMR and MD Studies of U4 snRNA. **William H. Gmeiner**<sup>1</sup>, Jian-xin Goa<sup>2</sup>, Luis Commoli<sup>3</sup>, Nick Ulyanov<sup>3</sup>, and Thomas James<sup>3</sup>. <sup>1</sup>Department of Biochemistry, Wake Forest University School of Medicine, <sup>2</sup>Camitro Corporation, <sup>3</sup>UCSF.

**11:00, 08-NMR.** Structural insights into Rac1 Signaling. **Roopa Thapar** and Sharon Campbell. Department of Biochemistry, UNC-CH.

**11:20, 09-NMR.** Protein Dynamics and the Promiscuity of DNA-Binding. **John Cavanagh**. Department of Molecular & Structural Biochemistry, NCSU.

**11:40, 10-NMR.** Structural Studies of Larger Proteins and Complexes. **Ronald A. Venters**<sup>1</sup>, Geoffrey A. Mueller<sup>2</sup>, Leonard D. Spicer<sup>3</sup>, W.Y. Choy<sup>2</sup>, and Lewis E. Kay<sup>2</sup>. <sup>1</sup>Duke University NMR Center, <sup>2</sup>University of Toronto, <sup>3</sup>Dept. of Biochem., Duke University.

**NMR POSTER SESSION**

Dabney Hall, First Floor

8:30 am 12:00 pm (posted times)

9:40 am 10:20 am (discussion times)

**11-NMR.** Probing the Limits of Detection of CryoProbe™ Technology. **Kimberly L. Colson** and C. Anklin. Bruker Instruments, Inc.

**12-NMR.** 19F NMR Study of Fluorocarbons. **Clarence W. Murray** and Edward T. Samulski. Dept. of Chem. UNC-CH.

**13-NMR.** The Interaction of MRI Contrast Agents with Phospholipids. **Anthony Ribeiro**<sup>1</sup>, Gordon Jendrasiak<sup>2</sup>, and Ralph Smith<sup>2</sup>. <sup>1</sup>Duke University, <sup>2</sup>East Carolina University.

### PHYSICAL CHEM. POSTER SESSION

Dabney Hall, First Floor

8:30 am - 12:00 noon (posted times)

11:00 am - 12:00 am (discussion times)

**01-PHYS.** New Homologous Series of Non-Linear LC Mesogens with a Central Core Based on 1,3,4-Oxadiazole Group. **Jirakorn Thisayukta** and Edward T. Samulski. Department of Chemistry, UNC-CH.

**02-PHYS.** In search of the Smectic C Liquid Crystalline Phase: A Computer Simulation Study. **Ian M. Withers**<sup>1</sup>, Maureen P. Neal<sup>2</sup>, and Douglas J. Cleaver<sup>3</sup>. <sup>1</sup>Dept. of Chemistry, UNC-CH, <sup>2</sup>Dept. of Mathematics and Information Sciences, Coventry University, UK; <sup>3</sup>Dept. of Materials Research, Sheffield Hallam University, UK.

**03-PHYS.** Computational Investigation of Bioactivation Mechanisms of Toxicity Across Classes of Haloorganics: Bromination vs. Chlorination. **Paul D. Swartz**<sup>1</sup> and Ann M. Richard<sup>2</sup>. <sup>1</sup>UNC Curriculum in Toxicology, <sup>2</sup>US Environmental Protection Agency.

**04-PHYS.** Development of a Nonlinear Ultrafast Spectroscopic Technique for Investigating Surface Low-Frequency Motion. **David J. Styers-Barnett** and John M. Papanikolas. Department of Chemistry, UNC-CH.

### POLYMER CHEMISTRY (POLY)

Cox Hall, Room 204

10:20 am - 12:00 pm

**10:20, 01-POLY.** A New Method of Molecular Assembly on Elastomer Surfaces. **Kirill Efimenko** and Jan Genzer. Department of Chemical Engineering, NCSU.

**10:40, 02-POLY.** Time-Resolved FTIR/DMA Studies Show Evidence of Cluster Evolution in Cation-Loaded Nafion and Support for the EHM Model. **Yanqia Wang**<sup>1</sup>, Y. Kawano<sup>2</sup>, S. R. Aubuchon<sup>3</sup> and R. A. Palmer<sup>1</sup>. <sup>1</sup>Depart. of Chemistry, Duke University, <sup>2</sup>Department of Chemistry, University of Sao Paulo, and <sup>3</sup>TA Instruments.

**11:00, 03-POLY.** Inclusion Compound Formation and Characterization of PET and PET/PEN Blends in Gamma-Cyclodextrin. **Francis, E. Porbeni**, T. Bullions, M. Gerber, and A. Tonelli. Fiber and Polymer Science Program, NCSU.

**11:20, 04-POLY.** Molecular Dynamics Simulations of Semidilute Polyelectrolyte Solutions. **Qi Liao**, Andrey V. Dobrynin, and Michael Rubinstein. Dept. of Chemistry. UNC-CH.

**11:40, 05-POLY.** Phase Transitions in Dilute Polyelectrolyte Solutions. **Alexander Deshkovski**<sup>1</sup>, S. Obukhov<sup>2</sup>, and Michael Rubinstein<sup>1</sup>. <sup>1</sup>Dept. of Chemistry, UNC-CH, <sup>2</sup> Univ. of Florida.

### POLYMER CHEM. POSTER SESSION

Dabney Hall, First Floor

8:30 am - 12:00 pm (posted times)

8:40 am - 9:40 am (discussion times)

**06-POLY.** Compatibilization of Polymers via Coalescence from their Common Cyclodextrin Inclusion Compounds. **Min Wei** and Alan E. Tonelli. Fiber & Polymer Science Program, NCSU.

**07-POLY.** Molecular Structure, Network Formation and Gelation Efficacy of Dibenzylidene Sorbitol. **Elizabeth A. Wilder**, C.K. Hall, S.A. Khan, and R.J. Spontak. Dept. of Chemical Engineering, NCSU.

**08-POLY.** Liquid Crystal Behavior in CO<sub>2</sub>. **Chad J. Booth** and Edward T. Samulski. Department of Chemistry, UNC-CH.

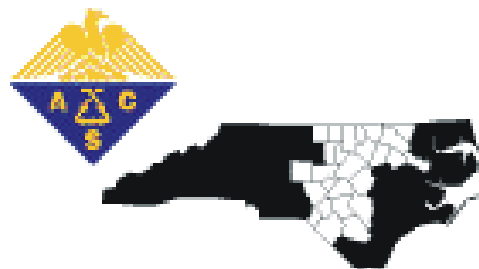
**09-POLY.** Preparing High-Density Polymer Brushes by Mechanically Assisted Polymer Assembly (MAPA). **Tao Wu**, Kirill Efimenko, and Jan Genzer. Department of Chemical Engineering, NCSU.

**10-POLY.** Monte Carlo Simulations for Pattern Recognition of Copolymers Near Heterogeneous Surfaces. **James J. Selmer** and Jan Genzer. Dept. of Chemical Engineering, NCSU.

**11-POLY.** Off-Lattice Computer Simulation of the Micellization Properties of Polymeric Surfactants. **Ian M. Withers**, Andrey V. Dobrynin, and Michael Rubinstein. Department of Chemistry, UNC-CH.

**12-POLY.** Effect of High-Pressure Carbon Dioxide on Polymer Blend Phase Behavior. **Teri A. Walker**, Richard J. Spontak, and Saad A. Khan. Dept. of Chemical Engineering, NCSU.

**13-POLY.** Properties of High Density Polyethylene Filled with Mixtures of Graphite and Carbon Fibers. **Wiriya Thongruang**<sup>1</sup>, C. Maury Balik<sup>1</sup>, and R. J. Spontak<sup>2</sup>. <sup>1</sup>Dept. of Material Sciences and Engineering, and <sup>2</sup> Dept. of Chemical Engineering, NCSU



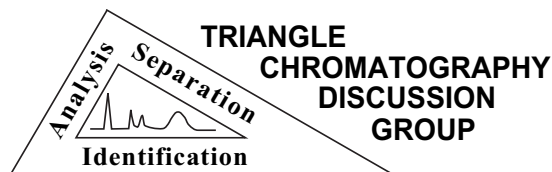


## SERMACS 2004 Organization Meeting

The NC-ACS will host the 2004 Southeastern Regional Meeting of the American Chemical Society (SERMACS). Believe it or not, it is time to start planning. SERMACS 1998, held in RTP, was one the most successful regional meetings ever in the history of ACS. Those of us who organized the meeting in 1998 are optimistic that we can make SERMACS 2004 even better. A site selection committee has identified potential sites and dates for the SERMACS 2004.

An organizational meeting will be held at 2:15 p.m., April 21<sup>st</sup> immediately following the general session/luncheon at the 115th Local Section Conference, in Dabney Hall on the campus of North Carolina State University (room124). Anyone interested, or thinking about being interested, is encouraged to attend. The organization of this meeting is a team effort. Those involved in the early stages of the planning will shape the ever so important technical program, as well as the other meetings activities. The committee structure will consist of a General Chair (or co-chairs) who will lead the efforts of the following committees: General Program, Symposium, Exhibition, Development, Finance, Publicity and Printing, Workshops, Banquets and Special Programs, Public Relations, Undergraduate Program, Registration, Housing and Transportation, and Facilities. A job description of each of the committee chairs can be found at [http://membership.acs.org/N/NCarolina/serm\\_job\\_descriptions.html](http://membership.acs.org/N/NCarolina/serm_job_descriptions.html)

If interested in participating in the organization of the meeting, please contact any member of the Executive Committee or Brad Sturgeon ([sturgeon@ncssm.edu](mailto:sturgeon@ncssm.edu), 919-286-3366 x223). Hope to see you there!



## The 18th Annual TCDG Symposium & Instrument Exhibit

Thursday May 17th, 2001  
At the  
Jane S. McKimmon Center  
North Carolina State University  
Raleigh, NC

### Invited Speakers:

**Irving W. Wainer**, Georgetown University  
"Immobilized Receptor-Based Liquid Chromatographic (LC) Stationary Phases: A New Paradigm for the Use of LC in Pharmacology and Drug Discovery"

**Christa Colyer**, Wake Forest University  
"Using Lasers To Determine Proteins in Capillary Electrophoresis"

**Roy Williams**, Old Dominion University  
"Applications of HPLC for Wine Constituents and Related Natural Products"

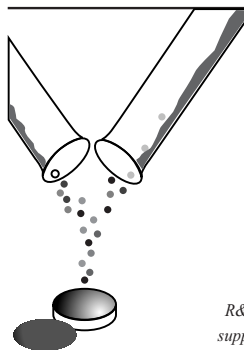
**Patricia A. Hyldborg**, Magellan Laboratories  
"Meeting FDA Expectations for Instrument Qualification"

**Gary D. Bowers**, GlaxoSmithKline  
"LC/MS(/MS) Methodologies for the Identification of Drug Metabolites in Complex Biological Matrices"

**Wil van Egmond**, ATAS International  
"Routine Rapid Large Volume Injections with Innovative Analytical Solutions for Hyphenated Techniques"

For More Information, See <http://RTPnet.org/tcdg>

**Please Plan to Attend!**



*EISAI INC., an international pharmaceutical company located in Research Triangle Park, NC, is committed to innovation through world class R&D facilities, programs and scientific staff. We currently have an opening for a professional who can make an immediate impact in our cutting-edge*

*R&D facility and who is also looking for a challenging and supportive environment.*

## RESEARCH ASSOCIATE PRODUCT DEVELOPMENT

The successful candidate will support parenteral formulation development from discovery to scale-up activities. This includes physicochemical characterization of new chemical entities (e.g., pKa, solubility, stability) to demonstrate formulation feasibility. Other requirements include investigating various techniques and excipients needed to develop parenteral formulations, participating in technical teams, and presenting data to internal and external audiences. Must have an aptitude to assist in experimental design, data interpretation, and in the preparation of reports describing scientific experiments. Strong oral and written skills along with the ability to work in a team environment are required.

Qualifications include a BS or MS in a relevant scientific discipline (e.g., chemistry, pharmaceuticals). Laboratory experience preferred.

**EISAI** offers intellectual challenges, state-of-the-art facilities and a generous benefit package in a growth-oriented environment. **EISAI** also offers a unique opportunity to shape the future of human health care for generations to come... a place where your individual innovation and accomplishments will be recognized and rewarded.

Please mail or fax your resume and academic transcripts to: **EISAI INC., 900 Davis Dr., P.O. Box 14505, Research Triangle Park, NC 27709; Fax: (919) 941-0511.** (No Calls, Please)  
Equal Opportunity Employer M/F.

[www.eisai.com](http://www.eisai.com)

© 2001 NAS  
(Media: delete copyright notice)  
Original Art

### Entry Level Organic Chemist

ARCADIS Geraghty & Miller, a dynamic international leader in the architectural engineering and environmental services industry is seeking the following professional to join our Durham Technology Office. We offer a great benefits package. EOE M/F/D/V

**AGM-01-035** - BS/BA Chemistry and 0-2 yrs experience or equivalent. Will prepare environmental samples for analysis using extraction and concentration procedures. Knowledge of gas chromatography a plus. Please send your resume, including salary history, in confidence to: Email to: [arcadis@rpc.webhire.com](mailto:arcadis@rpc.webhire.com)

ARCADIS Geraghty & Miller, P.O. Box 13109, RTP, NC 27709. Reference job code in response

**RESEARCH TRIANGLE INSTITUTE - CHEMIST 1**

Degree: BS degree in Chemistry

This individual will provide analytical chemistry support for toxicity studies. Laboratory tasks will primarily involve development of methods for quantitative analysis of test chemicals in biological matrices, validation of analytical methods, stability studies of test chemicals in biological matrices, analysis of test chemicals and metabolites in biological matrices, analysis of data, and report writing. Laboratory tasks may also include purity determination, development of methods for quantitative analysis of test chemicals in dose formulations, stability studies of test chemicals in dose formulations, and dose analysis. Techniques utilized will primarily be chromatographic (GC and HPLC) and rarely spectroscopic (UV, IR, NMR, and MS). This individual will contribute to lab maintenance and instrument personal computers (Windows 95/98/NT, Microsoft WORD, and Microsoft EXCEL spreadsheets at a minimum with use of automated chromatographic data acquisition systems preferred) and possess excellent math, writing, and organizational skills. For more information see: <http://membership.acs.org/N/NCarolina/jobs/rti01mar.pdf>

**Postdoctoral Position.**

Synthesis of pharmacologically active heterocyclic compounds and related activities. Experience in molecular modeling and CADD is helpful. The position is available immediately at 25-30 K and is potentially renewal depending on the availability of grant funds. To apply send CV and names of three references to Dr. Robert A. Izydore, Department of Chemistry, NCCU, Durham, NC 27707, or preferably send all information to rzydore@wpo.nccu.edu. See the Department of Chemistry, NCCU web site

(<http://www.nccu.edu/artsci/chemistry/izydor.html>)

for further information concerning the organic synthesis. NCCU is an equal opportunity employer.

**Organic Chemistry Lecturer at Duke University**

The Chemistry department at Duke seeks to fill a nine-month visiting lecturer position. The position will begin two weeks prior to the fall, 2001 semester. Duties will include lecturing, coordination of introductory organic chemistry sections, and supervision of associated laboratories. Salary will be based upon experience. For full consideration, interested candidates should forward curriculum vitae, three letters of recommendation, and a cover letter to:

Organic Lecturer Search  
P.M. Gross Chemical Laboratories  
Duke University  
Box 90346  
Durham, NC 27708

Duke University is an Affirmative Action / Equal Opportunity Employer and is eager to identify minority persons and women with appropriate qualifications.

**Hazardous Materials Manager**

The University of North Carolina at Chapel Hill is seeking a Hazardous Materials Manager to join our Health and Safety team. The position reports to the University Environmental Affairs manager. The selected candidate will be responsible for the management of all aspects of the University's RCRA Part B Treatment, Storage, and Disposal (TSD) facility, including supervision of four facility technicians, assisting in emergency spill responses, and management of a low-level radioactive waste program.

Minimum requirements include a Bachelor's degree in chemistry or a closely related field and two years progressive experience in hazardous material/waste management. Prefer prior experience managing a RCRA facility, conducting training of laboratory personnel, and implementing waste minimization programs.

For an application, phone (919) 962-2991 or apply at: Employment Department, Office of Human Resources, The University of North Carolina at Chapel Hill, CB #1045, 725 Airport Road, Chapel Hill, NC 27599-1045; or applications are available on the University website [www.job.unc.edu](http://www.job.unc.edu). For additional information, please contact Rich Miller, Environmental Affairs Manager at (919) 962-5718.

**Senior Associate Research Scientist in Analytical Development - Code # PACC1061**

needed immediately with Bayer Corporation's Plasma Manufacturing Facility located in Clayton, NC. This position provides analytical support for the development of new Biological Products. Responsibilities include the development and validation of analytical methods for protein-based pharmaceuticals. The individual selected will work closely with various groups involved in the characterization and testing of new and existing products, including Research, Product Development and QA/QC.

**Associate/Senior Associate Developmental Scientist**

Will provide analytical support for existing analytical methods in association with QC Biology and Biochemistry laboratories. Will direct validation studies for new assay methods including preparation of protocols and reports for such studies that are suitable for review by national and international regulatory agencies. Responsibilities will include writing test procedures, test method validation reports, method development reports and investigative reports. Will interact with various groups such as Compliance, Regulatory Affairs and Validation.

Please forward your resume along with referencing code number to: Bayer Corporation, Pharmaceutical Division, P.O. Box 3238, Scranton, PA 18505-0238. Fax: 1-888-805-7474. E-mail: [bayerpharma@alexus.com](mailto:bayerpharma@alexus.com).

In addition please E-mail your resume to [kathleen.fleming.b@bayer.com](mailto:kathleen.fleming.b@bayer.com) for direct consideration. For more information on Bayer, please visit our website at [www.bayerpharma-na.com](http://www.bayerpharma-na.com). No agencies or phone calls please.

# The TarHelium 31:4

Bradley E. Sturgeon, Editor  
North Carolina School of Science and Mathematics  
P. O. Box 2418, Durham, NC 27715

PRST STD  
US POSTAGE  
PAID  
RALEIGH, NC  
PERMIT #1854

## Executive Committee:

|  |                |   |
|--|----------------|---|
| C. M. Balik (NCSU), Chair, '01                               | 515-2126       | <i>balik@ncsu.edu</i>                   |
| S. C. J. Sumner (CIIT), Chair-Elect '01                      | 558-1343       | <i>sumner@ciit.org</i>                  |
| S. Levine (NCSU), Secretary '00-'01                          | 513-2585       | <i>slevine@pams.ncsu.edu</i>            |
| J. T. Bursey (ERG), Treasurer '01-'02                        | 468-7926       | <i>jburse@erg.com</i>                   |
| B. E. Sturgeon (NCSSM), TarHelium Editor '00-present         | 286-3366       | <i>sturgeon@ncssm.edu</i>               |
| A. L. Crumbliss (Duke), Councilor '01-'03                    | 660-1540       | <i>alc@chem.duke.edu</i>                |
| R. A. Palmer (Duke), Councilor '01-'03                       | 660-1539       | <i>rap@chem.duke.edu</i>                |
| J. L. Chao (IBM), Councilor '00-'02                          | 543-3054       | <i>jchao@us.ibm.com</i>                 |
| E. C. Bigham (GSK), Councilor '99-'01                        | 483-9844       | <i>ecb12781@glaxowellcome.com</i>       |
| R. W. Morrison, Jr. (NCSU), Councilor '99-'01                | 515-2549       | <i>robert_morrison@ncsu.edu</i>         |
| S. T. Purrington (NCSU), Alt. Councilor, '01-'03             | 515-2864       | <i>purringt@chemdept.chem.ncsu.edu</i>  |
| E. T. Samulski (UNC), Alt. Councilor, '01-'03                | 962-1562       | <i>et@unc.edu</i>                       |
| W. Powell (Meredith), Alt. Councilor '00-'02                 | 760-8619       | <i>powellw@meredith.edu</i>             |
| J. D. Martin (NCSU), Alt. Councilor '99-'01                  | 515-3402       | <i>jdmartin@chemdept.chem.ncsu.edu</i>  |
| W. L. Switzer (NCSU), Alt. Councilor '99-'01                 | 515-2945       | <i>bill_switzer@ncsu.edu</i>            |
| G. H. Wahl, Jr. (NCSU), Past Chair '99                       | 515-2941       | <i>george_wahl@ncsu.edu</i>             |
| R. J. Linderman (Pharmacia) Past Chair '98                   | (847) 982-8153 | <i>Russell.J.Linderman@monsanto.com</i> |
| M. M. Bursey (UNC), Ex Officio                               | 493-3025       | <i>mbursey@acs.org</i>                  |
| K. A. Cutler (Hillside High School), Project Seed Ex Officio | 560-3925       | <i>NCProjectSEED@aol.com</i>            |
| E. L. Eliel (UNC), Ex Officio                                | 962-6198       | <i>eliel@unc.edu</i>                    |
| T. A. Lehman (UNC-CH), Ex Officio                            | 966-0581       | <i>talehman@intrex.net</i>              |
| D. G. Morgan (GSK), TAMS, Ex Officio                         | 483-4291       | <i>dm19700@glaxowellcome.com</i>        |
| D. Canelas (Lord), PDG, Ex Officio                           | 469-2500       | <i>dorian_canelas@lord.com</i>          |
| P. Hyldburg (Magellan ), TCDG, Ex Officio                    | 465-8430       | <i>pahyld@magellanlabs.com</i>          |
| T. M. O'Connell (GSK), TMRDG, Ex Officio                     | 483-1535       | <i>tmo89509@glaxowellcome.com</i>       |
| D. S. Coleman (Eli Lilly) YCC, Ex Officio                    | 314-4352       | <i>dscoleman@lilly.com</i>              |

**Dated Material - Please Deliver Promptly**

---

## The TarHelium

The TarHelium is a publication of the North Carolina Section of the American Chemical Society. The views expressed herein are not necessarily those of the Section. Public lectures and seminars as well as announcements of interest to the ACS membership will be listed as deemed appropriate by the editor and as space permits. Short commentaries or contributed articles will also be considered. Also, we are happy to publicize, free of charge, any job openings for chemists. We also accept paid advertisements for more extensive recruiting announcements. The Deadline for each publication is usually the first of the month prior to publication.

## NC Section Electronic Communications

The NC Section of the ACS offers two services which may be of interest to members: 1) a listserver and 2) a web page: <http://membership.acs.org/N/NCarolina/>.

The listserver is used for ACS meeting announcements and for job announcements. Unlike some lists, the number of postings is quite limited--usually no more than 3 or 4 a month. This list is moderated, which means that all messages must be approved by the list owner before they are posted. If you have a valid opening within the NC Section, please mail an appropriate announcement to [bill\\_switzer@ncsu.edu](mailto:bill_switzer@ncsu.edu). Very occasionally openings outside of the NC Section are posted. If you wish to subscribe, address mail to: [listserv@listserv.ncsu.edu](mailto:listserv@listserv.ncsu.edu). The subject field is ignored, but in the message field type: `subscribe ncacs first_name last_name`. Your name is required; spaces are allowed. Your return address becomes your subscription address. These instructions as well as those for removing your name are linked to the web page.

If you have not looked at the web page recently, please do so. The Executive Committee is committed to making this page a useful resource. It is constantly being updated to include new information. Please feel free to suggest additional links and PLEASE offer to take responsibility for maintaining one or more of the local links. Contact: [bill\\_switzer@ncsu.edu](mailto:bill_switzer@ncsu.edu).

---