



Bradley E. Sturgeon, *Editor*

Judi Price, *Copy Editor*
Sol Levine, *Address Information*
Custom Mail Solutions,
Printing/Mailing



NCACS
EXECUTIVE
COMMITTEE

J. A. Myers, Chair 2003
D. S. Coleman, Chair Elect
S. Levine, Secretary
J. T. Burse, Treasurer

The TarHelium
Volume 33: Number 4
Bradley E. Sturgeon, *Editor*
4400 Currie Court
Raleigh, NC 27613

117TH NORTH CAROLINA-ACS SECTIONAL CONFERENCE



Saturday, April 26th, 2003
University of North Carolina
Kenan and Venable Halls

The program for the 117th NC-ACS Sectional Conference features 78 submitted papers (47 oral and 31 poster presentations) divided into eight concurrent sessions. The oral and poster presentations will take place from 8:20–11:40 am. The General Session will be held immediately after the technical program. During the General Session the 2003 Marcus E. Hobbs Award will be presented, in addition to other awards. The General Session will conclude with the 2003 NC-ACS Distinguished Chemist Lecture presented by Dr. Mansukh C. Wani of Research Triangle Institute, RTI International. Lunch will follow immediately.

REGISTRATION AND LUNCH RESERVATIONS

Everyone planning to stay for lunch please register online at the main NC-ACS web page: <http://membership.acs.org/N/NCarolina> or by contacting the program chair (Darrell Coleman) via phone (919-314-4352), FAX (919-314-4347), or email (dscoleman@lilly.com) no later than April 22, 2003. Please register promptly so that we have an accurate head count for lunch. Registration is free and includes a coffee break and a buffet luncheon provided by ARAMARK Services. The meeting registration table will open at 7:50 am. Upon arrival at the meeting, stop by the registration table to pick up a program, name tag, and your lunch ticket which is located in Kenan Laboratory the entrance way between Kenan Tower A and B (beside the underpass).

INSTRUCTIONS TO PRESENTERS

Please send program corrections to the program chair (dscoleman@lilly.com).

Oral Presentations

It is a professional courtesy to speak within your allotted time. All oral presentations will be 20 minutes; preferably a 15-minute presentation with 5 minutes for questions. The chair of the session will coordinate the session. Each room will be equipped with an overhead projector, and a solid pointer. If you prefer a laser pointer please bring your own. Only select rooms will be equipped with a computer-interfaced projection system.

Poster Presentations

Poster presenters are expected to be at their posters during the session "discussion times" (see the program). Poster boards will be set up in a designated area. The poster boards will be labeled with poster numbers and session abbreviations (i.e. 11-ANYL). Poster board dimensions are 4 feet by 5 feet; please bring your own tacks. Have your poster up by 8:30 am and please leave it up until lunch.

(continued on page 2)

UPDATE YOUR CHANGE OF ADDRESS

With each mailing of the TarHelium, there are always some returned to the section (at a fee) due to an incorrect or obsolete address.

To make sure you receive your local section information on time, notify the ACS with any address changes. To update your records online, just log onto

<http://center.acs.org/applications/addrupdate/addrchange.cfm>



**NCACS
EXECUTIVE
COMMITTEE**

J. A. Myers, Chair 2003
D.S. Coleman, Chair Elect
S. Levine, Secretary
J. T. Bursley, Treasurer
B. E. Sturgeon, Editor
A. L. Crumbliss
R. A. Palmer
J. L. Chao
E. C. Bigham
R. W. Morrison, Jr.
R. M. Forbis
S. T. Purrington
S. Sendlinger
E. T. Samulski
W. Powell
W. L. Switzer,
G. H. Wahl, Jr.
C. M. Balik
S. J. Summer
M. M. Bursley
K. A. Cutler
E. L. Eliel
D. G. Morgan, TAMS
K. Dawes, PDG
J. Hines, TCDG
T. M. O'Connell, TMRDG

DIRECTIONS/PARKING

Maps and driving directions are available at: http://www.chem.unc.edu/home_page/maps_and_directions.html

From Interstate 40 (from Raleigh and points east):

Take Exit 273-B (Hwy 54) towards Chapel Hill. Continue straight for 4 miles to the top of the hill. Park at UNC Visitor Parking Lot on right before traffic light*

From Interstate 85 (coming from Charlotte, Winston-Salem, and Greensboro):

take I-40 East towards Raleigh. Take Exit 273 and turn right at the end of the exit ramp. Continue straight for 4 miles to the top of the hill. Park at UNC Visitor Parking Lot on right before traffic light*

From Interstate 85 North (from Durham and points north):

Follow I-85 to intersection with Hwy 15-501 South. Follow 15-501 South towards Chapel Hill; the highway will divide. Remain on 15-501 South (Bypass) bearing left, away from Franklin Street. Turn right at Highway 54 Exit towards "UNC-Chapel Hill". Continue to the top of the hill. Park at UNC Visitor Parking Lot on right just before traffic light*

ACKNOWLEDGEMENTS

The NC-ACS Local Section gratefully acknowledges the University of North Carolina for hosting this event, and Dr. Dick Forbis and his colleagues of the Chemistry Department for coordinating the use of the UNC facilities.

Darrell S. Coleman
NCACS Program Chair
Eli Lilly - RTP
20 T.W. Alexander Drive
Research Triangle Park, NC 27709
dscoleman@lilly.com

TECHNICAL PROGRAM

Note: Posters will be displayed from 8:30–12:00 noon. Presenters will be available for discussion at poster presentation times below.

General Session

Awards, NC Distinguished Lecture 11:50 am – 1:10 pm
Lunch 1:15 pm

Analytical Chemistry (ANYL-1) - Venable Hall Room 223

Oral Presentations 8:00 am – 11:00 am
Poster Presentations During Sessions Break Time

Analytical Chemistry (ANYL-2) - Venable Hall Room 224

Oral Presentations 8:40 am – 11:40 am
Poster Presentations During Sessions Break Time

Biochem/Medchem/Organic (BMO) - Venable Hall, Room 221

Oral Presentations 8:20 am - 11:40 am
Poster Presentations During Sessions Break Time

Inorganic/Physical Chemistry (INOR/PHYS) - Venable Hall Room 222

Oral Presentations 8:00 am – 11:40 am
Poster Presentations During Sessions Break Time

Organic/Biochemistry/Med (ORGN/BIO/MED) - Venable Hall Room 221

Oral Presentations 8:20 am – 11:40 am
Poster Presentations During Sessions Break Time

NMR Discussion Group (NMR) - Venable Hall Rm 268

Oral Presentations 8:00 am – 11:40 am
Poster Presentations During Sessions Break Time

Polymer Chemistry (POLY/NMR) - Venable Hall Rm 222

Oral Presentations 9:40 am - 11:40 am
Poster Presentations During Sessions Break Time

Chemical Education (CHED) - Venable Hall Rm 308

Oral Presentations 8:30 am – 11:40 am
Workshop Presentations 2:00 pm – 5:00 pm

GENERAL SESSION*Lecture Hall Auditorium*

11:50 am – 1:10 pm, 1:15 pm Buffet Lunch*

John Myers, NC-ACS Chair, presiding

- Presentation of the 2003 Marcus E. Hobbs Award
- Recognition of the 50-year ACS Members
- Presentation of the 2003 Barbara Whittaker Award
- Recognition of the Undergraduate Scholarship Awards
- Recognition of the 2002 ACS ChemLuminary Award
- Presentation of the 2003 NC-ACS Distinguished Speaker Award to:

Dr. Mansukh C. Wani, Ph.D.
 Research Triangle Institute
 Research Triangle Park, NC 27709-2194

“Taxol: From Landfill to Landmark”

Taxol, a potent antitumor agent, was isolated from a tree, *Taxus brevifolia*, by procedures guided by bioactivity. Final isolation in pure form was accomplished using repeated Craig Countercurrent Distribution (CCD). The structure of Taxol was determined by a combination of chemical degradation and single crystal x-ray analysis. It is a diterpene ester with unique structural features and eleven asymmetric centers. The compound displayed considerable cytotoxic and antitumor activity, particularly toward B-16 melanoma. Taxol binds strongly to tubulin by a unique mechanism. Early clinical trials with patients with ovarian cancer showed remarkable efficacy resulting in complete and partial remissions. Taxol has received much chemical study, particularly in regard to structure/activity relationship (SAR), semi- and total synthesis. It is currently regarded as one of the best new anticancer agents. This lecture will present the salient features involved in the discovery of Taxol and will describe the 25-year efforts which transformed this compound from interesting plant secondary metabolites to a useful clinical chemotherapeutic agent.

Introduction by Nicolas H. Oberlies, Ph.D.
 Dept. of Chemistry, NCSU

*LUNCH will be served in the Kenan lobby beside the registration table immediately after the General Session and NC-ACS 2003 Distinguished Speaker's lecture.

**ANALYTICAL CHEMISTRY (ANYL-1)***Venable Hall, Room 223*

8:00 am – 11:00 am

8:00 01-ANYL. Band-Broadening in Isocratic Ultra-High Pressure Liquid Chromatography.

Jerkovich, Anton D., J. Scott Mellors, J. Will Thompson, James W. Jorgenson; UNC-Chapel Hill.

8:20 02-ANYL. Development and performance of radio frequency circuitry for an electrically tunable compensated cylindrical ion trap mass spectrometer. **Kaplan, Desmond A.**, Gary Glish; UNC-Chapel Hill.

8:40 03-ANYL. A Novel Method for Measuring Diffusion Coefficients using Capillary Electrophoresis and Diode Array Detection. **Theftord, Christine M.**, James W. Jorgenson; UNC-Chapel Hill.

9:00 04-ANYL. Analytical Methods for the Determination of 3,3',4,4'-Tetrachloroazobenzene and 3,3',4,4'-Tetrachloroazoxybenzene in Environmental Matrixes. **Heltsley, Rebecca M.**, Damian Shea; NCSU.

9:20 Break

9:40 05-ANYL. The Application of SUPREX to Large, High Molecular Weight Proteins. **Dai, Susie Y.**, Michael C. Fitzgerald; Duke University.

10:00 06-ANYL. Ultra-High Voltage Capillary Electrophoresis. **Henley, Wm. Hampton**, James W. Jorgenson, UNC-Chapel Hill.

10:20 07-ANYL. Electron Transfer in Networked Films of Monolayer Protected Clusters. **Brennan, Jennifer L.**, Jocelyn F. Hicks, Andrea Osiek, Royce W. Murray; UNC-Chapel Hill.

10:40 08-ANYL. A Tool for Screening the Food Supply for Arsenic and Mercury Contamination. **Essader, Amal**, G. Ross, K. Levine, R. Fernando; RTI, International.

ANALYTICAL CHEMISTRY (ANYL-2)*Venable Hall, Room 224*

8:40 am – 11:40 am

9:00 09-ANYL. Spectroelectrochemistry of Monolayer Protected Gold Clusters. **Harper, Amanda S.**, Victoria L. Jimenez, Dongil Lee, Robert L. Donkers, Royce W. Murray; UNC-Chapel Hill.

9:20 10-ANYL. Peptide Sequencing in a Quadrupole Ion Trap utilizing Thermally Assisted Collision Induced Dissociation. **Racine, Alawee H.**, Anne H Payne, Gary L. Glish; UNC-Chapel Hill.

GENERAL SESSION**ANYL-1**

 ANYL-2

9:40 11-ANYL. Study of Relative Collisional Cooling Rates in a Quadrupole Ion Trap using Thermally Assisted Infrared Multiphoton Photodissociation, **Black, David M.**, Anne H Payne, Gary L. Glish; UNC-Chapel Hill.

10:00 Break

10:20 12-ANYL. Ultra-High Pressure LC and MS of Peptides from Complex Mixtures. **Link, Jason C.**, James, W, Jorgenson; UNC-Chapel Hill.

10:40 13-ANYL. Vapor Sensing with MPC Films. **Georganopoulou, Dimitra.**, Robert L. Donkers, Michael C. Leopold, and Royce W. Murray; UNC-Chapel Hill.

11:00 14-ANYL. A MALDI Mass Spectrometry-Based High Throughput Screen for the Detection of Protein-Ligand Interactions in Solution. **Powell, Kendall D.**, Michael C. Fitzgerald; Duke University.

11:20 15-ANYL. Development and Application of a New H/D Exchange- and Mass Spectrometry-Based Protocol for the Thermodynamic Analysis of Protein Folding Reactions. **Tong, Yan**, Michael C. Fitzgerald; Duke University.

 ANALYTICAL CHEM. POSTER SESSION

Kenan Lobby (near registration)
During Session Breaks

16-ANYL. The Effects of Glucose Binding with Self-Assembled Monolayers containing Boronic Acid through an Electrochemical Method. **Allen, Angela M.**, Christopher B. Gorman, NCSU.

17-ANYL. A Study of Fluorescence of Gold Monolayer Protected Clusters. **Wang, Gangli.**, Jian Zhang, Robert Donkers; UNC-Chapel Hill.

18-ANYL. Photothermal Beam Deflection Spectroscopy Using Solid Deflection Media. **Gillikin, Angela M.**, Richard A. Palmer; Duke University.

 BIOCHEM/MEDCHEM/ORGANIC (BMO)

Venable Hall, Room 221
8:20 am - 11:40 am

8:20 01-BMO. A New Platform For Telomerase Inhibition. **Kepler, Brian R.**, Michael B. Jarstfer; UNC-Chapel Hill.

8:40 02-BMO. The Nascent DNA-Template RNA Interactions in the Telomerase Active Site Revealed with Nucleotide Analogs. **Jarstfer, Michael B.**, Pamela K. Dominick; UNC-Chapel Hill.

9:00 03-BMO. Nucleic Acid Recognition with Beta Hairpin Peptides. **Butterfield, Sara M.**, Marcey L. Waters; UNC-Chapel Hill.

9:20 Break

9:40 04-BMO. Ligand Density Control Surfaces - Stretching the Limits of Biomaterials. **Chaney, Bryce N.**, Andrea Liebmann-Vinson(1), Mohammad Heidarani(1), Jan Genzer(2), Kiril Efimenko(2); (1) BD Technologies (2) NCSU.

10:00 05-BMO. Electronic Structure of Biomolecular Systems (Nitrogenase, Fe-Porphyrin). **Bajdich, Michal**, Lubos Mitas, Zachary Helms; NCSU.

10:20 06-BMO. Antiviral Activity of substituted 1-Hydroxyacridones. **Lowden, Christopher T.**, Kenneth Bastow, UNC School of Pharmacy.

10:40 Break

11:00 07-BMO. Catalytic Enantioselective Diboration of Alkenes: Access to Versatile Reactive Chemical Intermediates. **Morgan, Jeremy B.**, Steven P. Miller, James P. Morcken; UNC-Chapel Hill.

11:20 08-BMO. Isotopically Chiral Probes for *in situ* High-Throughput Asymmetric Reaction Analysis. **Evans, Michael A.**, James P. Morcken; UNC-Chapel Hill.

 BIO/MED/ORG POSTER SESSION

Kenan Lobby (near registration)
During Session Breaks

09-BMO. The Template-Active Site Interaction in the T. thermophila Telomerase Enzyme. **Legassie, Jason D.**, Michael B Jarstfer, UNC-Chapel Hill.

10-BMO. Synthesis of Acyclonucleoside alpha-P-Boranotriphosphate and Evaluation as A Substrate for Retroviral Reverse Transcriptase. **Liu, Hongyan**, Ping Li, Hongyan Liu, Mikhail Dobrikov, and Barbara Ramsay Shaw; Duke University.

11-BMO. Novel Phenylaminotetralin Analogues Selectivity Activate Histamine H1 Receptors Coupled to IP vs. cAMP Signaling Pathways to Stimulate Tyrosine Hydroxylase. **Moniri, Nader H.**, Raymond G. Booth; University of North Carolina - Chapel Hill.

12-BMO. Design of Novel Histamine H₁ Agonists: (\pm)-2-Dimethylamino-5-phenyl-1,2,3,4-tetrahydronaphthalene. **Legere, Jacqueline A.**, Raymond G. Booth, Nader H. Moniri; Dept. of Medicinal Chemistry, UNC Chapel Hill.

13-BMO. Calcineurin is an inhibitor of phospholipase C-dependent inositol phosphate production in *Saccharomyces cerevisiae*. **Cornea, Anda M.**, John D York; Dept. of Biochemistry, Duke University.

 BMO

 ANYL POSTERS

INORGANIC/MATERIALS/PHYSICAL (IMP)*Venable Hall, Room 222***8:00 am – 11:40 am**

8:00 01-IMP. Synthesis and Characterization of Multi-Stable Co[bis(o-benzoquinone)(bpy)] Magnetic Molecules. **Bin-Salamon, Sofi**, David A. Shultz; NCSU.

8:20 02-IMP. Kinetics and Mechanism of Iron(III) Dissociation from a New Saccharide Based Exocyclic Trihydroxamate Analogue of Ferrichrome. **Dhungana, Suraj**, S. Heggemann(2), P. Gebhardt (2), U. Moellmann (2), A. L. Crumbliss(1), (1) Duke University, (2) Hans Knöll-Institut für Naturstoff-Forschung, Jena, Germany.

8:40 03-IMP. Temperature Dependence of Interligand Electron Transfer in OsII(bpy)₃²⁺. **Granger, Jeremy C.**, David Styers-Barnett (1), George Shaw (2), John Papanikolas (1); (1) UNC-Chapel Hill, (2) Argonne National Lab.

9:00 Break

9:20 04-IMP. Electrochemical Behavior of Novel Redox Active Azacrown Ethers. **Wirgau, Joseph I.**, J. W. Sibert (1), A. L. Crumbliss (2), (1) The University of Texas at Dallas, (2) Duke University.

9:40 05-IMP. Effects of Dendritic Architecture on Dendrimer Encapsulation. **Chasse, Tyson L.**, Qun Li, Zemin Li, Rakesh Sachdeva, Dr. Christopher Gorman; NCSU.

10:00 06-IMP. Iron Transport Across a Novel Polymer Inclusion Membrane. **Taheri, Saeed**, Joseph I. Wirgau, Alvin L. Crumbliss, Duke University.

10:20 Break

10:40 07-IMP. Lifting of Ions out of Solution by Laser Vaporization of non-Aqueous Aerosol Particles. Dessiaterik, Yury N., Teresa Nguen, Roger E. Miller, Tomas Baer; UNC-Chapel Hill.

11:00 08-IMP. Characterization of the Dynamics of Beta Sheet Formation by Time-Resolved Infrared Spectroscopy and Computational Modeling. Maness, Shelia J., Stefan Franzen (1), R. Brian Dyer (2); (1) NCSU, (2) Los Alamos National Laboratory.

11:20 09-IMP. Lipid Nanotube Arrays- a Spin-labeling EPR Study. Alaouie, Ali M., Alex I. Smirnov (1) and Oleg G. Poluektov (2); (1) NCSU, (2) Argonne National Laboratory.

INORG/MAT/PHYS POSTER SESSION*Kenan Lobby (near registration)*

During Session Breaks

10-IMP. The Effects of Au-Doping on Hydrogen-Saturated Silicon. **Helms, Zack**, Lucas Wagner(1),

Lubos Mitas(1), Munir Nayfeh(2), (1) NCSU, (2)University of Illinois at Urbana-Champaign.

11-IMP. Orientation of Liquid Crystals on Organized Molecular Films. **Russell, Joette M.**, Michi Nakata (1), Edward T. Samulski (2); (1) Tokyo Institute of Technology, (2) UNC-Chapel Hill

12-IMP. Polyacrylonitrile-based carbon nanofibers. **Zhang, Lei**, Bin Cheng, Edward T. Samulski; UNC-Chapel Hill.

13-IMP. Solution-phase Synthesis of One-dimensional Nanostructures. **Cheng, Bin**, Edward T. Samulski; UNC- Chapel Hill.

14-IMP. Supercritical CO₂ mediated intercalation of PEO in clay. **Zhao, Qian**, Edward T. Samulski; UNC-Chapel Hill.

NMR Discussion (NMR)*Venable Hall, Room 268***8:00 am – 11:40 am**

8:00 01-NMR. Solution structure of LpxC from Aquifex aeolicus in complex with a substrate analog inhibitor. **Zhou, Pei**, Brian E. Coggins, Xuechen Li, Ole Hindsgaul, Christian R.H. Raetz; Duke University Medical Center.

8:20 02-NMR. NMR Structure of the Targeting Domain of the Focal Adhesion Kinase (FAK) in Complex With a Paxillin Peptide. **Gao, Guanghua**, Kirk C. Prutzman(1), Michelle King-Brantley(2), Eugene F. DeRose(3), Robert E. London(3), Michael D. Schaller(2), Sharon L. Campbell(1); (1) Dept. of Biochem. & Biophysics, UNC-CH, (2) Dept. of Cell & Develop. Biology, UNC-CH, (3) NIEHS.

8:40 03-NMR. Rethinking the structure-function paradigm with SLBP and histone mRNA. **Thapar, Roopa.**, Department of Biochemistry and Biophysics, UNC-CH.

9:00 04-NMR. Dynamics of the RNase H Domain of HIV-1 Reverse Transcriptase in the Presence of Magnesium and AMP. **Mueller, Geoffrey A.**, Koteppa Pari, Eugene F. DeRose, Thomas W. Kirby, Robert E. London; NIEHS.

9:20 05-NMR. New Insights into Protein Energetics and Dynamics from a PDZ-Ligand Interaction. **Lee, Andrew L.**; Ernesto J. Fuentes (2); 07: University of North Carolina (1), Lineberger Comprehensive Cancer Center (2).

9:40 06-NMR. DNA Structural Studies by NMR. From Quadruplexes to Interstrand Cross-Links. **Webba da Silva, Mateus**, DUMC, Dept. of Medicine.

10:00 Break**IMP****NMR****NMR**

10:20 07-NMR. NMR of Lipid A (Endotoxin) from Bacteria by ^1H Observe, Selective ^{31}P Excite NMR Methods. **Ribeiro, Anthony A.**, Zhimin Zhou, M. Stephen Trent, Steven D. Breazeale and Christian R. H. Raetz; Duke University Medical Center.

10:40 08-NMR. Spectroscopic Validation of Structures Assisted By Prediction and Auto-assignment Algorithms - Verification Analysis of High-Resolution ^1H and ^{13}C NMR spectra. **Williams, Antony J.**, Brent Lefebvre, Mikhail Kvasha, Dmitry Mityushev, and Sergey Golotvin; Advanced Chemistry Development.

11:00 09-NMR. Deuterium NMR Studies on Rodlike and Bent-Core Liquid Crystals Using a Novel High-Temperature Rotation Probe. **Madsen, Louis A.**, Theo J. Dingemans, Edward T. Samulski; UNC-Chapel Hill Chemistry.

11:20 10-NMR. A High Pressure NMR study of Self-assembly Structures Formed with Phosphate Surfactants in Liquid CO_2 . **Xu, Bin**, Joseph M. DeSimone (1)(2), Charles S. Johnson, Jr. (1); (1) UNC-Chapel Hill, (2) Chem. Eng. Dept., NCSU.

11:40 10-NMR. Addressing Fundamental Questions about the Origin of Macromolecular Miscibility using Solid-State NMR. **Wolak, Justyna E.**, Xin Jia, Ed Stejskal, Hanna Gracz; NCSU.

NMR POSTER SESSION

Kenan Lobby (near registration)

During Session Breaks

12-NMR. Screening Analyte-Cyclodextrin Binding by ^1H ^{13}C Chemical Shift Mapping: Applications to Chiral Chromatography. **O'Connell, Thomas M.**, Michael P. Leblank, GlaxoSmithKline R&D.

13-NMR. Solution Structure of the 8 kDa Lyase Domain of Human DNA Polymerase Lambda. **DeRose, Eugene F.**, Thomas W. Kirby (1), Geoffrey A. Mueller (1), Katarzyna Bebenek (1), Miguel Garcia-Diaz (2), Luis Blanco (2), Thomas A. Kunkel (1), Robert E. London (1); (1) NIEHS, (2) Centro de Biología Molecular Severo Ochoa, Univ. Autonoma, Madrid, Spain.

14-NMR. NMR Studies of D-erythro and L-threo C16-Ceramides Under Physiological Conditions. **Gracz, Hanna**, Zdzislaw M. Szulc, Yusuf A. Hannun, and Alicja Bielawska, Department of Biochemistry and Molecular Biology, Medical University of South Carolina.

15-NMR. ^{15}N Chemical Shift Prediction - Databases, Algorithms, and Applications. **Williams, Antony J.**, Brent Lefebvre (1), Mikhail Kvasha (1), Dmitry Mityushev (1) Gary Martin (2); (1) Adv. Chem. Develop. (2) Pharmacia.

16-NMR. All Good Things to Those Who Wait - The Application of Automated Structure Elucidation Tools to Solve a Structure After 10 Years

of Human Effort!. **Williams, Antony J.**, Kirill Blinov(1), Mikhail Elyashberg (1), Gary Martin (2), Chad Hadden (2) Dave Russell (2); (1) Advanced Chemistry Development, (2) Pharmacia.

17-NMR. ^{13}C NMR Chemical Shift Prediction: A Comparison of Methods and a Case Study Analysis of Paclitaxel (TAXOL®). **Williams, Antony J.**, Brent Lefebvre; Advanced Chemistry Development.

18-NMR. Spectroscopic Validation of Structures Assisted By Prediction and Auto-assignment Algorithms - Verification Analysis of High-Resolution ^1H and ^{13}C NMR spectra. **Williams, Antony J.**, Brent Lefebvre, Mikhail Kvasha, Dmitry Mityushev, Sergey Golotvin; Advanced Chemistry Development.

19-NMR. The PACES Program: Protein NMR Sequential Assignment by a Computer-Assisted Exhaustive Search Method. **Coggins, Brian E.**, Pei Zhou; Department of Biochemistry, Duke Univ. Med. Center.

20-NMR. Acid-induced Rigidification of Eglinc at Low pH: Evidences from NMR Relaxation Experiment and MD Simulation. **Hu, Hao**, Jan Hermans (1,3), Andrew L. Lee (1-3); (1) UNC-Chapel Hill (2) School of Pharmacy (3) Depart. of Biochem. and Biophysics.

21-NMR. Clean Fuels Chemistry: Fundamental Mechanistic Investigations of Alkylate Formation by Solid State NMR. **Toporek, Stan S.**, Jeffery L. White, Matthew Truitt, Xingwu Wang; NCSU.

22-NMR. Dynamic Effects of Large-To-Small Mutations in Eglinc Extend to Non-Adjacent Side-Chains. **Clarkson, Michael W.**, Bin Cheng, Andrew L. Lee (1-3); (1) UNC-Chapel Hill (2) School of Pharmacy (3) Dept. Biochemistry and Biophysics.

23-NMR. New Strategies for Quantitative Spin-Diffusion Experiments in Amorphous Macromolecules. **Jia, Xin**, Justyna Wolak, J.L. White; NCSU.

24-NMR. Dynamic Response of a PDZ Domain Protein to Peptide Binding. **Fuentes, Ernesto J.**, Andrew L. Lee; UNC-Chapel Hill, School of Pharmacy.

POLYMERS (POLY)

Venable Hall, Room 222

9:40 am - 11:40 am

9:40 01-POLY. Benefits to Polymer Science by using Polymer-Cyclodextrin Inclusion Compounds. **Rusa, Cristian**, Tamer Uyar, Mariana Rusa, Alan E. Tonelli; College of Textiles, NCSU.

NMR
POSTERS

10:00 02-POLY. Encapsulation of Iron-Sulfur Clusters by Water-Soluble Dendrimers. **Cameron, Christopher S.**, Joseph Christopher B. Gorman, NCSU.

10:20 03-POLY. Monte-Carlo Study in Polymer Melt Dynamics. **Shirvanyants, David**, Michael Rubinstein; UNC-Chapel Hill.

10:40 Break

11:00 04-POLY. Synthetic Route To A Novel Acene-Type Conjugated Ladder Polymer. **Monceaux, Christopher J.**, Christopher B. Gorman, Christopher J. Monceaux, Won Jon Kwon, David A. Shultz; NCSU.

11:20 05-POLY. Synthetic Approaches to an Isostructural series of metal-trisbipyridine core dendrimers. **Hong, Young-Rae**, Christopher B. Gorman; NCSU.

POLYMER POSTER SESSION

Kenan Lobby (near registration)
During Session Breaks

06-POLY. Temperature-Dependent Dynamic Infrared Linear Dichroism Study of the Carbonyl Groups in Poly(ester urethane). **Wang, Yanqia**, Richard. A. Palmer (1), Steven R. Aubuchon (2); (1) Duke University, (2) TA Instruments, Inc.

07-POLY. Water Vapor and Carbon Dioxide Sorption in Cyclodextrin. **Hunt, Marcus A.**, Alan Tonelli (1), C. Maurice Balik (2(1) NCSU College of Textiles, (2) NCSU College of Engineering.

08-POLY. New Strategies for Quantitative Spin-Diffusion Experiments in Amorphous Macromolecules. **Jia, Xin**, Justyna Wolak, J.L. White; NCSU.

09-POLY. Dynamic Response of a PDZ Domain Protein to Peptide Binding. **Fuentes, Ernesto J.**, Andrew L. Lee; UNC-Chapel Hill, School of Pharmacy.

10-POLY. Reaction and Diffusion Kinetics in 'Icephobic' Epoxy-Siloxane Coatings. **Ayres, Jennifer A.**, C. M. Balik; NCSU.

11-POLY. Kinetics of Melt Complexation of Poly(ethylene glycol) into Solid-State Alpha-Cyclodextrin. **Peet, Jeffrey H.**, Jacqueline N. Gerken (1), Angelica M. Sanchez (2), Allan E. Tonelli (3), Charles M. Balik (1); (1) NCSU Materials Science and Engineering, (2) NCSU Chemical Engineering, (3) NCSU College of Textiles.

12-POLY. Preliminary Studies of Components for Two-Dimensional Ordering of Metallopolymers Through Linear Chain Interactions. **Allenbaugh, Rachel J.**, Cynthia K. Schauer and Ami Pateli; UNC-Chapel Hill.

13-POLY. Highly CO₂-Permeable and Selective Polymer Nanocomposite Membranes. **Patel, Nikunj P.**, Andrew C. Miller (1), Richard J. Spontak (2); (1) UIUC and (2) NCSU.

14-POLY. Entanglement studies in polymer solutions under theta condition **Chhajer, Mukesh.**, Michael Rubinstein; UNC-Chapel Hill

CHEMICAL EDUCATION (CHEMED)

Venable Hall, Room 308 (East Side & up steps)

8:30 am – 11:40 am

Moderator: Brad Sturgeon (UNC-Chapel Hill)

8:30, 01-CHEMED. Teaching General Chemistry Online. **Myra Halpin and Chuck Roser**; NC School of Science and Math, Department of Chemistry.

9:00, 02-CHEMED. Using Handheld Computers in the Chemistry Classroom. **Charles Ward**; UNC-Wilmington, Department of Chemistry.

9:30 03-CHEMED. Solution Incomplete Combustion with Candles: A Guided-Inquiry Experiment in the First-Year Chemistry Lab. **Lisa Volaric (1) and Joseph MacNeil (2)**; (1) UNC-Chapel Hill, Department of Chemistry, (2) Chatham College, Department of Chemistry.

10:00 Break

Chemistry and WebAssign Special Session

10:20 04-CHEMED. Introduction to Using WebAssign. **Bradley E. Sturgeon**; UNC-Chapel Hill, Department of Chemistry.

10:40 05-CHEMED. WebAssign Panel Discussion. **Moderator: Bradley E. Sturgeon (1); Panel: Myra Halpin (2), Chuck Roser (2), Zahra Syed (3), and Kay A. Sandberg (4)**; (1) UNC-Chapel Hill, Dept. of Chem., (2) NCSSM, Dept of Chem., (3) WebAssign, and (4) NCSU, Dept of Chemistry.

Chemical Demonstration Workshop:

2:00-3:30 06-CHEMED. Chemical Demonstration Workshop; Presented by the UNC-Chapel Hill Alpha Chi Sigma Fraternity (2 hrs).

3:30-4:30 07-CHEMED. Hands-On Demonstration of Handheld Computers in the Chemistry Classroom; Presented by UNC-Wilmington, Dept. of Chemistry (1 hr).

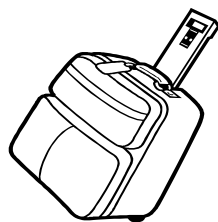
POLY

CHEMED

**EARTH
DAY**

**NEW NEW NEW BENEFIT FOR
YOU!!!!!!!**

The American Chemical Society announces its newest benefit for you the member. We are excited that we can offer you discounts on your next stay at any of the following hotels;



Ameri-Host
Days Inn
Knights Inn
Ramada Inn
Travelodge
Villager
Wingate Hotels

Take a minute and call 1-877-670-7088 to make your reservation, or call the hotel directly, mention the Society's discount #62871 and receive up to 20 percent off your next visit at any of the previously mentioned hotels.

**Patents — What Every
Chemist Should Know**

A new patent is granted every 3 minutes – 155,000 were granted by the U.S. government last year. The chemical sciences account for a significant portion of those patents. And for people in the chemical sciences, knowing how to register a patent or protect a patent is an important aspect of their professional skills.

To help chemists master the basics of intellectual property protection, the ACS Committee on Patents and Related Matters has released the printed version of the recently updated booklet, *What Every Chemist Should Know about Patents*. The booklet introduces important topics such as the basis for U.S. patent rights, an overview of the U.S. patenting process, how to obtain a patent, and how to extend patent protection to other countries.

Copies are available through the ACS Office of Society Services by calling 800-227-5558. The first copy is free, and additional copies are \$5 per copy. Bulk orders of more than 25 copies are \$3 each. The booklet is also available on the ACS Office of Legislative & Government Affairs Web site at <http://www.chemistry.org/government/patentprimer.pdf>

**CHEMISTS CELEBRATE
EARTH DAY, APRIL 22, 2003**

The American Chemical Society, Office of Community Activities, is pleased to invite you to join us as we celebrate Chemists



Celebrate Earth Day on April 22, 2003. The program is a joint effort between the National Chemistry Week Task Force, the Committee on Environmental Improvement, and the Green Chemistry Institute. Chemists Celebrate Earth Day provides volunteers with an opportunity to showcase chemistry's contributions to sustaining a healthy planet and environment as part of the annual Earth Day celebration.

The theme for Chemists Celebrate Earth Day 2003 is ChemisTree. As part of the celebration, the Office of Community Activities is sponsoring a poetry competition for students in grades K-12. Students in grades 3-12 are invited to write a poem in the haiku format related to the chemistry of trees. Students in grades K-2 may use any poetic style. As the unifying event, local sections are being asked to sponsor a tree planting ceremony in their community. Hands-on activities, as well as a sample press release, are available online at <http://chemistry.org/earthday>. For additional information, contact the ACS Office of Community Activities at 1-800-227-5558, ext. 6078.


Thought to Ponder

*If your ship doesn't
come in, swim
out to it.*

~Jonathan Winters, Comedian

American Chemical Society National Landmark Dedication and Celebration

The Natural Products Laboratory of Research Triangle Institute (RTI)
Research Triangle Park, NC

Wednesday, April 23, 2003

Schedule of Events for Special Invitees

11:30 a.m. – 12:15 p.m. Dedication and Presentation of Plaque by
Dr. Eli Pearce, Immediate Past President of
the American Chemical Society, Lawn of
Medicinal Chemistry Building, Research
Triangle Institute

Participants (in order of presentation):

Dr. Ernest L. Eliel, Past President, ACS
Dr. John A. Myers, NC Central University, Chair, ACS-NC
Dr. Eli M. Pearce, Immediate Past President, ACS
Dr. Victoria Franchetti Haynes, RTI, President & CEO
Dr. Mansukh C. Wani, RTI Principal Scientist & Honoree

Transportation to Charles Hamner Conference Center
North Carolina Biotechnology Center (NCBC)

SCIENTIFIC PROGRAM

2:00 p.m. – 5:00 p.m.

All lectures to be held in the General Assembly Auditorium,
Charles Hamner Conference Center, North Carolina Biotechnology Center
Chair: Dr. John A. Myers, Chair, North Carolina Section, American Chemical Society

2:00 p.m. – 2:45 p.m. **Lecture by Mansukh C. Wani, Ph.D.**, Principal Scientist,
Natural Products Laboratory, Research Triangle Institute

***“From Nature to Bench to Bedside: A Personal History of the Discovery
and Structural Elucidation of Taxol and Camptothecin***

2:45 p.m. – 3:45 pm **Lecture by Susan Band Horwitz, Ph.D.**, Professor, Molecular
Pharmacology, Albert Einstein College of Medicine of Yeshiva University,
Bronx, NY; Current President of the American Association for Cancer
Research (AACR)

***“Taxol, Tubulin and Tumors: Challenges in the New Era of Cancer
Therapeutics”***

3:45 p.m. – 4:00 pm **Coffee Break**

4:00 p.m. – 5:00 p.m. **Lecture by Paul A. Bunn, Jr., M.D.**, Professor of Medical Oncology,
Current and Founding Director of the University of Colorado
Comprehensive Cancer Center, University of Colorado Health
Sciences Center, Denver, CO; Current President of the American
Society of Clinical Oncology (ASCO)

“The Current Role of Paclitaxel and Irinotecan in Cancer Therapy”



**ACS
NATIONAL
LANDMARK
DEDICATION**

**Employment Aids
Available from
NCACS**

Employment Aids from the Local Section

As many of you are aware, the NC Section has a web page: <http://membership.acs.org/N/NCarolina/>. This page and the links therein are intended to be a resource for chemists in the Section. There are several links of interest particularly to those seeking employment. One link has a list of companies in the Section who hire ACS members; and another links to classified ads in the local paper and to a job search service for the area as well as to several other less targeted sources. Also there are links directly to company job opening web pages where we have been able to find them and links to some of the services offered on ACS web pages.

An additional resource for the most up-to-date job postings is the NCACS listserv. This listserv is operated as a public service of the NC Section and NCSU. There is no charge to anyone. It is operated as a moderated list, which means that only the list owner can approve posted material. This prevents the list from becoming overwhelmed with inappropriate messages. Only valid job openings and meeting announcements are approved. To subscribe, address mail to: listserv@listserv.ncsu.edu. Include a 1-line message saying: `subscribe ncacs <your name>`

The subject line is ignored and your return address is taken as the subscription address. Anyone having a valid job opening can contact Bill Switzer at: bill_switzer@ncsu.edu. To unsubscribe, reply to any posted message requesting that your name be removed.

Also contact Bill at the same address if you have suggestions for other links that might serve as useful resources on the web page or if you would be interested in taking responsibility for maintaining one or more pages

Employment Web Sites

**North Carolina State Bureau of
Investigation**

<http://webs.jus.state.nc.us/doj/hr/>

Magellan Laboratory

<http://excellentadventure.magellanlabs.com/>

News and Observer

<http://www.trianglejobs.com/>

Scynexis

<http://www.scynexis.com/pages/opps.html>

Research Triangle Foundation links to jobs in RTP including the following
(<http://www.rtp.org/local/jobs/home.html>)

Aventis

BASF

Bayer Biological Products

BD Technologies

Biogen

Chemical Industry Institute of Toxicology

Covance Biotechnology Services Inc.

Eisai Inc.

Eli Lilly

Glaxo SmithKline Inc.

International Business Machines Corporation
(IBM)

Lineberry Research Associates

Lockheed Martin Technical Services, Inc.

MCNC

National Institute of Environmental Health
Sciences

North Carolina Biotechnology Center

Paradigm Genetics

Research Triangle Institute

Underwriters Laboratories Inc.

U.S. Environmental Protection Agency

**These links can all be access through the NC-
ACS web site found at:**

<http://membership.acs.org/N/NCarolina/jobs.html>

If you would like your company's employment link added to this list please send an email to Brad Sturgeon at bes@unc.edu

Career Services at ACS Regional/National Meetings

Visit the Career Resource Center at these ACS regional meetings for an array of professional development programs and services. Features may include an employment clearing house (RECH), career management workshops, one-on-one resume critiques.

225th ACS National Meeting
March 23-27, 2003
New Orleans, Louisiana

For more information, job seekers and employers may visit the ACS website

www.chemistry.org/careers/calendar.html

or call 1-800-227-5558 x6208.

20th Triangle Chromatography Symposium and Instrument Exhibit

TCDG



Sponsored by

Triangle Chromatography Discussion Group
North Carolina Section of ACS

Thursday, May 15, 2003

McKimmon Conference and Training Center
NCSU, Raleigh, NC

The Symposium will feature state-of-the-art presentations in diverse areas of chromatography by nationally known experts in these areas. Attendees will have the opportunity to interact with symposium speakers on specific chromatography issues and laboratory problems as well as receive CLP-training and continuing education to maintain essential laboratory skills. A registration certificate will be provided for GLP training file.

The instrument exhibit features the area's largest vendor concentration for chromatographic instruments and supplies. You will have the opportunity to exchange ideas and communicate with local colleagues on trends in chromatography and related areas. Vendors to date include:

Advanced Chemistry Development, Inc	MicroSolv Technology Corp
Agilent Technologies	On Assignment Lab Support
Alltech Associates Inc.	Pall Life Sciences
Applied Separations, Inc.	PerkinElmer
Beckman Coulter Inc.	Phenomenex
Biotage	Polymer Laboratories, Inc.
Chiral Technologies, Inc.	Quantum Analytics
DraChrom Inc.	Restek
EMD Chemicals	Shimadzu Scientific Instr., Inc.
ESA, Inc.	Sun SRI
Government Scientific Source	Tekmar-Dohrmann
Hitachi Corporation	The Nest Group, Inc.
Hydro Service and Supplies, Inc.	Varian, Inc.
IN/US Systems, Inc.	Waters Corporation
MicroLiter Analytical Supplies, Inc.	Wheaton Science Products

Other activities to look forward to during this day include a free lunch which is served on-site as part of your registration fee; prize drawings (contributed by many of the TCDG exhibitors and a Grand Prize contributed by the TCDG); Exhibitor Seminars where presentations will be made on state-of-the-art topics; the TCDG elections of 2003 officers; and a Poster Contest competition for local students, local university and industry research and vendor developments.

20th Anniversary Symposium Speakers

Professor James Jorgenson, UNC-Chapel Hill
"Ultra-High Pressure Liquid Chromatography"

Dr. Ron Majors, Agilent
"Recent Advances in HPLC Column Technology"

Dr. Alfred V. Del Grosso, Food and Drug Administration, CBER
"Analytical Procedures: An FDA Regulatory Perspective"

Dr. Michael Ramsey, Oak Ridge
"Thinking Small About Chemical Separations and More!"

Dr. Arthur Moseley, Glaxo Smith Kline
"The Role of Chromatography and Mass Spectrometry in Proteomics"

For further information, visit the Triangle Chromatography web site at: <http://www.RTPnet.org/tcdg>

The TarHelium Volume 33: Number 4

Bradley E. Sturgeon, Editor
4400 Currie Court
Raleigh, NC 27613

PRST STD
US POSTAGE
PAID
RALEIGH, NC
PERMIT #1854

Executive Committee:

<i>J. A. Myers (NCCU), Chair '03</i>	560-6461	jmyers@upo.nccu.edu
<i>D. Coleman (Eli Lilly-Sphinx), Chair-Elect '04</i>	314-4352	dscoleman@lilly.com
<i>S. Levine (NCSU, Ret.), Secretary '02-'03</i>	676-3740	naturpix@mindspring.com
<i>J. T. Bursey (ERG), Treasurer '01-'02</i>	468-7926	joan.bursey@erg.com
<i>B. E. Sturgeon (UNC), TH Editor '00-present</i>	962-1616	bes@unc.edu
<i>A. L. Crumbliss (Duke), Councilor '01-'03</i>	660-1540	alc@chem.duke.edu
<i>R. A. Palmer (Duke), Councilor '01-'03</i>	660-1539	rap@chem.duke.edu
<i>J. L. Chao (IBM), Councilor '00-'02</i>	543-3054	jlchao@us.ibm.com
<i>E. C. Bigham (GSK), Councilor '02-'04</i>	483-9844	ecb12781@gsk.com
<i>R. W. Morrison, Jr. (NCSU), Councilor '02-'04</i>	515-2549	robert_morrison@ncsu.edu
<i>R. M. Forbis (UNC), Alt. Councilor, '02-04</i>	962-2096	dick_forbis@unc.edu
<i>S. Sendlinger (NCCU), Alt. Councilor, '02-04</i>	560-6297	ssendlin@wpo.nccu.edu
<i>S. T. Purrington (NCSU), Alt. Councilor, '01-'03</i>	515-2864	purringt@chemdept.chem.ncsu.edu
<i>E. T. Samulski (UNC), Alt. Councilor, '01-'03</i>	962-1562	et@unc.edu
<i>W. Powell (Meredith), Alt. Councilor '00-'02</i>	760-8619	powellw@meredith.edu
<i>W. L. Switzer (NCSU), Alt. Councilor '02-04</i>	515-2945	bill_switzer@ncsu.edu
<i>S. J. Sumner (CIIT), Past Chair '02</i>	558-1343	sumner@ciit.org
<i>G. H. Wahl, Jr. (NCSU), Past Chair '99</i>	515-2941	george_wahl@ncsu.edu
<i>C. M. Balik (NCSU), Past Chair, '01</i>	515-2126	balik@ncsu.edu
<i>M. M. Bursey (UNC), Ex Officio</i>	493-3025	mbursey@acs.org
<i>K. A. Cutler (NCCU), Project Seed Ex Officio</i>	530-7004	kcutler@wpo.nccu.edu
<i>E. L. Eliel (UC), Ex Officio</i>	962-6198	eliel@email.unc.edu
<i>D. G. Morgan (GSK), TAMS, Ex Officio</i>	483-4291	dm19700@gsk.com
<i>D. Canelas (Lord), PDG, Ex Officio</i>	469-2500	dorian, canelas@lord.com
<i>J. Hines (RTI), TCDG, Ex Officio</i>	541-6647	hines@rti.org
<i>T. M. O'Connell (GSK), TMRDG, Ex Officio</i>	483-1535	tmo89509@gsk.com

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. Very occasionally openings outside of the NC Section are posted. If you wish to subscribe, address mail to: 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. ■