



# The TarHelium

Volume 25, Number 3

November 1994

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## Molecular Modeling Group

2:30 p.m., Tuesday, November 1, 1994  
111 Beard Hall, UNC School of Pharmacy

Dr. Jeff Blaney, Chiron Company

### "Evolution of Molecules to Fit a Binding Site of Known Structure"

## The TarHelium

c/o William L. Switzer, Editor  
Department of Chemistry-8204  
North Carolina State University  
Raleigh NC 27695-8204

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A. Tropsha (UNC), TMMDG, <i>Ex Officio</i>	966-2955
R. Ghirardelli (ARO-Ret.), Co-chair SERM-98, <i>Ex Officio</i>	489-6306
W. L. Switzer (NCSU), Co-chair SERM-98, <i>Ex Officio</i>	515-2945

**Voicemail Information Line:** (919) 541-7183 in the RTP

Changes have been made in the voicemail system. Further instructions will hopefully accompany the December issue.

### National ACS meetings:

April 2-7, 1995, Anaheim  
March 24-29, 1996, Seattle

August 20-25, 1995, Chicago  
August 25-30, 1996, Boston

**Deadline for December Publication: November 12, 1994**

## Polymer Discussion Group

Thursday, November 10, 1994

Steven D. Smith

Procter & Gamble Company

### "Random Diblock Copolymers: A New Class Of Block Copolymers"

NCSU Faculty Club

4200 Hillsborough St., Raleigh

5:30 p. m. Social Hour

6:30 p. m. Dinner\* (members-guests:  
\$15; students \$8)

7:30 p. m. Lecture

\*Reservations by noon, November 8 with  
Richard Venditti in Raleigh at: 515-6185  
or richard\_venditti@ncsu.edu

Results of the Fall Elections were not  
available at publication time. They should  
appear in the December issue.

## TCDG Meeting

Dr. Lane C. Sander  
National Institute of  
Standards and Technology

"Shape Selectivity in  
Liquid Chromatography"

Tuesday, November 8, 1994

Camille Dreyfus Laboratory Auditorium  
Research Triangle Institute  
3040 Cornwallis Rd., RTP

11:30 - 1:00 Luncheon\*  
12:00 noon Presentation

\*Reservations are necessary. For \$6, a  
box lunch can be ordered or you may bring  
your own. For information or reserva-  
tions, call Judi Price (919) 541-8852, In-  
ternet: PRICE@RCC.RTI.ORG or John  
Hines (919) 541-6647, Internet:  
HINES@RCC.RTI.ORG by 5:00 pm Fri-  
day, November 4; cancel by same date and  
time. A waiting list will be kept in case  
of cancellation. Abstract: see p. 2

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W. L. Switzer, Editor

S. T. Purrington, Assistant Editor

P. A. Flowers, Advertising

*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.

Contributions for *The TarHelium*: Send to W. L. Switzer, Editor, Chemistry-8204, North Carolina State University, Raleigh NC 27695-8204. Phone: (919) 515-2945, Fax: (919) 515-5079 and Internet: bill\_switzer@ncsu.edu.

**Advertising:** All nine 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 four or more issues in a publication year which runs from September through April plus one issue in the summer. Contact Paul Flowers, Advertising Manager, Department of Physical Science, Pembroke State University, Pembroke NC 28372, Phone: (919) 521-6247 Fax: (919) 521-6649 and Internet: paul@nat.pembroke.edu.

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P. O. Box 3337  
Columbus, OH 43210  
meminfo@acs.org

When communicating electronically, include your membership number and a return telephone number in your message. You may request membership applications electronically, but when completing them please write NC Section in the blank labeled Local Section/Division Commission Claim in the lower right hand corner of the first page. You may also request add/drop subscriptions among other services.

If you wish to receive job announcements and announcements of Local Section ACS events by electronic mail, please subscribe to the NCACS list. Send e-mail to: listserv@listserv.ncsu.edu. Include a one-line message saying: subscribe ncacs <your name>. To remove your name, send a message to the same address saying: unsubscribe ncacs. Other features of the list can be obtained by sending mail to the same address with the one-line message saying: info ncacs. The info file includes on-line job search information and a list of companies in the Section who hire ACS members. Questions may be addressed to the *TarHelium* Editor.

To subscribe to a Local Section bulletin board to discuss general topics of interest to the chemical profession, follow the same procedure described above, but include the one-line message saying: subscribe ncacsdialog <your name>. To post to the list, send mail to ncacsdialog@ncsu.edu.

To communicate with the entire Executive Committee, send mail to: acsexcomm@ncsu.edu.

On-line copies of recent issues of *The TarHelium* are now available on the Triangle FreeNet at the University of North Carolina, Chapel Hill. One may telnet to: tfnet.ils.unc.edu with login: freenet and password: guest Issues are archived under:

4. Business/
3. Professional organizations/
  1. ACS American Chemical Society/
  1. ACS TarHelium (newsletter)/

Alternatively one may reach the server by gopher. From the State of North Carolina:

University of North Carolina at Chapel Hill, Info system  
Other information services  
Triangle Free-Net development gopher  
Business  
Professional organizations  
ACS American Chemical Society  
ACS TarHelium (newsletter)

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## Phoenix Award

The Section was nominated for the Phoenix Award for best activity in a museum or library during the 1993 National Chemistry Week. The Section wants very much to thank to Erin Keating at the Museum of Life and Science in Durham for her work in organizing this program.

## TCDG Meeting Abstract

Dr. Lane C. Sander from the National Institute of Standards and Technology will speak on "Shape Selectivity in Liquid Chromatography". Date, time and reservation information give on front cover.

**ABSTRACT:** The chromatographic discrimination of compounds on the basis of molecular structure is described as "shape selectivity". More than any other single effect, shape selectivity is influenced most strongly by the type of bonding chemistry used in the production of the stationary phase. Operational parameters provide additional control over shape selectivity, and dramatic changes in selectivity occur with changes in temperature. Smaller changes result from differences in mobile phase composition. In this presentation, shape selectivity effects will be compared for a variety of classes of solutes, including polycyclic aromatic hydrocarbons, polychlorinated biphenyl congeners, and carotenoid isomers. Molecular shape recognition will be examined for several types of reversed-phase columns including: monomeric and polymeric C18 columns, a new column developed specifically for the separation of carotenoid isomers, and columns based on self-assembled monolayer technology. Concepts relating phase order with shape recognition will be discussed.

**Future Event:** 12<sup>th</sup> Triangle Symposium & Instrument Exhibit - May 18, 1995 at the McKimmon Center, North Carolina State University.

Micron Inc. - p.

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Analytical Services

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5 3815 Lancaster Pike

6 Wilmington DE 19805

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8 (302) 998-1184

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## Purrington Appointed Councilor

Local Section Chair, Mike Crimmins, announced that he had received a letter of resignation from William F. Little, Councilor '93. With regrets the Executive Committee accepted his resignation. In accordance with the Section by-laws, the councilor's position is filled by appointment until the next election. The Committee unanimously approved the appointment of Dr. Suzanne T. Purrington, Alternate Councilor '93, to fill the unexpired term for Dr. Little. This position will be filled by election in 1995 for a term beginning in 1996.

Beckman Instruments, Inc. - p.

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3 Chemical Instrumentation

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5 Howard Rosenberg, Ph. D.

6 1210 Ashbrooke Dr.

7 West Chester PA 19380

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9 (215) 429-1375 (PA)

10 (201) 818-8900 (NJ)

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## Area News

**Duke: Todd E. Woerner**, Manager of the Duke Chemistry Advanced Undergraduate Laboratories, presented a talk entitled "Scanning Tunneling Microscopy in the Advanced Undergraduate Laboratory" at the Symposium on NSF-Catalyzed Innovations in the Undergraduate Laboratory at the recent ACS National meeting in Washington DC. His co-author was L. A. Coury, Jr., who co-authored a recent NSF-ILI grant with Dr. Catherine Heyer awarded to Duke for purchase of the STM instrument.

**Louis A. Coury, Jr.** has given talks recently at East Carolina University, Temple University, Miami University and UNC-CH. In addition, he was co-organizer of a symposium on Electrochemistry and Novel Materials at the recent FACSS meeting in St. Louis and was a feature speaker at the Ultrasonic Industry Association 25<sup>th</sup> Annual Symposium in Columbus, OH.

**NCSU:** This past year **Professor Robert D. Bereman** was named the first Center Fellow at the National Sigma Xi Headquarters in the Research Triangle Park. He became Associate Dean in the Division of Undergraduate Studies effective July 1, 1994, and is serving as the Interim Director of the Academic Support Program for Student Athletes until January 1, 1995. He also just finished a year of service as the Chair of the Undergraduate Environmental Sciences Faculty and was named to the Board of Editors for the Journal of Coordination Chemistry

**Dr. James D. Otvos** recently received a U.S. patent entitled: "Method and Apparatus for Measuring Blood Lipoprotein Levels by NMR Spectroscopy".

**Suzanne T. Purrington**, Associate Professor of Chemistry and Local Section councilor, is the recipient of the 1994 NCSU Libraries Faculty Award. The award is presented annually to a faculty member who has notably and consistently contributed to the development of the Libraries. She is actively engaged in chemical research that involves her directly with the libraries and she has been instrumental in integrating the use of literature and the library in the graduate and undergraduate curriculum.

**Elizabeth Theil** visited the University of Montpellier, France in June as part of a joint NSF-CNRS sponsored study of ferritin during plant development. She also was invited to talk at the PAMM (Program Against Micronutrient Malnutrition) Symposium at Wageningen University, The Netherlands.

Galbraith Laboratories - p.

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3 Microanalysis Services

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5 PO Box 51610

6 Knoxville TN 37921-1750

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8 2323 Sycamore Dr

9 Knoxville TN 37921-1750

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11 (615) 546-1336

12 (615) 546-7209

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**RTI: R. K. M. Jayanty** was named a fellow of the Air & Waste Management Association. The Association, which has approximately 15,000 members, has so honored 40 members in its 87-year history. Dr. Jayanty is the manager of the RTI Environmental Methods and Standards Department of the Center for Environmental Measurements and Quality Assurance.

The American Association for Cancer Research (AACR) has presented its Bruce F. Cain Award to RTI researchers **Monroe E. Wall**, PhD and **M. C. Wani**, PhD. The Cain Memorial Award is given annually to an individual or research team for outstanding preclinical research leading to the discovery of a significant new therapeutic agent for the improved care of cancer patients. The award was established by the Warner-Lambert Company to honor Bruce F. Cain, whose scientific interests involved the design, synthesis, and biological evaluation of potential anti-tumor drugs. Drs. Wall and Wani are most well-known for their discovery of taxol and camptothecin, two anti-tumor agents they isolated from natural products in the early 1960s.

RTI has funding from the NIEHS to research the mechanism of 2-methoxyethanol developmental toxicity. NIEHS has also provided additional funding for a combined endpoint germ-cell mutagenicity assay, studies of chemical disposition in animals, and chemistry support services of the National Toxicology Program.

For industrial clients, RTI is determining the mechanism of action of an insecticide, developing methods and conducting analyses for test compounds, developing a regulatory method to determine a compound or its marker residue in biological samples, conducting a dominant lethal assay, and providing toxicology screening. RTI also has additional Centers for Disease Control funding to provide mission support services for preparation of toxicological profiles.

RTI has additional EPA funding to develop, demonstrate and evaluate methods for analysis of environmental samples. Also

from the US Fish and Wildlife Service, RTI has additional funding to analyze environmental materials for residues of inorganic contaminants and funding from the National Park Service for sulfur dioxide analyses. The EPA has provided additional funding for quality assurance technical support, QA support for the Health Effects Research Laboratory, technical support in application of data quality objectives and QA for environmental pollutant monitoring. The National Institute of Standards and Technology has provided funding to develop and administer proficiency testing for asbestos laboratories.

Quantitative Technology Inc. - p.

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3 Elemental Analysis

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5 PO Box 470  
6 Whitehouse NJ 08888  
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8 (908) 534-4445

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## University Grants and Contracts

**Central Pharm Inc.:** "Characterization of the Nature of Several Proposed Polysaccharide Iron Complexes," **R. D. Bereman**, NCSU

**Georgia Institute of Technology:** "Southern Oxidant Study: Ozone Non-Attainment Atlantic Intensive", **V. P. Aneja**, NCSU

**EPA:** "Characterization of Emissions of Nitrogen Oxides from the Soils of the Southwest United States", **V. P. Aneja**, **V. K. Saxena** and **W. P. Robarge**, NCSU

**NCBC:** "Development and Optimization of Micro-LC FAB Mass Spectrometry for the Analysis of Phospholipids in Food Plants," **C. A. Haney**, NCSU

**NC Soybean Producers Association, Inc:** "Activation of Disease Resistance by Salicylic Acid in Soybean", **J. A. Knopp** and **J-S Huang**, NCSU

**NSF:** "Non-Stoichiometry in Semiconductor Heterostructure", **K. J. Bachmann**, NCSU; "FTIR Spectrometer System for Polymer Rheology and Membrane Science Research Program", **B. D. Freeman** and **S. A. Khan**, NCSU

**Perkin Elmer Corporation:** "Retention Time Prediction in High Performance Liquid Chromatography", **Charles H. Lochmüller**

**PHS:** "Synthesis and Synthetic Utility of 1-Acyldihydropyridines", **D. L. Comins**, NCSU

## Area Seminars

- Nov 1 Jeff Blaney, Chiron Company, "Evolution of Molecules to Fit a Binding Site of Known Structure", TMMDG  
Nov 3 Linda McPhail, Bowman Gray School of Medicine, "Signaling Mechanisms Involved in Activation of Neutrophil NADPH Oxidase", NCSU-BC

Huffman Laboratories, Inc. - p.

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3 Elemental Analysis

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5 4630 Indiana Street  
6 Golden CO 80403  
7 (303) 278-4455  
8 (303) 278-7012 (FAX)

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- Nov 4 David Askin, Merck Research Laboratories, "Diastereoselective Routes to Hydroxyethylene Dipeptide Isosteres: Synthesis of Clinically Interesting HIV-1 Protease Inhibitors", Duke  
Nov 7 John Markley, University of Wisconsin, Madison, "To be announced.", NCSU  
Nov 8 Lane C. Sander, National Institute of Standards and Technology, "Shape Selectivity in Liquid Chromatography", TCDG  
Nov 10 Steven D. Smith, Procter & Gamble Company, "Random Diblock Copolymers: A New Class Of Block Copolymers", PDG  
Nov 10 Jeffrey D. Milbrandt, Washington University, "Immediate Early Genes: The Biological Seismograph", Glaxo/NCSU-BC  
Nov 11 Mario B. Pinto, Simon Fraser University, "Towards a Vaccine for Group A Streptococcus", Duke  
Nov 14 Michael Maroney, University of Massachusetts, Amherst, "Insights into the Role of Nickel in Hydrogenases", NCSU

DIONEX c. - p.

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3 IC, Automation and HPLC

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5 1950 Lake Park Drive, Suite 175  
6 Smyrna GA 30080  
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8 (404) 432-8100 (voice)  
9 (404) 432-8300 (fax)

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- Nov 15 William A. Goddard III, California Institute of Technology, "Recent Advances in Simulations and Modeling of Materials: Applications to Biological and Polymeric Systems", Becton Dickenson Lecture; Duke
- Nov 17 Ellen Weiss, University of North Carolina, Chapel Hill, "Functional Domains of Rhodopsin: A Model for G-Protein-Coupled Receptors", NCSU-BC
- Nov 18 Sharon L. Neal, University of California, Riverside, "Characterizing Microheterogeneous Media via Wavelength Dependent Frequency Domain Fluorescence", Duke
- Nov 21 John Wheeler, Furman University, "New Directions in Microscale Separations: Sensitivity, Selectivity and Physico-chemical Measurements With Capillary Electrophoresis", NCSU
- Nov 30 Edward Stiefel, Exxon Research & Engineering, "Molybdenum and Sulfur in Cofactors, Catalysts, Complexes, and Clusters", NCSU

PDG-Polymer Discussion Group. Call Richard Venditti at NCSU: 515-6185 or richard\_venditti@ncsu.edu.

TCDG-Triangle Chromatography Discussion Group. Call John Hines 541-6647 (RTI).

TMMDG-Triangle Molecular Modeling Discussion Group. Call Alex Tropsha 966-2955 (UNC-CH).

Duke (Chemistry) Call Bonnie Turner at 660-1506.

NCSU (Chemistry) Call Joyce Weatherspoon at 515-2548.

NCSU-BC (Biochemistry) Call Pat Sullivan 515-2581.

## Exxon Valdez Oil Spill

On Friday, December 2, 1994, Dr. Edward Stiefel of Exxon Research and Engineering Company will present a seminar entitled: "The Exxon Valdez Oil Spill: The Bioremediation of Prince William Sound". Dr Stiefel's visit is funded by the Visiting Industrial Scientist Program of the North Carolina Biotechnology Center. In addition to the bioremediation seminar, which is intended for a lay audience, Dr. Stiefel will be giving a technical talks in the NCSU Department of Chemistry on Wednesday November 30, 1994: "Molybdenum and Sulfur in Cofactors, Catalysts, Complexes, and Clusters" and in the NCSU Department of Biochemistry on Thursday December 1, 1994: "Bacterioferritin: Iron, Heme, and Protein".

BETEC Laboratory - p.

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3 Laboratory Testing

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5 444 W. Country Rd. D

6 St. Paul, MN 55112

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8 (612) 631-9412

9 (612) 631-8405 (FAX)

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## High School Teachers

by Dr. Sarah Allen, Chair High School Committee

Well fellow High School Teachers, if you celebrated Mole Day in October and catch any of the NCSTA Convention in Raleigh November 9-11<sup>th</sup>, and participate in the ACS Satellite-TV Seminar on Materials Science, you have been busy! I have only one other thing which I'd like you to consider now, while things are somewhat less hectic.

We mentioned a Professional Development Scholarship awarded annually by the local ACS Section in the September issue and mentioned some details about previous awardees. The awards are announced in the spring and must be received by March 1, 1995. However, you might want to consider taking action before you break for the Holidays. The total amount available is \$1000, so the way it is awarded will be determined by the number of deserving applications. An application for is given in the next column. If you need more room, please attach the necessary sheets.

If you have news for this column, please write to Sarah Allen, NCSSM, 1219 Broad Street, Durham, NC 27705; (919) 286-3366 x225; Internet: allen@odie.ncssm.edu.

## New ACS Members

Gary William Adams  
 Armel Akouete Agbodjan  
 Iqbal Ahmad  
 Sameer Anand  
 Pawan Kumar Bali  
 Laura Bostick  
 Paul Daniel Boyle  
 Bradley B Brown  
 Dan Carlson  
 Connie Carothers  
 Allan John Carrano  
 Ping Yun Chen  
 Arthur R Clark  
 Lyn M Crosby  
 Charlotte R Dewan  
 John Charles Dicesar  
 Patrick Seamus Eaton  
 Adam M Eyring  
 Gang Fang  
 Brian Farkas

Stephen S Ferguson  
 Edward Foos  
 William Loyd Fornes  
 Yakov Samoilovich Freidzon  
 Joseph Renato Gibson  
 Dawn Angela Groenke  
 Lourdes Guerra-Weltzien  
 Kevin P Gwaltney  
 Christine M Havrilla  
 James Heinis  
 William G Hendricksdn  
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 Chin-Yi Huang  
 Lee M Hurer  
 Toru Kauita  
 Victor Vincent Kaminski III  
 George Kah Kangkolo  
 Darius A Kavaliunas  
 Christopher B Lagerholm  
 Donald G Lee

Wyn Lewis Bevan  
 Hong Li  
 Fangming Lin  
 Qicai Liu  
 Wentian Liu  
 Bounthon Loun  
 Eugene E Magat  
 Warren A Mc Allister  
 Molly H Meixner  
 David Earl Mills  
 Jarafshan Jamshed Mobeo  
 Michael Anthony Moody  
 David Mu  
 Jennifer Lee Nourie  
 Brian K Nunnally  
 Kristin Marie Omberg  
 Deremy Dohn Pietron  
 Harold W Pinnick  
 Michael G Pottmeyer  
 Darla Pruetten-Henderson

Candace Prusiewicz  
 Mukesh Ramchandani  
 Gary Kenneth Rowe  
 Stephanie Annie Ruefley  
 Timothy H Sanders  
 Laura B Scarola  
 Howard A Schneider  
 James J Spivey  
 Steve Stadelman  
 Oudith Ann Straub  
 Michael R Strommen  
 John Donald Summers  
 Lizhong Sun  
 Geof Trullinger  
 Richard Konrad Vetterl  
 Peng Wang  
 Stephen Alan Westcott  
 Kim White  
 Yaoqi Zhou

## Application

ACS Professional Development Award  
For High School Chemistry Teachers

Description of professional development activity:

Goal of professional development activity:

Budget:

Previous teaching experience:

Degrees held:

Applicant's signature and date:

School address:

County where you teach:

Principal's Certification: This applicant is scheduled to teach at least one chemistry class in the 1995-96 school year.

School principal's signature and date:

Mail to: Michael T. Riebe, Chair '95  
Glaxo INC., EP 2084  
5 Moore Dr.  
Research Triangle Park NC 27709

## Job Openings

All job announcements are broadcast immediately upon receipt to the NCACS recipients list. If you wish to be included, see subscription instructions given on the front inside cover. The INFO file for the NCACS bulletin board has instructions on searching job opening with the State of North Carolina, North Carolina State University and University of North Carolina, CH.

**Burroughs Wellcome:** Job Line (919) 315-8347.

**EPA-RTP:** Job line (919) 541-3014. Updated every Friday.

**Glaxo:** Job Line (919) 248-2565.

**RTI:** Contact: Research Triangle Institute, Office of Human Resources, PO Box 12194, Research Triangle Park NC 27709-2194. Phone: (919) 541-6466. For. An. Tox. III/Res. For. An. Tox. I F0455 64A B.S./B.A. in Chemistry or related area with at least 1-2 years experience with review/certification of GC/MS and immunoassay data and forensic chain of custody procedures. Postdoctoral Chemist F0446 63A Ph.D. in Chemistry with experience in organic synthesis. Will synthesize novel organic compounds. Postdoctoral Chemist F0447 63A Ph.D. in Chemistry with research experience in organic synthesis. Will conduct research in the synthesis of organic compounds. Postdoctoral Chemist F0450 63A Ph.D. in Organic Chemistry with experience or training in organic synthesis. Will conduct research to synthesize novel organic compounds. Postdoctoral Chemist F0462 63A Ph.D. in Organic Chemistry with research experience in organic synthesis. Will conduct research to synthesize novel organic compounds. Postdoctoral Chemist F0464 64A Ph.D. in Organic Chemistry with research experience in organic synthesis. Will synthesize haptens and conjugates for catalytic antibody programs. Some analytical (kinetics) work. Postdoctoral Chemist F0468 63A Ph.D. in Chemistry with research experience in synthetic organic chemistry. Will synthesize novel organic compounds. Postdoctoral Chemist F0472 63A Ph.D. in Organic Chemistry with research experience in organic synthesis. Will synthesize novel organic compounds.

ChemInnovation Software - p.

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3 Structure Drawing Software

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5 8190-E Mira Mesa Blvd., Suite 428

6 San Diego CA 92126

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8 (619) 566-2846

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Considerable resource information is given on the address page and on the front inside cover of each *TarHelium*. You will find how to:

- change your address with the ACS by mail or e-mail
- access voice mail announcements for each Local Section discussion group
- access on-line copies of *The TarHelium*
- subscribe to NCACS, a bulletin board for receiving Local Section meeting announcements and area job announcements
- subscribe to NCACSDIALOG, a bulletin board for those who might want to dialog on concerns about the chemical profession
- contact the Local Section Executive Committee individually by phone or as a group by e-mail
- submit announcements and advertisements for *The TarHelium*
- when and where future National ACS meetings are held