

# *The CSRA Chemist*

SAVANNAH RIVER SECTION  
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- ACS E-mail

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# The CSRA Chemist

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**Mailing Address:** Savannah River Section – American Chemical Society, c/o Lewis Baylor, Equitech Int'l, 218 Richland Ave., W., Aiken, SC 29801. All newsletter articles should be sent to this address. All subscriptions, ads, and payments should be sent c/o Brian Anderson.

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**Member Profile(s):** Joe Krupa is the Chair of the Membership Committee. This topic is a regular feature in the newsletter. The profile should include education, experience, accomplishments, hobbies and family items. To be featured, please send a 450 or less word profile, along with your telephone number, to the mailing address above. Profiles will be selected by the chairperson and printed in the order received.

**Meeting Announcements:** *The CSRA Chemist* will announce scientific meetings of interest to chemists and chemical engineers (when space is available). For information and deadlines, contact Lewis Baylor.

**Change of Address:** Send new address and member number to address above and ACS, PO Box 3337, Columbus, OH 43210. You may also send e-mail to ACS at [service@acs.org](mailto:service@acs.org).

## CHAIR'S THOUGHTS

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As I write this column, we are entering our final month of activities for 1998 – yes the Awards meeting on November 17 will wrap up our activities for the year. However, before we get to the end, there are many activities planned. We'll be at SEED shortly after you read this; we have a fine speaker scheduled on October 29<sup>th</sup>, and of course we have National Chemistry Week in early November. All these are outstanding opportunities to get involved with the Section, and stay in touch with chemistry.

I'd like to take some space here to encourage each one of you to exercise your right to vote! There are three (that's right, I said three) elections being held in the next few weeks. First, and most important from my perspective, is the annual election of Section officers. By this time you have received your ballot in the mail – please take the time to cast your vote and return your ballot to Dr. Stephanie Myers by October 25. The second election is that of ACS national for the year 2000 president. There are two fine candidates from academia running this year – do take the time to read about their positions and plans for the Society and cast your vote. The third election is that being held on the first Tuesday in November in which a variety of public offices will be filled. Do take the time and cast your vote for the candidates of your choice. The right to vote is a right granted by our Constitution to every adult American – and a right we often take for granted. Don't forget that many people on our planet do not have this privilege. Don't let yours wither and die – get out and vote!

As you read in last month's CSRA Chemist, our editor Chris Bannochie has resigned after three years in charge of the presses. I would like to thank him for a job well done! Chris' attention to detail assured the Section of a first-rate newsletter every time. Chris will still be in charge of the Section's web page – a job that can be handled from anywhere. I wish him good luck in his new work assignment in California – his energy and contributions to Section events will be missed.

It's about this point in my column where I start to run out of things to say. It's also at this point where my former editor would hound me for being so terse and start pasting in enormous graphics to fill the space allotted to me. Now, however, things are different! I can hound myself – it's much more convenient – and I can pick out graphics that I like to fill the empty space! Oops! I filled up the page.

# LOCAL SECTION NEWS

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## NATIONAL CHEMISTRY WEEK 1998

National Chemistry Week isn't just for chemists! Engineers, chemists, technicians, professors, teachers, and students are joining together to participate in CSRA National Chemistry Week events. **If you or someone you know would like to get involved, please contact Dr. Joyce Morningstar at 706-869-8587.**

This year National Chemistry Week, a grassroots outreach program of the American Chemical Society, will be celebrated from November 1-7<sup>th</sup>, 1998. This nationwide event is one of the most effective ways to let the public understand the importance that chemistry makes in all of our lives.

To demonstrate that chemistry is for everyone, a broad spectrum of employees from local chemical plants will be performing entertaining hands-on activities all day at Fort Discovery National Science Center on Saturday November 7. **If your company would like to get involved and sponsor a chemical demonstration table, please contact Dr. Joyce Morningstar at 706-869-8587 or Bill Trammel at 706-733-1844.** We can work with you to provide ideas, written materials, and training to help your company conduct a successful event.

Once again, the faculty and students in the chemistry departments at Augusta State University and University of South Carolina-Aiken will be reaching out to school children in Richmond, Columbia, and Aiken counties. **All sixth graders and their teachers in the CSRA area are invited to attend chemistry shows** which involve entertaining demonstrations of chemical principles – chemical analysis, acids and bases, and catalysts. After the show, educational materials explaining the experiments, procedures, and chemical principles will be available for teachers to take back to their classroom. **If you would like for your child to attend one of these informative events, please pass this information along to their teacher.**

The chemistry show at Augusta State University will be held at the Maxwell Performing Arts Theater on the ASU campus on Tuesday, November 24<sup>th</sup>, 1998. There will be two 60-minute shows; one at 10AM and one at noon. **For reservations or more information on the ASU chemistry shows, please call Dr. Stephanie Myers at 706-667-4514.**

The chemistry show at USC-Aiken will be held at the Student Activities Center on the USC-Aiken campus on Thursday, November 12<sup>th</sup>, 1998. There will be two 60-minute shows; one at 9:30AM and one at 11AM. **For reservations or more information on the USC-Aiken, please call Dr. Monty Fetterolf at 803-648-6815 ext. 3378.**

**For all teachers and adults in the CSRA area, there will be a class teaching how to plan and perform chemical demonstrations for the classroom.** The workshop will be held at Fort Discovery and is open to anyone who would like to learn how to perform demonstrations. Two sessions have been scheduled, one on Friday, October 16<sup>th</sup> at 4:45PM and one on Saturday, October 17<sup>th</sup> at 9AM. There is no charge or entry fee for the workshops. **If you or your teachers have questions about the workshops, call Dr. Joyce Morningstar at 706-869-8587 or Bill Trammel at 706-733-1844.**

We'd like everyone to participate in National Chemistry Week. Visit your child's school or volunteer for one of the events described above. Let us know what you'd like to do and you need.

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## September Meeting Update

Congratulations to all the participants in Chemical Jeopardy night in September. Teams from Augusta State University, University of South Carolina (Aiken) and Davidson Fine Arts all participated in the event. As you probably already know, or have guessed, Chemical Jeopardy pits the contestants in a battle of wits over chemistry knowledge, but otherwise is modeled after the popular television game show of a similar name. All the participants were good sports and answered questions shaded to the industrial side of life. In the end ASU was victorious.

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## SEED is almost Here

The Section is sponsoring a booth at SEED (Science Education Enrichment Day) at USC-Aiken on Saturday October 24. This annual event exposes the public to the many wonderful branches of science – from CHEMISTRY to biology, from mathematics to astronomy, and many more. It is primarily geared towards students in grades 4-8, though 'students' of all ages are welcome to attend. We are still looking for volunteers to talk about color, change and chemistry. Contact Roy Beck at (803) 208-6478 if you would like to help.

# NATIONAL NEWS

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## Tennessee and Kansas Host NSF-Sponsored Summer Research Programs for Small-School Analytical Faculty

The National Science Foundation Surface and Analytical Chemistry Program sponsors two AMacro-ROA@ (Research Opportunity Award) programs to provide collaborative summer research opportunities for faculty teaching analytical chemistry at non-Ph.D.-granting colleges and universities. These long-standing programs at the University of Tennessee-Knoxville and the University of Kansas-Lawrence have aimed to develop a strong regional infrastructure for sharing ideas among analytical chemistry faculty, and to increase the number and improve the preparation of chemistry majors at small institutions by invigorating the research interests and activities of faculty visitors. The goal of the program is to help participants establish or expand undergraduate research programs at their home institutions.

Participants in the UT program are paid \$1,100/week and provided with furnished apartments (those bringing families may need to make alternative housing arrangements). First-time participants generally spend 8-10 weeks in Knoxville, choosing a time convenient to the visitor and the UT collaborator; flexibility is a hallmark of the program. Shorter return visits (<5 weeks) can be arranged with support from the program and other resources. To receive the short application form or other information, contact Prof. Kelsey Cook, Department of Chemistry, University of Tennessee, Knoxville, TN 37996-1600 (phone 423-974-8019; fax 423-974-3454; e-mail [kcook@utk.edu](mailto:kcook@utk.edu)), or visit <http://www.chem.utk.edu/~acsec>. Applications are due by February 15, 1999, but will be evaluated as completed. As there are a limited number of appointments available, timely response is encouraged.

The program at KU features a ten-week summer research experience in bioanalytical or environmental analytical chemistry. Participants also have the opportunity to engage in collaborative research for a second summer at their home institution facilitated by follow-up support through this program. For applications or for more information, contact Prof. Cindy Larive, Department of Chemistry, University of Kansas, 2010 Malott Hall, Lawrence, KS 66045 (phone 785-864-4269; fax 785-864-5396; e-mail [clarive@caco3.chem.ukans.edu](mailto:clarive@caco3.chem.ukans.edu)), or visit our web site at <http://www.chem.ukans.edu/macroroa/macroroa.html>.

## Now you can reach ACS via email!

Moving, changed your phone number, recently got an e-mail address? Now you can let the ACS know by sending a quick and easy e-mail to [service@acs.org](mailto:service@acs.org).

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### The Younger Chemists Committee Turns Silver!

In celebration of the YCC's 25<sup>th</sup> Anniversary, special programming and events designed to highlight the achievements of younger chemists will be sponsored at ACS events throughout 1999. In addition to commemorative 25<sup>th</sup> Anniversary pins, YCC ribbons will be placed on posters contributed by younger chemists at the SciMix events in both Anaheim and New Orleans. YCC is striving to co-sponsor symposia with all of the ACS technical divisions including a special Biotechnology Symposia at the New Orleans meeting. Also in New Orleans, there will be a special reception entitled "Looking Back to the Future." This reception will include a short program where speakers will give perspectives on the past, present and future of the YCC. Visit the YCC web site for more information on these special 25<sup>th</sup> Anniversary events as the meetings draw nearer, <http://www.chem.hawaii.edu/ycc>. Help make the YCC's 25<sup>th</sup> Anniversary celebration a big success by planning to attend these special events!

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### New Journal in 1999

The American Chemical Society and the Association of Research Libraries are collaborating on the launch of a new journal in organic chemistry. The first issue of *Organic Letters* will debut in July 1999. Each biweekly issue will offer rapid communication of original and timely reports of significant research in the field. *Organic Letters* will provide creative approaches and improvements to existing methods in a broad range of organic chemistry research.

*Organic Letters* will be available in both print and Web Editions. The Web Edition will include all the benefits and features currently available for other ACS Web Editions. These online enhancements include: Articles ASAP (As Soon As Publishable), Articles on Command, full text searching, links to appropriate databases, categorization of articles by reaction type, and options for experimental details and supporting information. Subscriptions are available to both ACS members and libraries. For more information, call Member & Subscriber Services at 800-333-9511.

## EDITOR'S CHOICE

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Welcome to the October issue of *The CSRA Chemist*. This issue finds your new editor at the helm and struggling mightily with Adobe PageMaker. Please bear with me for the next few issues, while I get this beast under my control! Our former Editor, Chris Bannochie, had warned me that the 'newsletter gremlins' would strike, and he has been correct. Already, the Adobe cross-platform converter has balked at changing Chris' Mac files over to Windows files – thus I have no template from which to work. I hope to have this resolved in time for the November newsletter. Who knows what other monsters lurk out there, especially with Halloween fast approaching!

Some of you may wonder why I took on this extra responsibility with still two months left in my term as Chair. Well, I guess I have this sort of thing in my blood – my father worked as a newspaper reporter and editor for many years, and then closed his career as a public information director at a small Pennsylvania college. So, I've always thought about doing the newsletter editor's job, and when Chris' California assignment arose, I decided to take advantage of the impending vacancy. I look forward to providing you with informative and quality newsletters in the coming year. Of course, I would appreciate any comments or contributions that you may have.



# OCTOBER MEETING

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## Computer-Assisted Drug Design Methods

- Date:** Thursday, October 29, 1998
- Location:** The Partridge Inn  
2110 Walton Way, Augusta
- Schedule:** 6:30 PM Social  
7:00 PM Dinner  
7:45 PM Speaker: **Dr. J. Phillip Bowen**
- Menu:** Pork Loin  
or  
Boneless Chicken Breast Stuffed w/ Pecan Rice
- Cost:** \$27 per person; no student discount available.

*Reservations:* Deadline Tuesday, October 27 at 12:00 PM. Contact Roy Beck at (803) 208-6478. Leave a message on voice mail if necessary, indicating the names of those attending, the spelling of the names as they are to appear on the name tags, and your entrée selections.

*Abstract:* Hand-held mechanical models have been indispensable aids in understanding conformational problems and predicting chemical reactivity. Based in part on these mechanical models, chemical principles, and biological data, conceptual models have been used to predict biological activity. Despite their positive impact, however, mechanical models have inherent limitations that may adversely influence researchers. The advent of computers has ushered in a new and exciting age of molecular design, where it is now possible to calculate molecular properties accurately prior to laboratory preparation of the compounds. Molecular modeling-computational chemistry coupled with computer graphics-has become an increasingly important tool in chemistry-particularly medicinal chemistry, where it serves to gain insights into biochemical mechanisms and to assist in the design of molecules with specific biological activities. This presentation will focus on computer-assisted drug design methods that are used in academic and industrial laboratories.

*Continued on next page.*

*Our Speaker:*

J. Phillip Bowen is Professor of Chemistry in the Department of Chemistry and Co-Director of the Computational Center for Molecular Structure and Design (CCMSD) at the University of Georgia. He has over fifty (50) peer-reviewed research publications and five (5) book chapters. Dr. Bowen has been an invited lecturer on the topic of molecular modeling in the United States, Canada, and Europe.

Dr. Bowen received his BS in chemistry at Piedmont College, Demorest, Georgia, in 1979. Bowen studied synthetic organic chemistry under Professor David Goldsmith at Emory University and received his Ph.D. in 1984. Dr. Bowen has always been interested in theoretical organic chemistry. He accepted a postdoctoral research position with Professor Norman L. Allinger at the University of Georgia. In 1986, he accepted a faculty position as Assistant Professor in the Division of Medicinal Chemistry and Natural Products, School of Pharmacy, University of North Carolina at Chapel Hill.

While at the University of North Carolina, Professor Bowen developed a computational chemistry and molecular modeling teaching and research program that has been widely recognized and emulated by a number of other universities. For his efforts in creating this unique program, in 1988 he was given the Order of the Long Leaf Pine, the highest North Carolina nonmilitary award, by Governor James Martin. He was Director, Laboratory for Molecular Modeling (1987-1990) and held a Research Scientist appointment in the UNC School of Medicine (1987-1990). In 1990, Dr. Bowen accepted a faculty position (at the tenured rank of Associate Professor) at the University of Georgia and moved his laboratory into newly renovated research space. In 1997, Dr. Bowen was promoted to Professor of Chemistry.

Professor Bowen's research interests span the fields of organic and computational chemistry. Eleven students have received their doctorates under his direction, and two students who have completed their masters degrees. He is also one of the most highly rated teachers at the University of Georgia.

Professor Bowen plays an active role in community affairs. He is a Southern Baptist Deacon. He is a member of the North Clarke County Civic Association, where he served as president for the last three years. He is also a member of the Board of Trustees of Piedmont College. He has an active interest in American history, particularly the military events during the Civil War years.

# ACTIVITIES CALENDAR

February 3	Avondale Company Tour	Graniteville	Gregg Division
February 25*	SRS Technical Day	Augusta	Civic Center
February 27	Dr. J. Marquart "Caves – Worlds Within The World"	Augusta	Damon's
March 28*	Girl Scout Roundup	Augusta	Farmer's Market
April 27	Dr. J. Nagyvary "Chemistry and Violin Making – Past and Present"	Aiken	Willcox Inn
May 18	Dr. M. Reichmanis "Intellectual Property Rights in the Information Age"	Augusta	Rio Bravo
September 15*	CSRA College Night	Augusta	Civic Center
September 19-20*	Arts In The Heart	Augusta	Riverwalk
September 29	Chemical Jeopardy	Augusta	Augusta State
October 24*	SEED	Aiken	USC-Aiken
October 29	Dr. J. P. Bowen "Computer Assisted Drug Design Methods"	Augusta	Partridge Inn
November 1-7*	National Chemistry Week	CSRA	Various
November 17	Awards Banquet	Aiken	Aiken Brewing

\* ACS-SR booth or activity, volunteers needed.

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