

## ACS Meetings and Expositions – Regional Meeting Final Report



### I Introduction and General

General Co-Chairs – Tracy Hamilton (Alabama) and Xinyu Zhang (Auburn)

Program Co-Chair – Anne Gorden (Auburn) and David A. Dixon (Alabama)

#### I (a) Executive Summary

The 72nd Southeastern Regional Meeting of the American Chemical Society was held in Birmingham, AL November 10 – November 13, 2021 at the Birmingham Jefferson Convention Center (BJCC) . The last SERMACS hosted by the Alabama Section was in 1994. There were 1258 registered participants in attendance with 1224 presentations in 75 invited or contributed oral sessions and 15 poster sessions across four (4) days of technical and educational programming. Four (4) plenary sessions were held from an array of diverse and notable speakers. A variety of special events were held, in addition to the plenary addresses: an exposition with 15 vendors , an undergraduate student program, a graduate school fair with 30 participants, an awards luncheon, a K-12 teacher workshop with three parallel tracks with luncheon and demo, a Fermentation Chemistry social at a local brewery, a WCC social on the Chemistry of Absinthe with tasting, senior chemists breakfast, project SEED symposium, Women in Stem discussion. Two in person workshops: ACS CHAS, the Molecular Sciences Software Institute, were offered. Merck sponsored and ran a virtual workshop the Monday before the meeting. Two (2) Leadership Development courses were offered but were cancelled.

#### **I (b) Site and Date Selection**

The site selection process was initiated prior to the award of SERMACS 2021 in 2016 to the Alabama and Auburn Local Sections. Contact was made with the Director of Events (Jennifer Greer) at the Birmingham Sheraton Hotel and our ACS meeting planner (Michelle Stevenson) . There was turnover in the ACS position ( Starleeta Gaddis-Parker became our ACS meeting planner) before the contract was signed by Tracy Hamilton on June 11, 2018. The Birmingham Sheraton is adjacent to the Convention Center and created some confusion as to where the actual meeting rooms were located. The BJCC is able to handle very large conventions, so we only needed the East meeting rooms.

SERMACS meetings are traditionally held between mid-October and mid-November. We selected the first week in November to avoid conflicts with other regional meetings, and weather is generally good. We did not realize until shortly before the meeting that a large veteran's Day parade would be nearby.

#### **I (c) Committee Members**

**Tracy P. Hamilton**, General Co-Chair, is Associate Professor of Chemistry at the University of Alabama at Birmingham, and Councilor for the Alabama Local Section for the past 11 years. Tracy recruited the other members of the organizing committee and served as the primary interface with ACS National. [hamilton@uab.edu](mailto:hamilton@uab.edu) (which now re-directs to [t\\_p\\_hamilton@yahoo.com](mailto:t_p_hamilton@yahoo.com) since retirement).

**Xinyu Zhang**, General Co-Chair, is a Professor of Chemical Engineering at the University of Auburn. Xinyu was the primary Auburn liaison for the committee; taking the point on posters and on logistics. [xzz0004@auburn.edu](mailto:xzz0004@auburn.edu)

**Anne Gorden**, Program Co-Chair, is a professor at Texas Tech University. Most of the time she was in this role, she was a professor in the Auburn Chemistry Department. By agreement, Auburn handled most of the technical programming. Anne was instrumental in organizing the outstanding technical program along with her program co-chair. She served as the primary point of contact with ACS MAPS. [Anne.gorden@ttu.edu](mailto:Anne.gorden@ttu.edu)

**David A. Dixon**, Program Co-Chair, is a Robert Ramsay Chaired professor at the University of Alabama. Dave has extensive experience with MAPS as well, being a divisional (FLUO) councilor. He was responsible for being the contact with our largest sponsor – Oakwood Chemical. [dadixon@ua.edu](mailto:dadixon@ua.edu)

**Cindy Coshatt Pearson** (Cindy Willingham), Exposition Chair, is a Program Instructor/Chemistry Specialist at University of Alabama at Birmingham in the Science in Motion Program. She also obtained educational sponsorships and helped with K-12 programming. [ciwillin@uab.edu](mailto:ciwillin@uab.edu)

**Emily Menard**, K-12 Program Chair, is also a Program Instructor/Chemistry Specialist at University of Alabama at Birmingham in the Science in Motion Program. She recruited K-12 teachers and did programming on Friday (day after Veterans Day). She was key in getting us to realize that teachers would prefer Friday so that they would have a 4 day weekend. [emenard@uab.edu](mailto:emenard@uab.edu)

**Morgan C. Ponder**, Treasurer, is Professor (retired) of Chemistry at Samford University and an ALACS Treasurer for many years both past and present. Morgan is extremely detail oriented and responsive. [mcponder@samford.edu](mailto:mcponder@samford.edu)

**Pravin Kotian**, Awards Committee Chair, is a Principal Scientist at Biocryst Pharmaceuticals. Pravin began his duties on the SERMACS, Inc. Awards Committee with the 2019 regional meeting, and will continue through the 2022 meeting. He chaired the selection committee this year and also developed the awards program brochure and conducted the Awards Luncheon. [pkotian@biocryst.com](mailto:pkotian@biocryst.com)

**Jackie Nikles**, Undergraduate Program Chair, is an organic chemistry professor at UAB. Jackie coordinated the undergraduate program including symposia, poster sessions, and undergraduate social event at McWane Science Center. She is the faculty advisor for the UAB student Affiliate, who helped with poster setup along with UAB graduate students. [nikles@uab.edu](mailto:nikles@uab.edu)

**Kate Hayden**, Sponsorship Chair, is a professor at Birmingham Southern College (she will soon be at the University of Montevallo). Kate Helped with the sponsorship solicitation late in the process. All members of the organizing committee assisted with fund raising. [khayden@bsc.edu](mailto:khayden@bsc.edu)

**Vincent Ortiz**, Diversity Chair, is the Ruth Molette Professor and ex-chair of the Auburn Chemistry Department. His advice was invaluable, since he had experience as program Chair for a Midwest Regional meeting. Vince coordinated with Merck to arrange for a virtual symposium the Monday before the in-person meeting, and for a breakfast with targeted minority students with Merck representatives. [ortiz@auburn.edu](mailto:ortiz@auburn.edu)

**Jordan Harshman**, Secretary and Webmaster, is an Associate Professor in the Auburn Chemistry Department, maintained and updated the website which was hosted by Weebly with our own domain name. This website [www.sermacs2021.org](http://www.sermacs2021.org) will remain active for at least two more years so that future meeting webmasters can look for design ideas. [jth0083@auburn.edu](mailto:jth0083@auburn.edu)

**Catherine Situma**, Safety Co-chair, is a Laboratory Safety Program Manager at the University of Auburn. She was instrumental in planning and running safety workshops, and brought in another experienced safety expert. [cns0013@auburn.edu](mailto:cns0013@auburn.edu)

**Samuella B. Sigmann**, Safety co-chair, is the Chemical Safety Officer at Appalachian State University. She is the 2019 Howard Fawcett Chemical Health and Safety Award winner in the ACS Division of Chemical Health and Safety. Sammye oversaw safety protocols for the demos that were done for K-12 programs, and helped run the safety workshops. [sigmannsb@appstate.edu](mailto:sigmannsb@appstate.edu)

**Konrad Patkowski** , Graduate School Booth Chair, is a Professor in the chemistry Department of Auburn. kjp0013@auburn.edu

**Larry Krannich**, ex-officio, past District IV ACS Board Member, was the only person who had any involvement with planning the last SERMACS in Birmingham. krannich@uab.edu

**Starleetah Gaddis-Parker**, Meeting Planner, was of tremendous assistance in navigation meeting logistics. She in particular was invaluable in the meeting registration process. During the covid19 pandemic, ACS staff were not allowed in their offices the whole time that she was helping with the meeting, making certain tasks very difficult.

#### **I (d) Organizing Committee Meeting Operations**

The joint nature of the meeting added complications to oversight of operations, since the natural ultimately responsible party is the local section executive committee. In the days before Covid19 we would meet every six months in between the centers of the two sections, in Montgomery, AL. It was agreed at the first meeting that the Alabama Local Section manage most of the tasks which required visiting facilities, and Auburn would do most of the work on the technical program. The General and program co-Chairs all attended the Regional meetings track at the ACS Leadership Institute in Atlanta in 2020.

When covid19 started in Feb 2020, we started meeting quarterly as a whole committee by Zoom. The first vaccine was approved and available to the public in early 2021. We set a date for a drop dead decision by April 1, 2021 whether to proceed in-person, hybrid, or virtual. The vote was 11 for in-person , 3 for hybrid. The main argument against hybrid was the lack of experience, and prohibitive costs of doing it right. The whole committee started meeting every three weeks by Zoom after that date.

Many members of the committee were not experienced in the roles they held, but they were willing to work hard and do what was asked. Everything at the local level was rebuilt anew, and the help, advice and examples of other SERMACS members was invaluable. It has been suggested that current and recent past SERMACS chairs meet with their corresponding chairs in person at each SERMACS meeting, as part of the official program.

#### **I (e) Budget Development**

Most budget decisions were made by the executive committee (General co-chairs, Program co-chairs, Treasurer and Secretary). We based the budget development on the prior SERMACS budgets. Registration fees were \$5 more than the SERMACS 2019 meeting for regular member and nonmember rates, and the same as SERMACS 2019 for lower fee categories such as postdocs, K-12 teachers and students. The major expenses of Food and Beverage, and meeting rooms, were well estimated and fixed by the contract. The cost of AV was only a bit higher than expected. Traditional incentives which were used for symposium organizers to recruit speakers. An organizer of a half-day symposium could receive \$500 if they recruited five speakers, and an additional \$500 match if they obtained matching external funds.

This final meeting budget was approved by a Zoom meeting of the SERMACS, Inc. board (a first, since the 2020 joint SE/SW meeting in New Orleans was canceled).

## II Meeting Program

II (a) The full technical Program and Event Program is in Appendix A. While MAPS is used to generate a full technical program, we were not aware of how to automatically include social and other events, and did not have manpower available to combine the two. Starleeta used CVENT as a substitute for the app – this was universally panned. Paying an app provider is expensive, but worth it for engaging attendees who are familiar with the app.

### II (b) Plenary Speakers

Plenary talks were extremely well attended. They were scheduled to be after most symposia were finished but before supper. Snacks here were generally overbudgeted, and funds should have been applied more toward coffee in the expo/grad school recruiting hall. We focused on speakers with a local connection (former UA post-doc, UAB radiochemist, former Jacksonville State undergraduate football player, and UAB astronaut specialist), with the intent of exposing students to inspirational and perhaps careers that are not common.



## PLENARY TALKS

**Wed, Nov 10**



**Chang-Guo Zhan**  
Endowed College of Pharmacy Professor in Pharmaceutical Sciences, Department of Pharmaceutical Science, University of Kentucky  
*"Drug Discovery and Development via Structure and Mechanism Based Rational Design"*  
<https://pharmacy.uky.edu/people/chang-guo-zhan>

**Thu, Nov 11**



**Suzanne E. Lapi**  
Professor, Departments of Radiology and Chemistry  
University of Alabama at Birmingham  
*"From Isotopes to Images:  
Development of radiometal agents in medicine"*  
<http://www.lapilab.com/>

**Fri, Nov 12**



**Gregory H. Robinson**  
Foundation Distinguished Professor, Department of Chemistry  
University of Georgia  
*"From N-Heterocyclic Carbenes to Dithiolene-based Radicals: Recent developments in Main Group Chemistry"*  
<https://www.gregoryhrobinson.com/>

**Sat, Nov 13**



**Larry DeLucas**  
Principle Scientist, Aerospace Corporation  
*A Career in Science, Expect the Unexpected*  
<https://aerospace.org>

### II (c) Workshops

Most Merck scientists were prohibited from attending due to covid19 travel restrictions imposed by their company (National labs also had travel restrictions during this time).

### **Nov 8 (Monday) virtual Merck workshop**

9:00 am – 11:00 am CAREER WORKSHOP (topic TBD)

11 am – 12 pm BREAK

12:00 pm – 12:05 Brief Introduction

12:05 – 12:30 Yuping Bao (University of Alabama)

12:30 – 12:55 Subharekha Raghavan (Merck enabling tech)

12:55 – 1:45 Tom Kodadek (DEL)

1:45 – 1:55 BREAK

1:55 – 2:20 Dan Wyss (STING)

2:20 – 2:45 Frances Rodriguez-Rivera (micromapping)

2:45 – 3:10 Gregory Szwabowski (University of Memphis)

3:10 – 3:35 Michaelyn Lux (Skeletal rearrangements)

3:45 – 3:55 BREAK

3:55 – 5:00 Career Panel/closing remarks

**Nov 10 MOLSSI workshop** (120 registered, about 80 attended), on Python programming in computational Chemistry

### **Nov 12 Safety Workshop - Integrating Risk Assessment into Undergrad Teaching Labs**

The safety Workshop should have had a minimal fee, refundable if people to attend. This was planned but did not get implemented in the registration system.

This was also true of the MOLSSI workshop, but so many attended it exceeded our initial expectations. High attendance for MOLSSI was not particularly surprising, as there were non-overlapping theoretical symposia throughout the meeting.

## II (d) Award Presentations

Pravin Kotian was in charge, and did a great job. He did need a lot of advice from past Awards chairs, particularly Jordan Poler. Angela Wilson, gave the Awards talk, on very little sleep.



**Keynote Speaker**  
**Dr. Angela K. Wilson, ACS President-Elect**  
Angela K. Wilson is a John A. Hannah Distinguished Professor of Chemistry, Associate Dean for Strategic Initiatives and Director of the Center for Quantum Computing, Science and Engineering (MSU-Q) at Michigan State University. She earned her bachelor's degree in chemistry at Eastern Washington University and her Ph.D. in chemical physics from the University of Minnesota. She was a postdoctoral fellow at Pacific Northwest National Laboratory. From 2016-2018, she led the Division of Chemistry at the National Science Foundation. She has been a member of ACS since 1989.



**2021**

**Southeast Regional**

**ACS AWARDS PROGRAM**

**E. ANN NALLEY REGIONAL AWARD FOR VOLUNTEER SERVICE TO THE AMERICAN CHEMICAL SOCIETY**  
Recognizes the volunteer efforts of individuals who have served the ACS, contributing significantly to the goals and objectives of the Society through their regional activities  
**Robert C. Wingfield, Jr. (2021)**

**PARTNERS IN PROGRESS & PROSPERITY**  
Recognizes partnerships among industry, academia, government, small businesses and/or other organizations that result in impactful outcomes  
**Travis Throgmoll (2021)**

**ACS DIVISION OF CHEMICAL EDUCATION SOUTHEAST REGION AWARD FOR EXCELLENCE IN HIGH SCHOOL TEACHING**  
Recognizes, encourages, and stimulates outstanding teachers of high school chemistry  
**Evelyn Baldwin (2021)**

**SERMACS AWARDS COMMITTEE (2021)**  
Miguel Santiago  
Jordan Poler  
Pravin Kotian

**SERMACS PLANNING COMMITTEE (2021)**  
Tracy Hamilton, General Co-Chair  
Xinyu Zhang, General Co-Chair  
Anne Gordon, Program Co-Chair  
David Dixon, Program Co-Chair

**SPECIAL THANKS TO THE SERMACS EXECUTIVE BOARD**  
for their generous help and support of the awards program



**NOVEMBER 10-13, 2021**  
Hosted by the Alabama & Auburn Local Sections of ACS

**2021 SERMACS**  
Chemistry in the Magic City  
BIRMINGHAM, AL



**2021**

Southeast Regional

**ACS AWARDS PROGRAM**

## Program Agenda


## Award Recipients

**12:00 PM**  
Welcome Remarks & Meal Service

**12:30 PM**  
Introduction of Keynote  
Keynote Speaker:  
Dr. Angela Wilson, ACS President-Elect

**1:00 PM**  
Presentation of the Southeast Regional ACS Awards  
Recognition of the SERMACS Local Organizing Committee


**1:30 PM**  
Closing Remarks




**E. ANN NALLEY REGIONAL AWARD**  
**2021**

Dr. Robert C. Wingfield Jr. is currently serving as an Associate Professor of Chemistry at Fisk University (where he has served since 1985). He is the Director of the Fisk Community Environmental Toxicity Awareness and Sustainability Program, which is funded by NIEHS through the Midwest Consortium. He has had over twelve years industrial experience in chemical process and product development. He served as External Process Leader and Co-Chair of a statewide Steering Committee to develop an Environmental Justice Strategic Plan for the Tennessee Department of Environment and Conservation (1998-2000). From July 2003 to October 2004, he chaired the Nashville Health Disparities Coalition. Also, in 2003, he was appointed by the Mayor of Nashville to the Healthy Nashville 2010 Leadership Council to help lead the city in establishing strategic priorities and mobilizing community initiatives to achieve significant improvements in the city's health by 2010. In 2009 he was appointed by Governor of State of Tennessee to the Compliance Advisory Panel to provide support to the TDEC Small Business Environmental Assistance Program. He has served as an appointed member of the Metropolitan Nashville-Davidson County Wastewater Hearing Authority since 1999. He served on the Committee on Science of the American Chemical Society from 2003 to 2012. He is currently serving as Chair of the Nashville Section, American Chemical Society and serves on the Executive Committee of the Middle TN Group of the TN Chapter of the Sierra Club. During 2020, he served on the Climate and Energy Subcommittee of the Mayor of Nashville's Sustainability Advisory Committee for the development of a Nashville Climate Action Plan. Since April 2006, he has served as co-host on the WFSK 88.1 FM, "Health Watch: Pathway to Better Health" weekly radio show.

**PARTNERS IN PROGRESS & PROSPERITY**  
**2021**



Dr. Travis Thorpe is a research physical scientist at the US Army Engineer Research and Development Center (ERDC) in Vicksburg, MS. He received his BS in Polymer Science from the University of Southern Mississippi (USM) in 2013 and his PhD in Materials Engineering from Purdue University in 2018. Dr. Thorpe joined ERDC as a researcher in 2018 in the Concrete and Materials Branch of the Geotechnical and Structures Laboratory where he plans and conducts research in Military Engineering with internal and external partners. Through a partnership with the USM, Dr. Thorpe oversees research and academic collaboration between ERDC and USM that produces internship and employment opportunities for undergraduate and graduate students. His research interests are in the synthesis and characterization of stimuli-responsive polymers and development of multi-functional composites.



**Excellence in Highschool Teaching**  
**2021**

Evelyn Baldwin received her BS and MEd in science education from North Carolina State University and currently teaches at a STEM early college in Wake County, North Carolina. She is an ASSIST (Advanced Self-Powered Systems of Integrated Sensors and Technologies) RET (Research Experience for Teachers) fellow, a Kenan Fellow, a Lockheed Martin Fellow, and a National Board-Certified Teacher in Adolescent and Young Adulthood Education. She has been a secondary science educator in the Wake County Public School System for twenty-six years. At Wake STEM Early College High School, she teaches honors chemistry and honors physics and is the leader of the tenth-grade teaching team. Mrs. Baldwin sponsors the STEM Science Olympiad team and a junior chapter of NCSU's Women in Science and Engineering. Her focus is on empowering underrepresented students and first-generation college students to enter and be successful in STEM fields. Outside the classroom, she is an educational outreach liaison for the NCSU ASSIST center where she works with teachers to incorporate current STEM research into their lessons and enables students to conduct authentic research in research labs. Evelyn also supports online learning as a teacher, course leader, and content creator for the NC Virtual School.

**ACKNOWLEDGEMENTS**

ACS Committee on Minority Affairs  
ACS Division of Chemical Education

## II (e) Hotel and Venue Performance Issues

The hotel had not been open during covid, and had only opened June 1, 2021. The problems with staffing turned out to be a nationwide problem during the epidemic. Customer service was not up to Sheraton standards. Angela Wilson had been flight delayed and her room given away. Many of the hotel restaurants were closed, and we provided a list of restaurants that did takeout delivery. We were also unaware that the electronic signage outside each meeting room was not working – the explanation we were given was that work on the new stadium next to the convention center was somehow responsible.

## II (f) A/V arrangements

PSAV was the original vendor of choice, and gave us a 20% discount. We had to pay extra for microphones for the larger rooms, and for talks which had a significant online component. Responsibility for running a session as hybrid was fully the responsibility of the symposium organizers. The original estimate was \$40,000, and the final cost was \$44,722. PSAV had a technician on site, who responded quickly to requests and problems.



## II (g) Electronic Abstract Service

Both program co-chairs had previous MAPS experience, which was invaluable. There were a few chairs of the general sessions which did not return excel workbooks, probably from ignorance. These sessions were assigned by the program chairs after the window for submission. For some reason, a few sessions were not being assigned and numbered in MAPS. Anne Gorden was diligent and persistent in making sure every talk was sessioned correctly. When workbooks are created, columns for sponsorships should be added even if the system is unaware of any – because a sponsor may be late in providing funding for an event.

## II (h) Sponsorships

We had no experienced person as sponsorship chair, which impacted fundraising. The uncertainty surrounding covid19 also made some sponsors reluctant. Some organizations that would normally send representatives, donated a small amount to be a general sponsor. Sponsorships were acknowledged on the website, symposium signage, major sponsors were acknowledged in slides sent to the chairs of that day's sessions, with space for them to add specific symposium sponsors. Logos for each sponsor was placed on the website, with a link. Some links may have been missing. The sponsor benefits package is listed below:



### Sponsor Benefits

#### Platinum: \$10,000+

- Program App advertisement (premium time and duration)
- Five (5) attendee passes
- Exposition Booth
- Opportunity to address the attendees (5 minutes maximum)
- Website logo and link

#### Gold: \$ 5,000 - \$9,999

- Program App advertisement (superior time and duration)
- Three (3) attendee passes
- Opportunity to address the attendees (2 minutes maximum)
- Website logo and link

#### Silver: \$ 2,500 - \$4,999

- Program App advertisement
- Two (2) attendee passes
- Website logo and link

#### Copper: \$1,000 - \$2,499

- Program App advertisement
- One (1) attendee pass
- Website logo and link

#### Iron: \$500 - \$999

- Website logo and link

#### Aluminum: < \$500

- Recognition on Sponsor signage

Major sponsors were

Oakwood Chemical – Platinum

Merck, NSF, Auburn College of Math and Science – Gold

AMSTI and Avanti Polar Lipids – Silver

All session organizers and organizing committee members were responsible for finding sponsors for the meeting. This proved effective at meeting our sponsorship fund raising target. Individuals used their personal and business relationships to leverage support for the meeting.

### **III Meeting Finances**

#### **III (a) Budget**

See Appendix B for the proposed budget, and actual revenues and expenses. The meeting revenues were

Revenues      \$233,350.65

Expenses      \$167,425.80

Net              \$ 65,924.85

SERMACS, Inc share \$ 13,184.97

Auburn Section share      \$26,369.94

Alabama Section share      \$26,369.94

SERMACS, Inc for \$13,684.97 will be brought to the SERMACS 2022 meeting. The extra \$500 is the difference between the SERMACS loan of \$5,500 and the Merck sponsorship of \$5,000.

During covid19, we changed the estimated number of attendees for the registration budget from 1200 to 1000 to be conservative. The number of onsite registrations was very high because people were waiting to see if the meeting would proceed. Nevertheless, we exceeded the original registration revenue projection by >\$18K, with 1258 registrations and revenue at \$149,850. (refer to Appendix B: SERMACS 2021 Budget).

The rest of the estimated revenues were about the same as projected, with a much greater number of corporate sponsorships (from symposium and SERMACS organizer fundraising, and much less Expo revenue)

#### **III (b) Financial Accounts Used by the Meeting**

A SERMACS 2021 account was opened with Regions Bank, which also holds the checking account for the Alabama Local Section. The Alabama Local Section bank account with Regions is “American Chemical Society”, so the separate SERMACS account also was required to be “American Chemical Society”. Solicitations asked for checks to be made out to “American Chemical Society” with SERMACS 2021 in the memo line. The Alabama section

applied for a line of credit and direct billing with the Birmingham Sheraton, and was approved for \$65K. The Alabama local section made loans to the SERMACS 2021 account when fund balances were getting low, and registration fees hadn't come in yet.

Authority for financial transactions was only Morgan Ponder, Alabama section and SERMACS 2021 Treasurer

Morgan was the only person who wrote checks (199 as of Oct 12, 2022), and he was the only person who transferred funds to and from the account that the ACS escrowed from online registrations and sponsorships.

### **III (c) Fundraising for the Meeting**

Sponsorships were collected both by checks sent to the Treasurer, and later from the CVENT site. This did cause some problems with making sure that sponsors are acknowledged. It also made the Treasurer's job unnecessarily complicated. We had a person step up in the Fundraising role late in the game, it was difficult to find a person suited for the role who was also willing. Most fundraising was done by the committee and symposium organizers.

### **IV Expo and Graduate School Fair**

The SERMACS 2021 Expo was very small, with 14 booths rented. An additional booth was given to Agilent due to a confusion on their part between a sponsorship and expo booth. The expo solicitation process was very stressful given uncertainties due to covid19, and lack of personal contacts from the prior meeting. The organizing committee plan was to have most of the organizers attend the 2020 SW/SE combined meeting. No central list was kept of which vendors had been contacted. The graduate school fair was filled at 30, we could have easily taken more. The list of Expo Vendors and list of Graduate school booths is in Appendix C.

Getting the prospectus to hand potential vendors was too long delayed, which in turn delayed contacts with industry, and finally incorporation into the program. The map for the locations of booths was in the program, but the list of which sponsor was only on the website. ACS regional Meeting staff should be proactive with organizers on this during the year of the previous meeting. Having an experienced Expo Chair to help next time should result in a more systematic and successful effort.

We did not do any direct survey of the vendors, but traffic to the area seemed busy, and I know of no specific complaints. The poster location in the same hall, and coffee breaks, helped. It also helped that the hall was visible from the registration desk.

Appendix D contains forms and rules for expo and graduate school booths.

### **V Publicity**

The organizers publicized the meeting primarily through C&E News, ACS emails targeting all members in the SERMACS Region, and having an active, informative website well in advance. ACS emails apparently did not reach all members in the area – the list of local

sections contained in the SERMACS region needs to be double checked. A list of officers of each local section in the SERMACS region should be provided in the Spring after Fall elections have been held. We did not have the usual booth available for publicizing the next SERMACS. Below is the C&E News Announcement from Sept 24, 2021.



Credit: Shutterstock

Birmingham, Alabama

**T**he Auburn and Alabama Local Sections will host the Southeast Regional Meeting of the American Chemical Society (SERMACS) Nov. 10–13 at the Sheraton Birmingham Hotel in downtown Birmingham, Alabama. [Details, including COVID-19 protocols, can be found at sermacs2021.org.](https://sermacs2021.org)

**Technical program.** Plenary talks will be held daily in the early evenings. Speakers will include Chang-Guo Zhan, professor of pharmaceutical sciences at the University of Kentucky, on Wednesday evening; Suzanne E. Lapi, professor of radiology and chemistry at the University of Alabama at Birmingham, on Thursday evening; Gregory H. Robinson, professor of chemistry at the University of Georgia, on Friday evening; and Larry DeLucas, principal scientist with the Aerospace Corporation, on Saturday evening.

Over 1,250 abstracts have been submitted, and more than 60 half-day sessions of invited technical programming will span all the disciplines of chemistry. [View all the symposia at sermacs2021.org/symposia.](https://sermacs2021.org/symposia)

#### SERMACS 2021 AT A GLANCE

- **Dates:** Nov. 10–13
- **Location:** Birmingham, Alabama
- **Information contacts:** General cochair Tracy Hamilton  
[hamilton@uab.edu](mailto:hamilton@uab.edu)
- **Website:** [sermacs2021.org](https://sermacs2021.org)



**Workshops.** SERMACS 2021 offers two ACS Leadership Development courses: Collaborating across Boundaries on Thursday morning and Leading without Authority on Saturday morning. A Molecular Sciences Software Institute Workshop will cover how to create publication-quality graphs and visualizations using Python and the Jupyter Notebook and may be of interest to computational chemists. A safety workshop, "Integrating Risk Assessment into Undergraduate Teaching Labs," will be held on Friday. Merck will host a virtual career workshop and a technical symposium before the meeting on Monday, Nov. 8.

**Undergraduate programming.** The session "Women in STEM" will take place Friday afternoon, and "Careers in Industry" will be held on Saturday afternoon. Both sessions will end with a panel discussion. A special undergraduate poster session will be held at the McWane Science Center on Friday evening. The entire first floor will be open, and all attendees and their families are invited. Student chapters can [enter a virtual demo contest at sermacs2021.org/undergraduate.html](https://sermacs2021.org/undergraduate.html). On Saturday, DeLucas will close undergraduate programming with his plenary talk, and an undergraduate pizza party will follow.

**Exposition and graduate school fair.** The expo will kick off on Thursday morning and run through Friday, offering a great opportunity to learn about the latest products on the market. Applications for exhibitors are available on the meeting website. A graduate school fair will take place on Saturday morning, coinciding with two undergraduate poster sessions. **Applications for the expo and graduate fair can be found at [sermacs2021.org/exhibitors.html](https://sermacs2021.org/exhibitors.html).**

Exhibitors SERMACS 2021 - SERMACS 2021

**Awards.** Several awards will be presented at the meeting. These include the Stanley O. Inder Regional Award for Advancing Diversity in the Chemical Sciences, Regional Awards for Excellence in High School Teaching, and the E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society. The awards luncheon will take place on Thursday.

**Social events.** Among the social highlights of SERMACS 2021 will be the Younger Chemists Committee Brewery Event on Thursday night on the covered porch at Cahaba Brewing. Participants are also invited to attend the awards luncheon and the senior chemist breakfast at which Steve Burgess from Avanti Polar Lipids will discuss lipid nanoparticle technology in mRNA vaccines. On Wednesday, Ted Breau, chemist and founder of Jade Liqueurs, will lead an absinthe tasting at a Women Chemists Committee "Just Cocktails" event.

**Lodging and registration.** Early-bird registration for the meeting ends at 11:59 p.m. (EDT) on Sept. 29, but you can register at the on-site rate through the end of the meeting. You can reserve a room at a reduced rate at the Sheraton Birmingham Hotel through the SERMACS 2021 website.



## VI Website and Logo

The website was the most effective method of advertising the meeting. SERMACS attendees know to check the meeting websites for the latest information. A meeting app is increasingly more important as well, but web sites still exist for their clear advantages. Vendors probably did use the website to obtain information on who to contact, and initiated contacts, and sometimes specifically mentioned not having booths next to a competitor. Many vendors had no budgets for expos in 2021 due to covid19 travel restrictions.

Our website design was modeled after the 2018 and 2019 SERMACS meetings. We concur with the prior reports, and wish to emphasize that having a website early DOES NOT interfere with other meetings or confuse attendees. To quote the 2018 report:

“Future regional meetings need to launch their websites years BEFORE their meeting is scheduled to begin. The recent ACS Regional Meeting Office guidance that one cannot publicize an upcoming meeting website until AFTER the proceeding meeting is short sighted. It is important to build interest in the future meetings because sessions, sponsors, and exhibitors cannot be secured in a single year, this effort takes years of effort. A future meeting needs to look professional in order to attract sponsors and vendors. The biggest disservice a regional meeting does to itself is launch and build out its website too late for it to be an effective marketing tool.”

The logo was designed by a graduate student of Anne Gorden , Julie Niklas. It is a minimal design. Birmingham's nickname is the Magic City (because it grew quickly as if by magic). We tried variations on Magic and Chemistry, and settled on the more direct reference to the Magic City. The colors are ACS yellow and blue, the zero in 2021 is a flask, and the one in 2021 is a magic wand. The hexagonal bipyramid is a balance for the text, and more obviously a chemical graphic.



The pandemic did give us a unique give-away which we hope most people can put away fondly, never to be used again. Again, in the colors to match ACS blue and yellow. Supply issues did make us nervous about delivery in time. The feel was very soft and satiny, attendees loved them.



## VII Arrangements

Given the increasing availability of Uber and Lyft, and prohibitive costs of buses, we decided against providing travel arrangements.

Pizza was purchased from Post Office Pies for the Wednesday night WCC Social “The Chemistry of Absinthe” presented by world expert and analytical chemist Ted Breau. Ted provided the absinthe for the tasting. This event did not make it into the registration site, so we had attendees pay at the door. We made announcements through emails, daily announcement slides before symposia, and word of mouth. We also invited the general public. The event sold out – we had to turn people away. The space was donated by Avondale Brewing in the Sour Room. Unfortunately, some attendees were late because a notorious train crossing had a train stopped for 15 minutes.

The fermentation social on Thursday night had sandwiches from the Publix bakery which was picked up by volunteers. Drink tickets were issued for two beers or wines or one mixed drink. This was also well attended, around 80 attendees participated. The event was on an open air front porch, which alleviated covid19 concerns.

The Friday night event at McWane Science Center was a few blocks from the convention center, walkable in good weather – which we fortunately had. The walk gave attendees a good feel for the revitalization of Birmingham downtown. The next SERMACS in Birmingham will see an even more vital downtown area. The downtown was renovated in order to create the best impression for attendees of the World Games (which was canceled in 2021 and moved to 2022). Sandwiches and chips were again provided, though through an oversight a vegetarian option was not ordered.

The Saturday night undergraduate social was a ticketed event – we sold tickets for 40 (the capacity of that restaurant minus the bar area for walk-ins) but about half showed up at Tortugas. This was at the end of the conference, so it is probably something that should be expected in the future.

## Appendix A

# SERMACS 2021 Technical Program

For Workshops, Expo, Graduate Fair, Social Events and Meal events see the SERMACS 2021 Event Program

Maps are at the end of the technical program

## WEDNESDAY AFTERNOON

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

### Biochemistry

#### Poster Session

J. Zhang, *Organizer*

#### 1:00 - 3:00

**2.** Investigation of Protein Complexes Involved in the Activation of Methyl-coenzyme m Reductase. **S. Yavari**

**3.** Thermodynamics of the Competition Between Netropsin and AT-hook Peptides for AT-rich sites. **T. Townsend**, M. Fuenmayor Llanos, K.L. Buchmueller

**4.** Screening of EndoV variants as a tool for mapping A-to-I editing. **A. Scott**, S. Knutson, **A. Quillin**, J.M. Heemstra

**5.** Partial Formation of a Protein-based Cofactor in *M. tuberculosis* KatG and Its Impact on Catalysis. **T. Aziz**, **D.C. Goodwin**

**6.** Investigating the Interactions Between DNA Oligomers and Gemini Surfactants. **E. Boatwright**, A. Ginegaw, H. Nembaware, R.D. Sheardy

7. Probing Conformational Dynamics of GQ Formation in Varying Na<sup>+</sup>/K<sup>+</sup> Ratios. **A. Lacen**, H. Lee
8. Expression, Purification, and Crystallization of a Putative Monooxygenase Key to Global Sulfur Cycling. **H.C. Frohock**, M. Culpepper, S. Bober
9. Testing the Methylation Ability of Mmp10, a New Radical SAM Methyltransferase. **K. Clohan**, N. Shao, W.B. Whitman, E.C. Duin
10. Allosteric Regulation of Human Epithelial 15-lipoxygenase-2. **A. Ohler**, E. Patel, A.R. Offenbacher
11. Role of Intrinsically Disordered Electronegative Clusters in RNA-binding Proteins. **S.M. Zaharias**, T. Fargason, Z. Zhang, T.M. Paul, J. Zhang
12. Ionic Liquid Loaded Nanoparticles to Deliver drug Candidates to Mammary Carcinomas. **G.S. Dasanayake**
13. Active Pharmaceutical Ingredient-Ionic Liquid (API-IL) Drug Loaded Polymer Nanoparticles for Targeted Drug Delivery Applications.. **G. Singh**, E.E. Tanner
14. Characterization Initiation of Alternative Splicing: The Interaction of SR Proteins and the U1 Spliceosomal Complex. **T.M. Paul**, T. Fargason, s. jamal, Z. Zhang, J. Zhang
15. Biophysical Studies of Genomic West Nile virus RNA G-quadruplexes. **T. Le**, A. Paul, W. Wilson, M.W. Germann
16. Determining the Mechanistic Role of the A12.2 Subunit in the Kinetics of Multi-nucleotide Addition Catalyzed by RNA Polymerase I. **K. Fuller**, D. Schneider, A.L. Lucius
17. Using X-ray Structures to Probe the Molecular Properties of the Specific Binding of Heterocyclic Diamidines in AT-Rich DNA Sequences. **E. Ogbonna**, A. Paul, A. Kumar, a. Farahat, D.W. Boykin, W. Wilson
18. Determining the Role of Metal Ions in Inhibiting Topoisomerase II $\alpha$ . K.R. Lyons, W. Medawala, **E.C. Lisic**, X. Jiang
19. Mechanistic insights into photochemical processes of a de novo designed artificial metallopeptide hydrogenase. **S. Maliyam Parambath**, A.E. Williams, L.A. Hunt, D. Selvan, N. Hammer, S. Chakraborty

- 20.** Characterization of the substrate binding site for the poly(aspartic acid) hydrolase PahZ2 from *Sphingomonas* Sp. KT-1. **A. Jansch**, M. Weiland
- 21.** Development of Spectroelectrochemical Techniques for Redox-Active Neurotransmitter Detection. **P.A. Evans**, B. Sharma
- 22.** Synthesis and Cytotoxic Evaluation of 15-deoxy-Prostamide J<sub>2</sub> and Related Derivatives. **D. Halatek**, R. Van Dross, C. Burns
- 23.** Crystallographic Examination of Inhibition by Diamidine Minor Groove Binders on the Transcription Factor PU.1. **J. Terrell**, A. Paul, G. Poon, W. Wilson
- 24.** Observations and Conformational Changes of Zinc Dependent AdcR by Structurally Inspired Inhibitors. **A. Cutright**, J. Emerson
- 25.** Role of Outer-Sphere H-bond Donation on the 3-Mercaptopropionic Acid Dioxygenase (3MDO) Transition State. **A. Schmittou**, N. York, M. Lockart, B.S. Pierce
- 26.** Analysis of Microbial Colonization Patterns of Forensically Important Flies. **C. Huhn**, S. Bucheli
- 27.** Analysis of Green Fluorescent Protein using Polarized Resonance Synchronous Spectroscopy. **K.R. Carter**, S. Stokes, D. Zhang, J. Emerson
- 28.** Insights into the Local Structural Impact of Neighboring Nucleotides in Duplex DNA. **S.T. Brenden**, M.W. Germann
- 29.** Investigating the Production and Biosynthesis of Coenzyme F<sub>430</sub> Variants in Methanogenic Archaea. **K. Boswinkle**, K. Allen
- 30.** A suicide diiron oxygenase in *p*-aminobenzoate biosynthesis in *Chlamydia trachomatis*. **R.S. Wooldridge**, K. Allen
- 31.** *Ribonucleotide damage near a replication fork. Enzymatic and structural consequences.* **S.T. Brenden**, R.M. Brosh, M.W. Germann
- 32.** Stimuli-responsive Nucleic acid Activation via Catalyzed Glyoxal Decaging. **D. Karloff**, A. Sanford, S. Knutson, J.M. Heemstra
- 33.** Elucidation of the Structural Mechanism for RNA Recognition of SR Proteins. **N.U. De Silva**, T. Fargason, Z. Zhang, J. Zhang

- 34.** Interactions of RRM Motifs of SRSF1 Proteins. **E. King**, J. Zhang, T. Fargason
- 35.** Characterization of the Interaction Between U2AF35 and SRSF1 in RNA Splicing. **Z. Zhang**, J. Zhang
- 36.** NIR Donor Acceptor Fluorophores: Stability, DNA Interactions, and DNA Photocleavage. **C.P. Seudieu**, G.E. Ozmen, D.T. Brewer, E.O. Ahoulou, M. Henary, K.B. Grant
- 37.** Synthesis and Antiviral Evaluation of 6-Azauridine Prodrugs. **S.D. Karyakarte**, L.D. Bratton, O. Moukha-Chafiq, J.L. Smith, K. Keith, N. Haese, F. Ahmad, Y. Martinez-Gzregorzevska, L. Rasmussen, B. Ying, M. Diamond, H. Xia, P. Shi, B. Tekwani, R. Bostwick, D. Streblow, A.J. Hirsch, C.E. Augelli-Szafran, A.K. Pathak
- 38.** Hepatic Genomic Assessment of Dietary Ingestion of 2-Aminoanthracene in Sprague Dawley Rats. **A.M. Cisse**, W.E. Gato, J. Erber
- 39.** 4-Substituted-2-Thiazole Amides as Viral Replication Inhibitors of Alphaviruses and Flaviviruses. **A. Garzan**, S. Ahmed, N. Haese, S. Zhang, N. Tower, F. Ahmad, L. Rasmussen, V. DeFilippis, A.J. Hirsch, J.L. Smith, B. Tekwani, R. Bostwick, C.E. Augelli-Szafran, M.J. Suto, T. Morrison, M. Heise, D. Streblow, A. Pathak
- 40.** Analysis of the Optical Properties and DNA Photocleaving Abilities of NIR Carbocyanine Dyes Containing a Triphenyl Phosphonium Moiety. **D. Brewer**, E.O. Ahoulou, K. Ilina, M. Henary, K.B. Grant
- 41.** Characterization of the Flavin-dependent Tryptophan 7-halogenase (PrnA) from *Burkholderia ambifaria*. **M. Akter**, M.R. Uddin, J. Emerson
- 42.** Enhanced Structural Characterization of Multi-stranded Nucleic Acid Nanoparticles. **L.A. Rolband**, M. Chandler, C. West, D. Beasock, I. Danai, J. Krueger, K. Afonin
- 43.** Environment Matters: Lipid Composition and Stability of Staphylococcal Membrane Preparations from Supplemented Growth Media. **A. Pokorny Almeida**, D. Raskovic, G. Alvarado, K. Hines, C. Gatto, L. Xu, B. Wilkinson
- 44.** Redox Inactive Chloride Salts can Enhance the Ability of Methylamine Polycyclic Aromatic Hydrocarbons to Photosensitize ROS Production. **A.M. Ugboya**, K.B. Grant, M. Safarian

- 45.** Computational Studies Evaluate Experimentally Observed Binding of Novel glycopeptide Antibiotics to Bacterial Cell Wall Analogs. **K.L. McWhorter**, V.T. Chioti, M.R. Seyedsayamdost, K.M. Davis
- 46.** Thermodynamic, Dynamic Light Scattering, and Hydrogen-Deuterium Exchange Investigation of Fatty Acid Regulation of Soybean Lipoxygenase Reveals Dynamically Driven Allostery. **D. Roberts**, A. Benton, S. Lindsay, Y. Li, A.M. Spuches, A.R. Offenbacher
- 47.** Experimental Validation of Computationally Generated Structure-Based Pharmacophores. **M. Guerrero**, G. Szwabowski, K. Ruddick, A.L. Parrill-Baker, D.L. Baker
- 48.** Surface energy profiling of adhesin proteins. **P. Ayres Galhardo**, M. Phan, A. Brown
- 49.** Synthesis and Evaluation of Novel, Small Molecule Inhibitors of Spermine Oxidase as Neuroprotective Agents. **A. Furbish**, P.M. Woster
- 50.** Exploring Microsphere Suspensions for High throughput detection of label-free RNA. **M.C. Adams**, V.T. Milam
- 51.** Quantum Dot Tracking Illuminates the Role of Membrane Microdomains in Serotonin Transporter Function and Cell Surface Dynamics. **L. Bellocchio**, O. Kovtun, I.D. Tomlinson, S. Rosenthal
- 52.** Synthesis and Evaluation of KDM4B inhibitors for the Treatment of Inflammation in Periodontal Disease. **K. Garrabrant**, J. Gerasco, C. Novince, P.M. Woster
- 53.** Controlled Disorder: Phosphorylation tunes Intramolecular Interactions of the Protein SRSF1. **T. Fargason**, E. King, Y. Thompson, I.U. De Silva, Z. Zhang, T.M. Paul, S. Zaharias, J. Zhang
- 54.** Quantum Dot Tracking Uncovers D2 Dopamine Autoreceptor-dependent Dynamic Rescue of Bipolar Disorder-associated Dopamine Transporter Mutant. **R. Torres**, O. Kovtun, I.D. Tomlinson, S. Rosenthal
- 55.** Kinetic Mechanism of Translocation of ClpB, an Hsp100 Protein, on Protein Substrates. **J. Banwait**, A.L. Lucius
- 56.** Evaluation the Efficacy of Various Hydrophobic Degrons for PROTAC-Mediated Degradation of the Androgen Receptor. **J. Crowe**



- 57.** Comparison of sequence and Structural Features of Fish and Mammalian Protamine using Multiple Trajectory MD Simulation to Understand their Role in DNA Condensation. **H. Shadman**, C. Gallops, J. Ziebarth, Y. Wang
- 58. Withdrawn.** Tracking Individual Endogenous Dopamine Transporters using Antagonist-conjugated Quantum Dots. **B. DeMarco**, R. Torres, O. Kovtun, I.D. Tomlinson, S. Rosenthal
- 59.** Uncovering the Unique Biochemical Properties of RNA Polymerases I, II, and III. **R.Q. Jacobs**, Z.M. Ingram, A.L. Lucius, D. Schneider
- 60.** Structures Of Repressor: DNA Complexes From Different Mycobacteriophage Subclusters Reveal The Molecular Details Of Heteroimmunity Phenotypes. R. McKinney, M.D. Gainey, **J. Wallen**
- 61.** Identifying the tolerance of CRISPR-Cas10 to mismatches in the crRNA-target duplex. **S. Khweis**
- 62.** Engineering Reversibly Thermo-Responsive Gold Nanoparticles for Photothermal Therapy. **D. Amarasekara**, C. Kariyawasam, M. Hejny, N.C. Fitzkee
- 63. Withdrawn.** SWiCAM (Sliding Window Comparative Alignment Metrics): An open-source program for visualizing differential amino acid enrichments in subsets of homologous protein families. **A. Schoeffler**, E. Hill, **A. Hill**
- 64.** Secondary Amine Selective Petasis Bioconjugation. **O. Nwajiobi**, M. Raj
- 65.** Synthesis of Hibiscone C. **M. Turnipseed**
- 66.** Interactions Between Emerging Per and Poly-fluoroalkyl Substance (PFAS) with Human Serum Albumin (HSA). **D. Perera**, K.E. O'Shea, J. Miksovska
- 67.** Development of Molecular Probes for Imaging of CD206 Positive Macrophages in Cancer. **C. Parker**, A. Bin Salam, C. Yates, S.E. Lapi
- 68.** Characterization of Radical SAM Aminomutases Involved in Compatible Solute Biosynthesis in Methanogenic Archaea. **T. Tunckanat**, A. Gendron, K. Allen
- 69.** Growth Outcomes of Pseudomonas Aeruginosa after Knockout and Restoration of the Inhibitor of Vertebrate Lysozyme in Conditions Mimicking the Cystic Fibrosis Lung. **A. Gaddy**, T. Leeper

**70.** Recombinant Expression of Methyl-coenzyme M Reductase Reveals the Importance of Accessory Proteins for Proper Assembly. **A. Gendron**, K. Allen

Birmingham Jefferson Convention Center  
East Meeting Room F

## **Bioinorganic Chemistry**

B. S. Pierce, *Presiding*

**1:00** Introductory Remarks.

**1:05 71.** Iron-sulfur (Fe-S) Cluster Biogenesis: Studies of the Suf Pathway in *E. coli*. **F. Outten**, C.E. Fisher, T.D. Carter

**1:25 72.** Site-Directed NiS<sub>3</sub> type Model of the Proximal Ni of the A Cluster of Acetyl Coenzyme Synthase / ACS using a De Novo Designed Trimer Peptide. **D. Selvan**, S. Chakraborty

**1:45 73.** Investigating the Biosynthesis of N-Nitroglycine. **G. Padilla**, R. Lake, D.E. Graham, J.D. Caranto

**2:05 74.** Biomimetic Polyimidazole Chelates Investigating Mn<sup>2+</sup> Affinity in Immune Protein Calprotectin. **R.B. Gaynor**, S. Creutz

**2:25 75.** Platinum Indazole Complexes with Potential Anti-cancer Activity: Synthesis, Characterization, and Reactivity. **R.E. Bachman**, K. Wills, K. Barwick, G. Ferrence, K.A. Wheeler

**2:45** Intermission.

**3:15 76.**

Connecting Conformational Entropy Changes to Zinc(II) and Copper(II) Binding in Human Carbonic Anhydrase II. **J. Emerson**

**3:35 77.** Manganese Complex with a Redox-active Ligand acts as an Efficient Superoxide Dismutase Mimic. **S. Karbalaeei**, D.D. Schwartz, I. Ivanović-Burmazović, C. Goldsmith

**3:55 78.** Ferric-superoxo Intermediate of the TxtE Nitration Pathway Resists Reduction, facilitating its Reaction with Nitric Oxide. **C.P. Martin**, M. Chen, M. Martinez, Y. Ding, J.D. Caranto

**4:15 79.** H<sub>2</sub> Evolution by Rationally Designed Biomolecular Catalysts: Insights into Electron and Proton Transfer Processes. **S. Chakraborty**, S. Malayam Parambath, D. Selvan, P. Prasad

**4:35 80.** Two Nickel Binding De Novo Designed Tetramer as an Artificial Hydrogenase: The Role of Cooperative Bimetallic Active Sites in Increasing Hydrogen Production. **P. Prasad**, S. Chakraborty

**4:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room A

## **Biophysics of Macromolecular Machines**

A. L. Lucius, *Presiding*

**1:00** Introductory Remarks.

**1:05 81.** Structural Analysis of the *Legionella pneumophila* Dot/Icm type IV Secretion System. **C. Durie**, M. Sheedlo, M. Swanson, D.B. Lacy, M. Ohi

**1:30 82.** Elucidating the Role of Zinc in Salmon Sperm Nuclear DNA Packaging. **M. Dinar**, A. Drake, S. Rankin, J.E. Derouchey

**2:20** Intermission.

**2:40 83.** Defining and Exploiting Unique Properties of Eukaryotic RNA Polymerases. R.Q. Jacobs, Z.M. Ingram, K. Fuller, S. Cooper, A.L. Lucius, **D.A. Schneider**

**3:05 84.** Falling off: ClpB and Hsp104 Operate as Non-Processive Translocases. **A.L. Lucius**

Birmingham Jefferson Convention Center  
East Meeting Room D

## **Chemical and Biochemical Approaches to the Investigation of Lipid Membranes**

Financially supported by Avanti Polar Lipids, T&T Scientific  
M. Best, *Presiding*

**1:00** Introductory Remarks.

**1:05 85.** Stimuli-Responsive Liposomes via Engineering of Membrane Properties. **M. Best**, J. Lou, R. Sagar, M.L. Qualls, J. Schuster, F. Barrera

**1:30 86.** Natural Products as Selective Glucocorticoid Signaling Modulators. **F. Rivas**

**1:55 87.** Toward Applications of Synthetically Evolved, Membrane-permeabilizing Peptides That Form Macromolecule-sized Pores. L. Sun, E. Wu, K.A. Hristova, **W.C. Wimley**

**2:20 88.** Delivery of Recombinant SARS-CoV-2 Envelope Protein into Human Cells. **C.R. Sanders**, J. Hutchison, R. Capone, D. Luu, W.D. Van Horn

**2:45** Intermission.

**3:00 89.** A picture Worth a Thousand Words: Optimizing cryo-EM for Membrane Structural Studies. **F.A. Heberle**, D.A. Welsch, E. Chaisson, E. Crumley, M. Doktorova, N. Waxham

**3:25 90.** New Approaches to Uncover how Membrane Rafts and Caveolae Form and Function. **A. Kenworthy**

**3:50 91.** Coupling between Protein Condensates and Membrane Domains Regulates T Cell Membrane Structure and Protein Organization. **I. Levental**

**4:15 92.** A General Approach to Understand Lipid Interactions in Membranes. **P.F. Almeida**

**4:40** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room J

## **Discovery of Therapeutic Agents for Emerging Viruses**

Corinne E. Augelli-Szafran, *Presiding*

**1:00** Introductory Remarks

**1:05 93.** Small Peptide Inhibitors of SARS-CoV-2 3-chymotrypsin-like Protease. **J. Stewart**, M. Halim

**1:35 94.** Design and Synthesis of Potential Drug Candidates for SARS-CoV-2 using Molecular Hybridization Approach. **S.S. Panda**

**2:05 95.** Vinyl Sulfone-based Inhibitors of Non-structural Protein 2 Block the Replication of Venezuelan Equine Encephalitis Virus. **I.V. Ogungbe**, H. Zhang, M. Harmon

**2:35 96.** Discovery and Optimization of BCX 5191 a Novel Nucleotide RNA Dependent RNA Polymerase Inhibitor of Hepatitis C virus. **P.L. Kotian**, M. Wu, S.K. Vadlakonda, Y. El-Kattan, X. cheng, X. Chen, S. Bantia, T. Lin, P. Chand, Y.S. Babu

**3:05** Intermission

**3:25 97.** Structural Analyses Reveal the Mechanism of Inhibition of Influenza virus NS1 by two Antiviral Compounds. **C. Petit**

**3:55 98.** Pyrimidone inhibitors targeting Chikungunya Virus nsP3 macrodomain by fragment-based drug design. **M. Wu**, S. Zhang, A. Garzan, N. Haese, R. Bostwick, Y. Martinez-Gzregorowska, L. Rasmussen, M.I. Sosa, D. Streblow, M. Heise, A.K. Pathak, C.E. Augelli-Szafran

**4:25 99.** Computer-Aided Drug Discovery of Anti-Alphavirus and Anti-Coronavirus Agents. **S. Zhang**, A. Garzan, N. Haese, R. Bostwick, Y. Martinez-Gzregorowska, L. Rasmussen, M.I. Sosa, D. Streblow, M. Heise, A. Pathak, C.E. Augelli-Szafran, M. Wu

**4:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room L

## **General Session - Energy and Fuels**

S. Pan, *Organizer*

**1:00** Introductions.

**1:10 100.** Improvement of Weibull Breakdown Strength in Single-Phase Multiferroic Films with High Dielectric Constant for Supercapacitors. **R. Harry**, S. Zainuddin, S. Jeelani

**1:30 101.** Ethanol Upgrading to Olefins Over Metal-containing Beta Zeolites: Characterization and Catalysis. **N. Samad**, J. Zhang, E.C. Wegener, S. Purdy, K.A. Unocic, D. Liu, Z. Li, J.W. Harris

**1:50 102.** Pyrolysis of Butyl Acetate Isomers Inside a Shock Tube. F. Arafin, **S. Vasu**

**2:10 103.** Computational Studies of the Substituent Effect on Fe(II) Arylisocyanide Complexes. **M. Deegbey**, E. Jakubikova

**2:30** Intermission.

**3:00 104.** Main Group, Alkali, and Alkaline Earth Metal Amine Borane-based Chemical Hydrogen Storage Molecular Systems. **M.P. Confer**, D.A. Outlaw, D.A. Dixon

**3:20 105.** “The Use of Lithium ion Conducting Sulfonate MOFs as Anode Materials for Li-S Batteries.”. **D.K. Panda**

**3:40 106.** The Prediction of Diesel Fuel Economy and Emissions Using Python Machine Learning Tools.. **D.T. Daly**

**4:00 107.** Asymmetric glycerol derivatives: Synthesis, properties, and application in CO<sub>2</sub> absorption. **S. Qian**, J.E. Bara

**4:20 108.** Free-base Porphyrin Polymer for Bifunctional Electrochemical Water Splitting. **Y. Ge**, D. Villagran

**4:40** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room E

### **General Session - Environmental Chemistry**

Financially supported by Nashville Local Section of the ACS

R. C. Wingfield, *Presiding*

**1:00** Introduction .

**1:05 109.** Community based Participatory Research in Monitoring of Criteria and Toxic Air Pollutants in Environmental justice Communities and Vulnerable Populations. **D. Padgett**

**1:25 110.** Silica Fiber-based Visible Colorimetric Method for On-site Polycyclic Aromatic Hydrocarbons Detection. C. Duprey, H. Rouhi, Y. Lu, M. Elliott, **E.K. Wujcik**

**1:45 111.** Synthesis and Studies on Photophysical Properties of Rhodamine dyes and their Metal Complexes for Application in Dye Sensitized Solar Cell. **O. Oloyede**, F. Abebe, W. Gahnn, J. Uddin

**2:05 112.** Spectroscopic Studies (Raman, FTIR) of Boron in Aqueous Solutions. **J. Mierzwa**, R. Avedananda, R. Mumbi, S. Rakshit

**2:25 113.** In-situ Synthesis Nanoscale Zero-valent Iron-decorated Biochar for Water Remediation. **X. Zhang**, J. Zhang

**2:45 114.** Effect of Ultrasonicated Sustainable Biochar Reinforcement on Mechanical and Thermal Properties of Polypropylene Biocomposite.. **Z. Mohammed**, S. Jeelani, V. Rangari

**3:05** Intermission.

**3:20 115.** Preparing Vulnerable Populations for the Impacts of Climate Change Amid a Global Pandemic: The Path Forward to Building Sustainable and Resilient Communities. **R.C. Wingfield**, N. Lake, A. Searce, B. Holmes, A. Lee



**3:40 116.** CO<sub>2</sub> Reduction in Acetonitrile Enhanced by Electrolyte-assisted Mass Transport of Water. **A.J. Wilson**

**4:00 117.** Simultaneous Sorption of Multioxyanions (arsenate, phosphate, selenate, and chromate) using Magnetic Douglas Fir Biochar. **P.M. Rodrigo**, C. Navarathna, T. Mlsna

**4:20 118.** Immobilization of Lead in Simulated Polluted Soil by Douglas Fir Biochar-supported Phosphate. **B. Arwenyo**, J. Varco, A. Dygert, F. Afstar, S. Sabrina, R. Thirumalai, C.U. Pittman, T. Mlsna

**4:40 119. Withdrawn.** Effective Removal of Anionic Dyes (Remzol Brilliant blue and Remzol Reactive black) from Aqueous Solution by Novel Ozone Oxidized Hydrochar Treated with Polyethyleneimine.. **S. Madduri**, I. Elsayed, E.M. Hassan

Birmingham Jefferson Convention Center  
East Ballroom B

## **High Performance Computing Applications in Chemistry 1**

T. P. Straatsma, *Presiding*

**1:00** Introduction .

**1:00 120.** High Performance Computing for Rapid Generation of Benchmark-quality Quantum Chemistry Data. **C.D. Sherrill**

**1:35 121.** Multilayer Linear-scaling Coupled Cluster Methods. **D. Bykov**, A. Barnes, D. Lyakh, T. Straatsma

**2:10 122.** Fast Coulomb matrix Construction via a Hierarchical Block Low-rank Representation of the ERI Tensor. **E. Chow**, X. Xing, H. Huang

**2:45** Intermission.

**3:05 123.** ACE2 Glycans Preferentially Interact with SARS-CoV-2 spike Protein Over SARS-CoV. **A. Acharya**, D.L. Lynch, A. Pavlova, Y. Pang, J.C. Gumbart

**3:40 124.** Mechanistic Investigations into Benzylic Amine-Directed C-H Borylation with Iridium. **N. Le**, N. Chuang, C. Oliver, A. Samoshin, K.B. Morris, S. Hyland, H. Guan, T.B. Clark, C.E. Webster

**4:15 125.** Exploiting Graphical Processing Units (GPUs) to Enable Large-scale Quantum Chemistry of Molecules in Realistic Environments. **F. Liu**

Birmingham Jefferson Convention Center  
East Meeting Room C

### **N-Heterocyclic Carbenes in Synthesis, Catalysis and Material Science**

K. Marichev, *Presiding*

**1:00** Introductory Remarks.

**1:10 126.** Tweaking NHC Ligand Design for Gold Nanoparticle and Surface Applications. I.M. Jensen, J.F. DeJesus, S.L. Strausser, R.K. Borsari, L.M. Sherman, N.L. Dominique, J.P. Camden, **D.M. Jenkins**

**1:45 127.** Merging Single-electron Processes with Carbene Catalysis. **A.V. Bay**, K.P. Fitzpatrick, G.A. Gonzalez-Montiel, A.O. Farah, P.H. Cheong, K. Scheidt

**2:05 128.** N-Heterocyclic Carbenes as a Surface-Functionalization Platform for Molecular Sensing. **J.P. Camden**

**2:40 129.** Experimental and Theoretical Investigations of a Copper(II) Bipyridyl-*N*-Heterocyclic Carbene Macrocyclic. **S. Sahil**, K.M. McCardle, P. Magueres, J. Panetier, J.W. Jurss

**3:00** Intermission.

**3:20 130.** Organometallic Polymers Comprising Janus bis(*N*-heterocyclic carbenes) Linkers and Metal-sulfur Cubane-type Clusters. **C. Beijer**, J. Gillen, M. Vuong

**3:55 131.** Metal Carbenes in Synthesis of Chiral Carboxylic Acid Derivatives and Natural Products using Strain Release Methodology. **K. Marichev**

**4:30 132.** Study of Effect of Polyethylene Glycol Chain Lengths in the Synthesis of Water-Soluble Metal phthalocyanines, and Incorporation into Hierarchically Porous Carbon Monolith Catalysts. **A. Shrestha**

**4:50** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room K

### **General Session - Polymer Chemistry**

V. Thomas, *Organizer*  
D. Lerew, *Presiding*

**1:00** Introduction .

**1:10 133.** Structure Property Relationships in Imidazolium Ionenenes: Effects Of Linkage and Anion Structures. **S. Chatterjee**, J. Bridges, J.E. Bara, K.E. O'Harra, K.N. West

**1:25 134.** Anionic Ring-opening Copolymerizations of Sulfonylaziridines to Afford Previously Insoluble Linear Polysulfonylaziridines. **S. Sisk**, P. Rupa

**1:40 135.** Ion-Exchange Cellulose Nanoresins for Water Purification. **S. Schmal**, A. Sahu, S. Elmore, J.C. Puler

**1:55 136.** Upper Critical Solution Temperature Behavior of Linear and Star Polymers. **A. Aliakseyeu**, R. Hlushko, S.A. Sukhishvili

**2:10 137.** Synthesis and Characterization of Sulfonimide Based Anionic Ionenenes. **K. Watson**, P. Rupa

**2:25 138.** Anionic Polyimide Ionomers with Ionic Liquids Through Cation-exchanges for Gas Separation Membranes. **J. Chang**, G. Dennis, J.E. Bara, P. Rupa

**2:40** Intermission.

**3:00 139.** Phenothiazine Based Polymer as a Mimic of Polyaniline for Optoelectronics Application. **H. Giri**, C.N. Scott

**3:15 140.** Synthesis of Branching-controlled Comb Polymers via Thiol-yne "click" Chemistry. **B.J. Curole**, A. Nadeem, W. Broussard, S.M. Grayson

**3:30 141.** Triphenylene-Enchained Perfluorocyclobutyl Aryl Ether Polymers: Blue-Light Emitters with High Thermal-Oxidative Stability. **E. Borrego**, B. Farajidizaji, S. Athukorale, C.U. Pittman, D.W. Smith

**3:45 142.** Synthesis of semi-fluorinated polyaryl ethers via direct Friedel-Crafts polymerization of aryl ethers and hexafluoroacetone hydrate. **G. Munoz**, K.M. Chamberlain, S. Athukorale, C.U. Pittman, D.W. Smith

**4:00 143.** Synthesis of Biobased Novolac Phenol-Formaldehyde Wood Adhesives from Biorefinery-Derived Lignocellulosic Biomass. **A. Bansode**, M.L. Auad

Birmingham Jefferson Convention Center  
East Meeting Room B

### **Single Molecule Approaches to Chemistry and Biology**

K. Welsher, *Presiding*

**1:00** Introductions.

**1:05 144.** Single molecule imaging approaches to study the mechanochemistry of living systems. **K. Salaita**, H. Ogasawara, A. Blanchard, Y. Duan, Y. Hu, R. Ma

**1:30 145.** Active Feedback Three-dimensional Tracking of Single Polymer Particles in the Solution Phase. **D. Yu**, A. Garcia IV, S. Blum, K. Welsher

**1:50 146.** Covalently-Linked Rhodamine B Dimers: Stereochemistry and Photophysical Interplay. **K. Fogarty**

**2:10 147.** Indestructible Tension Probes for Measuring High-force Mechanical Events in Cells. **R.L. Bender**, Y. Duan, A.V. Kellner, B. Deal, J. Heemstra, Y. Ke, K. Salaita

**2:30 148.** Unraveling the Molecular Details of Bacterial Type 3 Secretion by Tracking Single Biomolecular Complexes in Living Cells. J. Prindle, O.I. de Cuba, Y. Wang, **A. Gahlmann**

**2:55** Intermission.

**3:05 149.** 3D Intra-Organellar Transport of Toxins Inside Live BHK cells using Phase Engineered Optical Microscopy. **C. Dutta**, J. Zepeda O., A. Misiura, S. Sarkar-Banerjee, C.F. Landes

**3:30 150.** Recursive Bayesian Position Estimation for Active Feedback Single-Molecule Tracking in Complex Environments. **A.J. Niver**, K. Welscher

**3:50 151.** Chemical-to-mechanical Molecular Computation Using DNA-based Motors with Onboard Logic. **S. Piranej**, A. Bazrafshan, K. Salaita

**4:10 152.** Understanding Cells at the Molecular Level using Light Sheet Single-molecule Super-resolution Microscopy in 3D. **A. Gustavsson**

**4:35 153.** Single-Molecule Orientation Localization Microscopy: Visualizing Molecular Rotational Dynamics at the Nanoscale. T. Ding, T. Wu, **M.D. Lew**

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

## **Analytical Chemistry**

### **Poster session**

A. Ghosh, S. Pan, *Organizers*

**3:00 - 5:00**

**154.** Peroxidase-Like Activity of Platinum-Group Metal Nanoparticles. **H. Crawford**, A. Biby, X. Xia

**155.** Evaluating Structural Heterogeneities of Amyloid Aggregates in Alzheimer's Disease Tissues with Infrared Microscopy. **A. Foes**, S. Walker, J. Holmquist, A. Ghosh

**156.** Exploring the Biological Relevance of Some Synthesized Heterocyclic Compounds in Model Biomimetic Environment. **E.T. Fasusi**, S.M. Landge, D. Ghosh

- 157.** Digestive Ripening Yields Atomically Precise Au Nanomolecules.. **S. Eswaramoorthy**, A. Antonysamy
- 158.** Investigation of Polymerization Reactions via Dual Spray ESSI-MS. **J. Griggs**, M. Gilliland
- 159.** Chemical Profiles of Weathered Ignitable Fluids Based on GC/MS, Raman, and Infrared Spectroscopic Analysis. R. Boyce, S. Perna, M. Zhang, **N.S. Chong**
- 160.** Investigating the Photophysical Changes of a Prodrug in Cationic Micelles. **A. Merhar**, E. Dobson, K.S. Aiken, S.M. Landge, D. Ghosh
- 161.** Label-free discrete frequency infrared imaging of beta sheet aggregates in Alzheimer's Disease. **T.B. Maupin**
- 162.** Investigating Nanoscale Heterogeneities of Self-assembled Monolayers with AFM-IR for Area-selective Atomic Layer Deposition. **M. Hasan Ul Iqbal**, H. Yan, Q. Peng, A. Ghosh
- 163. Withdrawn.** Authenticating Aspirin Brands Through LC-MS/MS. **W. Than**
- 164.** Ionic Liquid-Solvated Indolizine Squaraine Sulfonate Dyes for Enhanced Emission in the Presence of Blood. **D.S. Darlington**, A.N. Mahurin, W.E. Meador, J.H. Delcamp, E.E. Tanner
- 165. Withdrawn.** Transferring Solid Phase Elution Methods from TomTec Quadra 4 SPE to Zephyr G3 SPE Workstation: Applications in HPLC. **S. Fisher**, L. Nguyen, C. Green, J. LaPalme, E. Bair, N. Epie
- 166.** Evaluation of a Targeted Multiple Reaction Monitoring Lipidomics Approach to Assess Various Sphingolipid Species. **S.C. Swiderski**, N.A. Chung, T.A. Clemons, R.A. Robinson
- 167. Withdrawn.** Gas Chromatography Rapid Automation and Quantitative Procedure for the Measurement of Hydrogen Cyanide in Whole Blood. **P. Brito**, J. LaPalme, E. Bair, N. Epie
- 168.** Analysis of Guanine Content on DNA detection, Induced Oxidative Damage, and Hydrolysis using Complementary Square Wave Voltammetry and LC-MS/MS. **T. Hindi**, **K. Cheek**, E. LaFave, E. Hvastkovs

**169.** Morphological and Structural Studies of RGD and VEEV based-Tetraphenylalanines. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu

**170.** Energy Harvesting from Enzymatic Glucose Biofuel Cell Utilizing Meso-porous Two Dimensional Reduced Graphene Oxide. **M.H. Kabir**, W. GHANN, J. Uddin, M.M. Ali, H.Z. Msimanga, M. Thompson, A. Poyraz

**171.** Interfacial Interaction Between cellulose nanofibrils (CNFs) and Fipronil. **S.W. Freij**, M.C. Iglesias, T. Ciaramitaro, M.S. Peresin

## **WEDNESDAY EVENING**

Birmingham Jefferson Convention Center  
East Ballroom B

### **Plenary**

D. A. Dixon, *Presiding*

**5:30 172.** Drug Discovery and Development *via* structure and Mechanism Based Rational Design. **C. Zhan**

## **THURSDAY MORNING**

Birmingham Jefferson Convention Center  
East Meeting Room I

### **Contemporary Fluorine Chemistry in the Southeast 1**

Cosponsored by FLUO  
D. A. Dixon, T. Lectka, *Presiding*

**8:00** Introductory Remarks.

**8:05 173.** Synthesis of Difluorinated Alcohols and Halohydrins. **D.A. Colby**



**8:35 174.** Advances in Trifluoromethoxylation and Electrophilic Fluorination. **G.B. Hammond**, T. Umemoto, Z. Lu

**9:05 175.**

C-F Bonds in tight spaces: Getting fluorine to do what it may not want to do. **T. Lectka**, S. Harry, M. Kazmin

**9:35** Intermission.

**9:50 176.** New, One-step Synthesis of the Anesthetic Agent Sevoflurane,  $(\text{CF}_3)_2\text{CHOCH}_2\text{F}$ . X. Liu, C. Liu, A.V. Matsnev, P.V. Jog, M. Ulman, **J.S. Thrasher**

**10:20 177.** Real-time Dermal Sorption of  $^{18}\text{F}$ -labeled Perfluorinated Alkyl Substances in Immunocompetent Mice. **J.L. Bartels**, S.R. Fernandez, M. O'Malley, G.F. Peaslee, S.E. Lapi

**10:50 178.** Direct Fluorination of Tetrafluoroethylene and the Effect of  $^{60}\text{Co}$   $\gamma$ -radiation on the Tetrafluoroethylene/ Perfluoro(methyl vinyl ether) Copolymer. **M.P. Confer**, S.R. Allayarov, D.A. Dixon

**11:20 179.** Comparison of  $^{18}\text{F}$ FDG with  $^{18}\text{F}$ -labeled amino acids for PET imaging of breast cancer. **U. Akca**, P. Song, D.A. Devalankar, N. Yasui, A. Sorace, J.E. McConathy

Birmingham Jefferson Convention Center  
East Meeting Room E

## **Frontiers in Nucleic Acids**

K. L. Hayden, R. M. Wadkins, *Presiding*

**8:00** Introduction.

**8:10 180.** Conjugation of the Synthetic Anthracycline Chemotherapeutic Pixantrone with an Apurinic Site in DNA. **M.P. Stone**, A.H. Kellum, P. Pallan, Y. Fu, J. Terrell, B. Noh, M.V. Voehler, C.J. Rizzo, M. Egli

**8:30 181.** Structural Effects of Incorporation 6-oxo- $\text{M}_1\text{dG}$  DNA Adduct into DNA Duplex. **Y. Fu**, P. Kingsley, R. Richie-Janetta, L.J. Marnett, M.P. Stone

**8:50 182.** Coloring DNA Strands with Silver Clusters. **J.T. Petty**, D. Lewis, C. Couch, M. Branham, K. Thomas, Y. Zhang, B. Kohler, I. Santos, J. Brodbelt

**9:10 183.** Can anything Stabilize a DNA i-motif?. **R.M. Wadkins**

**9:30** Intermission.

**9:55 184.** The Interaction of DNA with Gemini Surfactants. E. Boatwright, D. Aguilar, **R.D. Sheardy**

**10:15 185.** Programmable Approach for Specific Recognition of Adjacent GG Base Pairs by Modular Synthetic Diamidines. **A. Paul**, P. Guo, A. Farahat, D.W. Boykin, W. Wilson

**10:35 186.** Dynamic and Hydration Properties of DNA Site Selection by Nucleoproteins. **G. Poon**, J. Terrell

**10:55 187.** Influence of Pre- and Post-transition Baselines on the Uncertainty and Reliability of Thermal Denaturation Parameters Extracted from DNA Melting Curves. **R. Bishop**

**11:15** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Ballroom B

## **High Performance Computing Applications in Chemistry 2**

T. P. Straatsma, *Presiding*

**8:00** Introduction .

**8:10 188.** Simplifying Multilevel Quantum Chemistry Procedures through Psi4 and QCArchive. **L.A. Burns**, C.D. Sherrill

**8:45 189.** Scalable GPU-accelerated Computational Infrastructure for Parallel Tensor Processing in Quantum Many-body Theory. **D. Lyakh**

**9:20 190.** Accelerating Density-Functional Tight-Binding Using Graphical Processing Units. **S. Irle**, V. Vuong, C. Cevallos, B. Aradi, C. Camacho

**9:55** Intermission.

**10:15 191.** High-Performance Density Fitting Technology on Accelerated Computed Platforms. **E.F. Valeev**, A. Asadchev

**10:50 192.** GronOR: Scalable and Accelerated Non-Orthogonal Configuration Interaction for Molecular Fragment Wavefunctions. **T.P. Straatsma**

**11:25 193. Withdrawn.** Computational investigations of Aromatic Borylene-type Systems. **U. Gaillard**, K. Donald

Birmingham Jefferson Convention Center  
East Meeting Room J

### **Inorganic Electron Transfer Reactions for Energy Storage**

Financially supported by **Cell Reports Physical Sciences**

B. H. Farnum, *Presiding*

**8:00** Introductory Remarks.

**8:05 194.** Advanced Scanning Electrochemical and Spectroelectrochemical Methods for Analyzing Surfaces of Catalytic Electrode Materials. **S. Pan**

**8:25 195.** Molecular Z-Scheme for H<sub>2</sub> Production via Dual Photocatalytic Cycles. **K. Hanson**, P.J. Avare, N. Watson, A.K. Vannucci

**8:45 196.** Characterization of a New Class of Platinum Bipyridyl Complexes with Blue to Cyan Emission. **J. McCarthy**, M.J. McCormick, J.H. Zimmerman, W.M. Thomas, P.S. Wagenknecht

**9:05 197.** Redox Hopping Promoted Water Oxidation by a Metal-Organic Framework. **A.J. Morris**

**9:25 999.** CHASE Hybrid Photoelectrodes for Water Oxidation **G. Meyer**

**9:45** Intermission.

**10:00 198.** Improving 2e<sup>-</sup> Redox Chemistry of Nickel Dithiocarbamates for Application in Redox-Flow Batteries. **B.H. Farnum**, M. Mazumder

**10:20 199.** Cr Complexes for the Electrocatalytic Reduction of Carbon Dioxide. S. Hooe, J. Moreno, A. Reid, **C.W. Machan**

**10:40 200.** Ligand-to-Metal Charge-Transfer Photochemistry and Photophysics of d<sup>0</sup> Titanocenes. **H. London**, D. Pritchett, C. McMillen, G.C. Shields, P.S. Wagenknecht

**11:00 201.** Self-Sensitized Photocatalytic CO<sub>2</sub> Reduction by a Series of Ruthenium Complexes Under Visible-Light Irradiation. A. Devdass, K.M. McCardle, A. Dorris, D.K. Buettner, N. Hammer, J. Panetier, **J.W. Jurss**

**11:20 202.** Metalloenzyme Mimics: Iron Carbonyl Clusters Tethered to Non-Innocent Aromatic Ghiolate Groups. **C.A. Mebi**

**11:40 203.** Excited State Proton Transfer and Electron Transfer in Complexes Exhibiting Intramolecular Reversible Energy Transfer. **F. Zhang**, J.J. Paul, R.H. Schmehl, J. Stash

Birmingham Jefferson Convention Center  
East Meeting Room G

### **Measuring More than Mass: Innovations in Mass Spectrometry Experiments and Applications**

Financially supported by **Mississippi State University**

A. L. Patrick, *Presiding*

**8:00** Introductory Remarks.

**8:05 204.** Application of Liquid Chromatography Tandem Mass Spectrometry for Analysis of Complex Mixtures. **Z. Popovic**, L.C. Anderson, C. Weisbrod, H. Chen, D. Butcher, G.T. Blakney, X. Zhang, L. Babcock-Adams, R. Boiteau, N. Coffey, P. Morton, T.B. Kelly, A. Dispenzieri, S. Dasari, C.P. Hutchinson, P. Chance, C. Reimers, J. Li, B.N. Granzow, M. Acker, M.R. Stukel, D.R. Griffith, D.J. Repeta, R. Zubarev, D.L. Murray, D. Barnidge, A.M. McKenna, C. Hendrickson, A.G. Marshall

**8:40 205.** Determining the Structure of Neuregulin by Multi-dose FPOP Coupled with Computational Modeling. N.A. Khaje, C.K. Mobley, A. Eletsy, S.E. Biehn, S.K. Mishra, R.J. Doerksen, S. Lindert, J. Prestegard, **J.S. Sharp**

**9:15 206.** Comparing Lipid Normalization Methods for Label-free Quantitative Lipidomic LC-MS/MS. **L.S. Bailey**, K.B. Basso

**9:50** Intermission.

**10:10 207.** Resolving Diagnostic Isomeric Lipids with Liquid Chromatography, Ion Mobility Spectrometry and Tandem Mass Spectrometry. **A.M. Hamid**

**10:45 208.** Derivatizing Reagents for Improved Analysis of Performance Enhancing Drugs with IM-MS. D.C. Velosa, S.P. Neal, **C.D. Chouinard**

**11:20 209.** Advancing Chemical Liability Assessments and Biogeochemical Interpretations of Aquatic, Soil, and Oil Organic Matter by FT-ICR MS. **J. D'Andrilli**, C. Romero, P. Zito, D. Podgorski, R. Payn, S. Sebestyen, A.R. Zimmerman, F.L. Rosario

**11:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room A

### **New Directions in Metal-Catalyzed Reactions 1**

Financially supported by Organic Reactions, Biocryst, VWR

K. H. Shaughnessy, *Presiding*

**8:00** Introductory Remarks.

**8:05 210.** Ruthenium-Catalyzed Enantioselective Functionalization of Carbon–Hydrogen Bonds. **X. Cui**

**8:35 211.** Metal-mediated Approaches Toward the Formation of the Synthetically Challenging 2-pyridyl bond. Z.Z. Gullledge, G.D. Waters, J.W. Cleveland, A. Chin, M.L. Tedder, **J.D. Carrick**

**9:05 212.** Applications of Platinum-Catalyzed Carbene Formation toward Heterocycle Synthesis. **E.M. Ferreira**

**9:35** Intermission.

**9:50 213.**

Synthesis of Pyridyl Triazole Ligands With Transient Directing Groups For Meta and Para C-H Activation of Aryl Aldehydes, Ketones, and Aryl Amines. **T. Ricks**

**10:20 214.** Mechanistic Study of Enantiomer Selectivity C–H bond Functionalization catalyzed by Ruthenium complexes. **N. Le**, C. Hetti Handi, N. Udayanga, X. Cui, C.E. Webster

**10:50 215.** New Catalytic uses for Gallium in the Oxidation of Hydrocarbons. **C.R. Goldsmith**, A.C. Saunders

**11:20 216.** Pincer Ligand Cobalt Chromophores for Selective Radical Trifluoromethylations. **J.D. Soper**

Birmingham Jefferson Convention Center  
East Meeting Room L

## **Electrocatalysts and Solar Cell For Clean Energy Conversion Part 1**

S. Pan, *Presiding*

**8:00** Introduction .

**8:10 217.** Bifunctional Nickel and Copper Electrocatalysts for CO<sub>2</sub> Reduction and the Oxygen Evolution Reaction. **H. Pan**, C. Barile

**8:30 218.** Photocatalytic Reduction of CO<sub>2</sub> to Formic Acid by Rhenium(I) Dicarbonyl Complexes. **E. Asempa**, E. Jakubikova

**8:50 219.** Photocatalytic Carbon Dioxide Reduction with Nickel Complexes Supported by Redox-active Macrocycles with Extended Conjugation. **S. Bhattacharya**, A. Devdass, J.W. Jurss

**9:10 220.** Electrocatalytic CO<sub>2</sub> Reduction with Nickel Complexes Supported by Redox-Active Macrocycles with Extended Conjugation. **A. Devdass**, A. Richmann, J.W. Jurss

**9:30 221.** Thickness Dependent OER Electrocatalysis of Epitaxial LaFeO<sub>3</sub> Thin Films. **A. Burton**, R. Paudel, B. Matthews, S. Spurgeon, M. Sassi, B.H. Farnum, R. Comes

**9:50** Intermission.

**10:10 222.** Activation of Methane to Produce Methanol Over a Vanadium Single Site MCM-41 SiO<sub>2</sub> Amorphous Mesoporous Quantum Photocatalyst. **C. Evrard**, L.M. Thompson

**10:30 223.** Molybdenum Ditelluride and Sulfotelluride with Graphene Support as Cathodic material for hydrogen generation. **A. Ali**, S. Sarwar, D.R. Pollard, X. Zhang, A.J. Adamczyk

**10:50 224.** Electrochemical CO<sub>2</sub> Reduction and Water Splitting Reactions at NanoCOT Electrodes for Clean Energy Conversion and Storage. **A. Ashaduzzaman**, S. Pan

**11:10 225.** Automated Structure Generation and Theoretical Predictions for Potential Near-Infrared (NIR) Dye Sensitized Solar Cells. **T. Santaloci**, A. Wallace, R.C. Fortenberry

**11:30 226.** Highly Active and Robust Ruthenium Photocatalysts for CO<sub>2</sub> Reduction: Exploring Electronic and Steric Effects for both Sensitized and Self-Sensitized Catalysts. **E.T. Papish**, S. Das, C.E. Webster, J.H. Delcamp

Birmingham Jefferson Convention Center  
East Meeting Room O

## **Polymer Assemblies: from Fundamental to Applications 1**

E. P. Kharlampieva, G. Schneider, *Presiding*

**8:00** Introductory Remarks.

**8:05 227.** Dynamics of Semiflexible Colloidal Polymer Chains. **S.L. Biswal**

**8:30 228.** Advanced Time-Temperature Scaling in Polymer Melts. K. Bichler, B. Jakobi, **G. Schneider**

**8:55 229.** Mesoscale Modeling of Controlled Degradation and Erosion of Polymer Networks. V. Palkar, **O. Kuksenok**

**9:20 230.** Unentangled Vitrimer Melts: Generalized Rouse Theory Reveals Influence of Cross-link and Backbone Chemistry on Linear Viscoelasticity. **R. Ricarte**, S. Shanbhag

**9:45** Intermission.

**10:00 231.**

Polymer Salogels for Shape Stabilization of Inorganic Phase Change Materials. **S.A. Sukhishvili**, X. Zhu, K. Rajagopalan

**10:25 232.** Precision Synthesis of Acrylamide Block Polymers with Degradable Thioester Junctions. **W. Gutekunst**

**10:50 233.** Anionic Ring-Opening Polymerization in Ionic Liquids. **c. giri**, P. Rutar

**11:05 234.** Manipulating Structure and Membrane Properties of Nano-scale Model Membrane Systems of Amphiphilic Polymers and Lipids. **R.M. Perera**, G. Schneider

**11:20 235.** Development of Rapid, Colorimetric Sensors to Detect SARS-CoV-2 viral Particles in Environmental and Human Samples. **C.T. Stueber**, B. Cochran, J. Northcutt, P. Dawson, T.W. Hanks

Birmingham Jefferson Convention Center  
East Meeting Room B

### **Small Molecules for the Disruption of Bacterial Processes 1**

Financially supported by Clemson University

D. C. Whitehead, *Presiding*

**8:00** Introductory Remarks.



**8:10 236.** Eradicating Resistant and Tolerant Bacteria with Phenazine Antibiotic Inspired Small Molecules. **R.W. Huigens**

**8:45 237.** Targeting Bacterial Polysaccharide Metabolism of Gut Microbes with Small Molecules. **D.C. Whitehead**

**9:20 238.** Slaying Superbugs One Natural Product at a Time. **W.M. Wuest**

**9:55** Intermission.

**10:10 239.** Antiinfective Properties of Human Milk. **S.D. Townsend**

**10:45 240.** Disruption of Salmonella Biofilms In Vitro and In Vivo. **C. Melander**

**11:20 241.** Plant Natural Products as a Resource for Antibiotic Drug Discovery. **C. Quave**

Birmingham Jefferson Convention Center  
East Meeting Room D

### **Structure-Property-Function Relationships in Polymers**

*C. Zhao, Presiding*

**8:00** Introduction .

**8:10 242.** Toughing the Elastomers, Go Beyond the State-of-Art. Z. Zhang, **P. Cao**

**8:40 243.** Structure-Property-Function of Polypentenamer Systems. **J.G. Kennemur**

**9:10 244.** Structure-property Relationships in Self-healable Ultra-stretchable Electronic Polymers for Wearable Strain Sensors. **E.K. Wujcik**

**9:40** Intermission.

**9:55 245.** Investigation of the Doping Effects of Small Molecule Acids on Self-healable, Stretchable PANI/PAAMPSA Conductive Polymer Complexes. **N. Penners**, K. Webb, J. Jeon, Y. Lu, E.K. Wujcik

**10:25 246.** Solvent Vapor Annealing Processing to Control Properties of Semi-crystalline Polymers in Thin Films. **J. Albert**, S. Bliesner, J. Strzalka, Q. Zhang, T. Parker, G. Kelly

Birmingham Jefferson Convention Center  
East Meeting Room K

### **Supramolecular and Biomolecular Chemistry**

Financially supported by the Louisiana Local Section of the ACS and the Tulane Chemistry Department

J. Jayawickramarajah, *Presiding*

**8:00** Introductory Remarks.

**8:05 247.** The Expansion of Bilingual Peptide Nucleic Acids: Decoding the Nucleic Acid and Protein interaction for the development of Self-Assembling and Stimuli-Responsive Biopolymers.. **H. Argueta-Gonzalez**, C. Swenson, S. Sterling, G. Song, J. Heemstra

**8:20 248.** Unravelling the Structural Organization of Individual Alpha-Synuclein Oligomers Grown in the Presence of Phospholipids. **D. Kurouski**

**8:40 249.** Development of Supramolecular Hosts Targeting Phospholipids Commonly Found in Gram-positive Bacteria. **N. Busschaert**

**9:05 250.** Recognition of GC rich Nucleic Acids. **D.P. Arya**

**9:30 251.** Carbon Monoxide: The Good, the Bad, and the Ugly. **B. Wang**

**9:55 252.** Synthesis, Self-Assembly, and Dynamic Behavior of DNA Sequences Appended with Supramolecular Host and Guest Moieties. **D. Walpita Kankanamalage**, S. Pandey, J. Jayawickramarajah, H. Mao, L.D. Isaacs

**10:10** Intermission.

**10:40 253.** Increasing the Membrane Permeability of Carboxylic Acid-containing Drugs using Synthetic Transmembrane Anion Transporters. **R. Salam**, S. Marshall, N. Busschaert

**10:55 254.** Bilingual Peptide Nucleic Acids: Encoding the Languages of Nucleic Acids and Proteins in a Single Self-assembling Biopolymer. **J.M. Heemstra**

**11:20 255.** Supramolecular Assemblies as Key Contributors to the Origin of RNA. **N.V. Hud**

**11:45 256.** *RE*-SELEX: Restriction Enzyme-Based Evolution of Structure-Switching Aptamer Biosensors. **A. Sanford**, A.E. Rangel, T.A. Feagin, R. Lowery, H.S. Argueta-Gonzalez, J.M. Heemstra

Birmingham Jefferson Convention Center  
East Meeting Room F

### **The Magic of Spectroscopy**

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, *Presiding*

**8:00** Introductory Remarks.

**8:10 257.** Theoretical Investigations of Oxygenated Hydrocarbons for Matrix Isolation Infrared Spectroscopy Experiments. **A. Gunn**, M. Sakalosh, A.L. Smalley, J. Dovi

**8:35 258.** Reactivity, Coordination Behavior, and DFT Challenges for Transition Metal-acetylene Complexes Revealed via Infrared Laser Photodissociation Spectroscopy.. **A.D. Brathwaite**, J. Marks, A. Batchelor, M.A. Duncan

**9:15 259.** Ultrafast Spectroscopy with Frequency Combs: Enabling new Measurements of Dilute Species in Molecular Beams. **M.A. Reber**, N.D. Cooper, W.M. Jones

**9:55** Intermission.

**10:10 260.** Vibrational Fingerprints of Substituted Ketenes. E. Sparks, K. El-Shazly, K. Narkin, H. Legg, **L.R. McCunn**

**10:50 261.** Shining Light on the Avian Compass Sense: An Investigation of the Magnetic Sensitivity of Cryptochrome 4 from a Migratory Bird using Cavity-enhanced Spectroscopies. **L. Jarocho**, J. Xu, K. Henbest, C. Timmel, S. Mackenzie, H. Mouritsen, P. Hore

**11:30 262.** Vibrational Spectroscopy of Aqueous Solutions: A Tale of Two Bases. **C. Pibel**, J.D. Ametepe, B.S. Pibel

Birmingham Jefferson Convention Center  
East Meeting Room C

### **Total Synthesis of Complex Molecules**

J. M. Smith, *Presiding*

**8:00** Introduction .

**8:05 263.** 21st Century Cope Rearrangements Inspired by the Historical Report.. **A.J. Grenning**

**8:40 264.** Innovative Reactions and Strategies for the Synthesis of Complex Natural Products. **J.G. Pierce**

**9:15 265.** Dearomative Alkaloid Synthesis. **J.M. Smith**

**9:50** Intermission.

**10:10 266.** Venturing Outside Flatland: Formation of Hindered Bonds in Aliphatic Systems. **T. Qin**

**10:45 267.** Synthesis of Illudalic Acid and Analogous Phosphatase Inhibitors. **G.B. Dudley**

**11:20 268.** Photoassisted Total Synthesis of Architecturally Complex Diterpenes. **J. Frederich**

**11:55** Concluding Remarks.

## THURSDAY AFTERNOON

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

### Environmental

#### Poster Session

R. C. Wingfield, *Organizer*

**12:30 - 2:30**

**269.** Investigating Adsorption Kinetics and Isotherm Studies of In-House Biochar for the Removal of Emerging Chemical Contaminant from Water. **J. Lennox**, L.D. Moore, A. Saha, P. Bhoi

**270.** Jar Test Studies on Simulated Raw Water Containing Microplastics: Monitoring Turbidity, pH and Added Metal Salts. J. Outten, **M.C. Koether**, A. Gruss

**271. Withdrawn.** Application of Microbial Communities for Bioremediation of Uranium Contaminated Sites. **J.R. Hoyle-Gardner**, V. Ibeanusi, G. Chen, V. Badisa, B. Mwashote

**272.** Modification of a Fast, Reliable Microplastics Quantification Method: Visualizing Plastic Particles in Freshwater with Nile Red. **J. Forakis**

**273.** Origin of Oxalate-rich Rock Coatings. **S. Ginsberg**, **L. Rayburn**, **A. Bray**, **F. Nuñez-Parker**, **A. Dowling**, J. Russ

**274.** GC/MS Analysis of Volatile Organic Compounds (VOCs) Emitted During Wildfires by Using Cryogenic and Sorbent Pre-concentration. **J. Mann**, S. Pham, Z. Li, M. Zhang, N.S. Chong

**275.** Boronic Acid-based ferrocene Complexes Towards Fluoride Ion Sensing. **P.I. Fernando**, **G. Kosgei**, M. Glasscott, G. George, E. Alberts, C. Bresnahan, L. Moores

**276.** Computational Study of the Thermal Degradation of Perfluoroalkyl Carboxylic Acids. **C. Paultre**, A.M. Mebel, K.E. O'Shea

**277.** Point-of-need Qualitative or Quantitative Detection of Trihalomethanes in Environmental Water Samples Using a Highly Sensitive and Selective Fiber-based Preconcentration System. H. Rouhi, C. Duprey, L. Terry, M. Elliott, **E.K. Wujcik**

**278.** Method Improvement of Microplastic Weathering Resulting in Improved Modeling of the Behavior of Heavy Metal Laden Microplastics through Drinking Water Treatment Plants. **S. Diehl**, M.C. Koether, A. Gruss

**279.** Nitric Acid and Base (Ammonia and Dimethylamine) Calculations of Gibbs Free Energies for Nucleation: A Computational Analysis for Aerosol Formation. **M. Joines**, T. Odbadrakh, G.C. Shields

**280.** A Computational Study of Atmospheric Aerosol Formation . **G. Mazaleski**, T. Odbadrakh, G.C. Shields

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## **Organic**

### **Poster Session**

L. Yet, *Organizer*

**12:30 - 2:30**

**281.** “Real-World” Medicinal Chemistry is Possible with Undergraduate Research Students. **L. Yet**

**282. Withdrawn** Furan Synthesis via a One-Pot enol Silane Formation-alkylation-cyclization-aromatization Cascade. **C.W. Downey**

**283.** "Unzipping" a Corannulene Bowl: Harnessing Strain Energy for Promoting Novel Structural Transformations. **G. Leith**, N.B. Shustova

**284.** Rapid Synthesis of Primary Amines by Radical C-H Amination. **R.J. Comito**, M. Hu, S.K. Ghosh

- 285. Withdrawn.** Ion-responsive Release of Contents from Liposomes for Cellular Delivery. **R. Sagar**, A. Watson, J. Lou, M. Best
- 286.** Regioselective 6-*endo* or 5-*exo* Radical Cyclization of *N*-Hetrocycles via Photoredox Catalysis. **M. Maust**, S. Blakey, C. Hendy, N. Jui
- 287.** Synthesis, Characterization and Antimicrobial Activity of N,N-substituted Triazolium Salts with Lipophilic Substituents on Triazole and Benzotriazole Rings. J. Wilson, Z. Lin, I.C. Rodriguez, D. Fico, S. Sanders, J. Gorden, M. Frazier, L. King, **K.S. Taylor**
- 288.** NMR Studies of Temperature and Solvent Effects on Dimerization of 4-*tert*-butylnitrosobenzene. **C.H. Rogers**, S.C. Blackstock
- 289.** Mechanism of Thiol-catalyzed Hydrolysis of P-Nitrophenyl Acetate Ester: Towards Novel Method for Chemical Recycling of Polyesters. **A. Nisathar**, V. Popik
- 290.** Development of Inhaled PLGA Encapsulated Ivermectin for the Treatment of SARS-CoV-2. **S. Sood**, S. Jha, S. Rayalam, S. Taval, V.V. Mody
- 291.** Development of Inhaled PLGA Encapsulated Aloin for the Treatment of SARS-CoV-2. **S. Jha**, S. Sood, S. Rayalam, S. Taval, V.V. Mody
- 292.** The Development of a DNA Aptamer with Isozyme Selectivity for Human Carbonic Anhydrase II. **E.B. Atuk**, J. Jayawickramarajah, N. Beltrami, M.M. Ismail, D. Hook, Z. Pursell, M.F. Ali, N. Nguyen
- 293.** Exploring the Substrate Scope of the E1 subunit of the 2-oxoglutarate Dehydrogenase Complex for Abiological catalysis. **R. Peterson**, E. Reynolds
- 294.** Rhodium-Catalyzed Asymmetric Dearomatization Strategy for the Total Synthesis of Nuphar Alkaloids. **K.G. Ortiz**, R. Karimov
- 295.** Synthesis of (±)-Hibiscone C. **A. Wildgen**
- 296.** Efforts Toward the Development of Non-Nucleoside *MraY* Inhibitors for the Treatment of Tuberculosis. **T. Berida**, S. Chatterjee, S. Mckee, P. Pandey, C. Ducho, R.J. Doerksen, S. Roy
- 297.** Towards the Total Synthesis of Ambuic Acid and Analogues. **P.M. West**, A. Ustoyev, M.P. Croatt

- 298.** Bactericidal Urea Crown Ethers can Target Phosphatidylethanolamine Membrane Lipids. **S. Herschede**, N. Busschaert
- 299.** Stereoselective Desymmetrization of Nitriles to Lactones via the Pinner Reaction. **J. Frost**, K.S. Petersen
- 300.** Synthesis of Tetraarylphosphonium/Tetrakis(pentafluorophenyl)borate (TAP<sup>R</sup>/TFAB, R=1,2,3-TriOMe, and R=3,5-DiOMe) salts as Non-aqueous Electrolytes for Organic Redox Flow Batteries. **G. Mandouma**
- 301. Withdrawn.** Heteroacene-based Amphiphilic Fluorescent Nanoparticles for Bioimaging. **T. Ranathunge**, M. Loku Yaddehige, J. Varma, C. Smith, W. Kolodziejczyk, N. Hammer, G. Hill, A. Flynt, D.L. Watkins
- 302.** Growth and Structure of Nitrosoarene Electron Donor-acceptor Co-crystals. **S.A. Kelley**, V. Shuger, S.C. Blackstock
- 303.** Design and Synthesis of Kekulé and non-Kekulé diradicaloids Utilizing Radical Peri-annulation Strategy. **F. Kuriakose**, I. Alabugin
- 304.** Synthesis of Organic Fluorophore Ph<sub>2</sub>-IDPP for use in NIR-II Fluorescence Bioimaging. **K. McKinney**, D.L. Watkins, S.M. Vijayan
- 305.** Designer Liposomes for Phosphorylated Metabolite Triggered Release Through Conformational Changes of Synthetic Lipid Switches. **J. Lou**, J. Schuster, F. Barrera, M. Best
- 306.** Synthesis of Heterogeneous Green Catalysts for the Epoxidation Reaction. **J.C. Johnson**, M.H. San Soucie, S.M. Landge
- 307.** Design and Synthesis of pH-sensitive Benzothiazole Cyanine Dyes. **S. Casa**, M. Henary
- 308.** Synthesis of 6-(4-fluoro)-3,4-diphenylpyridazine. **T. Mallett**, J. Philp, A. Williams, C. Williams, V. Sittaramane, S.M. Landge
- 309.** New Molecular Designs for Solar Light Harvesting with Synthetic Bioinspired Pigments. **H. Jing**, N.C. Magdaong, C.R. Kirmaier, J.R. Diers, D.F. Bocian, D. Holten, J.S. Lindsey
- 310.** Rational Development of Activatable Donors for On-demand Delivery of HNO. **A. East**, R. Tapia Hernandez, N.W. Pino, J. Chan



- 311.** Killing Two Birds with One Stone: The Simultaneous Phosphorylation and Capturing of Phosphorylated Cyanide Ions Using a Single Fluorescent Chemodosimeter. **R. Mia**, K.J. Wallace
- 312.** Red Shifted Donor Acceptor Fluorophores as Potential Agents for Biomedical Applications. **G. Ersoy Ozmen**, Z. Essam, D. Setiawan, R. Hamid, R. El-Aalb, R. Aneja, D. Hamelberg, M. Henary
- 313.** Heterogeneous Catalysis: Cyclization Method via Self-assembled Monolayers. **A.H. Horchar** , K.S. Petersen
- 314.** Synthesis and Characterization of  $\beta$ -enaminoamides as Precursors for the Fabrication of ZnO Films for Application in the Microelectronic Industry. **G. Farris**
- 315.** Characterizing Biochemical Responses Originating from Leaf Pathogenic Stress: Spotlight on Red Spots. **B. McCormick**, **A. Ferraro**, M. Salley, N.M. Hughes, A.J. Wommack
- 316.** Synthesis of Phenylpropionic Acid using a Grignard Reagent. **A. Cronan**, R. Okoth
- 317.** Modification of a Hemicyanine Platform for Optimized Deep tissue Photoacoustic Imaging. **S. Gardner**, C. Brady, C. Keeton, A.K. Yadav, M.Y. Lucero, S. Su, J. Chan
- 318.** Stereoselective Synthesis of  $\alpha$ -Allyl- $\alpha$ -Trialkylsilyl- $\gamma$ -Alkyl- $\beta,\gamma$ -Unsaturated Carboxylic Acids via an Ireland-Claisen rearrangement. **C. Massey**
- 319.** Epoxidation and Ring Opening of  $\alpha$ -Trimethylsilyl- $\beta,\gamma$ -Unsaturated Esters. **L.M. Fealy**, M.P. Jennings
- 320.** Synthesis and Screening of Near-infrared (NIR) Hemicyanine Dyes for Photoacoustic Imaging. **T. Tran**, W.M. MacCuaig, L. McNally, M. Henary
- 321.** Electrophilic Aromatic Substitution of Phenanthrene as a Precursor to Functional Porous Materials. **R.J. Van Demark**, B. Aguila
- 322.** Voltage-Sensitive Asymmetric Thiazolothiazole Dye for Molecular Probe Sensing Applications. **A.R. Brotherton**, N. Sayresmith, M.G. Walter
- 323.** Development of Novel Small Molecule Photosensitizers with Integrated Photoacoustic Readout. **C. Brady**, S. Gardner, J. Chan

- 324.** Activity-based Delivery of Chemotherapeutics and Imaging Agents to Target Cancer. **M.C. Lee**, M.Y. Lucero, J. Chan
- 325.** Donor-acceptor-donor NIR Xanthene-based Dye for Photoacoustic Imaging. **C. Rathnamalala**, N.W. Pino, C.N. Scott
- 326.** Boron-mediated Enantioselective Aldol Reactions of Substituted Phenylacetates. **J. Mather**, **S.K. Ferrufino Amador**, M.X. Yáñez Diaz, T.L. Walls III, P.B. Chanda
- 327.** Aluminum-catalyzed Intermolecular mono- and bis-hydroalkoxylation of Allenamides with Alcohols. **K. Alam**, T. Li, M.P. Croatt
- 328. Withdrawn.** Development of Photoactivated nanoMOF Drug Delivery Systems. **H.D. Cornell**, M. Nagai-Singer, I.C. Allen, A.J. Morris
- 329. Withdrawn.** Novel Synthesis of Macrophilones as Potential Treatments for Melanoma. **J. Cowan**, A. Sherwani, N. Yusuf, S.E. Velu
- 330.** Investigation of Self-assembling BODIPY-pyridine/imidazole acceptors with a Series of Zinc Porphyrin/phthalocyanine Donors and their Charge Separated States. **T. Blesener**, Y. Zatsikha, V. Nemykin, C. Bruckner, L. Harrison
- 331.** Aurones as *S. mutans* Gtf Inhibitors for Prevention of Dental Caries. **P. Ahirwar**, A. Law, B. Nijampatnam, E.M. Rojas, H. Wu, S.E. Velu
- 332.** An Efficient Synthesis of 3-Alkylpyridine Alkaloids Enables Their Biological Evaluation. **A. Kaplan**, C. Schrank
- 333.** Ligand Modification Strategies for the Synthesis of Cu(II) Catalysts for Allylic and Benzylic Oxidation Reactions in Water. **M. Guagliardo**, A.E. Gorden
- 334.** Design, Parallel Synthesis, and Crystal Structures of Biphenyl Antithrombotics as Selective Inhibitors of Tissue Factor VIIa complex: Structure Activity Relationship of the S' site. **A. Spaulding**, R. Krishnan, P. Chand, s. arnold, S. Gupta, R. Upshaw, A. Dehghani, B.G. Boudreaux, C. Parker, S. Bantia, Y. El-Kattan, T. Lin, S. Saini, Q. Zhang, S. Rowland, Y.S. Babu, P.L. Kotian
- 335.** Deaminative Nickel-catalyzed One-carbon Homologation of Alkyl Amines. **C. Twitty**, M.P. Watson
- 336. Withdrawn.** The Synthesis and Biocatalytic Reduction of Beta-keto Alkynes. **R.M. Francis**, B.D. Feske

**1119. Towards the Synthesis of Ambuic Acid & Analogues A. Ustoyev**

Birmingham Jefferson Convention Center  
East Meeting Room K

**Centennial of the Discovery of Insulin**

D. Rabinovich, *Presiding*

**1:00** Introduction.

**1:10 337.** Insulin 100: A Brief Philatelic History. **D. Rabinovich**

**1:40 338.** History of Diagnosing Diabetes and Monitoring Blood Sugar.. **T. Whiteside**

**2:10 339.** The Past, Present and Future of Metformin.. **C.W. Padgett**

**2:40** Closing Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room F

**The Magic of Spectroscopy 2**

Financially supported by ACS Division of Physical Chemistry, ThermoFisher Scientific

A. Gunn, *Presiding*

**1:00** Introduction .

**1:05 340.** Quantum Chemistry and Spectroscopy: A Match Made in the Heavens.  
**R.C. Fortenberry**

**1:45 341.** Application of Polarization Modulated Infrared Spectroscopy to Model Prebiotic Chemical Systems. **H.L. Abbott-Lyon**

**2:25 342.** Rotational Constants and the Effect of Step Size on Quartic Force Field Calculations for Astrochemically Relevant, Cyclic, Aluminum-containing Compounds. **O.A. Harwick**, R.C. Fortenberry

**2:50** Intermission.

**3:05 343.** Laboratory Analogs of Thermally Processed H<sub>2</sub>O-rich Ices Containing NH<sub>3</sub> and CO<sub>2</sub> Relevant to Astrophysical Environments. **D. White**

**3:45 344.** Spectroscopic and Thermal Assessment of the Influence of Copper Loading on Calcium Phosphate Bio-relevant Glasses. **J.A. Jimenez**

**4:25 345.** Hydrogen Binding and Dissociation in Metal Hydride Clusters. **J.T. Lyon**

**4:50** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Ballroom B

### **Theoretical chemistry: Method development and applications 1**

Financially supported by Auburn University  
E. Miliordos, *Organizer*  
J. V. Ortiz, *Presiding*

**1:00** Introduction .

**1:05 346.** Quantum Chemistry and Computer Science: A Tightly Connected Parallel Development. **H.F. Schaefer**

**1:35 347.** Psi4Education: Free and Open-Source Programing Activities for Chemical Education with Free and Open-Source Software. **B. Magers**, V.H. Chávez, B.G. Peyton, D. Sirianni, R.C. Fortenberry, A. Ringer McDonald

**2:05 348.** New Developments in the Basis Set Exchange. **S. Lehtola**, B.P. Pritchard

**2:25 349.** Local Dispersion for Symmetry Adapted Perturbation Theory. **Z. Glick**, C.D. Sherrill

**2:45** Intermission.

**3:00 350.** Accelerating the Convergence of Self-consistent Field Calculations using the Many-body Expansion. **K. Lao**, F. Ballesteros

**3:30 351.** Unraveling the Mechanism of the Hydroxide Transport between the Cobaltocenium groups in Polyelectrolytes. **S. Wickramasinghe**, T. Zhu, Y. Cha, C. Tang, Q. Wang, S. Garashchuk

**3:50 352.** Mechanistic Analysis on Non-enzymatic Dipeptide Hydrolysis and Applicability to Other Polyamide-based Materials and Composites. **K. Lawson**, A.J. Adamczyk

**4:10 353.** Computational UV Spectra for Amorphous Solids of Small Molecules. **A.M. Wallace**, R.C. Fortenberry

Birmingham Jefferson Convention Center  
East Meeting Room C

### **Methods and strategies for modern organic synthesis**

Financially supported by **Oakwood Chemical, VWR, Auburn University**

M. Chen, R. Karimov, *Presiding*

**1:15** Introductory Remarks.

**1:25 354.** Azadienes and Azatrienes for Catalytic Enantioselective Umpolung Synthesis of Chiral Diamines – Methods and Mechanism. **S. Malcolmson**, X. Shao, P. Zhou

**1:55 355.** Making Chiral Heterocycles Using Chiral Heterocycles as Ligands. **A. Aponick**

**2:25 356.** Oxidative C-H Functionalization. **S. Blakey**

**2:55** Intermission.

**3:15 357.** Polarity Reversal and Functionalization of Fluorinated Alkenes. **S. Roy**

**3:45 358.** Bisketene Equivalents as Diels–Alder dienes, and their Application in Natural Product Synthesis. **C. Newton**

**4:15 359.** Dearomative Coupling of Heteroarene Salts with Nucleophiles and Electrophiles. **R. Karimov**

**4:45 360.** The Flip Side of Click Chemistry: Breaking Bonds Reliably. **M. Finn**

Birmingham Jefferson Convention Center  
East Meeting Room J

### **Small molecule activation at biological or bio-inspired metal centers**

Financially supported by Agilent Technologies, Quark Enterprises, Chemglass Life Sciences, Thermo Fisher Scientific, ACS Division of Inorganic Chemistry, M Braun Inc

J. D. Caranto, G. B. Wijeratne, *Presiding*

**1:15** Introductory Remarks.

**1:20 361.** Cu-promoted Functionalization of C-H Bonds Using Directing Groups with Varying Denticity, Hydrogen Peroxide and Triethylamine.. **I. Garcia-Bosch**

**1:45 362.** Modulating O<sub>2</sub> Affinity and Reactivity in Sensor Globin Domains. **E.E. Weinert**

**2:10 363.** Towards Understanding why the TxtE {FeO<sub>2</sub>}<sup>8</sup> Intermediate Resists Reduction. **J.D. Caranto**, C.P. Martin, M. Chen, M. Martinez, Z. Ma, V.L. Davidson, Y. Ding

**2:35 364.** Native and Non-native Reactions Catalyzed by the Multifunctional Hemoglobin Dehaloperoxidase. **R.A. Ghiladi**, D. Yun

**3:00 365.** Kinetic, Thermodynamic, and Theoretical Investigations into Proton-coupled Electron Transfer Reactivities of Synthetic Heme Superoxide Intermediates. **P. Mondal**, G.B. Wijeratne

**3:20** Intermission.

**3:35 366.** Superoxide Dismutase Mimicry Across the Third Row Metals. **C.R. Goldsmith**, J.L. Moore, L. Senft, R.S. Boothe, J. Oppelt, A. Franke, A. Scheitler, D.D. Schwartz, I. Ivanović- Burmazović

**4:00 367.** Protic Ruthenium Anticancer Compounds: Describing the role of Ligand Charge in both Photodissociation and Singlet Oxygen Production. **E.T. Papish**, O.E. Oladipupo, Y. Kim

**4:25 368.** De Novo Designed Artificial Cu Proteins (ArCuPs) as a New Generation of Biocatalysts for O-H/O-O/C-H Activation Reactions. **S. Chakraborty**, S. Mitra, D. Prakash

**4:50 369.** Bioinspired Heme Mediated Monooxygenation of Indoles. P. Mondal, **G.B. Wijeratne**

**5:10 1903.** The role of tyrosine-159 hydrogen bond donation on 3-mercaptopropionic acid dioxygenase (3MDO) catalysis: a combined catalytic, spectroscopic, and computational investigation. N. J. York, M. Lockart, A. Schmittou, **B. S. Pierce**

Birmingham Jefferson Convention Center  
East Meeting Room E

### **Spatially resolved spectroscopy: Applications in Biomedical and Materials Imaging**

A. Ghosh, *Presiding*

**1:15** Introduction .

**1:20 370.** Phenotyping Extracellular Vesicles from Red Blood Cells Using Vibrational Spectroscopy and Imaging. **R.A. Dluhy**, A. Konutham, J. Oh, A. Gaggar, R. Patel

**1:50 371.** Discrete Frequency Infrared Imaging of Colorectal Cancer and Lipid Deposits in Alzheimer's Brain Tissue. **M.P. Confer**, A. Ghosh, R. Bhargava

**2:20 372.** Label-free Sensing and Imaging for Lipidome Analysis. **M.R. Gartia**

**2:50 373.** Disease Diagnosis using Mid-infrared Spectroscopic Imaging. **C. Gajjela**, R. Mankar, S. Afrose, D. Mayerich, R. Reddy

**3:20 374.** Simultaneous IR+Raman Microscopy Measurements, SIRRMM for the identification of microplastic contamination of <20 $\mu$ m. **J. Anderson**, M. Kansiz, F. Weston, C.A. Marcott

**3:50 375.** Nanoscale IR spectroscopy: From Principles to Nanoscale Imaging and Identification of Metal Soaps. **A. Centrone**

**4:20 376.** Challenges in Nanospectroscopy Techniques for Materials and Biological Applications. **J. Atkin**

**4:50 377.** Nanoscale Spatially Resolved Infrared Spectroscopy of Amyloid fibrils and Prefibrillar Aggregates. **A. Ghosh**

Birmingham Jefferson Convention Center  
East Meeting Room I

## **Contemporary Fluorine Chemistry in the Southeast 2**

Cosponsored by FLUO  
M. Etzkorn, *Presiding*

**1:30** Introduction .

**1:35 378.** Chemistry for Molten Salt Reactors – History and Perspectives. **S. Dai**

**2:05 379.** Semi-Fluorinated Aromatic ether Polymers from Step-growth Polymerization of Fluoroalkenes and Fluoroalkylation of Diphenyl Ether. G. Munoz, K.M. Chamberlain, K. Shelar, K.M. Mukeba, E. Borrego, S. Athukorale, C.U. Pittman, **D.W. Smith**

**2:35 380.** Fluorine's role in halogen bonding. **W.T. Pennington**, A. Peloquin, C.D. McMillan

**3:05 381.** Fluorinated Indene Derivatives as New Building Blocks for Organic Materials. **M. Etzkorn**, M.J. Elardo

**3:05** Concluding Remarks.



Birmingham Jefferson Convention Center  
East Meeting Room D

## **Design, Chemistry, and Application of Active, Functional Materials**

A. Koh, *Presiding*

**1:30** Introductory Remarks.

**1:35 382.** Electroactive Hydrogel actuators fabricated via Digital Light Projection Additive Manufacturing. Y. Wang, B. Beckingham, **M.L. Auad**

**2:15 383.** Photons, Electrons, and Polymer Design: Structure-processing-property Relationships for Radiation-induced Polymerization. **J.L. Jessop**

**2:55** Intermission.

**3:00 384.** Shape and Structure in Active Biopolymer Droplets. **K.L. Weirich**, K. Dasbiswas, D. Scheff, F. Schwarzendahl, P. Ronceray, A. Patel, T.A. Witten, S. Vaikuntanathan, M. Gardel

**3:40 385.** Galinstan Multi-material Dispersions for Deformable Electronics. **E. Bury**, A. Koh

**4:05** Intermission.

**4:10 386.** Mixed Heterocyclic Oligomers Based on Pyrazine, Thiophene, and Furan as Organic Semiconducting Building Blocks. **D. Karunathilaka**, D.L. Watkins

**4:35 387.** Enhancing the Sustainability of Pd-based Hydrogenation Catalysts. **A. Rahmani**, T. Jurca

Birmingham Jefferson Convention Center  
East Meeting Room G

**Ground truth: bridging knowledge gaps between computational and experimental enzymology**

Financially supported by **University of Memphis College of Arts & Sciences,**  
**University of Memphis Department of Chemistry**

N. J. DeYonker, *Presiding*

**1:30** Introductory Remarks.

**1:35 388.** Cassava as a Solution for Cancer: A Computational Approach. **S. Delwakkada Liyanage,** C. Ratnaweera, D. Gunasekera

**1:55 389.** Application of RINRUS in Studying Enzymatic Reactions. **Q. Cheng,** N.J. DeYonker

**2:20 390.** Structure-Guided Protein Engineering: Utilizing the *Sphingomonas* sp. KT-1 PahZ1 Structure to Create a Commercially Useful Bioreagent for Poly(aspartic acid) Degradation. **J.M. Miller,** T. Lamantia, A. Jansch, j. marsee, M. Weiland

**2:45 391.** Ensemble Docking and Exploration of the Coronavirus Protease Active Site: Developing Optimization Rules for SARS-CoV-2 M<sup>pro</sup> Antiviral drug development. **S. Stoddard**

**3:10** Intermission.

**3:25 392.** Coupling of Electrostatic Preorganization and Dynamic Allostery: Insights from Atomistic Modeling. M.M. Lawal, **V. Vaissier**

**3:50 393.** Ionic Atmosphere Effects: A Reminder to Consider Solution Ions in Computational Simulations. Y. Orozco-Gonzalez, B.D. Dratch, M. Kabir, G. Gadda, **S. Gozem**

**4:15 394.** A role for N99 in the “b-latch” regulatory mechanism of the type II cysteine desulfurase SufS from *Escherichia coli*. J.V. Conte, R. Gogar, J.A. Dunkle, **P.A. Frantom**

**4:45 395.** Ligand interactions that determine transcriptional outcomes. **C.D. Okafor**

Birmingham Jefferson Convention Center  
East Meeting Room A

**New Directions in Metal-Catalyzed Reactions 2**

Financially supported by Organic Reactions, Biocryst, VWR

X. Cui, *Presiding*

**1:30** Introduction .

**1:35 396.** Electronic Structure of  $\text{RhO}^{2+}$ , Its Ammoniated Complexes  $(\text{NH}_3)_{1-5}\text{RhO}^{2+}$ , and Mechanistic Exploration of  $\text{CH}_4$  Activation by Them. **N. Khan**, E. Miliordos

**2:05 397.** Development of a Ni-catalyzed Larock Annulation. **D. Wilger**

**2:35 398.** Synthesis, Characterization, and Reactivity of Redox-Active Polymerization Catalysts. N. Taylor, L.N. Baker, M. Gordinier, K. Young, **T. Brewster**

**3:05** Intermission.

**3:20 399. Withdrawn.** Copper-Catalyzed Aminoheteroarylation of Unactivated Alkenes through Distal Heteroaryl Migration. **Y. Kwon**, W. Zhang, Q. Wang

**3:40 400.** Enantioselective Lactonization by  $\text{P}^{\text{t}}$ -acid Catalyzed Allylic Substitution: a Complement to  $\text{P}^{\text{t}}$ -allylmetal Chemistry. **A. Kizhakkayil Mangadan**, J. Liu, A. Aponick

**4:00 401.** *E*-Substituted Polydentate Phosphine Complexes: Their Catalytic Activity and Incorporation into Metal Organic Frameworks. N.S. Abeynayake, L.J. Barrios, V. Ramkumar, C. Secrist, **V. Montiel-Palma**

**4:30 402.** Dipyridylarylmethane Ligands Enable Efficient Alkane C-H Borylation Catalysis. **N.D. Schley**

Birmingham Jefferson Convention Center  
East Meeting Room L

**Electrocatalysts, Solar cell and Electrochemical methods part 2**

S. Pan, *Presiding*

**1:30** Introduction .

**1:40 403.** Dye-Sensitized Solar Cells in Unbiased Water and CO<sub>2</sub> Electrolysis Systems. **J.H. Delcamp**, S. Pan, H. Cheema, J. Watson, R.R. Rodrigues, P. Shinde

**2:05 404.** *In situ* Surface Sensitive Vibrational Spectroscopic Probe of Catalyst Structures, Dynamics and Reaction Mechanisms at Electrochemical Interfaces. **T. Lian**

**2:30 405.** *Interfacing Photosystem I into Nanomaterials*. **D.E. Cliffl**, K. Wolfe, C. Stachurski, J. Williams

**2:55 406.** Electrocatalytic OER and ORR Studies with Single Crystal Perovskite and Spinel Oxides Grown by Molecular Beam Epitaxy. **B.H. Farnum**

**3:20** Intermission.

**3:35 407.** Electrochemically Triggered Interfacial Deposition/Assembly of Aqueous-Suspended Colloids. **W. Zhan**

**4:00 408.** Nanointerface-localized Electrical Field Enhancement in Energy Harvesting and Ion Separation: From Single Nanopores to AAO Membranes. **G. Wang**, D. Baram, M.M. Kvetny, W. Brown

**4:25 409.** Electrochemical and Light-driven Carbon Dioxide Reduction by Molecular Manganese Catalysts: Exploring the Positional Effect of Second-Sphere Hydrogen-Bond Donors. S. Sinha Roy, K. Talukdar, **J.W. Jurss**

**4:50 410.** Investigating Oxygen Evolution Reaction over Layered Intermetallic Electrocatalysts. D.K. Mann, A. Díez, O. Lebedev, Y. Kolenko, **M. Shatruk**

Birmingham Jefferson Convention Center  
East Meeting Room O

## **Polymer Assemblies: from Fundamental to Applications 2**

Financially supported by the National Science Foundation

B. Beckingham, Y. C. Simon, *Presiding*

**1:30** Introduction .

**1:35 411.** Supramolecular Crosslinking Strategies for Polylactone-based Nanocarriers for Theranostics. **D.L. Watkins**

**2:00 412.** Leveraging Connectivity in Block Copolymers to Control Assembly and Shape Transformation in Polymersomes.. **Y.C. Simon**, T. Chidanguro, L.D. Dugas, C.H. Liu

**2:25 413.** Responsive self-assembled nano- and microcapsules. **E.P. Kharlampieva**

**2:50 414. Withdrawn.** Incorporation of Polysaccharide Derivatives into Cellulose Particles for Enzyme Immobilization. L. Portilla Villareal, A. Bansode, J. Garcia Alonso, M.L. Auad, B. Via, **I. Vega Erramuspe**

**3:05** Intermission.

**3:20 415.** Microcapsule-based Self-healing for Additive Manufacturing. **B. Beckingham**, V. Shinde

**3:45 416.** All-aqueous Assembly of Highly Hydrophobic, pH-responsive Polyelectrolyte Multilayers. **J. Brito**, K. Asawa, A.K. Andrianov, C. Choi, S.A. Sukhishvili

**4:00 417.** Star Polyelectrolytes in Multilayer Assemblies. **A. Aliakseyeu**, J. Ankner, S.A. Sukhishvili

**4:15 418.** Free-Standing Multilayer Hydrogels. **M. Dolmat**, V.A. Kozlovskaya, E.P. Kharlampieva

**4:30** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room B

## **Small Molecules for the Disruption of Bacterial Processes 2**

Financially supported by Clemson University

D. C. Whitehead, *Presiding*

**1:30** Introductory Remarks.

**1:40 419.** Exploration of a Synthetic Retinoid Scaffold for the Treatment of Persistent MRSA Infections. **C. Schrank**, A. Cheng, I. Escobar, B. Haney, E. Mylonakis, W.M. Wuest

**2:05 420.** A Novel Antibiotic Adjuvant Scaffold Identified Through Fragment Screening that Potentiates  $\beta$ -lactam Antibiotics in MRSA by Dampening Transcription of key resistance genes. **M.S. Blackledge**, H.B. Miller

**2:30 421.** Computationally-guided Design of Promysalin Analogues to Overcome Resistance in *P. aeruginosa*. **A. Mahoney**, J. Khowsathit, J. Karanicolas, W.M. Wuest

**2:55** Intermission.

**3:10 422.** Synthesis and Characterization of Novel Diffusible Signal Factor Analogs for Analysis of Structure Activity Relationships. **R. Wiley**, D.L. Baker

**3:35 423.** Quantitative Analysis of Fatty acid diffusible signaling factors by HPLC-ESI-MS. **B. HOFFMAN**

**4:00 424.** Promysalin Analogs Reveal New Binding Cleft in Succinate Dehydrogenase. **S. Post**, C. Keohane, L.M. Rossiter, A. Kaplan, J. Khowsathit, K. Matuska, J. Karanicolas, W.M. Wuest

Birmingham Jefferson Convention Center  
East Meeting Room N

**How to Foster Diversity, Equity and Inclusion in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award**

R. Joseph, *Organizer*  
P. Gordan, *Presiding*

**2:30** Introduction .

**2:40 425.** Transformation of the LSU Chemistry Department. **I.M. Warner**

**3:05 426.** Diversity and Excellence: The Role of Senior Faculty. **J.V. Ortiz**

**3:30 427.** A Cuban Campesino in Chemistry's Academic Court. **R. Hernandez**

**3:55 428.** DEIR in Teaching and Research: Some personal Experiences, Challenges, and Opportunities. **D. Rabinovich**

**4:20** Panel Discussion.

Birmingham Jefferson Convention Center  
East Meeting Room K

## **Chemical Education**

### **The Plant Hunter**

C. Quave, *Organizer*

**3:00** Introduction.

**3:10 429.** Book Talk: "The Plant Hunter: A Scientist's Quest for Nature's Next Medicines". **C. Quave**

**4:00** Discussion and Questions.

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## **Inorganic**

### **Poster session**

J. E. Ritchie, *Organizer*

**3:00 - 5:00**

- 430.** Loss of Chromium(III) from Mixed Cr(III),Fe(III) Serum Transferrins. K.C. Edwards, **D.R. Graham**, D. Keith, J.B. Vincent
- 431.** Hydrothermal Synthesis of Rare Earth Ruthenates. **B. Patel**, M. Kolambage, C.D. McMillen, J.W. Kolis
- 432.** Gas-phase Oxidative Coupling of Alcohols and Amines over Bimetallic Solid Catalysts. **A. Minne**, J.W. Harris
- 433.** Heterometallic Metal-Organic Frameworks as a Platform for Gas-Phase Heterogeneous Catalysis. **A. Mathur**, D. Shakya, D.A. Chen, N.B. Shustova
- 434.** Designing Sublimable Lanthanide-Based Precursors for Quantum Information Processing. **S. Bisht**, M. Gakiya-Teruya, J. Vellore Winfred, M. Shatruk
- 435.** One-electron Oxidation of Methanesulfinic Acid (MSA) by Hexachloroiridate(IV). **Y. Yang**
- 436. Withdrawn.** Light-activated ruthenium polypyridyl  $\beta$ -diketonate complex is Cytotoxic within the Photodynamic Therapy Window. **R. Ryan**, R.J. Mitchell, D. Havrylyuk, D.K. Heidary, J.P. Selegue, P.C. Glazer
- 437.** Photophysical and Electronic Properties of Photoresponsive Metal-organic Frameworks. **G. Wilson**, C.R. Martin, N.B. Shustova
- 438.** Pyrrophenes and Pyrropyridines: Hexadentate Coordination systems for Uranyl  $\text{UO}_2^{2+}$ . **J. Ducilon**, A.E. Gorden
- 439.** Syntheses and Characterization of Valence Tautomeric Cobalt Complexes with Magnetic Transition at Room Temperature. **P. Wang**, M. Shatruk
- 440.** Investigation of Well-Defined Donor–Acceptor Fulleretic Materials. **G. Thaggard**, G. Leith, N.B. Shustova
- 441.** Exploring Metal-organic Frameworks: Reversible Gas Adsorption and Catalytic Activity. **P. Kittikhunnatham**, N.B. Shustova
- 442.** Synthesis and Metalation of Two Redox-active Ligands Functionalized with a Terminal Alkyne for Applications in Flow Chemistry. **A. Yu**, J. Bacsá, C.E. MacBeth
- 443.** Magnetic Structure of Chain Antiferromagnets  $\text{MBi}_4\text{S}_7$  ( $\text{M} = \text{Mn}, \text{Fe}$ ). **I. Campbell**, M. Shatruk, O. Garlea



- 444.** Synthesizing Organometallic Polymers from Metal-sulfur Cubane Clusters. **J. Gillen**, C. Bejger
- 445.** Titanium-45 for Development of PET Radiopharmaceuticals. **F. shefali**, I. Chaple, S.E. Lapi
- 446.** Biomimetic-inspired Polyimidazole Manganese Chelates. **B. McIntyre**
- 447.** Superacidic Nanostructured Materials. A.A. Kuvayskaya, **A. Vasiliev**
- 448.** Water-soluble Rhodium (III) and Cobalt(III) Porphyrin Complexes for the Biological Inactivation of Fentanyl. **H. Pal**, **A. Nina**, O.K. Nag, E. Oh, A. Burkus-Matesevac, C.D. Chouinard, K. Maiello, J. Delehanty, D. Knight
- 449.** To activate or not to activate? Experimental and computational studies of small molecule activation by copper- and zinc-based frustrated Lewis pairs. **K. Bledsoe**, L.K. Bennett, K.M. Clark
- 450.** Dimethyl zinc complexes supported by TBAM ligands: Exploration of ligand exchange thermodynamics and the mechanism of protonolysis. **L.K. Bennett**, K.M. Clark
- 451.** Magnetic and optical properties of  $\text{NaLnS}_2$  ( $\text{Ln} = \text{La, Ce, Pr, Eu, Er, Yb, Lu}$ ). **F.I. Danladi**
- 452.** Production of  $^{52}\text{Mn}$  using Natural and Enriched Chromium Targets with a Semi-Automated Purification System. **J. Pyles**, A.V. Massicano, J. Appiah, J.L. Bartels, A. Alford, S.E. Lapi, J. Omweri
- 453.** Radioscandium Isotopes of Clinical Interests: Production and Purification of High Purity  $^{43,47}\text{Sc}$  Radioisotopes via Enriched  $^{46,50}\text{Ti}$   $\text{TiO}_2$ . **S. Cingoranelli**, C.S. Loveless, J.L. Bartels, J.R. Blanoc, R. T, S.E. Lapi
- 454.** Mechanochemical Investigation of the Impact of Solvates on Organometallic Halide Metathesis. **H. DeGroot**
- 455.** Effect of Tethered, Axially Coordinated Ligands (TACLs) on Rh(II)-Catalyzed Cyclopropanation: A Linear Free Energy Relationship Study. **C. Zavala**, A. Darko
- 456. Withdrawn.** Ferromagnetic  $\text{Cd}_{(1-x)}\text{Cu}_x\text{Cr}_2\text{S}_4$  Thin Films: Synthesis, Characterization and First-principles Calculations. **J. ABBASI**, S. Regmi, A. Gupta

- 457.** Inelastic Neutron Scattering Study of Magnetic Exchange Pathways in MnS and MnSe. **J. Roth**, V. Yannello, A. Samarakoon, C. Ross, M. Uible, O. Garlea, M. Shatruk
- 458.** Optimization of a Microwave-assisted Reaction Method to Synthesize Europium-based Calcium Fluoride Nanoparticles for Potential Optical Imaging. **M. Fratarecangeli**, M. Rathbone, C. De Silva
- 459.** Zr-MOFs as a Platform for Nuclear Waste Sequestration. **K. Park**, N.B. Shustova
- 460.** Dynamically and Staticly Tailoring the Properties of Metal-Organic Frameworks. **C.R. Martin**, N.B. Shustova
- 461.** A Novel Magnetic Drug Screening Nanoplatform Based on Immobilized Transmembrane Proteins on Magnetic Superparticles. **S. Mansur**, J. Horne, S.E. Velu, Y. Bao
- 462.** Surface Functionalized Polyamidoamine (PAMAM) - Fatty Acid Amphiphilic Janus Dendrimers for Biomedical Applications. **M. Loku Yaddehige**, I. Chandasiri, D.L. Watkins
- 463.** Unprecedented Ag Doping and the Crystal Structure of  $\text{Au}_{30-x}\text{Ag}_x(\text{S}-t\text{Bu})_{18}$ . **K.H. Wijesinghe**, N. Sakthivel, T.C. Jones, A. Antonysamy
- 464.** Short-range Ordered 2D Phases and their Electronic Properties in  $\text{Nb}_x\text{V}_{1-x}\text{O}_2$ . **T. Rawot Chhetri**
- 465.** Structure-Function Correlation in InP-Based Quantum Dots. **S. Click**, J.R. McBride, K. Reid, S. Rosenthal
- 466.** Biodegradation of N-nitroglycine by the Heme Protein NnlA. **K.A. Strickland**, A. Holland, A. Trudeau, D.E. Graham, J.D. Caranto
- 467.** Reorganization Energy and Charge Transfer Rates from Quantum Dots to Cobalt Redox Mediators. **M. Fort**, S. Click, E.H. Robinson, F.M. He, P.V. Bernhardt, J. Macdonald, S. Rosenthal
- 468.** Synthesis and characterization of ultrasml superparamagnetic Iron Oxide Nanoparticles-encapsulated Liposomes as a Novel ph-responsive T1-weighted MRI Contrast Agent for Cancer Diagnosis. **S. Rahmati**

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## Multidentate Ligands in Inorganic Chemistry

### Poster session

W. E. Lynch, *Organizer*

**3:00 - 5:00**

**469.** Synthesis, Characterization and Structure of a *tetra*(acetonitrile)ruthenium(II) complex,  $[(\text{NCCH}_3)_4\text{RuPh}(\text{P}\{\text{OCH}_2\}_3\text{CEt})][\text{BArF}']$  and its Reactivity with Multidentate Ligands. **G. Durrell**, J. Bazemore, B.P. Quillian

**470.** Synthesis of New Nickel(II) CNC-Pincer Complexes as Catalysts for Carbon Dioxide Reduction. **S.Y. Manafe**, **S. Das**, **D. Nugegoda**, **J.H. Delcamp**, **E.T. Papish**

**471.** Synthesis of Symmetric Water Soluble N-Heterocyclic Carbene Ligands for AuNPs. **R. Borsari**, S.L. Strausser, I.M. Jensen, D.M. Jenkins

**472.** Systematic Investigation of Halogen Bonding Interactions in Dye-sensitized Solar Cells Using Cobalt Redox Shuttles Bearing Halogen Substituents. **S. Bhattacharya**, D. Nugegoda, J.H. Delcamp, J.W. Jurss

**473.** Catalytic Activity of NU-1000 based Catalysts Grafted with a Ni Organometallic Complex. **L.J. Barrios**, C. Secrist, V. Montiel-Palma

**474.** Synthesis of Heterobimetallic Arene Ruthenium Complexes Incorporating Aromatic N-Heterocycles and a Group 13 Metal. **G. Sanchez Lecuona**, V. Montiel-Palma

**475.** Synthesis of  $C_2$ -symmetric Chiral Diimidazoles for NHC Macrocyclic Construction for Catalytic Applications. **H. Brothers**, J.R. Russell, D.M. Jenkins

**476.** Light-responsive and protic ruthenium compounds bearing bathophenanthroline and dihydroxybipyridine ligands achieve nanomolar toxicity towards breast cancer cells. **O.E. Oladipupo**, S. Brown, R. Lamb, J. Gray, C. Cameron, A. DeRegnaucourt,

N. Ward, F. Hall, Y. Xu, C. Petersen, F. Qu, A. Shrestha, M.K. Thompson, M. Bonizzoni, C.E. Webster, S. McFarland, Y. Kim, E.T. Papish

**477.** Investigation of Phthalocyanine Synthesis for Catalysis in Zeolites. **J. Enguita**, A. Shrestha, A. Chowdhury, M.G. Bakker

**478.** Synthesis of New Pincer Ligands for Forming Ruthenium Photocatalysts for Carbon Dioxide Reduction. **W. Silprakob**, S. Das, D. Nugegoda, J.H. Delcamp, E.T. Papish

**479.** Synthesis and Characterization of Tri- and Tetra-cobalt Complexes Supported by 2,6-bis[(trimethylsilyl)Amino]pyridine. **L. Nguyen**, J. Bates, G. Guillet

**480.** Catalytic Hydrodeoxygenation of Vanillyl Alcohol with Ruthenium and Iridium Catalysts in Water and Other Green Solvents. **W. Yao**, S. Das, A.K. Vannucci, E.T. Papish

**481.** Synthesis, Characterization, and Catalytic Performance of Ru(II) Complexes Bearing 2,2'-bis(diphenylphosphino)Biphenyl (BIPHEP) Derivatives. **M.J. Goldberg**, **I. Alam**, **J.R. Stryker**, R.E. Black

**482.** Synthesis and Characterization of the Second Triiron Extended Metal Atom Chain Complex with Fe-Fe Bonding. **C.E. Mullins**, J.E. Bates, G. Guillet

**483.** Cobalt Catalyzed Regioselective Trifluoromethylation of C–H bonds. **C. Kuehner**, C.F. Harris, J.D. Soper

**484.** Development of Multidentate, Mixed O/S-donor Imidazole Thione Ligands. **R. Wolsleger**, M. Wetzler, J.L. Brumaghim

**485.** Small Molecule Activation by Ruthenium (BB)-carboryne Complex. **H. Jayaweera**, D.V. Peryshkov

## **THURSDAY EVENING**

Birmingham Jefferson Convention Center  
East Ballroom B

### **Plenary**

D. A. Dixon, *Presiding*

**5:30 486.** From Isotopes to Images: Development of Radiometal Agents in Medicine.  
**S.E. Lapi**

## **FRIDAY MORNING**

Birmingham Jefferson Convention Center  
East Meeting Room G

### **Research in Practice 1**

Financially supported by Wilson Dam Local Section of the ACS

S. Love-Rutledge, *Organizer*  
S. Johnson, *Presiding*

**8:00** Introductory Remarks.

**8:05 487.** Evaluating peer-led team learning in an online context: Is it still effective?.  
**J.D. Young**, S.E. Lewis

**8:25 488.** Uncovering the Chemistry behind Food: Intentional Course Design for Broadening Science Literacy in Nonmajors during a Global Pandemic. **J.A. Dabrowski**

**8:45 489.** How does task design affect student engagement in small group discourse?.  
**S. Fateh**, Z. Kirbulut, J. Reid, G.T. Rushton

**9:05** Intermission.

**9:20 490.** Uncovering Mindset Perspectives via Analysis of Undergraduate Views on Intelligence in Chemistry. **D. Santos**, H. Gallo, J. Barbera, S. Mooring

**9:40 491.** Socio-psychological Interventions to Promote General Chemistry Student Success. Y. Wang, G.A. Rocabado, J.E. Lewis, **S.E. Lewis**

**10:00 492.** Exploring the Relationship Between a Student's STEM Professional Identity and their Perception of Meaningful Learning in the chemistry Laboratory. **M.L. Head**, D. Dayani, A. Alkawam, E. Pearman

**10:20 493.** “I Felt Like I was Losing Like, an Hour of my Time”: Examining the Experiences of Pregnant and/or Parenting Women in STEM Doctoral Programs. **C. Wright**

**10:40** Discussion.

**11:00** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room I

### **Classroom Chemistry: Innovations in Practice**

Financially supported by Central Alabama Community College  
J. M. Carr, *Presiding*

**8:00** Introductory Remarks.

**8:05 494.** *Can Students Learn Chemistry on Their Phones? Opportunities and Challenges in Tech-Driven Learning.* **K.D. Revell**

**8:35 495.** Psi4Education: Free and Open-Source Programing Activities for Chemical Education with Free and Open-Source Software. **R.C. Fortenberry**, B. Magers, A. Ringer McDonald, C.D. Sherrill

**8:55 496.** Surveying Microplastic Pollution and developing Science Identity through Field Experience and Course-based Undergraduate Research. **J. Forakis**, J. March, M.A. Erdmann

**9:20 497.** Incorporating Concept Development Activities into a Flipped Classroom Structure: Reframing the Flipped Classroom as a Blended Learning Mode of Instruction. **J.F. Eichler**, E.J. Yeziarski

**9:40** Intermission.

**9:55 498. Withdrawn.** Flipped Classroom in Organic Chemistry: Significant Effect on Final Grades. **C. Cormier**

**10:15 499.** Lennard-Jones Plot Construction in General Chemistry: How Well Do Semiempirical  $\Delta H_f$  Values Accurately Estimate Covalent Bond Lengths in Simple Diatomics? **J.M. Carr**, C.A. Rock, Z. McClendon

**10:35 500. Withdrawn.** Model-Based Inquiry and Engineering Design in the Classroom. **C.A. Rock**, B.A. Whitworth

**11:00 501.** Online-simulation Modules as Pre-learning Material to Reduce Cognitive Overload in Guided Inquiry Labs. **D. Das**

**11:20** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room F

### **f-Element Chemistry and Applications**

Financially supported by University of Tampa College of Natural and Health Sciences, ACS Division of Nuclear Chemistry and Technology

A. E. Gorden, E. J. Werner, *Presiding*

**8:00** Introduction .

**8:05 502.** Alternative Methods to Generate High-Valent Transuranic Elements. M. Sheridan, J. McLachlan, J. Gonzalez-Moya, T.S. Grimes, **C. Dares**

**8:25 503.** Crystal Engineering with Imidophosphorane L ligands in High-valent Actinide Complexes. **J. Niklas**, J. Bacsá, H.S. La Pierre

**8:45 504.** Understanding tetravalent actinide oxide formation, stability, and dissolution under far field environmental conditions. **B.A. Powell**, K. Peruski, C.J. Parker, M. Maloubier, D. Kaplan, A. Kersting, M. Zavarin

**9:05 505.** Tailoring Redox Active Ligands for Probing the Reactivity of Actinides. **A.E. Gorden**

**9:25 506.** From Solution to Solid State: An Update on Hexavalent Actinide Co-Crystallization. **J.D. Burns**, J. Einkauf

**9:45 507.** Exploring the Nature of F-Element Soft Donor Interactions using Electronically Tunable Azolate Ionic Liquids. **R.D. Rogers**, H.B. Wineinger, G. Gurau

**10:05** Intermission.

**10:20 508. Withdrawn.** Use of Bis-lactam-1,10-phenanthroline Ligands as Selective Holdback Reagents for Improved Adjacent Lanthanide Separation. **K. Johnson**, I. Popovs, S. Jansone-Popova

**10:40 509.** Technetium Complexation with Halides. **N.A. Wall**, C. Eiroa-Lledo

**11:00 510.** Clean-up after F-element chemistry: Savannah River Site Tank Closure Cesium Removal (TCCR) In-Situ Cs-137 monitoring. **T. Whiteside**, D.P. Diprete, K.M. Fenker

**11:20 511.** Why Formal Oxidation States do not tell the Story of Magneto-structural Phase Transitions in Ce- and Eu-containing Intermetallics. J. Roth, V. Yannello, A. Rogalev, V.O. Garlea, **M. Shatruk**

**11:40 512.** Meso-unsubstituted Expanded Porphyrins: Synthesis and Applications. **J.L. Sessler**

Birmingham Jefferson Convention Center  
East Meeting Room D

## **Frontiers in Organic Synthesis and Catalysis 1**

Cosponsored by ORGN  
W. Santos, *Presiding*

**8:00** Introductory Remarks.

**8:05 513. Withdrawn.** Nickel-Catalyzed Deaminative Cross-coupling Reactions. **M.P. Watson**



**8:30 514.** Multifunctional aza-crown Ether Catalysts for Selective Hydroxyl Functionalizations. **B. Kim**

**8:50 515.** Ring Distortion of Indole Alkaloids as a Synthesis Platform for Drug Discovery. **R.W. Huigens**

**9:15 516.** Heterogeneous acid- and base-catalyzed Conversion of Unprotected Aldose Sugars to Furan Derivatives via the Garcia Gonzalez Reaction. **S.A. France**

**9:40** Intermission.

**9:55 517.** Leveraging Complex Molecule Synthesis as a Driver for Chemical and Biological Discovery. **J.G. Pierce**

**10:20 518.** Broadening Copper-catalyzed Boracarboxylation to include Unactivated  $\alpha$ -olefins by using Xantphos as a Secondary Ligand: Preliminary Insights from Catalytic and Stoichiometric Reactivity Studies. **B.V. Popp**, S.W. Knowlden, C.H. Gordon, N.N. Baughman

**10:40 519.** Transition Metal-Free Stereoselective Borylation Reactions. **W.L. Santos**

**11:05 520.** Beyond Cp\* - Mechanism guided design of a new rhodium complex for enantioselective C-H functionalization. **S. Blakey**

Birmingham Jefferson Convention Center  
East Meeting Room L

## **Main Group Chemistry and Inorganic Materials**

P. Rupar, *Presiding*

**8:00** Introductory Remarks.

**8:05 521.** Coordination Chemistry of Aromatic Boracyclic Anions. **C. Martin**

**8:25 522.** Effects of Heteroatoms on the Chemical and Electrochemical Stability of Some Polyaniline Derivatives. **C.N. Scott**, M.N. Almtiri, H. Gigi

**8:45 523.** Tetraarylphosphonium: A Versatile Platform for Green Chemistry Applications. **B. Wicker**, B.A. Atwater

**9:05 524.** Synthesis and Optical Studies of 4-coordinate Borafluorenes. **M. Pennington**, P. Rupar

**9:25 525.** Redox-active Ligands for the Rational Design of Electronically Delocalized Materials. **K.M. Clark**

**9:45 526.** Metal-free Bond Activation by Carboranyl Diphosphine. **G. Gange**, D.V. Peryshkov

**10:05** Intermission.

**10:20 527.** Accessing Structural Information across Different Length scales in Distorted Rutiles using Irreducible Representations and Total Scattering Methods. **J.M. Allred**, T.C. Douglas, M.A. Davenport, M. Krogstad, L.M. Whitt, T. Rawot Chhetri, R. Osborn, S. Rosenkranz

**10:40 528.** Connections between Synthesis, Physical Properties and Chemical Bonding in 3d Polar Magnets. **T.T. Tran**

**11:00 529.** Understanding Dendrite Formation in Mg-based Batteries. **R.D. Davidson**, A. Verma, S. Angarita-Gomez, F. Hao, J. Van Buskirk, O. Gonzalez, P. Balbuena, P.P. Mukherjee, S. Banerjee

**11:20 530.** Relationship between Local Crystallographic Order and Geometric Frustration within  $V_{1-x}Mo_xO_2$ . **T.C. Douglas**, M.A. Davenport, L.M. Whitt, T. Rawot Chhetri, M. Krogstad, S. Rosenkranz, R. Osborn, J.M. Allred

**11:40 531.** Possible Evidence for Incipient Magnetism in quasi-one-dimensional Chevrel Phases. **L.M. Whitt**, T.C. Douglas, S. Chi, K. Taddei, J.M. Allred

Birmingham Jefferson Convention Center  
East Meeting Room K

**Multidentate Ligand Systems in Inorganic Chemistry: Synthesis, Complexes, Structures and Reactions 1**

W. E. Lynch, *Presiding*

Financially supported by ACS Division of Inorganic Chemistry, and the Coastal Georgia Local Section of the ACS

**8:00** Introductory Remarks.

**8:05 532.** Trisimidazolyl Phosphine, a Versatile Tridentate Ligand for Bioinorganic and Catalytic Studies. **W.E. Lynch**, C.W. Padgett, B.P. Quillian

**8:30 533.** Polydentate bis(amidines) as Selective Molecular Locks for Embedding Coinage Metal Fragments. **M. Stollenz**, J. Arras, O. Ugarte Trejo, C. O'Dea, A. Calderón-Díaz, N. Bhuvanesh, C.D. McMillen

**8:55 534.** Heterobimetallic Complexes of Ru, Rh and Ir Incorporating a Group 13 Element and Formation of bi- and Polydentate Phosphinogallyl Ligands. G. Sanchez Lecuona, N.S. Abeynayake, **V. Montiel-Palma**

**9:20 535.** Trimetallic Extended Metal Atom Chain Complexes of Fe(II) with Fe-Fe bonds, Variation of Properties Derived from Ligand Composition. **G. Guillet**, K.Y. Arpin, C.E. Mullins, J. Bates

**9:45** Intermission.

**10:05 536.** The Generation of *Trans*-spanning Metallohedged Ligands. **J.A. Pienkos**, J.P. Lee, C.D. McMillen, S.L. McDarmont, L.D. Jaques, B.D. Nessel, S.E. Neglia

**10:30 537.** New hydroxy substituted Salen-type Pd and Pt complexes: Spectroscopical properties, Structural characterization, DFT calculations, and CO<sub>2</sub> reduction. **D.M. Pinero Cruz**, J.O. Rivera

**10:55 538.** Imidazole Thiones: Unique Sulfur-Containing Ligands for Metal Coordination. M.M. Kimani, M.T. Zimmerman, A.A. Gaertner, M.A. Abbas, R. Wolsleger, M. Wetzler, **J.L. Brumaghim**

**11:20 539.** Coordination Chemistry with Tridentate Pyridine/chalcogenone Mixed-donor Ligands. **D. Rabinovich**

Birmingham Jefferson Convention Center  
East Meeting Room E

**Polymer Membrane: Chemistry, Fabrication, and Application to Separations and Energy Devices**

B. Beckingham, *Presiding*

Financially supported by Polymers

**8:00** Introductory Remarks.

**8:05 540.** Tethered Electrolyte Active-layer Membranes (TEAMs): Expanding the Avenues for Polyelectrolyte Membranes. **C. Porter**, R. DuChanois, E. MacDonald, S. Kilpatrick, M. Zhong, M. Elimelech

**8:35 541.** Effect of PEGMA as a Comonomer in PEGDA Based Films for Controlling Fractional Free Volume and in Co-transport of Carboxylate Ions with Alcohols Through the Films.. **A. Mazumder, J. Kim, B. Hunter, B. Beckingham**

**8:50 542.** Advancing Forward Osmosis for Energy-efficient Wastewater Treatment towards Enhanced Water Reuse and Resource Recovery. **S. Zou**

**9:20** Intermission.

**9:30 543.** MOF- Functionalized Membranes with Enhanced Antifouling and Selectivity for Efficient Water Treatment. **M.R. Esfahani**

**10:00 544.** Poly(4-vinylpyridine)-*block*-poly(*tert*-butylmethacrylate) as a Promising Precursor System to Charge Mosaics: Nanostructured thin Films of Oppositely Charged Domains.. **J.G. Kennemur**, R. Verduzco, T. Terlier, B.A. Fultz, B. Dunoyer de Segonzac

**10:15 545.** Leveraging Insights from Transport and Co-transport Behavior in Anion Exchange Membranes to Improve Membrane Performance for Direct Urea Fuel cells. **B. Beckingham, J. Kim**

**10:45** Intermission.

**10:55 546.** Synthesis and Performance of New Vinylimidazolium Poly(Ionic Liquids) as Gas Separation Membranes. **S. Ravula, J.E. Bara**

**11:10 547.** Polynaphthalene Networks and High Yield Carbon-Carbon Composites via *Ortho*-Diynyl Arene (ODA) Resins. E. Borrego, S. Athukorale, S. Gorla, A.K. Duckworth, W. Johnson, H. Ahmad, S. Kundu, C.U. Pittman, **D.W. Smith**

**11:40** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Ballroom B

## **Theoretical chemistry: Method development and applications 2**

Financially supported by Auburn University  
E. Miliordos, *Organizer*  
K. D. Vogiatzis, *Presiding*

**8:00** Introduction .

**8:05 548.** Spin-forbidden processes and molecular magnetism: New theoretical tools for quantitative modeling and insight. **A. Krylov**

**8:35 549.** Flexible wavefunctions for strongly correlated systems: quasiparticle, coupled cluster, and seniority-based approaches. **R. Miranda Quintana**

**9:05 550.** Partitioning Correlation Mechanisms through Nonorthogonal Multiconfigurational Self-Consistent Field Theory. **L.M. Thompson**

**9:25 551.** New Method Developments for the Application of Correlated Electron Systems. **E. Kempfer-Robertson**, L.M. Thompson

**9:45** Intermission.

**10:05 552.** Identifying domains of applicability of machine learning models of quantum-mechanical properties. **C. Sutton**

**10:35 553.** Density Matrix Embedding Theory Methods for Non-equilibrium Electron Dynamics in Extended Systems. **J. Kretchmer**

**11:05 554.** (T)+EOM Quartic Force Fields for Theoretical vibrational spectroscopy of electronically excited states.. **M. Davis**, R.C. Fortenberry

**11:25 555.** Global Searching of Self-Consistent Field Solutions Extended to Large Systems. **X. Dong**, L.M. Thompson

**11:45 556.** Modeling of Macromolecules with Electric Fields. Y. Zheng, **V. Vaissier**

Birmingham Jefferson Convention Center  
East Meeting Room J

### **Women in Chemistry: Advances and Experiences in the Field A**

Financially supported by **ACS Women Chemists Committee**

S. K. Hamilton, *Organizer*  
X. Jiang, *Presiding*

**8:00** Introduction .

**8:05 557.** Providing Students with Interdisciplinary Research in Organic Synthesis and Computational Chemistry. **J.A. Pigza**

**8:35 558. Withdrawn.** Elucidating Molecular Mechanisms of Mental Illness with Quantum Dots. **S. Rosenthal**

**9:05 559.** “It's not the warmest environment”: How Women Navigate Pregnancy and Parenting Throughout the STEM Doctorate. **C. Wright**

**9:35** Panel Discussion.

Birmingham Jefferson Convention Center  
East Meeting Room A

### **STEM Education in K-12**

Financially supported by ACS Division of Polymer Chemistry, Alabama Science Teachers Association, Southern Research, Alabama Math Science and Technology Initiative, Birmingham Southern College

## **STEM K-12 1**

E. Menard, C. Willingham, *Organizers*

**9:00 560.** Ironclad Chemistry – from Supernovae to the Red Mountain iron ore. **S. Brande**

**10:00** Intermission.

**10:10 561.** Teaching Physical Science, Chemistry, and AP Chemistry in the Digital Realm. **K. Reaves, J. Firth, L. Swift**

**11:10** Intermission.

**12:40 562.** Ask the Professor. **J. March, K.L. Hayden, M.S. Ponder, K.H. Shaughnessy, J. Harshman**

**1:40** Intermission.

**1:50 563.** Particulate Diagrams in AP Chemistry. **L. McGaw**

**2:50** Intermission.

**3:00 564.** Acids, Bases and Buffers in AP Chemistry. **L. McGaw**

Birmingham Jefferson Convention Center  
East Meeting Room B

## **STEM Education in K-12**

## **STEM K-12 2**

E. Menard, C. Willingham, *Organizers*

**9:00 565.** The AMSTI/ASIM Program: An Overview. **A. Murphy**

**10:00** Intermission.

**10:10 566.** REasons for Geographic and Racial Differences in Stroke (REGARDS). **G. Howard**

**11:10** Intermission.

**12:40 567.** Developing a Particle Model of Matter using Modeling Instruction. **C. Manor**

**1:40** Intermission.

**1:50 568.** Proportional Reasoning to Describe (Qualitatively and Quantitatively) gas Behavior using Modeling Instruction. **C. Manor**

**2:50** Intermission.

**3:00 569.** The Science of Sloss Furnaces. **T. Malugani**

Birmingham Jefferson Convention Center  
East Meeting Room C

## **STEM Education in K-12**

### **STEM K-12 3**

E. Menard, C. Willingham, *Organizers*

**9:00 570.** Colorful and Sweet Chemistry. **A.A. Hazari**

**10:00** Intermission.

**10:10 571.** Changing an Atom. **K. Williams**

**11:10** Intermission.

**12:40 572.** Proficiency Scales in the Chemistry Classroom. **R. Poe**

**1:40** Intermission.

**1:50 573.** Uses of Radioactive Isotopes in Pharmacy. **J.D. Burns**



**2:50** Intermission.

**3:00 574.** FoodMASTER: Cooking with Chemistry. **T. Petrov**

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## **Energy and Fuels**

**10:00 - 12:00**

**575.** Analysis of Molten Salt Reactor Source Terms. **S. Creasman**, T.J. Harrison, L.H. Heilbronn

**576.** Copper Redox Shuttles Supported by Pentadentate Ligands for High Performance Dye-Sensitized Solar Cells. **A. Devdass**, J. Watson, J.H. Delcamp, J.W. Jurss

**577.** Electrochemical and Ce(IV)-driven Water Oxidation with Dinuclear Ruthenium Complexes Featuring Dipyrityl- or Dipyrimidyl-Pyridazine Bridging Ligands. **S. Sahil**, J.W. Jurss

**578.** Plasmon-Exciton Coupling Effect in Nanostructured Arrays for Optical Signal Amplification and Application in Nucleic Acid Detection. **F. Tukur, A. JAYAPALAN**, J. Wei

**579.** Novel Cobalt Oxide @ N-carbon Dots Core-shell Nanocomposite Synthesis as Efficient Electrocatalysts in Oxygen Reduction Reactions. **A. JAYAPALAN**, F. Tukur, J. Wei

**580.** MnO<sub>2</sub>-MWCNT Nanocomposite for High Energy Supercapacitor Applications. **M.H. Kabir**, M. Thompson, W. GHANN, J. Uddin, A. Rodriguez, A. Poyraz

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

## **Undergraduate Research 2**

## Poster Session Undergraduate Research 2

J. A. Nikles, *Organizer*

**10:00 - 12:00**

**581.** Surface Modification of Titanium to Support Soft Tissue Growth. **M. Roberts**, S.G. Dennis-Little, M. Yost, T.W. Hanks

**582.** Effects of Co-doping and Alternate Sulfur Sources on Polyol Synthesized Cu-Sb-S Systems. **J.E. Daniel**, M. Jensen, T.R. MacAlister, M.E. Anderson

**583.** Effect of Flanking Sequence on AT-hook peptide Motif Binding Action. **E.A. Durham**, M. Tedrick, K.L. Buchmueller

**584.** Screening of a Small Library of Phenolic Compounds as Inhibitors of Melanoma and Non-melanoma Skin Cancer Cells. **M. Agbo**, S. Boateng, T. Roy, J. Chamcheu, J. Fotie

**585.** Expression and Characterization of Lanthipeptide Components from the Marine Bacteria *Salinispora arenicola*. **A. Deen Sesay**, **D. Ellis**, E. Limbrick

**586.** Stereoselective Hydrosilylation of Alkynes Catalyzed by Dichloro(ethylenediamine) Platinum(II) under Heterogeneous Conditions – a Mechanistic Study. **T. Tolar**, M. Agbo, C. Huff, **J. Fotie**

**587.** A Comparative Study of Palladium on Charcoal and Palladium Nano-Dispersed in Organically Modified Silicate as Heterogeneous Catalysts for the Hydrosilylation of Aldehydes and Ketones. **H. Drago**, M. Agbo, T. Tolar, C. Huff, **J. Fotie**

**588.** Cobalt, Nickel, Iron, Platinum and Palladium Individually Dispersed and Stabilized in Organically Modified silicate as Catalysts for a Reductive Functionalization of CO<sub>2</sub>. **C. Huff**, M. Agbo, T. Tolar, H. Drago, **J. Fotie**

**589.** Synthesis and Spectroscopic Analysis of Liquid State Hydantoin Derivatives. **B.C. Copeland**, O.A. Cojocar

**590.** Synthesis and Analysis of Self-Assembling Small Organic Molecules for Rectifiers and Biosensors. **R. Ma**, M.E. Welker, R. Sullivan, O. Jurchescu

- 591.** Photochemical Annulation of 2-pyridone via Photocycloaddition–oxidative Cyclobutane Fragmentation. **E. Hardwick**, C. Slough, M.E. Daub
- 592.** Method Development of MC-LR Detection in the Liver and Brain of the Mummichog. **M.K. Klumb**, A. Aga, W. Silander, D. Hollis, J.F. Wheeler, S.K. Wheeler
- 593.** Mycoremediation of the herbicide Atrazine with Various White-rot Fungi via Ultra Performance Liquid Chromatography (UPLC). **J.S. Wirth**, M.K. Klumb, C.S. Webber, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 594.** Analysis of Atrazine Degradation and Metabolite Formation after Mycoremediation Utilizing the Fungus *Pleurotus ostreatus*. **J.R. Wilson**, H.E. Burney, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 595.** Atrazine Degradation in Soil by a Mixed Inoculum and White-Rot Fungi. **C.S. Webber**, **M.L. Schroder**, M.K. Klumb, J.S. Wirth, J.R. Wilson, L.H. Olson, J.F. Wheeler, S.K. Wheeler
- 596.** Quantification of Heavy Metals in Commercial Tuna. **M. McCormack**, J.D. Leyba
- 597.** Synthesis of Styrenes from Aldehyde-Aldehyde Aldol Coupling Products. **M. Rodriguez**, **T.G. Chong**, G. Dixon, C.W. Downey
- 598.** One-pot Synthesis of Furans from 3-(trimethylsilyl)propargyl Carboxylates. **A.V. Helbling**, D. Sklar, C.W. Downey
- 599.** Enol Silane Formation-allylation Reactions Promoted by Trimethylsilyl Trifluoromethanesulfonate. **R. Coyle**, E.D. Heafner, X. Lin, H. Zhong, C.W. Downey
- 600.** Addition of Indoles to Nitrones via Friedel–Crafts Silyloxyaminoalkylation. **H.L. Xia**, Z. Oracheff, C. Poff, S.E. Isaacson, C.W. Downey
- 601.** Synthesis of 2,3-Dihydroisoxazoles from Ketones and N-benzyl Nitrones. **R.M. Goodner**, C.W. Downey
- 602.** Determination of Cannabidiol in Tennessee Hemp Bud and Trim. **M.A. Lutey**, G.E. Potts
- 603.** Withdrawn
- 604.** Withdrawn

- 605.** Modifying SurMOF Thin Film Morphology: Examining the Effect of Deposition Parameters on Nucleation and Growth. **B.N. Diederich**, F.G. Gonzalez, A.M. Weeks, M.E. Anderson
- 606.** Correlating the Regioselectivity of Bromohydrin Formation from Unsymmetrical Alkenes with Bromonium ion C-Br Bond Lengths. N. Johansen, **B. Tutkowski**
- 607. Withdrawn.** Synthesis of Biaryl Phosphatane Ligands for Transition Metal-Catalyzed Cross-Coupling Reactions. **Z.K. Abro**, **V.A. Osenga**
- 608.** Analysis of Hormone Agonists on the Differentiation of Oligodendrocytes Precursor Cells. **N. Campbell**, M.C. Zupan, I. Parish, A. N.D. Punchi Hewage, M.D. Hartley
- 609.** Ampicillin-induced Biophysical Changes of *Escherichia coli* Cells Over Multiple Generations. **A. Carranza-Parras**, K. Dungey
- 610.** Halogen Bonding Capable Functionalized Gold Nanoparticles – an Avenue for Molecular Detection Schemes. **Q. Dang**, **K. Lalwani**, **S.T. Gilmore**, M.C. Leopold
- 611.** Sintering-Based In-Situ Synthesis of Noble Metal Nanoparticles for Ceramic Glaze Color Control. **K. Lalwani**, N. Dinh, M.C. Leopold, R. Coppage
- 612.** Design and Application of an Immobilizable Protein Kinase. **T. Cope**, D. Deane, T. Bennett, R.M. Hughes
- 613.** Analysis of Commercial Glow Sticks. **T. Kanipe**, **H.E. Sasko**, C.E. Dahm
- 614.** Analysis of Colored Golf Balls. **J.A. Nolasco**, **C.E. Dahm**
- 615.** Colorimetric and Fluorometric Dual Sensor for the Detection of Copper and Aluminum Ions. **A. Foret**, E. Fasusi, S. Westervelt, D. Ghosh
- 616.** Suspension of Pt(II) Complexes in PMMA Films: Photophysical Effects. **J.H. Zimmerman**, M.J. McCormick, P.S. Wagenknecht
- 617.** Search for Blue Emitters with High Phosphorescence Quantum Yield. **W.M. Thomas**, M.J. McCormick, J.H. Zimmerman, C.D. McMillen, P.S. Wagenknecht
- 618.** Photochemistry and Computational Modelling of Titanocene Complexes. **T.J. Whittemore**, H.C. London, A.G. Gale, G.C. Shields, P.S. Wagenknecht

- 619.** Preparation and Analysis of Vanadium–Amoxicillin Complexes. **R. Overend**, J.A. Dabrowski
- 620.** Synthesis, Characterization, and Cytotoxic Activity of Asymmetric *N,N'*-bis-substituted 1,2,3- Triazolium Salts. **D. Fico**, I.C. Rodriguez, J. Wilson, R.V. Clamor, S. Sanders, J. Gorden, M. Frazier, L. King, K.S. Taylor
- 621.** Reverse Engineering as a Freshman Chemistry Research Experience. **M. Morris**, N. Edge, J.K. Konzelman
- 622.** Novel Synthesis of Gamma Lactones from Dinitriles. **K. Youngblood**, K.S. Petersen
- 623.** *Selenium heterocycles and the enzymatic inhibition of SARS-CoV-2's  $M^{protease}$ .* **R.E. Panella**, M. Donahue, J. Kessl, F. Bai
- 624.** Investigating the Role of Disulfide Interface in Metal Binding for Psoriasis Using Molecular Dynamics Simulations. **Y. Chen**, A. Acharya, D. Das
- 625.** Synthesis, Characterization, and Reactivity of Copper Complexes Supported by a Tripodal Amidate Ligand. **Y. Zhang**, E. Liu, J. Bacsá, C.E. MacBeth
- 626.** Developing a Biodegradable Collagen Mimic for Applications in Wound Healing. **A. Tarlton**, S. K. Hamilton
- 627.** Recycling Plastic Materials by Solvent-targeted Recovery and Precipitation. **B. Martin**, C. Tirla, J. Locklear
- 628.** The Chemical Depolymerization of Poly Lactic Acid (PLA) Plastic Accelerated by Microwave Heating.. **B. Murphy**, J. Cooper, J. Konzelman
- 629. Withdrawn.** Monitoring Ivyp1 Active Site Loop Structure and Dynamics using Variable Temperature NMR. **J. Durham**, K. Letsinger, T. Leeper
- 999.** Synthesis and Reaction Pathways Cu-Sb-S Systems for Sustainable Energy Production. **M. Jensen**, T. MacAlister, M. Anderson

Birmingham Jefferson Convention Center  
East Meeting Room J

**Women in Chemistry: Advances and Experiences in the Field B**

Financially supported by ACS Women Chemists Committee

S. K. Hamilton, *Organizer*

J. M. Murphy, *Presiding*

**10:00** Introduction .

**10:10 630.** Thiosemicarbazone Inhibition on Topoisomerase II $\alpha$ . **X. Jiang**, W. Medawala, L. Ngo, W. Morris, E.C. Lisic, J. Deweese, E. Driggers

**10:40 631.** Bloom Where You are Planted: Growing Outreach Programs as an Early Career Chemist. **E.E. Hardy**

**11:10 632.** Encouraging Representation of Women in STEM: Organizing Arkansas' first Virtual Women in STEM Conference. **S.E. Hubbard, S.K. Hamilton**

**11:40** Panel Discussion.

## **FRIDAY AFTERNOON**

Birmingham Jefferson Convention Center  
East Meeting Room G

### **Research in Practice 2**

Financially supported by Wilson Dam Local Section of the ACS

S. Johnson, *Organizer*

S. Love-Rutledge, *Presiding*

**1:00** Introductory Remarks.

**1:05 633.** Comparison of Laboratory Notebooks in Three Contexts - Traditional Laboratory, CURE, and Research. **A. Hagwood**, M.G. Koufas, W.E. Allen, **J.P. Walker**

**1:25 634.** Assessing the Scientific Practices: Lessons Learned about Content and Context. **J.H. Carmel**, E. Day, N.S. Stephenson, M. Cooper, D.G. Herrington

**1:45 635.** Using Classical Test Theory and Rasch Modeling to Improve General Chemistry Exams on a Per Instructor Basis. **K. Hanson**, B. Sorrenson

**2:05 636.** Engaging Metabolic Pathways: Infographics to Promote Creativity and Multimodal Learning in Biochemistry. **S.T. Love-Rutledge**, **S. Johnson**, J. Robinson

**2:25** Intermission.

**2:40 637.** Understanding how Representations of Chemical Bonding Influence the Paths Students Engage in while Predicting Molecular Shape. **A. Farheen**, S.E. Lewis

**3:00 638.** Organic Chemistry students' Reasoning and Representational Competence Skills in the Context of Dash-wedge Diagrams and Newman Projections. **M. Popova**

**3:20 639.** Using EEG and Eye Tracking Data to Characterize Learner Cognitive Processes During 3D Modeling Tasks in General Chemistry. K. Barbee, T. Gordon, H. Knoefel, T. McCullough, A. Randolph, C. Terrell, **K.J. Linenberger Cortes**

**3:40** Discussion.

**4:00** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

## **COMP**

### **Poster session**

T. P. Hamilton, *Organizer*

**1:00 - 3:00**

**640.** Computational comparison of atmospheric clusters:  $\text{H}_2\text{SO}_4\text{-HCOOH-H}_2\text{O}$  and  $\text{H}_2\text{SO}_4\text{-HNO}_3\text{-H}_2\text{O}$ . **L. Juechter**, S. Harold, T. Odbadrakh, G.C. Shields

**641.** Computational Analysis of Prebiotic Triglycine Formation in Atmospheric Microdroplets. **S. Harold**, S. Warf, T. Odbadrakh, G.C. Shields

- 642.** Calculating the Concentrations of Hydrated Sulfuric Acid Clusters. **L. Kurfman**, S. Vanovac, T. Odbadrakh, G.C. Shields
- 643.** Computational Study of Hydrated  $\text{H}_2\text{SO}_4\text{-NH}_3\text{-(H}_2\text{O)}_n$  Clusters. **V. Fowler**, T. Odbadrakh, G.C. Shields
- 644.** Triglycine Formation in Atmospheric Nano Droplets of Water. **S.L. Warf**, S. Harold, T. Odbadrakh, G.C. Shields
- 645.** Computational Calculations of Radical pair EPR Parameters for Avian Magnetoreception. **C. Bready**, C. Kerpel, T. Odbadrakh, L. Jarocha, G.C. Shields
- 646.** Design and Computational Study of Cyanide Bridged Platinum-iron Complex as Anti Cancer Prodrugs. **A. Kaspi-Kaneti**, S. Bhandari, A. Schubert, S. Huang, B.D. Dunietz
- 647.** Generating Spin-orbit Couplings for x-ray Absorption Spectra using a Simplified LR-TDDFT/ZORA Approach. **S. Pak**, D. Nascimento
- 648.** Determination of the Binding Affinities of Acridinyl, Quinoliny, and Pyridinyl Benzenesulfonamides with Enzymes in the *Plasmodium Falciparum* folate Pathway using Docking and Molecular modeling studies. **A. Mallia**, N.Y. Forlemu
- 649.** Electron Donating Group Effects on Halogen Bond donor  $\sigma$ -holes. **D. Devore**, T.L. Ellington, K.L. Shuford
- 650.**  $\sigma$ -Hole Flexibility in Chalcogen Bond Donors. **K.A. French**, T.L. Ellington, K.L. Shuford
- 651.** Statistical Analysis of Protein Similarity Measures. **K. Orellana**, **C. Dyer**, A.L. Parrill-Baker, D.L. Baker
- 652.** QM/MM studies of Xanthine Oxidase Inhibitors. **Y. Maghsoud**, C. Dong, G.A. Cisneros
- 653.** Pursuing type II Heterostructures Using low Dimensional Material Composites for Enhanced Photocatalytic Activity. **U. De Alwis**, K.M. Weerawardene, T.L. Ellington, K.L. Shuford
- 654.** Conventional Strain Energies of Three-membered Heterocycles. **R.P. Ivey**, M.M. Case, D.H. Magers



**655.** QM-cluster study of Reaction Energies in [Ni,Fe]-hydrogenase. **T. Suhagia**, T.J. Summers, Q. Cheng, M. Griffing, N.J. DeYonker

**656. Withdrawn.** Feasibility Studies of High Speed Molecular Information Processing. **K. Williamson**, D. Herr, Y. Mo, H.P. Rathnayake

**657.** Computed vs. Experimentally Derived Oscillator Strengths: A Benchmark Study of Excited-state Quantum Chemical Methods. **J. Garcia Alvarez**, A. Tarleton, A. Wynn, C. Awbrey, T. Roberts, S. Gozem

**658.** Understanding the Effects of Non-bonding Interaction on the Flavin's Absorption Spectra. **M. Kabir**, Y. Orozco-Gonzalez, S. Gozem

**659.** Benchmarking Dimer Contributions to Crystal Lattice Energies in Small Organic Crystals. **C. Sargent**, C.D. Sherrill

**660.** Free energy of  $\text{Fc}/\text{Fc}^+$  redox process in Ferrocene-terminated alkanethiol self-assembled monolayers on Au(100). **J. Hymel**, J.G. McDaniel

**661.** Dissociation Dynamics of Water Molecule on the Core-excited Potential Energy Surface. **A. Datar**, D. Matthews

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

## Physical Chemistry

### Poster session

T. P. Hamilton, *Organizer*

**1:00 - 3:00**

**662.** Methane to Methanol Conversion Facilitated by Anionic Transition Metal Centers: The Case of Fe, Ni, Pd, and Pt. **S. Sader**

**663.** Development of Solvated Electrons Precursors as a Novel Catalyst: Functionalization of  $\text{CO}_2$ . **B. Jackson**, E. Miliordos

- 664.** Benchmark Database of Accurate Nonadditive Interaction Energies of Three-body Complexes. **S. Ochieng**, K. Patkowski
- 665.** Investigations into the Physical Properties of Gemini Surfactants. **D. Aguilar**, A. Wisner, S.J. Bachofer, R.D. Sheardy
- 666.** Temperature Dependence of Fluorescence Emission of Polyaromatic Hydrocarbons: Effect of Excitation Wavelength, Emission Wavelength, and the Sample Matrix. **M. Wamsley**, W. Peng, X. Cui, D. Zhang
- 667.** Eliminating Spurious Multipoles in Intramolecular Symmetry-adapted Perturbation Theory. **D. Luu**, K. Patkowski
- 668.** QM-cluster Modeling of Chorismate Mutase Based on Sampling MD Simulation. **D.A. Agbaglo**, **T.J. Summers**, Q. Cheng, N.J. DeYonker
- 669.** Guest-Host Raman Under liquid Nitrogen Spectroscopy (GHRUNS) for the acquisition of improved vibrational spectra of solids. **E.C. Lambert**, C. Smith, R.N. Compton, N. Hammer
- 670.** Tunable Attosecond Charge Migration in Functionalized Environmentally Persistent Free Radicals. **N. Luedman**, **C.T. Papszycki**, A. Osborne, V.B. Baron, A. Bruner
- 671.** Electron Paramagnetic Resonance Studies of Transition Metal Phthalocyanines. **G.R. Rana**, M.G. Bakker
- 672.** Probing mixed ionic-electronic conducting polymers using ultrafast spectroscopy. **C. Grieco**
- 673.** Plasmonic Coupling of Silver and Gold Nanoparticles in Dimer Systems: Investigating the Near-field Spectra. **S. Gomrok**, J. Barr, E. Chaffin, X. Huang, Y. Wang
- 674.** Pro-drug Encapsulation by Cyclodextrin in a Model Biomimetic System. **S.E. Westervelt**, K.S. Aiken, S.M. Landge, D. Ghosh
- 675.** Observing Belousov-Zhabotinsky Oscillating Reactions in Acoustically-Levitated Droplets. **K. Everitt**, H. McCardle, E.R. Duranty
- 676.** The Ideal Gas Thermodynamic Properties of PtC. **L. Biolsi**

**677.** Solvent Polarity-induced SPAAC Rate Enhancement of the Most Reactive Cyclooctyne: Synthesis and Photo-click Kinetics of a Water Soluble Cyclopropenone-caged Triazole-fused Dibenzocyclooctyne. **C.J. Molnar**, V. Popik

**678.** Self-assembly, Gelation, and Mechanical Properties of Molecular Gels Based on Tyramine based Alkanamides and N-(4-hydroxyphenyl)alkanamides as Low Molecular Mass Gelators. **J. Miller**, **A. Mallia**

**679.** Investigation of Carbene Formation in Ionic Media with Physics-based, Neural Network Force Fields. **J. Stoppelman**

**680.** Exploring Excited States of Ruthenium Polypyridine Chromophores by Ultrafast Transient Absorption and 2D-spectroscopy. **S.E. Dominguez**, M.A. Hermosilla-Palacios, L. Baraldo, V.D. Kleiman

**681.** Helmholtz Capacitance of Aqueous Solution at Au (100) Electrode Under Applied Voltage. **S. Park**, J.G. McDaniel

**682.** Solid Lipid Nanoparticles of Cannabidiol (CBD): A Brief Survey on Emulsifying Ingredients. **M. Valizadehderakhshan**, A. Shahbazi, A. Bhowmik, M. Azami, F. Khaleseh

**683.** Effect of Deposition Parameters and Constrained Area on the Characteristics of Langmuir Films of Nanoparticles. **C.V. Nguyen**, J.J. Weimer

**684.** Preparation And Characterization Of Microcrystalline Cellulose From Raphia Farinifera Inflorescence. **E. Agboeze**

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

## **Polymer Chemistry**

### **Poster session**

V. Thomas, *Organizer*

**1:00 - 3:00**

- 685.** Self-assembly of Single-chain Polymer–fluorophore Nanoparticles in Physiological Milieu. **S. Liu**, J.S. Lindsey
- 686.** Multilayer Hydrogel Particles for Controlled Delivery. **D. Inman**, M. Dolmat, V.A. Kozlovskaya, P. Dickens, E.P. Kharlampieva
- 687.** Simplifying the Synthesis of Conjugated Polymers Utilizing Dihydropyrrolo[3,2-b]pyrrole as a Novel, Tailorable Building Block. **K.J. Bell**, A.M. Kisiel, G.S. Collier
- 688.** Understanding the Solution Behaviors of Ionenenes in Ionic Liquids using Dynamic Light Scattering. **C. Patton**, J.E. Bara, K.E. O'Harra, G. Thompson
- 689.** Synthesis of new Diketopyrrolopyrrole Scaffolds for High-performance Organic Electronic Device Applications. **R. Wahalathantrige Don**, C.N. Scott
- 690.** Highly Swellable Hydrogels Prepared from De-aromatized Lignin. **J. Hwang**, D. Goodlett, M. Ganewatta, M. Kent, C. Tang
- 691.** Co-transport of Methanol and Carboxylates in Cation Exchange Membranes: Effect of Poly(ethylene glycol) Phenyl Ether Acrylate as a Blocking Group. **P. Parasakthi Aravindhan**, J. Kim, B. Beckingham
- 692.** Polyaddition with Dimaleiimides and Aminomaleiimides. **N.Z. Singleton**, T.I. Robinson, A.J. Caroland, **H.J. Schanz**
- 693.** Dimaleihydrizide: Synthesis and Polyaddition with Diamines. **K.M. West**, N.Z. Singleton, H.J. Schanz
- 694.** Main-chain Metallo-Polyelectrolytes for Alkaline Anion-Exchange Membranes. **H. Lin**, C. Tang
- 695.** General Access to Allene-containing Polymers using the Skattebøl Rearrangement. **N. Galan**, J.N. Brantley
- 696.** Effect of Bicyclohexyl Regioisomer Ratios on the Physical Properties of Poly(bicyclohexyldimethylene terephthalate). **A. Coley**, T.N. Thompson, M.D. Schulz

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

**Polymer Materials Science and Engineering**

## Poster session

V. Thomas, *Organizer*

**1:00 - 3:00**

**697.** Capacitive Electrode Printed Using Silver Nano-Ink on Plasma Modified/Functionalized PET for Potential Organic Pollutants Sensing from Water. **R. RAJAN PILLAI**, S. Gardner, S. Sunilkumar, S. Sanas, M. Haider, V. Thomas

**698.** Crystallization Kinetics of Mixtures of Polypropylene Homopolymer and Impact Copolymer. **P. Wang**, S. Liu, Y. Peng

**699.** Effects of Functional Groups and Anions on the Properties of Polyamide-Ionenes. **J. Bridges**, S. Chatterjee, K.E. O'Harra, J.E. Bara

**700.** Optimizing polyHIPE Foams for PFAS Removal from Wastewater and Groundwater via the Implementation of Surfmers. **I. Dorsey**, A. Koh

**701.** Development of a Scalable, Organic Solvent-free Process for PCDA Liposome Formation. **M. Head**, T.W. Hanks

**702.** Chemical “Activation” of Polyvinyl Chloride for Upcycling and Depolymerization. **M. Bepari**, A. Alshaikh, J.E. Bara

**703.** Tröger's Base Containing Polymers Membranes For Separation of CO<sub>2</sub> From other gases  
. **C. Baltier**, S. Chatterjee, J.E. Bara, C. Patton, K.N. West

**704.** Non-releasing, Enzymatic Layer-by-layer Coatings with Antibacterial Activity. **J. Brito**, I. Alvarado, A.K. Andrianov, S.A. Sukhishvili

**705.** Competition-Enhanced Aptamer Selection Against A Chiral Lipid. **S. Ochoa**, M.C. Adams, A. Saad-Falcon, D. Hufnagel, V.T. Milam

**706.** Processing Carbon-Carbon Composites from Ortho-diynylarene Resins. **W. Johnson**, E. Borrego, S. Gorla, S. Athukorale, A.K. Duckworth, H. Ahmad, S. Kundu, H. Toghiani, C.U. Pittman, D.W. Smith

**707.** Electrospinning Parameters and Chemical Additives in Fabricating PVA Electrospay Fibers. **M. Ucak Astarlioglu**, T. Thornell, H. George, E. Alberts, K. Klaus, S.E. Morgan

**708.** Dynamics of Bottlebrush Polymers. **K. Bichler**, B. Jakobi, G. Schneider

**709.** Agglomeration Behavior in Case of Bottlebrush Polymer. **B. Jakobi**, K. Bichler, G. Schneider

**710.** AFM Investigation of the Effects of Disinfection Treatments on Polypropylene Personal Protective Equipment (PPE) Materials. **T.G. Chambers**

**711.** Renewable Semifluorinated Polymers. **K. Mills**, K. Shelar, K.M. Mukeba, D.W. Smith

**712.** Bis-*ortho*-diynylarene Performance Optimization via Expansion of Processing Window and Post-Cures in Air. **A.K. Duckworth**, E. Borrego, S. Athukorale, S. Gorla, W. Johnson, C.U. Pittman, D.W. Smith

**713.** Effect of Nanoparticle Size on Internalization and Transport Across the Corneal Barrier. **M. Azadi**, A.E. David

**714.** Improved Nanoformulation of *Linear-Dendrimer Block-co-Polymer* Materials for Red Blood cell Hitchhiking with *Ionic Liquids*. **C. Hamadani**, I. Chandasiri, M. Loku Yaddehige, G.S. Dasanayake, I. Owolabi, A. Flynt, D.L. Watkins, E.E. Tanner

Birmingham Jefferson Convention Center  
East Meeting Room J

### **Women in Chemistry: Advances and Experiences in the Field C**

Financially supported by the Women's Chemist Committee of the ACS

S. K. Hamilton, *Organizer*  
S. E. Hubbard, *Presiding*

**1:00** Introduction .

**1:05 715.** From AP Certification to PhD in six (intense) years: Obstacles and Advantages to Second-career PhD Students in Chemistry. **J.M. Murphy**

**1:35 716.** Equity in Parental Leave? or You Have a Baby...In a Pandemic!. **S. Zingales**

**2:05 717.** Changing the Academic Culture as a Woman in STEM. **J.L. Brumaghim**

**2:35 718.** Empowering the Next Generation of Chemists Through Academic Advising, Mentoring, and Cohort Building. **A.J. Carroll**

**2:35 719.** Resilience of Women in Chemistry: Lessons Learned. **L. Tribe**

**3:05** Panel Discussion.

**3:35** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room F

## **Women in STEM**

### **Undergraduate Discussions: Women in STEM**

Financially supported by UAB Department of Chemistry, UAB Educational Foundation

J. M. Meyers, *Presiding*

**1:00** Introduction .

**1:10 720.** Career built on collaborative investigations of membrane protein structure, function, and ligand discovery. **A.L. Parrill-Baker**

**1:35 721.** Dance to central dogma with physical chemistry at the single molecule level. **H. Lee**

**2:00 722.** Chemical tools for selective detection of monomethyl lysine PTMs. **M. Raj**

**2:25** Intermission.

**2:40 723.** How did I get here? From Chemistry to Biology and motherhood. **M. Frazier**

**3:05 724.** Biomolecules do amazing things and I get to work with amazing people.  
**J.M. Heemstra**

**3:30** Panel Discussion.

Birmingham Jefferson Convention Center  
East Meeting Room I

**Active Learning Strategies in Remote Learning Environments: Successes and Lessons Learned**

M. S. Reeves, *Presiding*

**1:15** Introductory Remarks.

**1:20 725.** Remote Mentoring of Undergraduate Research Students (ReMentURS).  
**S.M. Ladge**, E. Sargent, K. Marriott, D. Cannon-Rech, M.A. Lnu

**1:45 726.** Collaborative Classroom and Laboratory Experiences Incorporating Online Simulations and Animations for Gas Chromatography. **A. Le**

**2:10 727.** Online Hands-on First-Semester Biochemistry Lab Course: It is Possible.  
**K.R. Willian**

**2:35 728.** From in-person to online: The Evolution of POGIL-PCL Workshops. **S.S. Hunnicutt**, A. Grushow, M.N. Muniz, R.M. Whitnell

**3:00** Intermission.

**3:15 729.** Engaging Students in a Remote Learning Environment. **N.F. Campbell**, T.L. Demeritte

**3:40 730.** What a great idea! Let's try it online.... **M. Tourne**

**4:05 731.** Flipped General Chemistry Instruction in the Time of COVID. **L. Hibbard**

**4:30 732.** Strategies for Making Feedback Useful in Online Courses. **S. Zingales**

**4:55** Concluding Remarks.



Birmingham Jefferson Convention Center  
East Meeting Room E

## **Optoelectronic Materials**

Financially supported by Mississippi EPSCoR

C. N. Scott, *Presiding*

**1:15** Introduction .

**1:25 733.** The Development of a Conjugated Polymeric Electrochemical Memristor for Neuromorphic Computation, Boolean logic, and Elementary Algebra. **B. Grant**, S.H. Foulger, I. Bandera

**1:45 734.** The Design, Synthesis and Application of Photoacoustic Imaging Probes for Companion Diagnostic Applications. **J. Chan**, M.Y. Lucero

**2:05 735.** Colloidal Quantum Dots and Gold Nanorods in Imaging and Photothermal Applications. **H.N. Jayawardena**

**2:25 736.** The Hole Problem. M. Fort, S. Click, A.D. Lacroix, K. Reid, E.H. Robinson, E.A. Hernandez-Pagan, S. Rosenthal, **J. Macdonald**

**2:45** Intermission.

**2:55 737.** High Refractive Index and Fully Degradable Polymers Prepared Using Radical Polymerization. **W. Gutekunst**

**3:15 738.** Photo-Electroswitchable Arylaminoazobenzenes. **C.J. Saint-Louis**, D. Warner, K.S. Keane, M. Kelley, C.M. Meyers, S.C. Blackstock

**3:35 739.** Surface Functionalization for Mid-infrared On-chip Gas Sensing.. **D. Al Hussein**, J. Zhou, R. Gutierrez-Osuna, G. L. Coté, P. Lin, S.A. Sukhishvili

**3:50 740.** Solvent Effects on Properties and Spectra of Xanthene-based dyes - DFT studies. **J.M. Saloni**, C.N. Scott, W. Kolodziejczyk

**4:10** Intermission.

**4:20 741.** Chromogenic Thiazolothiazole Hydrogel Devices Exhibiting Electrochromism, Electrofluorochromism, and Photochromism. **T.J. Adams**, A.R. Brotherton, M.G. Walter

**4:35 742.** Modular, Simple, and Efficient Synthesis of Electron-Rich Pyrrolopyrroles for Novel and Tailorable Conjugated Polymers. **G.S. Collier**, K.J. Bell, A.M. Kisiel, E.M. Wagner

**4:55 743. Withdrawn.** Enhanced Perovskite Solar Cells Performance by Organic Materials. **Q. Dai**

Birmingham Jefferson Convention Center  
East Ballroom B

### **Theoretical chemistry: Method development and applications 3**

Financially supported by Auburn University  
E. Miliordos, *Organizer*  
R. C. Fortenberry, *Presiding*

**1:15** Introduction .

**1:20 744.** Exploiting GPU-Accelerated Ensemble Density Functional Theory to Enable Efficient Photochemistry Simulations of Large Molecules. **F. Liu**

**1:50 745.** Resonant Inelastic x-ray Scattering Simulations from Simplified Time-dependent Density Functional Theory Approaches. **D. Nascimento**

**2:20 746.** A Critical Comparison of Direct Methods for Computing Metastable States. **T. Sommerfeld**, J. Davis

**2:40 747.** Multi-surface Quantum Dynamics with the QTAG Method. **M. Dutra**, S. Wickramasinghe, S. Garashchuk

**3:00** Intermission.

**3:20 748.** Strong Light-matter Interaction Effects on Molecular Systems. **R.F. Ribeiro**

**3:50 749.** Electronic spectroscopy of the  $\tilde{A}-\tilde{X}$  transitions of jet-cooled calcium methoxide ( $\text{CaOCH}_3$ ) and calcium ethoxide ( $\text{CaOC}_2\text{H}_5$ ) radicals: Vibronic structure of nonlinear alkaline earth monoalkoxide radicals as candidates for direct laser cooling. A.C. Paul, K. Sharma, H. Telfah, A. Reza, T.A. Miller, **J. Liu**

**4:10 750.** Systematic Catalyst & Ligand Design for C-H Bond Activation: A Computational Approach. **E.E. Claveau**, E. Miliordos

**4:30 751.** F12-TZ-cCR: A Methodology for Faster and Still Highly-Accurate Quartic Force Fields. **A. Watrous**, B.R. Westbrook, M. Davis, R.C. Fortenberry

**4:50** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room D

## **Frontiers in Organic Synthesis and Catalysis 2**

Cosponsored by ORGN  
W. Santos, *Presiding*

**1:30** Introduction .

**1:35 752.** Synthetic Methodologies Inspired by Complex Natural Products. **S.M. Wilkerson-Hill**, N.F. Cok, A.J. Zahara

**2:00 753.** Aerobic Oxidation Chemistry of Catalytically-relevant Cobalt-aminophenol Complexes. **J.M. Hoover**

**2:25 754.** Amine-Catalyzed Site- and Chemoselective C-H Hydroxylation. **M.K. Hilinski**

**2:50 755.** Determinants of Selectivity in Hydrosilylative Alkyl Ether Cleavage.. **N.D. Schley**

**3:10** Intermission.

**3:25 756.** Developing New Alkene Difunctionalization Reactions. **Q. Wang**

**3:50 757.** Carbohydrate Derived Macrocycles in Catalysis. **G. Wang**

**4:15 758.** Forging Dissonant Functional Group Pairs through Cu-catalyzed Asymmetric Reductive Coupling Reactions of *N*-Substituted Allenes. **J.D. Sieber**

**4:40 759.** (3+2) Cycloadditions Using Photocatalysis Based on Earth-Abundant Metals with Heterocyclic Ligands. **E.M. Ferreira**

Birmingham Jefferson Convention Center  
East Meeting Room K

## **Multidentate Ligand Systems in Inorganic Chemistry: Synthesis, Complexes, Structures and Reactions 2**

W. E. Lynch, *Presiding*

Financially supported by ACS Division of Inorganic Chemistry, and the Coastal Georgia Local Section of the ACS

**1:30** Introduction .

**1:35 760.** How a Pair of Extra “CH<sub>2</sub>’s” Unlocks Stability Versus Reactivity for Macrocyclic Tetra-N-heterocyclic Carbene Complexes. J.F. DeJesus, X.B. Carroll, M.R. Anneser, K.M. Blatchford, G. Elpitiya, **D.M. Jenkins**

**2:00 761.** Nickel Complexes with Multidentate N/S-ligands as Synthetic Models of Nickel-containing Superoxide Dismutase (NiSOD). **T.C. Harrop**, P.T. Truong, L. Howell

**2:25 762.** Copper-based Redox Shuttles Featuring Preorganized Polydentate Ligands for Dye-Sensitized Solar Cells. A. Devdass, J. Watson, R.R. Rodrigues, J.M. Lee, N.S. Taylor, H. Cheema, L. Chen, R.C. Fortenberry, J.H. Delcamp, **J.W. Jurss**

**2:50 763.** Ruthenium Complexes Supported by *bis*(pyrazolyl)acetate and its Derivatives: Synthesis, Structure, Characterization and Reactivity. **B.P. Quillian**

**3:15** Intermission.

**3:35 764.** Structural Inspiration for New Opportunities with Azamacrocyclic Ligands: Rethinking their Synthesis and Facile Access to Multiple Substituents. M.M. Sibley, I. Ruohoniemi, M. Wasilewski, **M. Wetzler**

**4:00 765.** Tethered Axial Coordination as a Control Element on Dirhodium Paddlewheel Complexes. **A. Darko**

**4:25 766.** Poly(pyrazolyl)aluminates and their TM complexes. **M.A. Muñoz-Hernandez**

**4:50 767.** First Row Transition Metal Photocatalysts for CO<sub>2</sub> reduction: control of the coordination environment. **E.T. Papish**, C.M. Boudreaux, C.E. Webster, J.H. Delcamp

Birmingham Jefferson Convention Center  
East Meeting Room L

### **Risk Management in Teaching and Research Settings**

S. B. Sigmann, C. N. Situma, *Organizers*

Financially supported by ACS Division of Chemical Health & Safety

**1:30** Introductory Remarks.

**1:35 768.** Data Analytics and Information Sharing as a Tool for Managing Safety in Academic Labs. **C.N. Situma**

**2:05 769.** Evolution of a risk Assessment Curriculum for Undergraduate and Beginning Graduate Student Researchers. **M.C. Box**, E.D. Blue

**2:35 770.** Staying Ahead of the Curve- Changing World of Laboratory Risk Assessment During Covid. **K. Jacob, J. McBride**

**3:05** Intermission.

**3:20** Discussion.

**4:05** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room M

### **Intellectual Property Basics**

A. Hoeher, *Presiding*

**2:30** Introduction.

**2:40 771.** Intellectual Property Basics. **A. Hoeher**

**3:15** Discussion and Questions.

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

### **Chemical Education**

#### **Poster Session**

**3:00 - 5:00**

**772.** Get involved with the ACS Division of Chemical Education. **S. Johnson, D.S. Boucher**

**773.** Determination of Caffeine in Beverage Samples using the Gas Chromatograph-Mass Spectrometer for an Undergraduate Non-majors Kitchen Chemistry Course.  
**H.V. Clontz**, B. Xiong, N. Johansen

**774.** Studies of Photochemical Thiol-ene Cyclization in Biological Model Systems. **A. Purvis**, A.J. Wommack

**775.** Developments in Remote Teaching and Use of Instruments with Zoom's Remote Control Feature. **D.R. Zuidema**

**776.** Strategies for Enhancing the Virtual Lab Experience. M. Atteya, J. Caton-Williams, J. Gonzales-Roman, **V.A. Mativo**, D. Paschal, **L. Strange de Soria**, **A. Sukhu**, **M. Vanegas**

**777.** Comparison of Particle-in-a-Box Measurements with Molecular Modeling. **J.W. Hall**, S.K. Hutchison

**778.** Synthesis of Isoxazole and Isoxazoline Heterocycles as Potential Inhibitors of Lysyl Oxidase. **M. Goulart**, D.M. Solano

**779.** Video Assignments Improve Self-reported Sense of Community in an Online Undergraduate Chemistry Course. **S. Post**, C. Schrank, K.J. McKnelly

**780.** Synthesis and Characterization of Tripodal Amines. **A. Marsh**, L. Wonnum, K. Lupton, C.R. Whitlock

**781.** Investigation of Anti/pro-oxidant Effects of Carbon Nanodots (CNDs) Doped with Different Heteroatom Elements. **M. Azami**, J. Wei

**782.** Utilizing Student Attitude in Introductory STEM Courses: A Closer look into General Chemistry I (CH-131). **C. Glenn**, P. Clevenger, D. Williams

**783.** How Features of Molecular Representations Impact General Chemistry Students' Correct Prediction of Shape and Polarity. **A. Farheen**, S.E. Lewis

**784.** A Longitudinal Perspective on General Chemistry Students' Differentiation of Covalent Versus Ionic Models of Bonding. **S.E. Lewis**, K.A. Bowe, C.F. Bauer

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

### **Undergraduate Research 3**

J. A. Nikles, *Organizer*  
A. E. Gorden, *Presiding*

**3:00 - 5:00**

- 785. Withdrawn.** Systematic Approach to Evaluate Ruthenium-Based Anti-cancer Agents. **S. Robinson**, K. Enkhbold, L. Paul, M.R. Norris, J.A. Pollock
- 786. Withdrawn.** Expression, Purification, and Assay Development to Study STK1, a Kinase Implicated in Antibiotic Resistance. **M. Callender**, M.S. Blackledge, H.B. Miller, J.A. Pollock
- 787. Withdrawn.** Using Biochemical Tools to Probe the Complexity of MEMO1 Function. **C.A. Bayas**, **C.T. Corl**, S.T. Gilmore, M.C. Leopold, J.A. Pollock
- 788.** Photocatalytic removal of Tetracycline from Simulated Wastewater Lagoons using Compound Parabolic Reflectors. L. Borton, E.R. Gaston, **J.E. Boyd**
- 789.** Photocycloaddition–Cyclobutane Fragmentation for the Synthesis of Annulated Pyridones. **C. Slough**, E. Hardwick, M.E. Daub
- 790.** Development of an Oxidative [3+2] Photocycloaddition of 4-hydroxy-2-pyrones. **C. Sar**, J. Mackey, M.E. Daub
- 791.** Progress Towards an Oxidative [3+2] Photocycloaddition for the Synthesis of Europyridone Natural Products. **J. Mackey**, C. Sar, M.E. Daub
- 792.** Removal of Cobalt(II) Aqueous Ions via Hydrogel Formation of Sodium Alginate in Synthetic Waters of Varying Harnesses. **P.N. Smith**, J.L. Hawk
- 793.** Using Sodium Alginate Hydrogels to Remove Cu<sup>2+</sup> Contaminants from Various Aqueous Solutions. K. Spalding, **J.L. Hawk**
- 794.** Optimization and Characterization of Phosphonium Salts. B. Wicker, **M.B. Miller**
- 795.** Stereoselective Trisubstituted Alkene Synthesis Using Ni-catalyzed Alkyne Hydroarylation. **L.E. Hutchinson**, D. Wilger
- 796.** Electrostatic Tuning Maps: Intuitive Tools to Represent the Effect of an Environment on a Molecule's Properties. **J. Gay**, S. Gozem
- 797.** Isolation and Characterization of a Putative Dimethyl Sulfide (DMS) Monooxygenase in *Arthrobacter globiformis* . **T. Weishaar**, M. Culpepper
- 798.** DMSO Impacts the Reduction of the Metal Containing Anti-Cancer Drug KP1019. **M. Campbell**, E. Garrett, L.K. Stultz



- 799.** Suppression of Key Antibiotic Resistance Genes in MRSA with Small Molecule Adjuvants. **B. Viering**, T. Cunningham, A. King, M.S. Blackledge, H.B. Miller
- 800.** Molecular Dynamics Simulation of Poloxamer 188 and POPC Membranes. **D. Singhi**, S.G. Dennis-Little, M. Yost, T.W. Hanks
- 801.** Dopant Release from Polypyrrole Films and Nanoparticles Controlled by Poly(ethylene glycol) Surface Modification. **G. Richter**, T.W. Hanks
- 802.** Schlieren Effect Usage for Portable Qualitative Analysis. **J.A. Fields**, H. Park
- 803. Withdrawn.** Using CRISPR-Cas9 to Delete *stkI* in MRSA. **A. Anthony**, V. Federico, G. DiGiacomo, H.B. Miller
- 804.** Modulating the Properties of Iridium and Rhenium Complexes Using N-oxide Formation. **E. Stumbo**, J.A. Pienkos, C.D. McMillen
- 805.** Silver Cluster Luminescence. **K. Thomas**, J.T. Petty
- 806.** Silver Cluster Luminescence using (C<sub>2</sub>A)<sub>6</sub>. **M. Branham**, J.T. Petty
- 807.** DNA-Bound Silver Clusters using Modified Oligonucleotides. **C. Couch**, J.T. Petty
- 808. Withdrawn.** N-Heterocyclic Carbene Complexes of Nickel: An Examination of Synthetic Options and Targets. **M. Richter**, R.M. Meier
- 809.** Effect of CMPO Ligand Scaffold Variation on Lanthanide Extraction and Luminescence Properties. **B. Lake**, W. Larrinaga, S.M. Biros, E.J. Werner
- 810.** Synthesis, Scope, and Application of Tetra-aryl Phosphonium Salts. **D.J. Schwaibold**, **M.B. Miller**, B. Wicker
- 811.** Exploring the Scope of Pnictogenium Syntheses. **J.S. Davies**, B. Wicker
- 812.** Application of 1,8-ANS Fluorescent Probe to Identify Hydrophobic Patches on Surface of EF-hand Protein, Human Cardiac Troponin C (hcTnC) Upon Heavy Metal Binding. **O.R. Warfel**, A.M. Spuches
- 813.** Isolating the Opened and Closed Forms of a Rigid Dimer of the Fluorescent dye Rhodamine B. **A.J. Pierre**, P. Lundin, B. Stratton, K. Fogarty

- 814.** Efforts Towards the Design and Synthesis of a New Aminotroponimate Supported Zinc Complex for Hydroamination. **E.J. DiBlasio**, R.J. Harris
- 815.** Investigations on Organobarium Chemistry: Novel Carbon-Carbon Bond Formation, Novel Mechanistic Concepts and Synthetic Applications. **M. Gorman**, J.C. Donnelly, M.L. Smith, R.N. Salvatore
- 816.** Computational Study of the Structure, Vibrational Spectra, and Hydrogen Bonding of  $\text{H}_5\text{O}_2^+$  and its Methylated Derivatives. **S. Sprouse, D. Herbert, B. Freeman, M. Kaledin**
- 817.** Synthesis of Hyperbranched Polymers via Metal-free Self-condensing ring-opening metathesis polymerization. **G. Dinges**, M.D. Schulz, H. Almuzaini
- 818.** Development of a Protecting Group Scheme for the Synthesis of Modified Deep-Cavity Cavitands. **T. Nsubuga**, M. Meadows
- 819.** Optimization of Synthesis and Spectroscopic Analysis of Vanadium–tetracycline Complexes. **S. Eastman**
- 820.** Effects of Pdr1 Phosphorylation Variants on Azole Resistance in *Saccharomyces cerevisiae*. **C.S. Burdette**, M.E. Breen
- 821.** Mapping Pho85-Pho80 Phosphosites in the *Saccharomyces Cerevisiae* transcription factor Pdr1. **R.E. Singer**, M.E. Breen
- 822.** Investigation of the Phosphorylation Status of the *Candida Glabrata* Pdr1 Transcription Factor. **J.R. McCallum**, M.E. Breen
- 823.** Detection of Nicotine Vapor through Photoacoustic Spectroscopy. **B. Freeman**, H. Park
- 824.** Development of Field Test for Identification of Cocaine with TLC. **E. Schrider**, J.O. Boles
- 825.** Predicting Protein Function in *Pythium Insidiosum* using Computational Techniques. **R.H. Gray**, S. Johnson
- 826.** Anion Effect on Octaethyltetraphenylporphyrin Protonation. **M. Swanson**, M. Ballester, V. Castro
- 827.** Recycling Plastic Materials by Solvent-targeted Recovery and Precipitation. **J. Locklear, C. Tirla, B. Martin**

**828.** Gas-phase Acidities of Cyanobenzene and Dicyanobenzene Isomers. **R.A. Firth**, T. Dimino, W.K. Gichuhi

**829.** Ethanolic Extraction of American Oak Wood. **N. Johansen, C. Baumgardner**, K.S. Kroeger

**830.** Gas Chromatographic Analysis of Commercial Whiskeys. **C. Baumgardner**, K.S. Kroeger

**831.** Synthesis, Characterization, and Evaluation of a Novel Coumarin Derivative as a Nerve Gas Sensor. T. Liontis, **S. Freitag**, A. Weerasinghe

**832.** Preparation, Characterization, and Chemical/antimicrobial Activity of 6-ethoxy-6-phenyl-6H-chromeno[3,4-b]quinoxaline Derivatives. **G.R. Lee, H.N. Watkins**, A. Brown, S. Gremillion, B.P. Quillian

**833.** A Metathesis Route Towards Sarcodictyin Analogs. **K. Estes**, N.M. Brandau, P. Wiget

**834. Withdrawn.** Synthesis, Characterization, and Reactivity of Phenylated *para*-cymene ruthenium(II) iodo Complexes Supported by Phosphorus Ligands. **K.D. Cartrette**, G. Durrell, B.P. Quillian

**835.** Simple, Green, Applied Chemistry Research with Undergraduate Scientists of all Career Stages and Disciplines: the Construction and use of Silver Nanoparticle, Pencil Graphite Electrodes for the Detection of Milli-ampere Changes in Cell Solutions. **R. Brosky**, V. Sudhakar, A. Bramblett

**836.** Hofmeister Anion Interactions with Coumarin. **O. Mumma**, Y. Zhang

**837.** Solid-phase Extraction of Rare-earth Elements using Phosphonated Polymer Resins. **A. Fiorito**, S. Winn, W.R. Archer, M.D. Schulz

**838.** Investigation of Quinolines as HIV-integrase Inhibitors. **J. Patterson**, M. Donahue

**839.** Identification of Economical Cross-coupling Catalysts by Small Scale Reaction Screening with Gas Chromatography-Mass Spectrometry. **A.L. Akers**, P. Lundin, S. Geyer

**840.** Synthesis and Characterization of New Earth-abundant Chalcogenide Perovskite Nanomaterials. **O. Parks**, D. Zilevu, S. Creutz

- 841.** Grafting-through Synthesis of Aziridine-based Bottlebrush Polymers. **P. MacNicol**, G. Dinges, W.R. Archer, M.D. Schulz
- 842.** Investigation of Pomalidomide-Derived HaloPROTAC Tool Compounds. **S. Nelson**, B. Ody, R. Liu, C. Dodd, J. Yin, M.L. Turlington
- 843.** Metabolite-responsive Liposomes via a Synthetic Lipid Switch. **S.E. Bottcher**, J. Lou, M. Best
- 844.** Analysis of the UVA/UVB Degradation of Lotions with Additives Through Raman Spectroscopy. **I. Dancer**, A. Wood, B. Sharma
- 1902.** Methodology Optimization for the Synthesis of Novel Carbazole Derivatives Utilizing the Chan-Evans-Lam Coupling Reaction to Target Antibiotic Resistance. **J. Emrich**, S. Gregory, M.S. Blackledge

Birmingham Jefferson Convention Center  
East Ballroom A

#### **Undergraduate Research 4**

J. A. Nikles, *Organizer*

**3:15 - 5:15**

- 845.** Homology Modeling and Molecular Dynamics Studies of the CDK Pho85: a Possible Source of PDR1 Activation in *Candida Glabrata*. **J.M. Dudley**, T. Odbadrakh, M.E. Breen, K.N. Kirschner, G.C. Shields
- 846.** Bioconjugation Studies of Polyethylene Glycol (PEG)-lysozyme and Small Laccase using ESI-MS and click-enabled Fluorescence. **H. Givhan**, W. Browning, M. Sullivan, B. McKinley, B.W. Gregory, C.M. Johnson
- 847.** Metal-Organic Complexes for Hydrogen Sulfide Coordination. **E. Cain**, C.M. Wallen
- 848.** Efforts Toward the Development of an N-heterocyclic Carbene Supported Zinc Catalysts for Hydroamination. **R.J. Alexander**, R.J. Harris

- 849.** Towards the Synthesis of a Simple Alkyl-substituted meta-poly(arylene ethynylene). **C. Bontempo, J. Faircloth, P. Lundin**
- 850.** qRT-PCR Assay Development for Campus-Wide Asymptomatic COVID-19 Screening on Undergraduate Campus. **M. McGuire, L. Evans, D. Manning, K. McKinney, R. Bishop, B. Magers, J. Neiswinger, S.A. Smith**
- 851.** Facile Chitosan Isolation for Heavy Metal Remediation. **R. Tikkala, B. Corbett**
- 852.** Investigating the C–H Arylation of Furan using a Carbazole Derivative as a Photocatalyst. **K. Ribeiro, A.R. Longstreet**
- 853.** A Carbazole Derivative as a Photocatalyst in the C–H Arylation of *N*-Methylpyrrole. **N.A. Reece, A.R. Longstreet**
- 854.** Storage of Carbon Dioxide in Basalt: An In-Depth Study of the Reaction Kinetics and Products of Enstatite Carbonation. **L.J. Hardee, B. Aguila**
- 855.** *Experimental analysis of double-stranded DNA cleavers on bacterial cells.* **T. Fraley, J. Heath, W. Yang**
- 856.** *Small molecules stabilizing the secondary structure of CCG repeat expansion.* **L. Wise, W. Yang**
- 857.** Effect of Initiator Structure on Poly(3-hexylthiophene) Polymerization and Aggregation Properties. **O.J. Armendarez, P. Lundin**
- 858.** Ionic Liquids to Enhance the Fluorescence of Organic Dyes for Bloodstain Detection. **A.N. Mahurin, D.S. Darlington, W.E. Meador, J.H. Delcamp, E.E. Tanner**
- 859.** Withdrawn
- 860.** Fabrication of Structures on Surfaces: From the Macro to the Molecular Scale. **P. Perdikis, B.H. Augustine**
- 861.** Joro Spider Webs as Bio-accumulators of Polycyclic Aromatic Hydrocarbons (PAHs) in North Georgia. **J. Casey, H. Cole, M. Smith-Roden, I. Agyekum, J. Driver**
- 862.** Evaluation of Polymer Surface Modification as an Inhibitor of Methicillin-resistant *Staphylococcus aureus* (MRSA) Biofilm Formation **M. Mauer, A. L. Akers, A. Copeland, M. S. Blackledge, P. Lundin**

- 863.** Determination of Metal Binding Specificity and Stoichiometry to a Monooxygenase Involved in Sulfur Cycling. **K. Zammit**, Z. Adamson, M. Culpepper
- 864.** Comparing Correlation Energy Approximations Derived from TDDFT within the Asymmetric Hubbard Dimer. **L. Everhart**, J.E. Bates
- 865. Withdrawn.** Fabrication of Microfluidic Devices Used for Electrophoretic Separations. **A. Wohlwend**, P. Lundin, K. Fogarty
- 866.** Withdrawn
- 867.** Time-resolved Protein-protein Interactions of Coronavirus nsp2 Constructs using a Trifunctional Small-molecule Probe. **M. Sullivan**, C. Cameron, L. Plate
- 868.** Synthesis of Biheteroaryls Through the Use of a Novel Imidazopyridine Phosphine Ligand in Pd-Catalyzed Suzuki-Miyaura Reactions. **A. Kantzler**, S.A. Jacoby, N.W. Harris, L. Yet
- 869.** Understanding the World at a Molecular-level: Use of the Johnstone Triangle to Determine if Students have Crossed the IMF Threshold. **D. Li**, B. Harmon, N.L. Powell
- 870.** Morphological Comparison of Grafted Bentonite to Various Nanoclays for Improvement of Fracture Toughness. **M.H. San Soucie**, M. Kimutai, J. Johnson, E. Koricho, S.M. Landge
- 871.** Hirshfeld and Void Surface Analysis in Halogen/chalcogen Bonded Crystalline Materials. **S. Alapati**, A. Peloquin, C. McMillen, **W.T. Pennington**, T.W. Hanks
- 872.** Understanding the Fluorescent Properties of Fluorescein Amide Derivatives. **R. King**, P. Lundin, K. Fogarty
- 873.** Reversible Colorimetric pH Sensors. **E. Callis**, **T.W. Hanks**
- 874.** Design and Antibiotic Activity of Novel Hair-pin Peptides. C. Rose, **I. Becerra**, **E. Roller**, **A. Dillora**, **S.E. Collins**, **B. Jackson**, J.M. Meyers
- 875.** Introduction of Mindful Doodling into Chemistry Courses at Georgia Gwinnett College to help Reduce Stress and Improve Student Confidence in their Ability to Draw Chemical Images. **M.S. Morton**
- 876. Withdrawn.** Development and Optimization of microPADs for Iron Detection. **B. Kokes**, **A. Holmes**, M.E. Howard

## FRIDAY EVENING

Birmingham Jefferson Convention Center  
East Ballroom B

### Plenary

A. E. Gorden, *Presiding*

**5:15 877.** From N-heterocyclic Carbenes to Dithiolene-based radicals: Recent Developments in Main Group Chemistry. **G.H. Robinson**

McWane Science Center

### Student Chemistry Chapter Activities During Covid19 Poster Session at the McWane

Financially supported by UAB Department of Chemistry, UAB Educational Foundation, and Refresco

J. M. Meyers, J. A. Nikles, *Organizers*

### 7:00 - 9:00

**878.** Erskine Chapter of the ACS: Adapting During Uncertainty. **M. Clothier**

**879.** TNTech Student Chapter Activities During COVID-19. **C.E. LaPointe**, R.A. Firth, A.J. Carroll

**880.** Mississippi College student ACS chapter: Promoting chemistry during the pandemic. **L. Sisson**, **M. Stewart**, **B. Steen**, L.T. Ashley, E. Tullos, C. Stokes, T.D. Selby

**881.** Successes of the SMACS Chapter at Valdosta State University. **D.B. McKay**, K. Patel, L. De La Garza

**882.** Delivering Virtual Programming to Effectively Sustain Chapter Camaraderie and Educational Outreach During a Pandemic. **L. Jaskowski**, R. Adams, S. Hubbard, J.A. Nikles

**883.** Student ACS Chapter Activities During the COVID-19 Pandemic. **B. Robertson**

McWane Science Center

## **Undergraduate Research 1**

### **Undergraduate Research at the McWane Center**

Financially supported by UAB Department of Chemistry, UAB Educational Foundation, and Refresco

J. M. Meyers, J. A. Nikles, *Organizers*

**7:00pm 884.** Modeling and Investigating the Molecular Basis of Tay-Sachs Disease. **M. Denish**, K.M. Matera, T. Laakko Train

**885.** Developing an Alternative Diagnostic tool for Eosinophilic Esophagitis by Quantification of Modified Tyrosines in Urine Samples. **J. Germany**, M. Thomas, M. Gilliland

**886.** Physical Paper Modification for Detection of Antiretrovirals via Paper Spray Ionization Mass Spectrometry. **N. Cheyne**, M. Gilliland

**887.** Chemically Patterned Paper Substrates for Paper Spray Mass Spectrometry. **A. Arias**, M. Gilliland

**888.** Structural Expansion of a Novel Antibiotic Adjuvant Scaffold to Improve Aqueous Solubility and Biological Activity. **S. Gregory**, A. King, M.S. Blackledge

**889.** Method Developmental of High-throughput, Sensitive, Colorimetric Assay for Methanethiol Detection. **Z. Adamson**, C. Miller, M. Culpepper

**890.** Presumptive Forensic Test kit Differentiating Hemp and Marijuana. **C.E. LaPointe**, J.O. Boles



**891.** Chemical Investigations of Organics in the Chattahoochee River. **H. Carlisle**, K. Goodwin, E. Klar, K.S. Taylor

**892.** Optimizing Growth Conditions for the Recombinant Expression of P450 27A1. **J. Bartholomew-Schoch**, M. Reddish

**893.** Allosteric Inhibition of Cytochrome P450 27A1: A Potential Means for the Creation of Novel Cancer Therapies. **N.L. Arnold**, E. Harris, L. Snider, M. Reddish

**894.** Microfluidics-based Approach to PCDA Liposome Synthesis. **A. Chadwick**, T.W. Hanks

**895.** Exploring the Relationship Between a Student's STEM Professional Identity and their Perception of an Organic Laboratory Experience. M.L. Head, **D. Dayani**, **A. Alkawam**, **E. Pearman**

**896.** Naphthalimide-triazole Hybrid pH-sensitive Fluorescent Probe. **A. Powell**, R. Osbourn, D. McCall, E.A. Adogla

**897.** Ruthenium-catalyzed Microwave Oxidation of Benzyl Silyl Ethers and Analogues. **R. Peterson**, K. Darrigrand, K. Poythress, A. Cameron, B.C. Goess, S.K. Goforth

**898.** Iron Geochemistry at Glendale Shoals. **C. Hatchell**, **M. Santos**, C. Romanek, G. Lewis, G.E. Schwartz

**899.** The Impact of Iron Geochemistry on Carbon Degradation at Glendale Shoals. **M. Santos**, **C. Hatchell**, C. Romanek, G. Lewis, G.E. Schwartz

**900.** Synthetic Methods of 4,6- or 4,8-Disubstituted-quinoline-3-methylcarboxylates Inhibitors for HIV-1 Integrase (IN) Enzyme. **C. Glenn**, L.P. Dinh, L. Yet

**901.** Towards Transdermal Delivery of Thioridazine Double Salt Ionic Liquid Drugs. **C.E. Rust**, O. Cojocar

**902.** Spectroscopic, Elemental, and Surface Characterizations of Biochar made from Pine Biomass and Co-pyrolyzed with High-density Polyethylene. **L.D. Moore**, **J. Lennox**, A. Saha, N. Takas, P. Bhoi

**903.** Computational and Spectroscopic Studies of Nitrogen-containing Multipole-bound Anions. **N. Kruse**, N. Hammer

**904.** Infrared Reflection Spectroscopic Studies of UV-ozone Cleaning of Substrates for Self-assembly. **L.B. Spurgeon**, M. Milosevic, B.W. Gregory

**905.** Kinetic Characterization of GAPDH from Infectious Microorganisms. **M. Hurd, G. Thrash**, K.L. Hayden, D. Chattopadhyay

**906.** Phase Control in Cu<sub>2-x</sub>Se Nanoparticles Through Tailored Selenium Reactivity Across Ligand Groups. **J. Macdonald, E.A. Ho**, A.R. Peng

## **SATURDAY MORNING**

Birmingham Jefferson Convention Center  
East Meeting Room G

### **Analytical Chemistry**

#### **Advanced materials and Surfaces for Analytical Chemistry**

A. Ghosh, *Presiding*

**8:00** Introduction .

**8:10 907.** Developed Ag@PANI/MWCNTs/MXene Nanocomposite as a High-performance Electrochemical Sensor for Simultaneous Determination of L-arginine and L-cysteine in Real Samples. **M. Mehmandust**, N. Erk

**8:30 908.** Transparent Ultramicroelectrodes for Studying Interfacial Charge Transfer Kinetics of Photoelectrochemical Water Oxidation at TiO<sub>2</sub> Nanorods with Scanning Electrochemical Microscopy. **X. Li**, S. Pan

**8:50 909.** Indirect Surface-Enhanced Raman Spectroscopic-Based Detection of Hormone Biomarkers Associated with Polycystic Ovarian Syndrome. **A. Wood**, I. Dancer, B. Sharma

**9:10 910.** Size Exclusion Chromatography: An Indispensable Tool for the Isolation of Monodisperse Gold Nanomolecules.. **S. Eswaramoorthy**, N. Sakthivel, V. Jupally, K.H. Wijesinghe, P. Nimmala, C. Kumara, M. Rambukwella, T.C. Jones, A. Antonysamy

**9:30** Intermission.

**9:45 911.** Raman Spectroscopic Detection of Biosignatures in an Extraterrestrial Context. **G. Sarabia**, B. Sharma

**10:05 912.** Magnetic Fe<sub>3</sub>O<sub>4</sub> Biochar Hybrid for Methylene Blue Removal: Effect of Porous Structure and Surface Chemistry. **S.N. Nawalage**, H. Samaraweera, T. Mlsna

**10:25 913.** Comparison of One-dimensional Plasmonic Gold Nanostructures for Colorimetric Sensing. **G. Chen**, B. Sharma, T. Egan

**10:45 914.** Investigation of Hydrogen Diffusion in High Hardness Steels. **R.F. Awoyemi**, W. Williams, H. Rhee, D. Wipf

Birmingham Jefferson Convention Center  
East Meeting Room O

## **Biochemistry**

### **General Session Biochemistry 1**

J. Zhang, *Presiding*

**8:00** Introduction .

**8:05 915.** Next Generation Disinfectants to Combat Resistance in the Post-COVID Era. K. Sommers, **M.E. Michaud**, C. Hogue, A. Scharnow, S.J. Post, R.A. Allen, K. Morrison, L. Amoo, A. Petersen, R.G. Carden, W.M. Wuest, K.P. Minbiole

**8:25 916.**

Combating Antibiotic Resistance in Septic Infections with Choline Carboxylic Acid-Based Ionic Liquids. **C. Chism**, E.E. Tanner, G.S. Dasanayake

**8:45 917. Withdrawn.** Biophysical Characterization of Orthogonal Conjugated Polymer Catalysis by Mutagenic Variants of T4 Lysozyme. **W.D. Turner**, T. Leeper

**9:05 918.** Utilizing Multi-scale Simulation to Reveal Mechanisms of Molecular Motors' Motility. **L. Li**

**9:25** Intermission.

**9:40 919.** Experimental Predictions of Ribosomal Evolution. **J.W. Haynes**, K.A. Lanier, A. Petrov, L.D. Williams

**10:00 920.** Analyzing Interactions of Thermoresponsive Coacervate-forming biodegradable polyesters on protein structure and activity Utilizing Fluorescence and Nuclear Magnetic Resonance. **C. Casterline**, T. Leeper

**10:20 921.** Confirmed and Quantified *in vitro* glycosylation of Membrane Proteins. **G. Cook**

**10:40 922.** Biochemical and Therapeutic Actions of Cathepsin L (CatL) Inhibitors against Hepatocellular Carcinoma. **C. Olamide**, I.V. Ogungbe, F.K. Noubissi

**11:00 923.** Biochemical Characterization of the Radical SAM Methylase Involved in Tetrahydromethanopterin Biosynthesis. **J. McKinney**, T. Tunckanat, K. Allen

**11:20 924.** Hydrophobic Surface Patch Disruption to Produce Water-Soluble G-Protein Coupled Receptor Analogs. **C. Dyer**, A.L. Parrill-Baker, D.L. Baker

**11:40 925. Withdrawn.** Comparison of the Structure and Activity of *Pseudomonas aeruginosa* Proteins, Inhibitors of Vertebrate Lysozyme Classes I and II. **K. Letsinger**, T. Leeper

Birmingham Jefferson Convention Center  
East Meeting Room K

## **Chemical Education Oral Presentations 1**

J. March, *Organizer*

**8:00** Introduction .

**8:10 926.** Teaching Design of Experiments for Method Development in Analytical Chemistry. **R. Thompson**, R. Saylor

**8:30 927.** Supporting the Motivation of Engineering Students with Design Challenges in General Chemistry Laboratory. **M. Korolev**, K. Crippen, L. Imperial, C. Payne, B. Phil, C. Wu

**8:50 928.** Upper-level Survey Course on Nanoscience for Chemistry Majors. **P. Lundin**, B. Augustine

**9:10** Intermission.

**9:30 929.** Bridging Workforce Development to General Chemistry: Results from a Multi-Year Career Shadowing Program. **J.M. Carr**

**9:50 930.** A New Course to Increase the Success of Students in the First Semester of General Chemistry. **S.C. Blackstock**

**10:10** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room B

### **Engineering Solutions for Social Challenges: Renewable Materials and Resources 1**

Financially supported by **Center for Sustainable Nanotechnology - UW Madison, and Surface Measurement Systems**

M. L. Curry, L. A. Lucia, M. S. Peresin, *Presiding*

**8:00** Introductory Remarks.

**8:10 931.** Lignin Thermochemistry for Advanced Composite Materials. **C.E. Frazier**, S. Yazdi, L. Fang

**8:55 932.** On the Road to Developing Sustainable Alternative Materials for Long-lasting Insecticide Nets: Cellulose-based Insecticidal Fiber Yarn for Malaria Control. **S. Brake**, D. G&oacute;mez Maldonado, M.S. Peresin, S. Zohdy

**9:25 933.** Facile Preparation of Hydrophobic Papers Through Metal-ion-induced Modification of Conventional Hydrophilic Papers. **O.N. Rathnayaka Mudiyanse**lage, X. Zhang

**9:55** Intermission.

**10:15 934.** Geologic Carbon Dioxide Storage Through Pyroxene Mineral Carbonation. **B. Aguila**

**10:45 935.** Fabrication and Thermal and Mechanical Characterizations of Cellulose-based UHP-Ionene Composites. **J. Mitchell**, K.E. O'Harra, J.E. Bara, M.L. Curry

**11:15 936.** Using Cyclodextrin Grafted Chitosan as Coating of Delignified Wood Aerogels for the Removal of Microcystin-LR. **D. Gomez Maldonado**, A. Reynolds, R.J. Babu, D.J. Burnett, M.N. Waters, M.S. Peresin

Birmingham Jefferson Convention Center  
East Meeting Room J

## **Inorganic**

### **General Session Inorganic 1 - Ligands and Metals in Catalysis**

J. E. Ritchie, *Presiding*

**8:00** Introduction .

**8:05 937.** Tuning Hydrosilylation and Dehydrogenative Silylation Upon the Choice of Metal Center: Rh and Ir Silylphosphine Catalysts. **N.S. Abeynayake**, V. Montiel-Palma

**8:20 938.** Redox-Active Heterobimetallic Catalysts for Polymerization of Polyolefins. **N. Taylor**

**8:35 939.** Enhanced Reactivity for C-H Bond Functionalization Using a Dinuclear Iron(III) Oxo-Bridged Catalyst and Hydrogen Peroxide. **Z. Turner**, J.W. Jurss

**8:50 940.** Modular Bimetallic Main Group Catalysts for Cooperative Polymerization of Lactones. **R.J. Comito**, Z. Gu, M. Tansky

**9:05 941.** Synthesis and Characterization of the Complete Series of Chlorine Substituted Cobalt Acetylacetonate Complexes—[Co(acac)<sub>x</sub>(acac-Cl)<sub>3-x</sub>], x = 0-3. **R.E. Bachman**, E.E. Joslin, E. Amason, M.H. Jones, C. Keuk, G. Ferrence

**9:25 942.** Synthesis of Zwitterionic-Alkenylammonio and Alkenylphosphonio Ligands in Dirhenium Carbonyl Complexes.. R.D. Adams, **M. Kaushal**

**9:40** Intermission.

**10:00 943.** Ligand Aromatization/dearomatization in Pyridine and Pyrazine Diimine Complexes. **J.R. Billups**, S. Creutz

**10:15 944.** Effect of Donor Groups on Ruthenium CNC pincer Complex for Reduction of Carbon dioxide. **D. Nugegoda**, S. Das, F. Qu, C.M. Boudreaux, P. Burrow, M.T. Figgins, R. Lamb, C.E. Webster, J.H. Delcamp, E.T. Papish

**10:30 945.** Evaluating Photochemical C–H Bond Activation by Introducing Electronegative Substituents to W(VI) Dioxo Complexes. **S.M. Siddhiaratchi**, F. Fronczek, M.B. Chambers

**10:45 946.** Remote Directing Group for Para C-H Functionalization of Aromatic Aldehydes. **A. Mercado**, T. Ricks, N. Taylor, E. Vilorio, T. Brewster

**11:00 947.** Asymmetric Ligand Design for Increased Volatility of Spin-crossover Complexes. **M. Gakiya-Teruya**, X. Jiang, A. Hebard, D. Le, T.S. Rahman, M. Shatruk

**11:15 948.** De Novo Designed Cu Peptides for Abiotic C-H bond Functionalization and Small Molecule Activation. **D. Prakash**, S. Mitra, P. Prasad, S. Chakraborty

Birmingham Jefferson Convention Center  
East Ballroom B

## **Machine Learning in Computational Chemistry**

S. Irle, *Presiding*

**8:00** Introduction.

**8:10 949.** Machine Learning for Intermolecular Interactions. **C.D. Sherrill**

**8:40 950.** Genetic Algorithms for Inorganic Oxides. **E. Valencia**, R.C. Fortenberry

**9:00 951.** Reducing Uncertainty in Quantum Chemistry Discovery with Machine Learning. **F. Liu**

**9:20** Intermission.

**9:40 952.** Recent Developments in CLIFF: A Component-based, Machine-learned, Intermolecular Force Field. **J.B. Schriber**, D. Nascimento, A. Koutsoukas, S. Spronk, D.L. Cheney, C.D. Sherrill

**10:10 953.** Data-driven Acceleration of Quantum Chemical Methods. **K.D. Vogiatzis**

**10:40 954.** Making use of Small Data in Machine-learned Binding Free Energy Prediction. **D. Metcalf**, Z. Glick, C.D. Sherrill

**11:10 955.** Deep Predictive Visual Proteomics. **D. Bhowmik**

**11:30** Panel Discussion.

Birmingham Jefferson Convention Center  
East Meeting Room A

## **Nanomaterials 1**

S. Street, *Presiding*

**8:00** Introduction .

**8:10 956.** Inorganic Nanoscale Unnatural Product Synthesis. C.G. Sharp, S. Sarkar, E.H. Robinson, A. Koziel, E.A. Ho, R.B. Goldfarb, A.R. Peng, A.D. Lacroix, E.A. Hernandez-Pagan, A.Y. Nuriye, **J. Macdonald**

**8:30 957.** Lewis Acid Catalyzed Synthesis of Metal Oxide Nanocrystals via Hydroxide Transmetallation. **B.H. Farnum**, A.R. Combs Bredar, N.J. Gibson, N. Chakraborty

**8:50 958.** Metal Ion Doping in Lead Halide Perovskites for Efficient Blue and White LEDs. **M. Gangishetty**



**9:10 959.** Langmuir Methods to Cast Uniform Films of Nanoparticles. **J.J. Weimer**, C.V. Nguyen, J. Mitchell

**9:30** Intermission.

**9:50 960.** Development of Solution-Based Synthetic Routes to Ternary Group 4-Containing Sulfides as Colloidal Nanomaterials. **S. Creutz**, D. Zilevu, N.E. Ingram, O. Parks, B. Jordan

**10:10 961.** High Temperature Synthesis of x-ray Luminescent Nanomaterials for Biomedical Applications. **E. Zhang**, A. Dickey, H.W. Jones, I. Foulger, I. Bandera, J.W. Kolis, S.H. Foulger

**10:30 962.** Intermediate Shell Formation and Anion Sublattice Rearrangement in the Cation Exchange from  $\pi$ -SnS to Cu<sub>1.8</sub>S. **C.G. Sharp**, S. Sarkar, J. Macdonald

**10:50 963.** Synthesis and Characterization of Iron Complex-based Nanoparticles. **M. Hawkins**, Y. Bao

**11:10 964.** Chemical Ordering in Dimetallic Nanoparticles. **S. Street**, F. Acquaye, R. Mahat

Birmingham Jefferson Convention Center  
East Meeting Room E

## **Organic**

### **Natural Products/Biological Applications of Organic Synthesis/Heterocycles**

L. Yet, *Organizer*

**8:00** Introduction .

**8:05 965.** Biomimetic Cyclizations in Pursuit of Marine Natural Products. **E. Jones**, D. Lutin, S.A. France

**8:20 966.** Stereoselective Synthesis of Protected  $\beta$ -OH Dab Isomers for Natural Product Synthesis. **M. Dekarske**, W. Zhang, W.M. Wuest

**8:35 967.** Cyclic Thiosulfonates as Anticancer Agents: Structure-reactivity and Structure-activity Relationships. **A. Franceschini Ghilardi**, E. Yaaghubi, R. Ferreira, M.E. Law, M. Wang, B.J. Davis, Y. Yang, I. Ghiviriga, A.E. Roitberg, B.K. Law, R.K. Castellano

**8:50 968.** Semi-Synthesis of (5Z)-7-Oxozeaenol/Hypothemycin Analogues from Kinase Inhibition Towards Cancer Treatment. **T. Li**, M.P. Croatt, A. Ustoyev, P.M. West

**9:05 969. Withdrawn.** Design and Synthesis of New Modulators for the Downregulation of Liver Receptor Homolog-1. **R. Spurlin**, M.L. Cato, J. Cornelison, N. Jui, E. Ortlund

**9:20 970.** Targeting the Sphingosine-1-phosphate Transporter SPNS2 for the Treatment of Multiple Sclerosis. **D. Foster**, W.L. Santos, K. Lynch, R. Fritzemeier

**9:35 971.** Design and Synthesis of Taurine Conjugates as Potential Anticancer Agents. **K. Wyman**, S.S. Panda

**9:50** Intermission.

**10:05 972.** Pyochelin Biosynthetic Metabolites Bind Iron and Promote Growth in Pseudomonads Demonstrating Siderophore-like Activity. **A. Kaplan**, J. Musaev, W. Wuest

**10:20 973.** Synthesis of Empetroxepin Derivatives and Bis-Nitrogenous Adjuvants and Subsequent Investigations into Biological Activity. **K. Murphy**

**10:35 974.** Development of Novel Fluorinated Amino Ester Prodrugs to Improve Detection of Brain Tumors. **D.A. Devalankar**, N. Yasui, U. Akca, A. Hjelmeland, J.E. McConathy

**10:50 975.** Fe(III)-Catalyzed Amidomethylative Nucleophile-free Tandem Reactions: Formal Substitution of Multiple C–H Bonds for Building Complexity of Styrenes. **X. Qian**, H. Zhou, C. Hetti Handi, J. Lucore, X. Cui

**11:05 976.** Synthesis of Achiral and Chiral CCC-NHC Pincer Complex and its Application in C-H Functionalization of Indoles. **M. Rawat**

**11:20 977.** Friedel–Crafts Additions of N-alkylated Indoles to Nitrones to Form 1:1 Products. **C.W. Downey**

**11:35 978.** Total Synthesis of the Reported Structure of Cahuitamycin A and Isomers. J.A. Shapiro, **S. Post**, M.E. Michaud, G. Smith, W.M. Wuest

**11:50 979.** Electrophile-Initiated Cyclization of Chiral, Non-Racemic Homoallylic *N*-tert-butanefulfonamide Carbamates and Bis-Boc/Cbz Protected Guanidines. **G.J. Rustin**, M. Donahue

Birmingham Jefferson Convention Center  
East Meeting Room I

## Physical Chemistry

### General Session Physical Chemistry 1

M. G. Bakker, *Presiding*

**8:00** Introduction .

**8:05 980.** Long-lived Ag<sub>10</sub><sup>6+</sup> Luminescence and a Split DNA Scaffold. **D. Lewis**, S. Carnahan, D. Kim, J.T. Petty

**8:25 981.** Infrared Studies of the Effect of Hofmeister Ions on Model Drugs. **S.I. Busch**, G. Macdonald, Y. Zhang

**8:45 982.** EPR Spectroscopy to Probe the Incorporation of Phthalocyanines into Hierarchically Porous Carbon. M. Lockhart, R. Adhikari, **M.G. Bakker**, M.K. Bowman, K.H. Shaughnessy

**9:05 983.** Effect of Solvent, Time, and Mixing Speed on Self-Assembly of Thiols on Iron Microparticles for Improving the Colloidal Stability of Magnetorheological Fluids. **S. Thiagarajan**, A. Koh

**9:25 984. Withdrawn.** Investigation of Chemistry at Ice-Mineral Interfaces of Phosphorus-Containing Meteorite Analogues. **K.F. Meyberg**, H.L. Abbott-Lyon

**9:45 985.** Spectroscopic Investigation of Novel 3,4-ethylenedioxythiophene (EDOT) Derivatives and their Potential Aggregate Induced Emitter Behaviors. **A. Dorris**, N. Sparks, I. Chandasiri, D.L. Watkins, N. Hammer

**10:05** Intermission.

**10:20 986.** Quantifying Emission of NIR-I and NIR-II dyes via Fluorescence Quantum Yield. **C. Smith**, D. Ndaleh, J.H. Delcamp, N. Hammer

**10:40 987.** Advances in CaLevIR: Observations of Droplet Heat Transfer via a High-Speed Thermographic Camera. **H. McCardle**, K. Everitt, K. Abbuhl, E.R. Duranty

**11:00 988.** Upconversion and Quantum Yield Studies of PdOEP-DPA System in the sPS/THF Polymer Gel. **A. Shaik**, B. Davis, Y.C. Simon, N. Hammer

**11:20 989.** Using 2D Spectroscopy to Explore Excited State Dynamics in Ruthenium Complexes. **M.A. Hermosilla-Palacios**, S.E. Dominguez, B. Aramburu-Trošelj, V.D. Kleiman, L. Baraldo-Victorica

**11:40 990.** Understanding the Microenvironment of Ionic Liquids. **S. Dutta**

Birmingham Jefferson Convention Center  
East Meeting Room C

## **Polymer Materials Science and Engineering**

### **General Session Polymer Materials 1 - Polymeric materials and composites**

D. Dean, *Presiding*

**8:00** Introduction .

**8:00 991.** Withdrawn.

**8:15 992.** Evaluation of the Dielectric Properties of Radar Absorbing Materials. **D. Wedgeworth**

**8:30 993.** Photomechanical Response from a Stilbene Polymer via Triplet Sensitization. **D. Beery**, E. Stanislauskis, G. McLeod, A. Das, W. Oates, K. Hanson

**8:45 994.** Covalent Anthracene Incorporation into Hydrogel Encapsulated Crystalline Colloidal Arrays for Radioluminescent Properties. **S. Mell**, H.W. Jones, I. Bandera, S.H. Foulger

**9:00 995.** Upcycling of Single-Use Polyethylene into High Strength Materials via Reactive Compounding. **A. Ghosh**, A.C. Kannan

**9:15** Intermission.

**9:25 996.** Synthesis of Alicyclic Polyesters: Examination of the Effect of Regioisomer Ratios on Physical Properties. **T.N. Thompson**

**9:40 997.** Semi-fluorinated Arylene Vinylene Ether (FAVE) Telechelic Polymers from Polycyclic Aromatic Hydrocarbon Bisphenols and Trifluorovinyl Aryl Ethers. **K.M. Mukeba**, B. Farajidizaji, K. Shelar, C.U. Pittman, D.W. Smith

**9:55 998.** Pretreatment of Asphaltene for Carbon Fiber Development. **J. Hinkle**, N. Alizadeh, A. Bansode, A. Bass, J. Thornhill, N. Tram, F. Leiva, E. Triggs, R. Farag, M.L. Auad

**10:10 999.** Isosorbide-based Semifluorinated Polymers. *Where Green meets Mean..* **K. Shelar**, K. Mills, K.M. Mukeba, D.W. Smith

**10:25 1000.** Dynamic Mechanical and Mechanical Analysis of Ionic Liquid Regenerated Cellulose Aerogels Loaded with Hexagonal-Boron Nitride (h-BN). M. Arafat, B.L. Sadiku, **S. Chakraborty**

Birmingham Jefferson Convention Center  
East Meeting Room F

## **Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging**

M. Henary, *Presiding*

Financially supported by Molecules, De Gruyter

**8:00** Introductory Remarks.

**8:10 1001.** Illuminating Biological Copper with Synthetic Fluorescent Probes. **C.J. Fahrni**

**8:40 1002.** Imaging and Tracking mRNA in Live Mammalian Cells via Fluorogenic Photoaffinity Labeling. **J.M. Heemstra**

**9:10 1003.** Bifunctionality of Neodymium (III) Complexes as Luminescent and Single Molecule Magnets (SMMs). R. Vincente, A. Tubau, S. Speed, F. Mautner, F. Bierbaumer, R. Fischer, **S.S. Massoud**

**9:40** Intermission.

**9:50 1004.** Fluorescent Detection of Protein Lysine Acetyltransferase Activities. **Y. Zheng**

**10:20 1005.** Fluorescence and Electroluminescence Spectroelectrochemistry Studies of Perovskite Quantum Dots. **S. Pan**, J. Yadav

**10:50 1006.** Synthesis and Applications of Near-Infrared Fluorescence Probes Based on Cyanine Dyes. **M. Henary**, **H. Choi**

**11:20** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room D

## **Project SEED**

A. Mallia, D. Masterson, *Presiding*

**8:30** Introductory Remarks.

**8:35 1007.** History, Progress, and Outlook of the Project SEED Program. **B.W. Boudouris**

**9:00 1008.** Implementation of Project SEED in a small two-year college. **J.W. Hartman**

**9:25 1009. Withdrawn.** A Divergent and Persistent Approach to Educating Economically Advantaged Students. **C. Tang**

**9:50 1010.** How to Leverage Science Competitions with Project SEED Students and Funding Opportunities. **D.S. Masterson**

**10:15 1011.** Assessing the ACS Project SEED Virtual Summer Camp for High School Students: Can a Virtual Program Increase STEM Identity, Professional Identity, and College Preparation?. **L.S. Nadelson**, R.C. Jamison, E. Soto, D.L. Warner

**10:45** Panel Discussion.

**11:45** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## **Undergraduate Research 1**

### **Poster Session**

J. A. Nikles, *Organizer*

**10:00 - 12:00**

**1012.** Characterization of Dewatered Nanocellulose for Commercial Application. **E. Pearson**, M.C. Iglesias, T. Ciaramitaro, A. Alawode, I. Vega Erramuspe, B. Via, M.S. Peresin

**1013.** Dynamic Patterns of Particle Size Distribution of Nonliving Natural Organic Matter. **K.E. Slamen**, K.N. Mealio, H.A. Stretz, M.J. Wells

**1014.** Synthesis and Computational Study of Semi-fluorinated Polyaryl Ethers via Friedel-Crafts Polymerization of Aromatic Hexafluoropropanol Derivatives. **K.M. Chamberlain**, G. Munoz, S. Athukorale, C.U. Pittman, C.E. Webster, D.W. Smith

**1015.** Metal Thiolate N-heterocyclic Carbenes for the Reductive coupling of Carbon Monoxide. **C. Carpenter**, N. Dodd, J.P. Sadighi

**1016.** Does the Environment Around the Carotenoid Change its Oxidation Potential and Thus its Scavenging Ability?. **D. Fountain**, A.L. Focsan

**1017.** LC-MS Identification of Serum Proteins Adsorbed onto Ionic Liquid-Coated Nanoparticles. **A.M. Hoang**, E.E. Tanner

- 1018.** Analysis of Different Types of Alcohol using gas Chromatography. **A.C. Gaquere, A. Cormier,** A. Watson
- 1019.** Theoretical Studies of Benzoquinone Reactivity in Acidic and Basic Environments. **N. Majoras**
- 1020.** Role of the Cation in Ionic Liquid-Facilitated Transdermal Transport. **A.N. Hunter,** E.E. Tanner
- 1021.** Synthesis of Nano Carbon Microspheres (nCMS) from Natural Materials for the Removal of Water Pollutants. **E. Banks,** M.M. Moyer
- 1022.** Forensic Odontology: Cleaning Chemicals on Molar Remnants Using Infrared Spectroscopy. **A.E. Kelly,** J. McCutcheon
- 1023.** Antioxidant Properties of a Zinc Complex With a Macrocyclic Redox-active Ligand. **A. Jordan,** S. Karbalaei, C.R. Goldsmith
- 1024.** Improved LC-MS Methodology for Determination of Endocrine-disrupting Chemicals (EDCs) in Southwest Florida Waterways. **M. Sciancalepore,** D. Paull, N. Demers
- 1025.** Designer Ionic Liquids for in situ Red Blood Cell Hitchhiking. **J. Randall,** C. Hamadani, E.E. Tanner
- 1026. Withdrawn.** Diffusion of Nanoparticles in Mucus for Nasal Drug Delivery. **J. Marzette,** E.E. Tanner
- 1027.** Incorporating a Collagen Analog and a Bioengineered Protein into Modern Wound Dressings. **J. Spiva,** S.K. Hamilton
- 1028.** Towards the Study of Flow and Mass Transport of Species in a Two-phase Flow Inside a Microreactor using Computational Fluid Dynamics. **O. Ayeni**
- 1029. Withdrawn.** New Electron Donor-acceptor (DA) Complexes of Pyridine-N-oxides Donors with Electron Poor Olefin Acceptors. **C. Fricken,** S.C. Blackstock
- 1030.** Regioselective Asymmetric Akynylation and Arylation of Pyridiniums. **A. Subhit,** T.A. Grigolo
- 1031.** Optimizing Rhodamine B Encapsulation in ZIF-8 Metal Organic Frameworks. **E. Stravolo**



**1032.** Computational Studies of Properties of 10,11-Diphenylcyclobuta[5,6]pyrazino[2,3-f][1,10]phenanthroline. **J. Powell**, R. Saadein, S. Nkomo

**1033.** Europium-based Nanoparticles Functionalized with Melanocortin Stimulating Hormone-4 peptide for Potential Cellular Imaging. **M. Rathbone**, M. Fratacangeli, C.R. De Silva

**1034.** Exploring Hydrogen Fuel Production using a Ruthenium-platinum Complex. **F.C. Wilson**, G.B. Ray

**1035.** Phytoremediation of Copper and Iron by Water Hyacinth (*Eichhornia crassipes*) and American Water Willow (*Justicia americana*). **R. Moore**, M. Hage, S. Nkomo

**1036.** Self-assembly, Gelation, and Spectroscopic Studies of 4-hydroxy-1-anthraquinonylalkanamides. **B. Dang**, J. Ivbaze, A. Mallia

**1037.** Synthesis, Characterization, and Spectroscopic Studies of Acridinyl and Quinolinylnyl Derivatives of Aminobenzenesulfonamides. **K. Figueroa**, N.Y. Forlemu, A. Mallia

**1038.** Modeling, Characterization and Analysis of Human WNT1-inducible-signalling pathway and Netrin receptor protein. **N. Luthcke**, G. Calderon, K. Edwards, K. Kasetty, S. Stoddard, K. Whalum, S. Stoddard

**1039.** Derivatives of 1,2,3-triazoles as Potential Drug Candidates. **G.S. Blount**, V.S. Smith, R. Dodson, A. Henderson, N. Nkengbeza, A. Stewart, J. Kocerha, R.R. Ramoutar, K.S. Aiken

**1040.** Characterization of a Novel Model for Rotational Acceleration-induced Traumatic Brain Injury. **R. Adams**, A. Umfress, J. Bibb

**1041.** Simulating the Two-dimensional Electronic Spectra of Organic dyes with vibronic coupling and internal solvation dynamics. **V.A. Suarez**, M.A. Hermosilla-Palacios, V.D. Kleiman

**1042.** Spectroscopic and Electrochemical Characterization of Iron(III) Oxide Electrodes for Photoelectrochemical Cells. **D.B. McKay**, L. De La Garza

**1043.** Gold Nanoparticle Immobilization for Photodynamic Therapy in Cancer Cells. **S. Crowder**

- 1044.** Synthetic Pathway Toward Generation of  $\alpha$ -ketoalkynes. **J. Gonzalez, B.D. Feske**
- 1045.** Novel Analogs of Sildenafil to Prevent Colorectal Cancer.. **C. Miller, M. Williams, D. Lyons, H. Ramos, I. Lebedyeva**
- 1046.** Development of Sildenafil Analogs as Selective PDE5 Inhibitors.. **H. Ramos, D. Lyons, C. Miller, M. Williams, I. Lebedyeva**
- 1047.** Photocatalytic Degradation of Imidazolium Based Room Temperature Ionic Liquids. **A. Parris, M. Moscatelli, T.R. Hayden**
- 1048.** Designing an undergraduate forensic chemistry experiment on the levels of amphetamine in urine using two different methods. **M. Teigen, M. Popkin, W. Medawala**
- 1049.** Developing a Synthetic Strategy Toward  $\beta$ -ketoalkynes. **K. Glorioso, R. Francis, B.D. Feske**
- 1050. Withdrawn.** Computational contributions to the design of new metal-organic framework materials (MOFs) with improved opto-electronic properties. **C. Crawford, D.A. Clabo**
- 1051. Withdrawn.** Computational Investigations of the Stereoselective Reduction of Dicarboxyls with Borohydride. **J. Butler, D.A. Clabo**
- 1052.** Supported Ionic Liquid Strategy for Emergent Liquid Asthma Medications. **D.M. Cotter, O.A. Cojocar**
- 1053.** Hydrogen Production Using Nickel Complexes with Substituted Thiosalen Ligands. **A. Hemphill, J.m. Briant, N.T. Hames, W.T. Eckenhoff**
- 1054.** Investigation of Group 6 M(III) Complexes with Diimine Ligands for Solvatochromism. **M.A. Davis, E.E. Dove, S.D. Helland, W.T. Eckenhoff**
- 1055.** Investigation of  $\text{Ni}(\text{EtImPDI})^{2+}$  as a Catalyst for Light-driven Hydrogen Production. **R.G. Musicante, L.M. Rhodes, W.T. Eckenhoff**
- 1056.** Nickel Complex with Pyridinediimine Ligands Bearing Pendant Base for Light-Driven Hydrogen Production. **S.A. Wicker, M. Kiker, W.T. Eckenhoff**

**1057.** Progress toward the Synthesis of Antibacterial Aomounds to Avoid efflux-mediated resistance in Gram-negative bacteria. **G. Krisanic**, J.D. Greenberg, E.J. Chow, E.A. Fontana, L.W. Peterson

**1058.** Using Extended DLVO Theory to Characterize Primary Colonization of Bacteria. **N. Pathak**, T.B. Cavitt

**1059. Withdrawn.** Fluorinated molecularly imprinted polymer: monomer and polymer synthesis for PFOA sorption. S.M. Durbin, A.M. Loucks, J.C. Meyer, **S.T. Hobson**

**1060.** Optimization of Synthesis of 3, 4-dihydroxycinnamic acid Analogues to Test Dioxygenase Activity. **J. Steiner**, G. Xhafkollari, R. Marasco, M. Betonio, K.L. Colabroy, L.W. Peterson

**1061.** Screening quaternary ammonium and phosphonium cations as precursors for juglone ionic derivatives. **R. Paris**, O.A. Cojocaru, T.W. Majors

**1062. Withdrawn.** Effect of dietary supplements and flavonoids of N-methyl-N-nitrosourea mediated methylation of guanine. M. McCoy, C.H. Rippey, L.B. Autrey, **S.T. Hobson**

**1063.** Use of a full-color 3D printer to create chemical objects for research and teaching. **K. Floyd**, D.A. Clabo

**1064.** Reaction Mechanism of *Streptomyces sclerotialis* *L-DOPA* dioxygenase with Varied Substrates. **K. Klugh**, P. Jones, D. Muxue, L.W. Peterson, K. Colabroy

**1065.** 3,6-dimethoxyxanthone from 2,2',4,4'- tetrahydroxy-benzophenone via Microwave-Assisted Annulation. R.E. Lee, **F.R. Rosario**, **S.E. Knisely**, **S.F. Gebeyehu**, P.E. Heiple

**1066. Withdrawn.** Uncovering Determinants of Temperature Specificity in Extremophilic Bacterial Type II Topoisomerases. **A. Schoeffler**, **T. Littleton**, **A. Byrd**

**1067.** Design and Synthesis of Fluoroquinolone Conjugates as Potential Antimicrobial Agents. **A. Rocque**, S.S. Panda

**1068.** Design and Synthesis of Potential Drug Candidates for SARS-CoV-19. **R. Dobaria**, **J. Moore**, P. Surapaneni, K. Wyman, S.S. Panda

**1069.** A Salivary Hormonal study on Individuals of African Ancestry living in Different Socioeconomic Environments, in order to Understand Etiology of Prostate Cancer. **B. Jones**, R. Cundey, E. Kaninjing, W. Medawala

**1070. Withdrawn.** Synthesis of 4-(4-nitrophenoxy)-cyclohexanone and Preliminary Spectroscopic Analysis in its Reaction Towards Nucleophiles.. **H. Walker**, P. Wiget

**1071.** Energetics of the Ligand-binding Activities of Human Serum Albumin.. **B. Robertson**, **R. Bishop**

## **SATURDAY AFTERNOON**

Birmingham Jefferson Convention Center  
East Meeting Room J

### **Inorganic**

#### **General Session - Inorganic Chemistry 2 - Materials, Electrochemistry, and Solar Energy Conversion**

J. E. Ritchie, *Presiding*

**1:00** Introduction .

**1:05 1072.** Solvent Dependent Spectroscopic and Electrochemical Studies of Nickel (II) Diethyldithiocarbamate for Energy Storage. **R. Islam**, B.H. Farnum

**1:20 1073.** 2D Magnetism: from Layered Intermetallics to Exfoliated Ultrathin Magnets. **G. Sasi Kumar**

**1:35 1074.** Physical and Electrochemical Properties of Synthetically Optimized p-type  $\text{CuCrO}_2$ . **A. Chown**, B.H. Farnum

**1:50 1075.** Fabrication and Application of Zinc Oxide Modified Cellulose Networks as Gas Separation Membranes. **A. Kinnebrew**, **C. Rhoades**, **M.L. Curry**

**2:05 1076.** Electronic Properties and Thermodynamics Investigation of Heterometallic Actinide-Based Metal–Organic Frameworks with Retrievable-Structure. **J. Yu**, N. Shustova

**2:25** Intermission.

**2:45 1077.** Improving the  $2e^-$  Reversibility of a Ni(IV/II) Redox Couple for Application in Redox Flow Battery. **M. MAZUMDER**, B.H. Farnum

**3:00 1078.** Polyimidazole Manganese Complexes for Oxidation Catalysis of Water. **G. Mu**

**3:20 1079.** Impact of Ethyl Cellulose on Defining the Structural and Electrochemical Properties of CuGaO<sub>2</sub> Mesoporous Nanocrystalline Thin Films. **H. Yeasmin**, A.R. Combs Bredar, B.H. Farnum

**3:35 1080.** Photophysics and Electronic Studies of Acceptor-Integrated Covalent-Organic Frameworks. **B. Yarbrough**, N.B. Shustova

**3:50 1081.** Nickel(II) Bis(diethyldithiocarbamate) as a Novel Redox Mediator in Dye-sensitized Solar Cells. **N. Dalpati**, B.H. Farnum

Birmingham Jefferson Convention Center  
East Meeting Room F

## **Synthesis of Fluorescent Probes and Their Applications from Sensing to Imaging**

### **2**

M. Henary, *Presiding*  
Financially supported by Molecules, De Gruyter

**1:00** Introductory Remarks.

**1:05 1082.** The Force is Within You: Fluorescent Probes to Map the Molecular Forces in Cells. **K. Salaita**, Y. Duan, Y. Hu

**1:35 1083.** Chemical Sensing through Fluorescence Modulation in Conjugated Polymers. **M. Bonizzoni**

**2:05 1084.** Excited State Proton Transfer Dye with an Emission Quantum Yield up to 60% upon  $\text{Zn}^{2+}$  Coordination. **K. Hanson**, S. Ayad, E.S. Knorr

**2:35 1085.** Characterization and Applications of Binding of Cyanine Dyes to Biomolecules. **G. Patonay**, M. Henary, P. Ali

**3:05** Intermission.

**3:25 1086.** Development of Chemical Tools to Decipher the Role of Reactive Nitrogen Species in Cancer Progression. **J. Chan**, A.K. Yadav, M.Y. Lucero, M.C. Lee, A. East, S. Su

**3:55 1087.** Characterization of the Reactivity and Optical Properties of an Amide Dimer of Rhodamine B. **P. Lundin**, **K. Fogarty**

**4:25 1088.** Tuning Asymmetric Xanthene-based Sensors via Modification of the Xanthene Moiety. **C. Stephenson**, M. Bratton, R. Brown, I. Andonie, M. Ohakwe

**4:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room E

## **Organic**

### **Organic Probes/Methodology/General**

L. Yet, *Organizer*

**1:15** Introduction .

**1:20 1089.** Highly Adaptable  $^{15}\text{N}$ -tag motif for Development of Novel Hyperpolarized Magnetic Resonance Imaging Probes. **H. Park**, G. Zhang, J. Bae, W.S. Warren, Q. Wang

**1:35 1090.** Photoacoustic Probe for biopsy-free Assessment of Copper Status in Murine Models of Wilson's disease and liver metastasis. **M. Lucero**, S. Su, J. Forzano, J. Chan

**1:50 1091.** SWIR Emissive Rosindolizine Dyes as Fluorescence Imaging Materials. **W.E. Meador**, S. Chatterjee, C. Smith, I. Chandasiri, M. Farid Zia, J. Nguyen, A. Dorris, A. Flynt, D.L. Watkins, N. Hammer, J.H. Delcamp

**2:05 1092.** Unique Reactivity of Meso-nitrile Oxide BODIPYs. **B.R. Schrage**, Y. Zatsikha, V. Nemykin

**2:20 1093.** Synthesis of Novel Xanthene Based NIR I Dyes to Develop as Biosensors. **I.N. Rajapaksha**

**2:35 1094.** Analysis of Torrefied Wood by Forrier-Transform Infra-red (FTIR) Spectroscopy, Atomic Absorbance, X-ray Diffraction, and Elemental Analysis. **G.W. Durrell**, A. Hulette, L. Richa, Y. Lin, F. Leconte, B. Colin, A. petrissans, W. Chen, M. Petrissans, R.L. Quirino

**2:50 1095. Withdrawn.** Molecularly Imprinted Polymer Based Real-time Sensor for PFOA. **S.T. Hobson**

**3:05** Intermission.

**3:25 1096.** Enantioselective Synthesis of Secondary Propargyl Amines. **K.N. Weeks**, A. Aponick

**3:40 1097.** (Diethylamino)Sulfur Trifluoride (DAST): A Versatile Reagent in Organic Synthesis. **M.A. Lnu**

**3:55 1098.** The Fascinating World of Nitrosobenzenes. **S.C. Blackstock**

**4:10 1099.** Radical Chain Reduction via Carbon Dioxide Radical Anion. **C. M Hendy**, G. Smith, Z. Xu, T. Lian, N. Jui

**4:25 1100.** Development of Sequence Defined Oligomers using Photo-SPAAC. **S. Sharma**, S. Minko, V. Popik

**4:40 1101. Withdrawn.** Ligand-Controlled Regiodivergence for Catalytic Stereoselective Semireduction of Allenes. **M. Hajiloo Shayegan**, Z. Li, X. Cui

**4:55 1102.** An Enantiomeric Excess Determination Using  $^1\text{H}$ -NMR of Isotope Labeled Substrates. **T.A. Owens**, D.S. Masterson

Birmingham Jefferson Convention Center  
East Meeting Room G

## **Analytical Chemistry**

### **Advanced Analytical Chemistry Studies of Biomolecule and Tissue Systems**

A. Ghosh, S. Pan, *Presiding*

**1:30** Introduction .

**1:40 1103.** Studying the Photophysical Modulation of Small Organic Molecules in Drug Delivery Vehicles. **D. Ghosh**, K.S. Aiken, S.M. Landge

**2:00 1104.** Analysis of Microplastics (MPs) and Perfluoroalkyl Substances (PFAS) in Marine Animal Tissues. **C. Navarathna**

**2:20 1105.** Mass Spectrometry Characterization of Deep Eutectic Solvents and their Impact on Protein Structure and Dynamics. J. Stewart, P. Gambill, M. Wewers, C. White, K. Galvez, M. Rahman, **M. Halim**

**2:40 1106.** X-ray Excited Luminescence Chemical Imaging (XELCI) based pH sensor for non-invasive Monitoring of Implant Associated Infections. **A. Rajamanthrilage**, C. Taylor, U. Uzair, J. Tzeng, J.N. Anker

**3:00** Intermission.

**3:25 1107.** Enhancing the Antioxidant Activity of Carotenoids-the Bioavailability Improvement. **A.L. Focsan**, Y. Gao, N. Polyakov, L. Kispert

**3:45 1108.** Fundamental Gas-Phase Chemistry of Beta2-agonists Using Mass Spectrometry: From Dissociation to Stereoisomer Discrimination. **M. Carlo**, A.L. Patrick

**4:05 1109.** UV-vis Extinction by Aggregated Proteins: Optical Absorption Induced by Charge Transfer or Light Scattering by the Protein Aggregates?. **P.D. Wathudura**, M. Wamsley, K.R. Carter, D. Zhang

**4:25 1110.** Optimization of a Prototype Analyzer for Trihalomethanes in a Drinking Water Distribution System. **M. Alfonso**, N. Boppana, M.A. Brown, P.S. Simone, G.L. Emmert



**4:45** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room O

## **Biochemistry**

### **General Session Biochemistry 2**

J. Zhang, *Presiding*

**1:30** Introductory Remarks.

**1:35 1111.** Surface Adsorption and Structure-Function Characterization of Autolysin-Amidase from *S. epidermidis*. **R. Yadav**, S. Yang, R. Somarathne, N.C. Fitzkee

**1:55 1112.** Understanding Binding Properties of Staphylococcal Autolysin Domains with Polystyrene. **R. Somarathne**, E. Chappell, Y. Perera, R. Yadav, J. Park, N.C. Fitzkee

**2:15 1113.** Synthesis, Characterization, Biological Analysis, and Molecular Docking Studies of DPDPE, a Delta Opioid Receptor Agonist and a Cyclic DPDPE Derivative Containing a Sonogashira Linkage. **K.R. Wilson**, M. Goertzen, J.C. Ouellette, T. McGomery, A. Williams, S. Majumdar

**2:35 1114.** Intrinsically disordered electronegative clusters improve stability and binding specificity of RNA-binding proteins. **J. Zhang**

**2:55** Intermission.

**3:15 1115.** Crystal Structure of a Mycobacteriophage Immunity Repressor Bound to DNA Sheds New Light on Transcriptional Silencing. **J. Wallen**, R. McGinnis, C. Brambley, B. Stamey, W.C. Green, K.N. Gragg, E.R. Cafferty, M. Hammel, T. Hollis, J.M. Miller, M.D. Gainey

**3:35 1116. Withdrawn.** Extending a Promising Aptamer Screening Platform to Gold Nanosphere Targets. **V.T. Milam**, M. Tapp, M.C. Adams, P. Dennis, R. Naik

**3:55 1117.** Asymptomatic COVID-19 Screening and Contact Tracing on an Undergraduate Campus. **S.A. Smith**, B. Magers, J. Neiswinger, R. Bishop, K. McKinney, L. Evans, M. McGuire, D. Manning

**4:15 1118. Withdrawn.** Targeting a Conserved Structural Element from the SARS-CoV-2 Genome Using Mirror Image Aptamers. **J. Li**, J.T. Szczepanski

**4:35 1119.**

Impact of Multivalency and Encapsulation of Affinity Reagents and Catalysts. **B. Manuel**, A. Sanford, S. Das, J. Heemstra, M. Finn

Birmingham Jefferson Convention Center  
East Meeting Room K

## **Chemical Education**

J. March, *Organizer*

## **Chemical Education Oral Presentations 2**

**1:30** Introduction .

**1:40 1120.** Improving Student Attitudes Towards General Chemistry I Laboratory as an Effect of Switching Lab Partners. **L. Smith**, D. Mlsna, T. Wei

**2:00 1121.** Measuring Internalized Stereotype Threat in Introductory Chemistry Courses Using a Customized Implicit Association Test (IAT). **T. Blue**, T.L. McGill

**2:20 1122.** Emerging Stronger through Resources Developed During the Pandemic. **B. Casselman**

**2:40** Intermission.

**3:00 1123.** Pre-COVID and during-COVID: A comparison of general chemistry instruction at the University of Florida. **M.T. Sumner**, S. Benjamin, S. Harris, S. Lopez, M. Veige

**3:20 1124.** Effects of a Preparatory Adaptive Module on Student Performance in General Chemistry I at University of Florida. **S. Benjamin**, S. Harris, S. Lopez, M.T. Sumner, M. Veige

**3:40** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room B

**Engineering Solutions for Social Challenges: Renewable Materials and Resources 2**

Financially supported by **Center for Sustainable Nanotechnology - UW Madison, and Surface Measurement Systems**

M. L. Curry, L. A. Lucia, M. S. Peresin, *Presiding*

**1:30** Introductory Remarks.

**1:35 1125.** Biobased Particles in Superstructured and Multiphase Materials. **O.J. Rojas**

**2:20 1126.** Cellulose Nanofiber-based Hydrogels for Rapid Removal of Methyl Blue dyes in Water. **Y. NAN**

**2:50 1127.** Effects of Hydrophobic-modified Cellulose Nanofibrils (CNFs) on the Physical and Chemical Properties of UHP PMDA Membranes. **M. Fair**, J. Mitchell, K.E. O'Harra, J.E. Bara, M.L. Curry

**3:20** Intermission.

**3:40 1128.** Downed Timber Degradation of Loblolly Pine in South Alabama and Potential Recovery of Natural Polymers for Value-added Applications. **J.A. Hernandez-Diaz**, M. Musah, B. Via, M.S. Peresin

**4:10 1129.** A Novel Method for Uniform Suspension of CNFs and Its Impact on the Fabrication and Thermal Stability of Cellulose-based Polymeric Composites. **D.H. White**, M.S. Islam, B. Frank, E. Laudadio, J.T. Buchman, E.M. Jackson, H. Fairbrother, R.J. Hamers, C.L. Haynes, M.L. Curry

**4:55** Concluding Remarks.

Birmingham Jefferson Convention Center  
East Meeting Room N

## **Industrial Careers in Chemistry**

### **Undergraduate Discussion: Industrial Careers in Chemistry**

Financially supported by Refresco  
J. A. Nikles, *Organizer*

**1:30** Introduction .

**1:40 1130.** The Unconventional Career path of a Chemist in Industry. **H.L. Davis**

**2:05 1131.** Technical challenges facing the food and beverage industry. **D.E. Ragland**

**2:30** Intermission.

**2:40 1132.** Chemistry Leads Beyond – Creating Your Career. **T. Tice**

**3:05 1133.** From a PhD in Biochemistry to the Director of Marketing: A Look at a Non-Traditional Career for your STEM Degree. **K. Sims**

**3:30 1134.** Successful Careers in the STEAM Field. **Y. Crawford**

**3:55 1135.** Transitioning from Academic Studies to an Industrial Career. **T.R. Totsch**

**4:20** Panel Discussion.

Birmingham Jefferson Convention Center  
East Meeting Room A

## **Nanomaterials 2**

S. Street, *Presiding*

**1:30** Introduction .

**1:40 1136.** Polymer Functionalized Zeolite - Green and Sustainable Ion Exchange Material. **J.C. Poler**, S. Elmore, C. Reid, S. Schmal

**2:00 1137.** Ionic Liquids as Antifouling Polymeric Nanoparticle Coatings. **E.E. Tanner**

**2:20 1138.** Using NMR to understand Protein Binding and Structure on Nanoparticle Surfaces. **N.C. Fitzkee**, J. Xu, R. Yadav, R.P. Somarathne, D.L. Amarasekara, Y. Perera

**2:40 1139.** Effect of Mass Transport Limitations on Gas Adsorption in Hierarchically Porous Carbons. **M.G. Bakker**, R. Adhikari

**3:00 1140.** Enhanced Harmonic Generation from Coupled Plasmonic Nanoparticle Films. **N. Spear**, J.M. Queen, S. Bailey, R.F. Haglund, J. Macdonald

**3:20** Intermission.

**3:40 1141.** A Facile Benchtop Reactor Design using Dendrimer-templating Technology for the Fabrication of PEI-coated CuO Nanoparticles on the Gram Scale. A. Ethridge, M.J. Gallagher, N. Hudson-Smith, D. Finley, A. Ahsan, H. Fairbrother, C.L. Haynes, R.J. Hamers, **M.L. Curry**

**4:00 1142.** Metal-Organic Frameworks: From Bulk to Thin Films. **A. Bajpai**, D. Speed, G.J. Szulczewski

**4:20 1143.** Characterization of Metal-organic Framework Thin Films using Laser Desorption/ionization Mass Spectrometry. **D. Speed**, A. Bajpai, G.J. Szulczewski

**4:40 1144.** Transport Features of Network Materials Built with Carbon Nanotubes Despite of Chiralities and Other Shape Factors. **S. Tang**

Birmingham Jefferson Convention Center  
East Meeting Room I

**Physical Chemistry**

**General Session Physical Chemistry 2**

T. P. Hamilton, *Organizer*

**1:30 1145.** Insights into Possible Halogen Bonding Effects in Dye Sensitized Solar Cells Studied via Nanosecond Transient Absorption Spectroscopy. **L. Hunt**, c. curiac, M. Sabuj, Q.Y. Li, A. Baumann, H. Cheema, y. zhang, N. Rai, N. Hammer, J.H. Delcamp

**1:50 1146.** Computational Analysis of the Spin-trapping Properties of Lipoic Acid and Dihydrolipoic Acid. **M. Bonfield**, S.J. Kirkby

**2:10 1147.** Correlating Stability of Substituted Cobaltocenium [bis(cyclopentadienyl)cobalt(III)] with Molecular Properties. **S.T. Wetthasinghe**, C. Li, H. Lin, T. Zhu, C. Tang, Q. Wang, V. Rassolov, S. Garashchuk

**2:30 1148.** Investigations of  $CF^+$  using High Accuracy Electronic Structure Theory Methods. **G. McCarver**, R.J. Hinde

**2:50 1149.** Computer Modeling of Size Effects in  $V_{1-x}M_xO_2$  ( $M = Mo, Nb$ ). **J. Phillips**, T.C. Douglas, J. Allred, M. Krogstad, T. Rawot Chhetri, M.A. Davenport

**3:10** Intermission.

**3:30 1150.** Understanding The Structural And Dynamical Properties Of Lignin Polymer In Dmso And Dmso/water Binary Mixtures. **N. Jahan**

**3:50 1151.** Transition-potential Coupled Cluster. **M. Simons**, D. Matthews

**4:10 1152.** Unusual Intramolecular Contacts in 2,3-Epoxycyclopentanol and their Analogs: Theoretical Evidence for Hydrogen Bonding. **J.M. Carr**, G.S. Tschumper

**4:30 1153.** Insight into Subsurface Adsorption from a Lattice-gas Model and Monte Carlo Simulations of Atomic Oxygen on the Silver Surface. **C. Mize**, L.D. Crosby, S.B. Isbill, S. Roy

Birmingham Jefferson Convention Center  
East Meeting Room C

**Polymer Materials Science and Engineering**

## **General Session Polymer Materials 2 - Polymeric Materials for Biological and Environmental purposes**

V. Thomas, *Presiding*

**1:30** Introduction .

**1:40 1154.** Poly(amino acid)s and PEGylated poly(amino acid)s in Biological Applications. U. David, J. Sanchez, **C. Scholz**

**2:00 1155.** Polymeric Tissue Scaffolds that Mimic the Structure, Composition and Function of the Extracellular Matrix. **D. Dean**, J. Ayariga

**2:20 1156.** Plasma Assisted Surface Polymerization Process for Nanoparticles Modified 3D Printed Polymer Scaffolds for Tissue Engineering Applications.. **V. Vijayan**, V. Thomas

**2:35 1157.** Supramolecular DNA Photonic Hydrogel for on Demand Control of Coloration with High Spatial and Temporal Resolution. **Y. Dong**, K. Salaita

**2:50 1158.** Differential Stiffness of Electrospun PLA Scaffolds Modulate Chondrocyte Behavior *in vitro*.. **J.A. Ayariga**

**3:05** Intermission.

**3:15 1159.** Synthesis and Characterization of PDMAEMA-g-CNT Composites. **T.L. Thornell**

**3:30 1160.** Recycling and Upcycling of Waste Plastics with Hemp Fibers. **Z. Wang**, Z. Vickery, E. Strickland

**3:45 1161.** Single-step Protease Immobilization in Solution Blown Polyethylene Oxide Nanofibrous Nonwoven Webs. **F. Asaduzzaman**, S.I. Salmon

**4:00 1162.** Fully Organic, X-ray Radioluminescent Crystalline Colloidal Arrays: Fine-tuning Color Characteristics via Photonic Bandgap Control and a Cascade of Energy Transfers. **H.W. Jones**, I. Bandera, E. Zhang, S.H. Foulger

**4:15 1163.** Anti-solvents Effects on Properties of Regenerated Cellulose from 1-butyl 3-methyl Imidazolium Chloride. **B.L. Sadiku**, C. Emehel, J.R. Alston

Birmingham Jefferson Convention Center  
East Exhibit Hall 1

## Undergraduate Research 5

J. A. Nikles, *Organizer*

**1:30 - 3:30**

**1164.** Exploiting Metallohedged *trans*-Bidentate Ligands for Cross-Coupling Reactions. **B. Nessell**, C.D. McMillen, J.A. Pienkos

**1165.** Biological Activity of Palladium Thiosemicarbazone. **E. Travers**, E.C. Lisic, J. Kim

**1166.** Attempts Toward Highly Electron-deficient Diimine Ligands and Expanding the Coordination Compounds of *N,N'*-bis(pentafluorophenyl)-2,3-butanediimine. **B. Newell**, J.P. Lee

**1167.** SDS-PAGE Studies on pH Dependent Lysozyme Modifications Induced by Naphthoquinones. **D. Madeksho**, J. Ewald, T.V. Albu, J. Kim

**1168.** Synthesis of Substituted Oxocanes to Probe Inductive Effects on Long-Range Hyperconjugation. **L. Middleton**, **J. Rivers**, **J. Hallford**, P. Wiget

**1169.** Pharmaceutical Drug Ligand Binding to Human Serum Albumin with Quantum Chemical Methods. **J.B. Baker**, A. Farmer, E. Mitchell, R. Bishop, B. Magers

**1170.** (Diethylamino)Sulfur Trifluoride (DAST) Mediated Oxidation of Alcohols and Amines to Carbonyl cCompounds. M.A. Lnu, **B. White**

**1171.** Synthesis of Trifluoromethyl Ketones by (diethylamino)sulfur trifluoride (DAST)-mediated nucleophilic trifluoromethylation of benzoic acids. M.A. Lnu, **M. Vescio**

**1172.** The Detection and Discrimination of Endocrine Disrupting Chemicals. **a. richardson**, M. Meadows



- 1173.** Defining the Mechanism of Inhibition of Thiosemicarbazone-metal Complexes on Topoisomerase II Alpha. **C. Greer**, K. Lyons, W. Morris, E.C. Lisic, J.D. Conner, X. Jiang
- 1174. Withdrawn.** Construction of an Instrument Capable of Two-color Fluorescence Correlation Spectroscopy:. **A. Lawrence**, K.H. Fogarty
- 1175.** Synthesis of Bioactive Juglone Compounds *via* aromatic Ammonium Cations. **H. Suddeath**, O.A. Cojocar, T.W. Majors
- 1176.** Synthesis of  $\alpha,\beta$ -unsaturated lactams via oxidative-elimination using  $\text{NaIO}_4$ . **D. Toman**, J.M. Plummer
- 1177.** Discovery of the Cryptic Allosteric Site on the CB1 Receptor. **D. Hunnicutt**, **A. Lee**, J. Shim
- 1178.** Potentiating Antibiotics to Target Multidrug Resistant ESKAPE Pathogens. **B.O. Allen**, R. Day, M.S. Blackledge
- 1179.** Theoretical Study of  $\text{Au}_{25}(\text{SCH}_3)_{18}^-$  and its Activation of  $\text{O}_2$  Molecules. **J. Pinkerton**, S. Havenridge, C. Aikens
- 1180.** Computational Investigations into Tetrahalogenated Tricyclooctanes and Tricyclodecanes. **R.A. Davy**, R.L. King, J.R. Boone, E.W. Reinheimer, C. Clinger
- 1181.** Synthesis and Characterization of Zeolite-Encapsulated Organometallic Complexes that Catalyze Selective Alkane Oxidation. **J.L. Groeber**, C.R. Diemer, E.P. Iaia, J.W. Harris, M.G. Bakker, G.R. Rana
- 1182.** Role of Quenching and Diffusion in the Magnetic Sensitivity of Micellar Thionine-aniline Radical Pairs. **A. McHorse**, A. Markham, D. Sowood, C. Timmel, L. Jarocho
- 1183.** Effects of Hydrophobic Modification and Electrostatic Interactions on the Sensitivity of Flavin-ascorbic Acid Radical Pairs to Weak Magnetic Fields. **E. Dowker**, E. Evans, C. Timmel, L. Jarocho
- 1184. Withdrawn.** Separation of Chiral Amino Acids Using Mass Spectrometry and Ion Mobility. **K.D. Hernandez Gomora**, H. Dossmann, S. Alves, D. Lesage
- 1185.** Seasonal Comparison of Metal Concentrations along the Alafia and Hillsborough Rivers. **R. Vernarsky**, K.A. Deister

**1186.** Preparation of Macrocyclic Polyphenylethynylarene Ethers. **B. Steen**, T.D. Selby

**1187.** Synthesis of Macrocyclic Diaminopolyphenylethynylarenes and Diaminopyridinylethynylarenes. **M. Stewart**, T.D. Selby

**1188.** Functionalizing Zeolite to Remove Hydrophilic Contaminants in Drinking Water. **S. Elmore**, S. Schmal, J.C. Poler

**1189.** Campus-wide COVID Screening Provides Non-Traditional Clinical and Laboratory Experiences for Students During Pandemic. **D. Manning, R.G. Ayres**, L. Evans, M. McGuire, K. McKinney, A. Farmer, M.L. Ayres, C.C. Bishop, E. Campbell, O. Haney, K. McKinney, M. Meadows, S. Roberson, R. Bishop, J. Neiswinger, B. Magers, S.A. Smith

**1190.** Chemical Analysis and Biototoxicity Assessment of Plastic Bioremediation using Tenebrio Molitor Larvae. **L. Sisson**, C. Stokes, S. Melton, T.D. Selby, S. Hearst

**1191.** Shear Rate Effects on Particle Size Distribution of Nonliving Natural Organic Matter. **K.N. Mealio**, K.E. Slamen, H.A. Stretz, M.J. Wells

**1192.** Protection of Alcohol Dehydrogenase Activity by a Tardigrade Cytosolic Abundant Heat Soluble Protein. **A. Burgess**, B.E. Christian

**1193.** Effect of Novel Fluoroquinolone-derived Inhibitors on DNA Gyrase Activity. **C. Plantz**, A. Rocque, S. Panda, A.C. Spencer

**1194.** A New Extraction and Quantification Method to Detect Polystyrene Plastics in Biological and Environmental Samples. **C. Stokes**, S. Melton, L. Sisson, T.D. Selby, S. Hearst

**1195.** Stabilization of Proteins in Solution by a Tardigrade Cytosolic Abundant Heat Soluble Protein. **L. Vaughn**, B.E. Christian

**1196.** Conventional Strain Energies of Thiaziridine and the Thiazetidines. **J.D. Gramm**, D.H. Magers

**1197.** Joro Spider Webs as Bioaccumulators of Heavy Metals in North Georgia. **M. Smith-Roden**, J. Casey, H. Cole, J. Driver, I. Agyekum

- 1198.** Boron-mediated diastereoselective aldol reactions of *N,N*-dialkylphenylacetamides. **B. Peco**, A. McCullough, **S. Reliford**, S.W. Primeaux, D.J. Cambre, P.B. Chanda
- 1199.** Analysis of Electronic Cigarette Liquids. **M. Deen**, L. Butler, V. Geisler
- 1200.** Influence of Spring Water on Two Rivers in Tampa Bay, Florida. **P. Mead**, K.A. Deister
- 1201.** Regioselectivity of Acid-catalyzed Epoxide Ring-opening Reactions. **B.R. Chastang**, D.H. Magers
- 1202.** The Conventional Strain Energies of Cyclopropylborane, Borirane, Boretane, the Diboretanes, Borolane, the Diborolanes, Borinane, and the Diborinanes. **K.E. Hood**, R.M. Rocray, D.H. Magers
- 1203.** Relative Stabilities of Derivatives of 9-methylantracene and 9-methylene-9,10-dihydroanthracene and Derivatives of 6-methylpentacene and 6-methylene-6,13-dihydropentacene. **E.P. Sullivan**, A.W. Plunkett, D.H. Magers
- 1204.** Ab Initio Analysis of Polarizability in Molecular Piezoelectric Response for Organic Dimer Systems. **D.L. Zetterholm**, D.H. Magers
- 1205.** Prediction of Chiroptical Spectroscopic Properties of Chiral Beta-lactone Heteroaromatics by Equation-of-Motion Coupled-Cluster Theory. **O. Haney**, H. McAlexander, R. Bishop, B. Magers
- 1206.** Design and Development of a Homogenous Protein-based Assay for the Detection of Organophosphates by Utilizing a Fusion Protein Between Organophosphorus Hydrolase (OPH) and Enhanced Green Fluorescent Protein (EGFP). **C.R. Schlaline**, **S. Knier**, L.G. Puckett
- 1207.** Structural Characterization of a Mutagenic 6-oxo-m1dg Adduct in DNA. **C.L. Wessel**, Y. Fu, L.J. Marnett, M.P. Stone
- 1208.** Comparison of Six Different Iron-Gall Ink Mixtures with Respect to Value of the Wet and Dried Inks as Determined using a Munsell Scale and Other Physical Properties. **M.S. Morton**, **J. Quesada**
- 1209.** Spin Trapping Reactive Oxygen Species Produced by X-ray Scintillating Nanoparticles. **I. Weaver**, E. Zhang, C. Kerpel, S.H. Foulger, L. Jarocho

- 1210.** Synthesis of Silver Phosphate Complexes. **T. Hussain**, N. Dodd, J.P. Sadighi
- 1211.** Characterization of Gamma Ray Imaging System for Use in Depleted Uranium Remediation Efforts: Shielding the Gamma Ray Imaging System. **C.E. McCormick**, B.P. Crider, R.J. Unz, L. Allen, B. Henkel, S. Lusby, S. Sansing, D.H. Magers
- 1212.** Synthesis of Homoepibatidine Derivatives for Smoking Addiction. **G. Womack**, S. Slauson
- 1213.** Are Halogenated Amino Acids from Plasma Proteins Correlated with Pediatric Eosinophilic Esophagitis?. **M. Thomas**, J. Germany, M. Gilliland
- 1214.** Using NMR Titrations and DFT Computational Modeling to Assess Halogen-Bonding Strength as a Function of Molecular Structure. **Q. Dang**, J. Simpson, C.A. Parish, M.C. Leopold
- 1215.** Biofouling Resistant ICP Films for Biologically Triggered Dopant Release. **A. Knepper**, P. Molino, T.W. Hanks
- 1216.** Nitrile Homoepibatidine Synthesis. **N.N. Al-Saadi**, S. Slauson
- 1217.** Characterizing *Brucella* FtrB: A New Class of Cupredoxin. **A. Kerkan**, S. Banerjee, D. Martin, S. Roy, B. Garcia, R. Roop
- 1218.** Analyzing Spectral Data of Rhodamine B dimer and related compounds. **B. Stratton**, A. Wolwhend, K. Fogarty, P. Lundin, A.J. Pierre
- 1219.** Mechanisms of Linoleic Acid Oxidation by Myeloperoxidase. **C. Powell**, K.M. Matera
- 1220.** Vapor Deposition Synthesis of Semiconducting Molybdenum Disulfide. **J. Arce**, P. Parajuli, A. Rao, R.E. Lee
- 1221.** Spartan18 QSAR Analysis of Ebselen-Type Heterocycles for the Inhibition of SARS-CoV2. F. Bai, **D. Cooper**, M. Donahue, J. Kessel
- 1222.** Resolution of Racemic Alcohol through the use of Mosher's Reagent for use in the Synthesis of Enantiopure Allosteric Inhibitors for HIV-1 Integrase. **L. Evans**, K. Patel, J. Patterson, J.A. Pigza, M. Donahue, J. Kessl
- 1223.** Effects of Self-assembled Monolayer Structure on Conjugated Polymer Morphology. **E. Silver**, P. Lundin

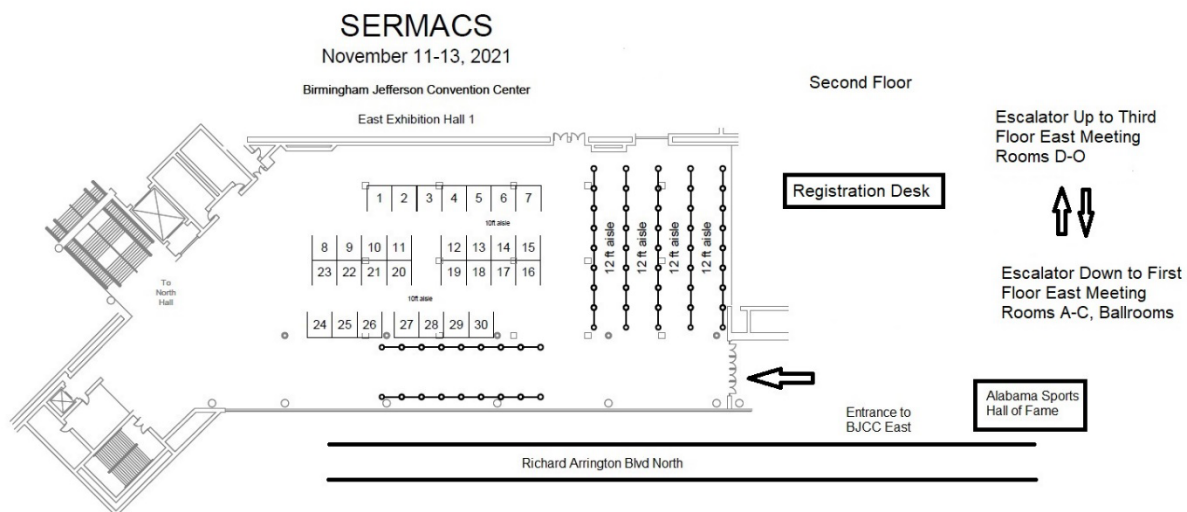
## SATURDAY EVENING

Birmingham Jefferson Convention Center  
East Ballroom B

### Plenary

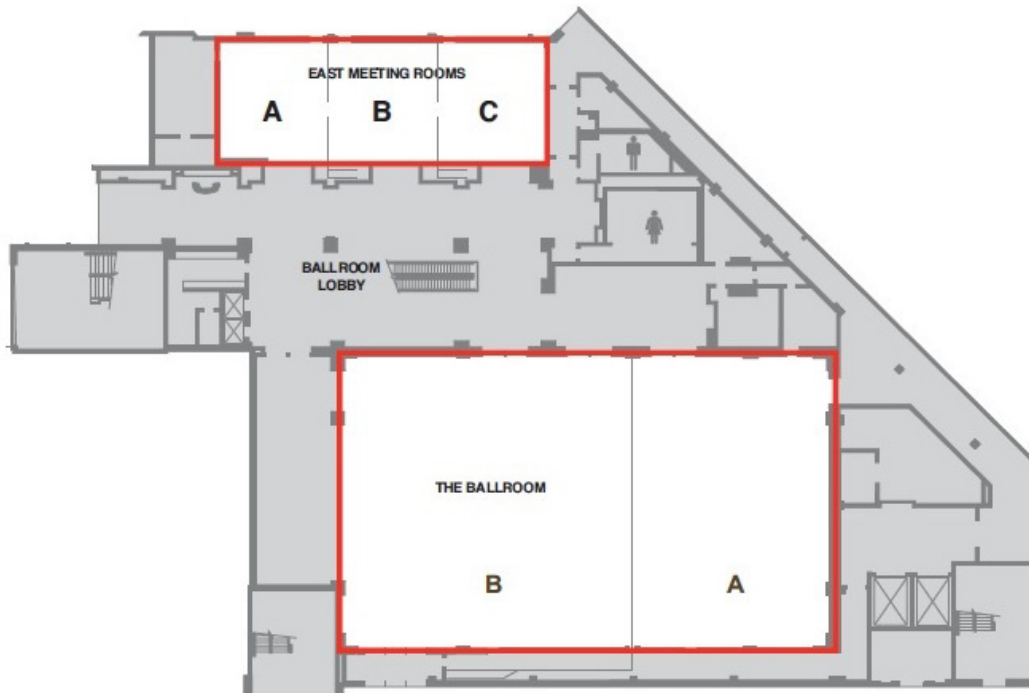
T. P. Hamilton, *Presiding*

**5:30 1224.** A Career in Science: Expect the Unexpected. **L.J. DeLucas**





Third Floor East Meeting Rooms



First Floor East Meeting Rooms

P5 is the recommended Parking Deck

Meetings are in East Meeting Rooms

Sheraton and Westin Hotels are also circled

Elevated walkway from Sheraton to Third Floor East





# SERMACS 2021 Event Program

Workshops, Expo, Graduate Fair, Social Events and Meal events

## WEDNESDAY MORNING

**9:00 am – 12:00 pm**

Birmingham Jefferson Convention Center  
East Ballroom A

### MOLSSI Workshop

Financially supported by the National Science Foundation  
Jessica Nash, *Organizer*

## WEDNESDAY EVENING

**5:30 pm – 6:30 pm**

Birmingham Jefferson Convention Center  
East Ballroom B

### Plenary

Drug Discovery and Development *via* structure and Mechanism Based Rational Design. **Chang-Guo Zhan, Endowed Professor in Department of Pharmaceutical Science, University of Kentucky**

D. A. Dixon, *Presiding*

## WEDNESDAY EVENING

**7:00 pm – 9:00 pm**

The Sour Room at Avondale Brewing, 205 41st St S

**Social Event:** Chemistry of Absinthe talk, and absinthe tasting by **Ted Breaux, Founder, Jade Liqueurs**

\$10 at the door. Contact [Hamilton@uab.edu](mailto:Hamilton@uab.edu) about availability, seating is limited

## **THURSDAY MORNING**

**8:00 am – 5:00 pm**

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

**Commercial Exhibitors** For a full list, go to  
<https://www.sermacs2021.org/exhibitors---commercial.html>

## **THURSDAY MORNING**

**8:00 am – 9:00 am**

Birmingham Jefferson Convention Center  
East Meeting Room N

### **Senior Chemists Committee Breakfast - \$20**

Financially supported by the ACS Senior's Chemist Committee  
Tracy Hamilton, *Organizer*

Get an update from **Arlene Garrison, Chair of SCC**, followed by a talk by **Steve Burgess, Managing Director, Avanti Polar Lipids** “mRNA Vaccines and the Future of Lipid Nanotechnology”

## **THURSDAY AFTERNOON**

**12:00 pm – 1:30 pm**

Birmingham Jefferson Convention Center  
East Meeting Room N

### **SERMACS Awards Luncheon - \$40**

Financially supported by SERMACS, Inc., ACS  
Pravin Kotian, *Organizer*

Meet and receive an update on ACS Diversity, Equity, Inclusion and Respect initiatives in the ACS from **Angela K Wilson, President-Elect of ACS**, followed by awards presentations. Stay for the special symposium from past Satnley Israel winners, in the same room after lunch.

## **THURSDAY AFTERNOON**

**2:30 pm – 5:00 pm**

Birmingham Jefferson Convention Center  
East Meeting Room N

**How to Foster Diversity, Equity and Inclusion in the Chemical Sciences: Lessons Learned and Taught from the Stories of Recipients of the Stanley C. Israel Award**

R. Joseph, *Organizer*  
P. Gordan, *Presiding*

**I.M. Warner, J.V. Ortiz, R. Hernandez, D. Rabinovich**

## **THURSDAY AFTERNOON**

**4:40 pm – 5:10 pm**

Birmingham Jefferson Convention Center  
East Ballroom B

**ACS Town Hall** Meet members of the ACS Board of Directors and other ACS Governance and learn about the new dues structure

## **THURSDAY EVENING**

**5:30 pm – 6:30 pm**

Birmingham Jefferson Convention Center  
East Ballroom B

### **Plenary**

From Isotopes to Images: Development of Radiometal Agents in Medicine. **Suzanne E. Lapi, Professor, Departments of Radiology and Chemistry, UAB**

D. A. Dixon, *Presiding*

## **THURSDAY EVENING**

**7:00 pm – 9:00 pm**

Cahaba Brewing, 4500 5th Ave S Building C

**Social Event: YCC Fermentation Social \$10**

## **FRIDAY MORNING**

**8:00 am – 4:00 pm**

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

**Commercial Exhibitors** For a full list, go to  
<https://www.sermacs2021.org/exhibitors---commercial.html>

## **FRIDAY MORNING**

**8:00 am – 12:00 pm**

Birmingham Jefferson Convention Center  
East Meeting Room M

### **Safety Workshop**

Financially supported by the Chemical Health and Safety (CHAS) Committee of ACS

### **Integrating Risk Assessment into Undergrad Teaching LabsCommercial Exhibitors**

Catherine Situma and Samuella Sigmann, *Organizers*

## **FRIDAY EVENING**

**5:15 pm – 6:15 pm**

Birmingham Jefferson Convention Center  
East Ballroom B

## **Plenary**

From N-heterocyclic Carbenes to Dithiolene-based radicals: Recent Developments in Main Group Chemistry. **Gregory H. Robinson, Foundation Distinguished Professor of Chemistry, University of Georgia**

Anne E. Gorden, *Presiding*

## **FRIDAY EVENING**

**7:00 pm – 9:00 pm**

McWane Science Center, 200 19th St N, Birmingham

## **Undergraduate Posters of Activities During Covid, Undergraduate Research**

Free admission to the McWane Science Center to any attendees, their families, or guests

Jackie Nikles and Jonathan Meyers, *Organizers*

## **SATURDAY MORNING**

**8:00 am – 12:00 pm**

Birmingham Jefferson Convention Center  
East Exhibition Hall 1

**Graduate School Fair** For a full list, go to <https://www.sermacs2021.org/exhibitors--graduate-school-fair.html>

## **SATURDAY MORNING**

**8:00 am – 12:00 pm**

Birmingham Jefferson Convention Center  
East Meeting Room N

**Closed meeting of the SERMACS, Inc Board and designated representatives from local section**

## **SATURDAY EVENING**

**5:30 pm – 6:30 pm**

Birmingham Jefferson Convention Center  
East Ballroom B

### **Plenary**

**A Career in Science: Expect the Unexpected. Larry J. DeLucas, Space Shuttle Astronaut; Principal Scientist, Aerospace Corporation; Founder of Soluble Biotech (now a Subsidiary of Predictive Oncology)**

T. P. Hamilton, *Presiding*

## **SATURDAY EVENING**

**7:00 pm – 9:00 pm**

Tortuga's - Birmingham, 1304 2nd Ave S, Birmingham

**Social Event: Undergraduate Networking Social \$10 (no seats available)**

## Appendix B – Financial Worksheets

### (I) Registration revenue

1	SERMACS WORKSHEET 2021										
2											
3				Registration Fee from 2017 Meeting	Registration Fee from 2018 Meeting	Registration Fee from 2019 Meeting	Registration Fee TPH estimate for 2021 Meeting		Actual # Registrants	Registration Fee	Total
4	Category	% Registrants	# Registrants								
5	50 Year Member	0.5	6	\$0	\$0	\$0	\$0	\$0	8	\$0	\$0
6	Member, Advance	25	300	\$165	\$165	\$180	\$185	\$55,500	268	\$185	\$49,580
7	Member, Onsite	2.3	27.6	\$200	\$200	\$225	\$230	\$6,348	103	\$230	\$23,690
8	Nonmember, Advance	3.5	42	\$220	\$220	\$250	\$255	\$10,710	24	\$255	\$6,120
9	Nonmember, Onsite	1	12	\$275	\$275	\$300	\$305	\$3,660	25	\$305	\$7,625
10	Guest of Registrant, Advance	1	12	\$25	\$30	\$30	\$30	\$360	11	\$25	\$275
11	Guest of Registrant, Onsite	1.2	14.4	\$50	\$40	\$40	\$40	\$576	0	\$25	\$0
12	Member Ret/Emeritus/Unemployed, Advance	1.2	14.4	\$10	\$40	\$40	\$40	\$576	6	\$40	\$240
13	Member Ret/Emeritus/Unemployed, Onsite	0.2	2.4	\$30	\$60	\$60	\$60	\$144	2	\$60	\$120
14	Member Precollege Teacher, Advance	1.8	60	\$10	\$30	\$30	\$30	\$1,800	13	\$30	\$390
15	Member Precollege Teacher, Onsite	0.3	5	\$25	\$50	\$50	\$50	\$250	3	\$50	\$150
16	Nonmember Precollege Teacher, Advance								17	\$30	\$500
17	Nonmember Precollege Teacher, Onsite								5	\$50	\$250
18	Member Graduate Student, Advance	18.5	222	\$75	\$70	\$80	\$80	\$17,760	144	\$80	\$11,520
19	Member Graduate Student, Onsite	2.1	25.2	\$100	\$90	\$100	\$100	\$2,520	72	\$100	\$7,200
20	Nonmember Graduate Student, Advance								113	\$80	\$9,040
21	Nonmember Graduate Student, Onsite								44	\$100	\$4,400
22	Member Post doctorate, Advance	2.2	26.4	\$100	\$100	\$120	\$120	\$3,168	21	\$120	\$2,520
23	Member Post doctorate, Onsite	0.3	3.6	\$135	\$135	\$140	\$140	\$504	7	\$140	\$980
24	Nonmember Post doctorate, Advance	0	0	\$120	\$120	\$140	\$140	\$0	9	\$140	\$1,260
25	Nonmember Post doctorate, Onsite	0	0	\$155	\$155	\$160	\$160	\$0	6	\$160	\$960
26	Member High School Student, Advance	1	12	\$10	\$10	\$10	\$10	\$120	1	\$10	\$10
27	Member High School Student, Onsite	1	12	\$10	\$10	\$10	\$10	\$120	0	\$10	\$0
28	Nonmember High School Student, Advance								6	\$10	\$60
29	Nonmember High School Student, Onsite								0	\$10	\$0
30	Member Undergraduate Student, Advance	30.4	364.8	\$30	\$50	\$60	\$60	\$21,888	113	\$60	\$6,780
31	Member Undergraduate Student, Onsite	5.5	66	\$50	\$70	\$80	\$80	\$5,280	58	\$80	\$4,640
32	Nonmember Undergraduate Student, Advance								112	\$60	\$6,720
33	Nonmember Undergraduate Student, Onsite								67	\$80	\$5,360
34	1 session "Family" of UG or Grad presenter	1	12	\$5	\$5	\$5	\$5	\$60			\$0
35	Adjustments*										\$ (540.00)
36	Number of registrants/total revenues	100	1200					\$131,344	1258		\$149,850

The registration adjustment is due to: 1) ACS reported an offline payment in the member category of \$310, which the treasurer cannot account for. 2) ACS reported that one pre-college faculty member paid \$20 instead of \$30. 3) On the revenue breakdown sheet of the ACS report, there is a difference of \$230 between the amount ordered and the amount collected online by ACS.

### (II) Total revenue

1	SERMACS 2021 Budget			
2	LINE ITEM	BUDGET	ACTUAL	NOTES
3				
4	REVENUES			
5	A. Corporate Sponsorships	\$ 5,000.00	\$ 42,991.37	
6	B. SERMACS, Inc loan	\$ 5,000.00	\$ 5,500.00	
7	C. Registration	\$ 131,344.00	\$ 149,850.00	See worksheet
8	D. Grants/Contributions	\$ 10,000.00	\$ 8,500.00	ACS Grants from Divisions
9	E. Sponsorships	\$ 10,000.00		funds from division, matching for ACS grant
10	Subtotal	\$ 161,344.00	\$ 206,841.37	Revenues not directly related to expenses. Should exceed subtotal for non-discretionary expenses.
11	F. Banquet tickets	\$ 4,750.00	\$ 2,809.28	Budget should equal expense line items in section H, minus any Complimentary or subsidies.
12	G. Luncheon Tickets	\$ -	\$ -	See banquet tickets
13	H. Mixer tickets cash bar	\$ 2,000.00	\$ -	Charge based on bar prices per drink, taxes, gratuities, & cost of bartender
14	I. Exposition	\$ 40,000.00	\$ 14,400.00	40 booths x \$1000 revenue/booth. See layout and contract for details
15	J. Advertising revenues	\$ -	\$ -	
16	K. Graduate fair booths	\$ 9,000.00	\$ 9,300.00	30 @ \$300
17	TOTAL REVENUES	\$ 217,094.00	\$ 233,350.65	

### (III) Total Expenses

1	<b>SERMACS 2021 Budget</b>			
2	<b>LINE ITEM</b>	<b>BUDGET</b>	<b>ACTUAL</b>	<b>NOTES</b>
12	G. Luncheon Tickets	\$ -	\$ -	See banquet tickets
13	H. Mixer tickets cash bar	\$ 2,000.00	\$ -	Charge based on bar prices per drink, taxes, gratuities, & cost of bartender
14	I. Exposition	\$ 40,000.00	\$ 14,400.00	40 booths x \$1000 revenue/booth. See layout and contract for details
15	J. Advertising revenues	\$ -	\$ -	
16	K. Graduate fair booths	\$ 9,000.00	\$ 9,300.00	30 @ \$300
17	<b>TOTAL REVENUES</b>	<b>\$ 217,094.00</b>	<b>\$ 233,350.65</b>	
18				
19	<b>EXPENSES</b>			
20	<b>A. Committee Expenses</b>			
21	1. Meetings	\$ -	\$ 31.61	
22	2. Postage, supplies, misc.	\$ 2,500.00	\$ 359.85	
23	3. Travel expenses 2020	\$ -	\$ -	covid canceled 2020 SWRM-SERMACS
24				
25	<b>B. Printing/Publicity</b>			
26	1. Regional Meetings APP	\$ 5,000.00	\$ -	To ACS for app
27	2. Flyers - printing/mailling/postage	\$ 2,000.00	\$ -	
28	3. Web page design	\$ -	\$ 182.83	
29	4. Ads in local section pubs	\$ 500.00	\$ -	check with CERM, D.C, etc different local sections
30	5. Call for Papers in C&EN	\$ 720.00	\$ -	
31	6. Promotional Items	\$ 5,000.00	\$ 3,375.00	Promotional Give-Aways, etc
32	7. Miscellaneous	\$ 2,000.00	\$ -	Miscellaneous
33				
34	<b>C. Meeting Site Expenses</b>			
35	1. Space Rental/Facility Charge	\$ 21,600.00	\$ 16,738.44	see contract ( + 23% service charge, then sales tax 10% on total)
36	2. Audiovisual Services - basics	\$ 40,000.00	\$ 45,840.05	PSAV contract with ACS, 20% discount
37	3. Audiovisual Services - special	\$ -	\$ -	Allowance for possible special requests from guest speakers and/or LCDs
38	4. Signage	\$ 1,250.00	\$ -	
39	5. Facility liability insurance	\$ -	\$ -	included in ACS umbrella package
40	6. Poster Sessions	\$ 2,000.00	\$ 930.55	Posterboard rental (need to check on cost)
41	7. Hospitality Suite*	\$ 500.00	\$ -	Room provided in contract; stock with water; soft drinks, and snacks
42	8. Internet Access	\$ -	\$ 1,253.70	Internet access in Meeting Rooms ?
43	9. Miscellaneous	\$ 2,000.00	\$ 349.30	
44				
45	<b>D. Program</b>			
46	1. Symposia Grants	\$ 25,000.00	\$ 38,583.78	50 session max @ \$500
47	2. Complimentary registrations			
48	2a. LOC	\$ 1,850.00	\$ -	10 at \$185
49	2b. Volunteers	\$ 3,850.00	\$ 900.32	10 at \$185 , 10 at \$80, 20 at \$60
50	2c. Symposium Chairs	\$ 8,325.00	\$ -	45 invited get one registration at \$185
51	3. Plenary Speakers	\$ 4,000.00	\$ 8,854.32	
52	4. Awards Expenses	\$ 1,000.00	\$ -	Plaques/Cash Awards
53	5. Postage for mailing plaques	\$ 200.00	\$ -	
54				
55	<b>E. Registration</b>			
56	1. Telephone lines	\$ -	\$ -	Local Access and 800 # Only for use at registration area
57	2. ACS -on-line registration processsing fee	\$ 4,800.00	\$ -	\$4 fee/registration
58	3. Credit card fees	\$ 1,700.00	\$ -	
59				
60	<b>F. Return of loan</b>	\$ 5,000.00	\$ 5,500.00	Equals item A and/or B under revenues.
61	<b>Subtotal - non-discretionary expenses</b>	<b>\$ 140,795.00</b>	<b>\$ 122,899.75</b>	
62				
63	<b>G. Exposition</b>			Offset by revenues
64	1. Decoration	\$ 3,500.00	\$ 2,865.50	
65	2. Exhibitor Prospectus Brochure	\$ -	\$ -	SERMACS Website
66	3. Postage, phone expense	\$ 300.00	\$ -	
67	4. Space Rental	\$ -	\$ -	see C. 1.
68	5. Security	\$ 500.00	\$ -	
69	6. Prizes/Contests	\$ 1,000.00	\$ -	
70	7. Miscellaneous	\$ 1,000.00	\$ -	



71				
72	<b>H. Special Events/Activities</b>			\$53,100 total including tax and charges
73	1. Diversity Luncheon*	\$ 1,400.00	\$ -	35 @ \$40
74	2. Awards Luncheon*	\$ 1,600.00	\$ 1,950.81	40 @ \$40
75	3. Steering Committee Breakfast*	\$ 1,200.00	\$ 3,315.40	40 @ \$30
76	4. Teacher Luncheon*	\$ 2,400.00	\$ 4,210.80	60 @ \$40
77	5. Undergraduate Program*	\$ 6,000.00	\$ 2,769.75	
78	6. Director's Ice Cream Social*	\$ 1,500.00	\$ -	
79	7. Complimentary events tickets	\$ 2,000.00	\$ -	Meals, receptions, special events where there is a fee.
80	8. Coffee Breaks*	\$ 15,000.00	\$ 28,251.70	
81	9. Undergrad Pizza Party and Graduate Fair*	\$ 1,000.00	\$ 432.14	Complimentary, registration required
82	10. Opening Reception for Expo*	\$ 20,000.00	\$ -	
83	11. YCC Social Fementation Chemistry*	\$ 1,000.00	\$ 729.95	100 @ \$10
84				
85	<b>TOTAL EXPENSES</b>	<b>\$ 200,195.00</b>	<b>\$ 167,425.80</b>	
86				
87	<b>NET</b>	<b>\$ 16,899.00</b>	<b>\$ 65,924.85</b>	
88				
89	* count towards contracted food and beverage minimum of \$34,000			minimum \$34,000 + 33% tax and charges = \$45220
90				
91	<b>Distribution</b>			
92	Regional Board	\$ 3,379.80	\$ 13,184.97	
93	Auburn Local Section	\$ 6,759.60	\$ 26,369.94	
94	Alabama Local Section	\$ 6,759.60	\$ 26,369.94	

## Appendix C – List of Expo Vendors and Graduate School Booths

Booth	Company
1	 Biotage
3	 Pine Research
5	 designed for scientists IKA
7	 Rikagu
9	 Elsevier
11	 Bruker Biospin
13	 Oxford Instruments
15	 Advion
17	 Jeol
19	 Oakwood Chemical
21	 Society of Catholic Scientists
23	 Nanalysis
26	 SERMACS 2022
30	 Jasco

<b>Booth</b>	<b>University</b>	<b>Booth</b>	<b>University</b>
1	University of Houston	16	Mississippi State University
2	Jackson State University	17	Texas A&M University
3	University of Southern Mississippi	18	University of Tennessee
4	University of Memphis	19	North Carolina State University
5	Georgia State University	20	University of Central Florida
6	City University of New York Grad Center	21	Augusta University
7	Auburn University	22	Florida International University
8	Florida State University	23	South University (Pharmacy)
9	UNC Greensboro (Chemistry)	24	Tulane University
10	West Virginia University	25	Vanderbilt University
11	University of Alabama (Chem. Eng.)	26	University of Missouri (Biochem)
12	University of Alabama (Chemistry)	27	University of Mississippi
13	UNC Greensboro, NC A&T St. (Nanoscience)	28	University of Louisville
14	Clemson University	29	UNC Charlotte
15	University of Alabama at Birmingham	30	Georgia Tech

## Appendix D – Expo Vendor and Graduate School Booth Forms and Rules

### SERMACS 2021 BOOTH APPLICATION AND CONTRACT

#### Graduate School Fair

November 13, 2021, Birmingham, AL

I (We) agree to abide by the EXPOSITION RULES AND REGULATIONS (included in this packet) and, in accordance with, also hereby apply for exposition space on November 13 at SERMACS 2021 to be held November 10-13, 2021 in Birmingham, AL.

BOOTH assignments cannot be made without this FORM and PAYMENT

BOOTH TYPE single \$300 [\$400 after Sept 30, 2021] double \$500 [\$600 after Sept 30, 2021]

Booth reservation number \_\_\_\_\_  
 1<sup>st</sup> choice \_\_\_\_\_ 2<sup>nd</sup> choice \_\_\_\_\_ 3<sup>rd</sup> choice \_\_\_\_\_  
*If you desire more than one contiguous booth, list all booths desired as one choice.  
 See website for booth numbers.*

Checks payable to American Chemical Society, put "SERMACS 2021 Grad Fair" in memo line

Payment by check VISA MC AmEx

Credit Card # \_\_\_\_\_ exp date \_\_\_\_\_

Credit Card Signature \_\_\_\_\_

Printed Name (as shown on card) \_\_\_\_\_

Send Application Form With  
 Payment Information To: Konrad Fatkowsky  
 Graduate Fair Chairman, SERMACS 2021  
 Department of Chemistry and Biochemistry  
 Auburn University  
 179 Chemistry Building  
 Auburn, AL 36849  
[kfp0013@auburn.edu](mailto:kfp0013@auburn.edu)

It is understood and agreed that SERMACS 2021 will endeavor to assign space in order of choice. If all spaces have been assigned previously, the Graduate Fair Chairman reserves the right to assign space as equitably as possible in accordance with the stated exhibitor preference.

	<b>Send Booth Confirmation and additional information to:</b>	<b>Person Responsible for Booth Set-up on Saturday Nov. 13:</b>
<b>Company</b>		
<b>Contact Person</b>		
<b>Address</b>		
<b>Phone/FAX</b>		
<b>email</b>		

Do you need a one-day exhibitor pass for Saturday (no extra charge)? If yes, list the name on this pass:

\_\_\_\_\_

Authorized Exhibitor Signature \_\_\_\_\_ Printed Name \_\_\_\_\_

## SERMACS 2021 EXPOSITION BOOTH APPLICATION AND CONTRACT

November 10 - 13, 2021, Birmingham, AL

I (We) agree to abide by the EXPOSITION RULES AND REGULATIONS (included in this packet) and, in accordance with, also hereby apply for exposition space on November 11 and 12 at SERMACS 2021 to be held November 10 - 13, 2021 in Birmingham, AL.

**BOOTH assignments cannot be made without this FORM and PAYMENT**

**BOOTH assignments cannot be made without this FORM and PAYMENT**

**BOOTH TYPE** single \$1000 [\$1200 after Sept 30, 2021] double \$1800 [\$2000 after Sept 30,

Booth reservation number      1<sup>st</sup> choice      2<sup>nd</sup> choice      3<sup>rd</sup> choice  
*If you desire more than one contiguous booth, list all booths desired as one choice.  
See website for booth numbers.*

Checks payable to      *American Chemical Society, place for SERMACS 2021 in memo*

Payment by      check      VISA      MC      AmEx

Credit Card #      exp date     

Credit Card Signature     

Printed Name (as shown on card)     

Send Application Form With      Cindy Willingham  
Payment Information To:      Exposition Chair, SERMACS 2021  
UAB AMSTI  
1720 2<sup>nd</sup> Ave South  
Birmingham, Alabama 35294

205-934-4011      [cwillin@uab.edu](mailto:cwillin@uab.edu)

It is understood and agreed that SERMACS 2021 will endeavor to assign space in order of choice. If all spaces have been assigned previously, the Exposition Chair reserves the right to assign space as equitably as possible in accordance with the stated exhibitor preference.

	Send Booth Confirmation and additional information to:	Person Responsible for Booth Set-up on Wednesday Nov. 10:
Company	_____	_____
Contact Person	_____	_____
Address	_____	_____

Phone/FAX	_____	_____
email	_____	_____

Names for Exhibitor Badges (1) \_\_\_\_\_ (2) \_\_\_\_\_

Authorized Exhibitor Signature \_\_\_\_\_

Printed Name \_\_\_\_\_

## **SERMACS 2021**

### **Rules and Regulations for Exposition Booths**

1. **Contract for Space.** The receipt by the SERMACS 2021 of your signed application accompanied by payment for the full amount of the exhibitor fee will constitute a contract for the right to use exhibit space at SERMACS 2021. Cancellations will be accepted only after all available exhibition space has been sold and another exhibitor agrees to purchase the cancelled space. In the event of a fire, strike, or other uncontrollable circumstance, which renders the exhibition area unavailable for use, this contract will not be binding. If such an event happens prior to September 30, 2021 SERMACS 2021 will issue a full refund of the exhibitor fee. If such an event happens after September 30, 2021 SERMACS 2021 will issue a full refund of the exhibitor fee. If SERMACS 2021 goes remote due to covid19, SERMACS 2021 will offer a virtual expo booth, with the difference in fees refunded, or for a full refund if the vendor declines a virtual expo booth.
2. **Space Assignment.** SERMACS 2021 will endeavor to honor your choice of exhibit space based on the date of receipt of the completed exhibitor application. In the event that your preferred choices have already been assigned, the SERMACS 2021 will assign booths as equitably as possible, in accordance with the exhibitor preferences. SERMACS 2021 reserves the right to rearrange booth space for flow. In such a case, as equivalent of a booth as possible will be assigned and your contact person consulted.
3. **Space Rental and Fees.** All booths will be 10 feet by 10 feet. Standard booth furnishings will include a 6-foot topped and skirted table, two banquet chairs, one wastebasket, one identification sign with booth number, and general overhead illumination. Prior to September 30, 2021, the rental fee for a single manned booth is \$1000, and for a double manned booth it is \$1800. On or after September 30, 2021, the rental fee for a single manned booth is \$1200, and for a double manned booth it is \$2000. Rental of a manned booth includes two complimentary exhibitor badges. The rental period for vendor expo booths will be from 8 am Thursday November 11 to 4 pm Friday November 12, 2021. The rental fee for a single manned graduate school booth is \$300 and a double booth is \$500. The rental period for graduate school booths will be from 8 am November 13 to 4 pm November 13, 2021.
4. **Additional Furnishings and Supplies.** Additional furnishings and supplies, internet and telephone access, and electrical power may be arranged in advance of the meeting through the Birmingham Sheraton (see SERMACS2021.org website for the required forms). A listing of these extra services and credit card authorization will be provided with your booth confirmation.
5. **Shipping and Handling of Shipping Crates.** Exhibitors have two options: A.) Bring your display materials with you when you arrive to set up your exhibit. Exhibitors should also bring equipment to move their materials to the exhibit area (e.g. cart or flat bed, etc). All materials must enter through the loading dock entrance. They should clear their vehicles from the loading dock area within 10 minutes. B.) Ship your materials to the Birmingham Sheraton to have them delivered at the time of setup. Shipments should arrive within five (5) business days of the event and be schedule for return shipment within 24 hours after the event. Handling fees will apply for all out bound shipments. Hotel shipping forms must be completed for out bound

shipments along with a form of payment. All shipping and handling costs are the responsibility of the exhibitor.

The same two options apply, in reverse, for removal at the end of the exhibition.

6. Installation and Dismantling of Exhibits. Vendor Exhibitors may set up their displays and other materials from 12:00 pm to 5:00 pm on Wednesday, November 10, 2021. All exhibit setup work should be completed before the exposition's opening time of 8 am on Thursday, November 11, 2021. Unoccupied exhibit space may be reassigned after 5:00 pm on Wednesday, November 10, 2021 without refund of any space rental fees that may have previously been paid for it. Dismantling of exhibits shall begin after the closing of the exposition at 4:00 pm on Friday, November 12, 2021. All exhibit materials must be removed by 6:00 pm on this same day. Graduate School Exhibitors may set up their displays and other materials on Saturday, November 13, 2021 beginning at 7 am and remove them by 4:00 pm Saturday, November 13, 2021.

7. Space Restrictions. All demonstrations, discussions, and other activities such as the distribution of descriptive literature of any kind, must be confined to the exhibitor's own booth or otherwise approved area. No exhibitor shall assign, sublet, or share the whole or any part of their assigned space without prior approval of SERMACS 2021. Booth displays should not be placed in such a manner as to interfere with other exhibitors. No tall sidewall shall project forward farther than 36 inches from the main back wall, and no equipment of abnormal height (greater than 8 feet) shall be allowed along the sides. There shall be no obstruction of the aisles.

8. Fire Precautions. All materials used for the displays must be flame retardant. Fire fighting and emergency equipment shall not be hidden or obstructed. All packing containers and similar shipping materials shall be removed from sight upon completion of the booth setup. Small items may be stored under the table, if hidden by a table skirt. Large items shall be stored by prior arrangement, in advance of the meeting, by the Birmingham Sheraton. All electrical work and wiring must be approved and installed in accordance with the underwriters code, local codes, and the directions of the Birmingham Sheraton.

9. Protection of Birmingham Sheraton Property. No items of any kind shall be glued, tacked, nailed, screwed, taped, or otherwise attached to the columns, walls, floors or other parts of the hotel or convention center building or to any of its furniture except that power cords may be duck-taped to the floor for safety purposes.

10. Liability. The exhibitor assumes the entire responsibility and liability for losses, damages, and claims arising out of the activities of the exhibitor and their agents. The exhibitor will indemnify and hold harmless the Birmingham Sheraton, the Auburn Local Section of the American Chemical Society, the Alabama Local Section of the American Chemical Society, SERMACS 2021, SERMACS, Inc., the American Chemical Society, and their agents and employees, from any and all such losses, damages and claims. The Birmingham Sheraton and its staff will provide a normal level of building security during the meeting. However, neither the SERMACS 2021 nor the Birmingham Sheraton can provide guarantees against losses of any kind.

11. Exhibitor's Badges. Each manned booth exhibitor will receive two exposition-only badges as part of registration. The names of each person should be listed on the booth

application form. The exposition chair, Cindy Willingham, should be notified of additions and deletions to this list. These meeting badges will admit exhibitor representatives to presentations of all SERMACS 2021 sponsored functions through Wednesday afternoon, except the technical sessions. However, exhibitor representatives with meeting badges will need to pay any extra event admission fees to “ticketed” events on the same basis as all other registered meeting attendees.

12. Admission to Exposition Area. Admission to the Exposition Hall will be limited to those wearing a SERMACS 2021 or Exposition-Only badge, except for staff and employees of the Birmingham Sheraton, who will also be admitted to the hall.

13. Exposition Hours. The two-day vendor exhibition is scheduled for Thursday, November 11, 2021 from 8:00 am until 5:00 pm, and Friday November 12, 2021 from 8:00 am until 4:00 pm . The graduate school fair is scheduled for Saturday, November 13, 2021 from 8:00 a.m. until noon. These exposition hours may be revised at a later date. Exhibitors of manned booths are expected to have at least one representative present at their booth during these hours, they are free to staff their booths with additional representatives as they see fit.