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 (Starleetah 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 (which now re-directs to 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

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

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

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

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**

Beatriz Vega , K-12 Program Co-Chair, is a Research Fellow in the Forest Products Development Center in the School of Forestry and Wildlife Sciences at Auburn University. ibv0002@auburn.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

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

Jackie Nikles, Undergraduate Program Co-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

Jonathan Meyers, Undergraduate Program Co-chair, is an associate chemistry professor at Columbus State University. Jonathan organized undergraduate symposia, and raised sponsors for them. meyers_jonathan@columbusstate.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

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

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 will remain active for at least two

more years so that future meeting webmasters can look for design ideas. 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

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

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. Starleetah 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.

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 physis 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.

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 Thornell (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)
MitKEl Santiago
Jordan Poler
Pravin Kotian

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

ACS Chemistry for Life®
American Chemical Society

2021

Southeast Regional

ACS AWARDS PROGRAM

NOVEMBER 10-13, 2021

Hosted by the Alabama & Auburn Local Sections of ACS

2021
Southeast Regional
ACS AWARDS PROGRAM

Program Agenda

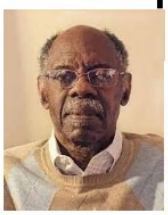
12:00 PM
Welcome Remarks & Meal Service

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



Award Recipients

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 Toxics 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.

ACKNOWLEDGEMENTS

ACS Committee on Minority Affairs
ACS Division of Chemical Education

PARTNERS IN PROGRESS & PROSPERITY 2021

Dr. Travis Thornell 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. Thornell 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. Thornell 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.

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

The 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**.

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.**

SERMACS 2021 AT A GLANCE

- **Dates:** Nov. 10–13
- **Location:** Birmingham, Alabama
- **Information contacts:** General cochair Tracy Hamilton hamilton@uab.edu
- **Website:** 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**. 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**.

Exhibitors SERMACS 2021 - SERMACS 2021

Awards. Several awards will be presented at the meeting. These include the Stanley C. Israel 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 Breaux, 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.

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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 Breaux. 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+/K+ 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 IIα. 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_2 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_{430} 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-Gzegozewska, 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, l. 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. Safiarian

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_3 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^{2+} 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. Karbalaei**, 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_2 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-chymotripsyn-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-Gzegozewska, 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-Gzegozewska, 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 Emssions Using Python Machine Learning Tools.. **D.T. Daly**

4:00 107. Asymmetric glycerol derivatives: Synthesis, properties, and application in CO_2 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. Scearce, B. Holmes, A. Lee

3:40 116. CO_2 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 Macrocycle. **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. Bejger**, 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 Ionenes: 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. Rupar

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

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 Ionenes. **K. Watson**, P. Rupar

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

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 lV, 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-Organelle 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. Welsher

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 VEVE 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 inTrifluoromethoxylation 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, $(CF_3)_2CHOCH_2F$. X. Liu, C. Liu, A.V. Matsnev, P.V. Jog, M. Ulman, **J.S. Thrasher**

10:20 177. Real-time Dermal Sorption of ^{18}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}Co γ-radiation on the Tetrafluoroethylene/ Perfluoro(methyl vinyl ether) Copolymer. **M.P. Confer**, S.R. Allayarov, D.A. Dixon

11:20 179. Comparison of [^{18}F]FDG with ^{18}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-M_1dG 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-FunctionalTight-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_2 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 $2e^-$ 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^0 Titanocenes. **H. London**, D. Pritchett, C. McMillen, G.C. Shields, P.S. Wagenknecht

11:00 201. Self-Sensitized Photocatalytic CO_2 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. Eletsky, 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 Lability 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. Gulledge, 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 Triflouromethylations. **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_2 Reduction and the Oxygen Evolution Reaction. **H. Pan**, C. Barile

8:30 218. Photocatalytic Reduction of CO_2 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_2 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 $LaFeO_3$ 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 SiO2 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_2 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_2 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. Rupar

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 Spectrocopy.. **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. Jarocha**, 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 Communites for Bioremediation of Uranium Contamined 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. Stereoseletive Desymmetrization of Nitriles to Lactones via the Pinner Reaction. **J. Frost**, K.S. Petersen

300. Synthesis of Tetraarylphosphonium/Tetrakis(pentafluorophenyl)borate (TAP^R/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_2-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 β-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 Phenylpropiolic 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 *α*–Allyl–*α*–Trialkylsilyl–*γ*–Alkyl–*β*,*γ*–Unsaturated Carboxylic Acids via an Ireland–Claisen rearrangement. **C. Massey**

319. Epoxidation and Ring Opening of α-Trimethylsilyl-β,γ-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_2O-rich Ices Containing NH_3 and CO_2 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. JimÃ©nez**

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 Heteroarenium 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_2 Affinity and Reactivity in Sensor Globin Domains. **E.E. Weinert**

2:10 363. Towards Understanding why the TxtE $\{FeO_2\}^8$ 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 Extracelluar Vescicles 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 <20µm. **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^{pro} 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 RhO^{2+}, Its Ammoniated Complexes $(NH_3)_{1\text{-}5}RhO^{2+}$, and Mechanistic Exploration of 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 Pi-acid Catalyzed Allylic Substitution: a Complement to Pi-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_2 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. Cliffel**, 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 β-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 β-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. Pyrrophens and Pyrropyridines: Hexadentate Coordination systems for Uranyl 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. Bacsa, C.E. MacBeth

443. Magnetic Structure of Chain Antiferromagnets MBi_4S_7 (M = Mn, 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 $NaLnS_2$ (Ln = La, Ce, Pr, Eu, Er, Yb, Lu). **F.I. Danladi**

452. Production of ^{52}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}Sc Radioisotopes via Enriched [^{46,50}Ti]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 $Cd_{(1-x)}Cu_xCr_2S_4$ 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. Fratarcangeli**, M. Rathbone, C. De Silva

459. Zr-MOFs as a Platform for Nuclear Waste Sequestration. **K. Park**, N.B. Shustova

460. Dynamically and Statically 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 $Au_{30-x}Ag_x(S\text{-}t\text{Bu})_{18}$. **K.H. Wijesinghe**, N. Sakthivel, T.C. Jones, A. Antonysamy

464. Short-range Ordered 2D Phases and their Electronic Properties in $Nb_xV_{1-x}O_2$. **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 ultrasmall 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, $[(NCCH_3)_4RuPh(P\{OCH_2\}_3CEt)][BArF']$ 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 Macrocycle 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. Yezierski

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 ΔH_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 igands in High-valent Actinide Complexes. **J. Niklas**, J. Bacsa, 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 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 α-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 Metallohinged Ligands. **J.A. Pienkos**, J.P. Lee, C.D. McMillen, S.L. McDarmont, L.D. Jaques, B.D. Nessell, S.E. Neglia

10:30 537. New hydroxy substituted Salen-type Pd and Pt complexes: Spectroscopical properties, Structural characterization, DFT calculations, and CO_2 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 Dipyridyl- 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_2-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 Heterogenous 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_2.. **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. Cojocaru

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 Phosphatrane 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 Psoriasin 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. Bacsa, 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 IIα. **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. Knoeferl, 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: H_2SO_4-HCOOH-H_2O and H_2SO_4-HNO_3-H_2O. **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 H_2SO_4-NH_3-$(H2O)_n$ 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. Kerpal, 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, Quinolinyl, 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 σ-holes. **D. Devore**, T.L. Ellington, K.L. Shuford

650. σ-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 Fc/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 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. Wiser, 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 Themodynamic 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 Ionenes 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_2 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 Electrospray 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. Landge**, 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 Husseini**, 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 ($CaOCH_3$) and calcium ethoxide ($CaOC_2H_5$) 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_2'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 Multidenatate 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 Azamacrocycle 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_2 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 Furopyridone 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^{2+} 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 *stk1* 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 $(C_2A)_6$. **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 Sytheses. **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 Aminotroponiminate 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 $H_5O_2^+$ 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. Diliora**, **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. Cojocaru

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 Cu2-xSe 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_2 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_3O_4 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. Gómez 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 Mudiyanselage**, 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. Gómez 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—$[Co(acac)_x(acac\text{-}Cl)_{3-x}]$, 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. Viloria, 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 Iteractions. **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 π-SnS to $Cu_{1.8}S$. **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 β-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 (5*Z*)-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-butanesulfonamide 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_{10}^{6+} 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. Stanisauskis, 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 Luminescencent 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. Fratarcangeli, 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 Quinolinyl 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 a-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 β-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 Dicarbonyls with Borohydride. **J. Butler**, D.A. Clabo

1052. Supported Ionic Liquid Strategy for Emergent Liquid Asthma Medications. **D.M. Cotter**, O.A. Cojocaru

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 $Ni(^{EtIm}PDI)^{2+}$ 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 Aompounds 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 sclerotialus 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 $CuCrO_2$. **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 $CuGaO_2$ 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 Zn^{2+} Coordination. **K. Hanson**, S. Ayad, E.S. Knorr

2:35 1085. Characterization and Applications of Binding of Cyanine Dyes to Biomoleules. **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}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}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 Opoid 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. Sczepanski

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-Epoxycyclopentanols 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. Viijayan**, 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 Cellullose 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 Metallohinged *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. Cojocaru, T.W. Majors

1176. Synthesis of α,β-unsaturated lactams via oxidative-elimination using $NaIO_4$. **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 $Au_{25}(SCH_3)_{18}^-$ and its Activation of 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. Jarocha

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. Jarocha

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 Biotoxicity 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 Enviromental 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-methylanthracene 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. Kerpal, S.H. Foulger, L. Jarocha

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

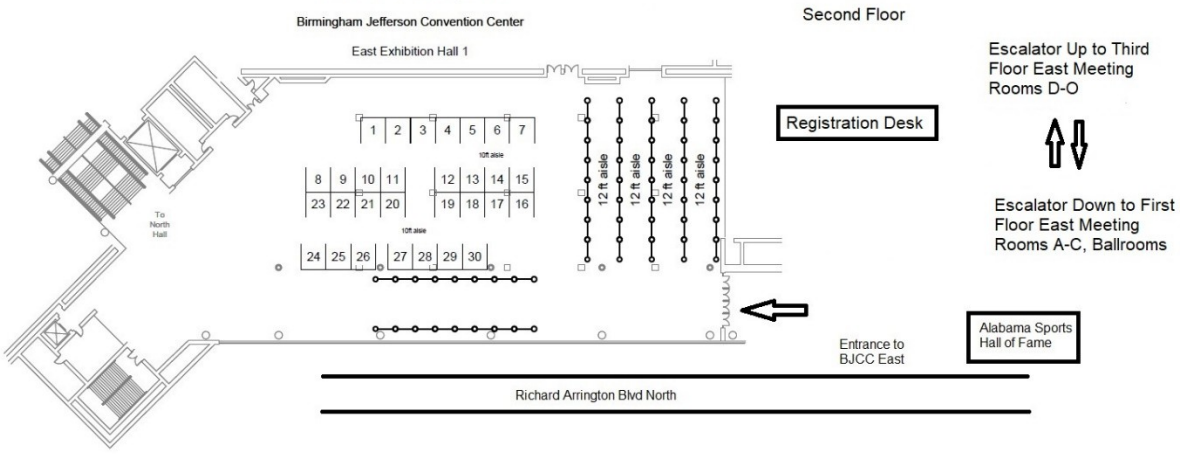
Plenary

T. P. Hamilton, *Presiding*

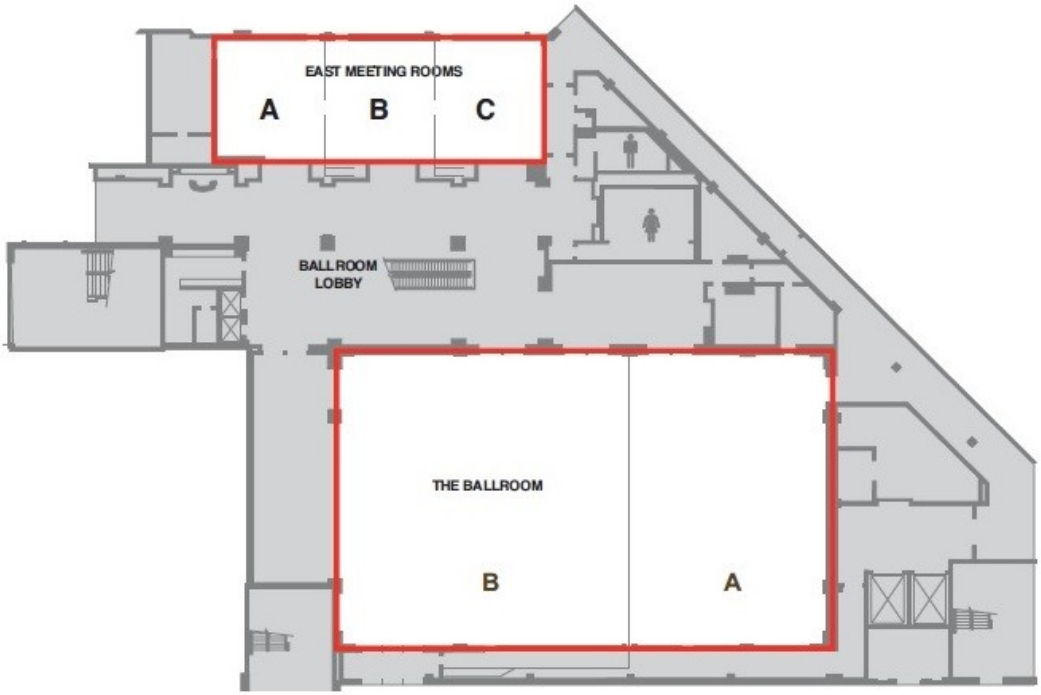
5:30 1224. A Career in Science: Expect the Unexpected. **L.J. DeLucas**

SERMACS

November 11-13, 2021



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 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 Garrision, 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

Intergrating 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

	SERMACS WORKSHEET 2021										
3	Category	% Registrants	# Registrants	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	50 Year Member	0.5	6	$0	$0	$0	$0	$0	8	$0	$0
5	Member, Advance	25	300	$165	$165	$180	$185	$55,500	268	$185	$49,580
6	Member, Onsite	2.3	27.6	$200	$200	$225	$230	$6,348	103	$230	$23,690
7	Nonmember, Advance	3.5	42	$220	$220	$250	$255	$10,710	24	$255	$6,120
8	Nonmember, Onsite	1	12	$275	$275	$300	$305	$3,660	25	$305	$7,625
9	Guest of Registrant, Advance	1	12	$25	$30	$30	$30	$360	11	$25	$275
10	Guest of Registrant, Onsite	1.2	14.4	$50	$40	$40	$40	$576	0	$25	$0
11	Member Ret/Emeritus/Unemployed, Advance	1.2	14.4	$10	$40	$40	$40	$576	6	$40	$240
12	Member Ret/Emeritus/Unemployed, Onsite	0.2	2.4	$30	$60	$60	$60	$144	2	$60	$120
13	Member Precollege Teacher, Advance	1.8	60	$10	$30	$30	$30	$1,800	13	$30	$390
14	Member Precollege Teacher, Onsite	0.3	5	$25	$50	$50	$50	$250	3	$50	$150
15	Nonmember Precollege Teacher, Advance								17	$30	$500
16	Nonmember Precollege Teacher, Onsite								5	$50	$250
17	Member Graduate Student, Advance	18.5	222	$75	$70	$80	$80	$17,760	144	$80	$11,520
18	Member Graduate Student, Onsite	2.1	25.2	$100	$90	$100	$100	$2,520	72	$100	$7,200
19	Nonmember Graduate Student, Advance								113	$80	$9,040
20	Nonmember Graduate Student, Onsite								44	$100	$4,400
21	Member Post doctorate, Advance	2.2	26.4	$100	$100	$120	$120	$3,168	21	$120	$2,520
22	Member Post doctorate, Onsite	0.3	3.6	$135	$135	$140	$140	$504	7	$140	$980
23	Nonmember Post doctorate, Advance	0	0	$120	$120	$140	$140	$0	9	$140	$1,260
24	Nonmember Post doctorate, Onsite	0	0	$155	$155	$160	$160	$0	6	$160	$960
25	Member High School Student, Advance	1	12	$10	$10	$10	$10	$120	1	$10	$10
26	Member High School Student, Onsite	1	12	$10	$10	$10	$10	$120	0	$10	$0
27	Nonmember High School Student, Advance								6	$10	$60
28	Nonmember High School Student, Onsite								0	$10	$0
29	Member Undergraduate Student, Advance	30.4	364.8	$30	$50	$60	$60	$21,888	113	$60	$6,780
30	Member Undergraduate Student, Onsite	5.5	66	$50	$70	$80	$80	$5,280	58	$80	$4,640
31	Nonmember Undergraduate Student, Advance								112	$60	$6,720
32	Nonmember Undergraduate Student, Onsite								67	$80	$5,360
33	1 session "Framily" of UG or Grad presenter	1	12	$5	$5	$5	$5	$60			$0
34	Adjustments*										$ (540.00)
35	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

	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

	SERMACS 2021 Budget			
	LINE ITEM	**BUDGET**	**ACTUAL**	**NOTES**
G. Luncheon Tickets		$ -	$ -	See banquet tickets
H. Mixer tickets cash bar		$ 2,000.00	$ -	Charge based on bar prices per drink, taxes, gratuities,& cost of bartender
I. Exposition		$ 40,000.00	$ 14,400.00	40 booths x $1000 revenue/booth. See layout and contract for details
J. Advertising revenues		$ -		
K. Graduate fair booths		$ 9,000.00	$ 9,300.00	30 @ $300
	TOTAL REVENUES	**$ 217,094.00**	**$ 233,350.65**	
EXPENSES				
A. Committee Expenses				
1. Meetings		$ -	$ 31.61	
2. Postage, supplies, misc.		$ 2,500.00	$ 359.85	
3. Travel expenses 2020		$ -	$ -	covid canceled 2020 SWRM-SERMACS
B. Printing/Publicity				
1. Regional Meetings APP		$ 5,000.00	$ -	To ACS for app
2. Flyers - printing/mailing/postage		$ 2,000.00	$ -	
3. Web page design		$ -	$ 182.83	
4. Ads in local section pubs		$ 500.00	$ -	check with CERM, D.C. etc different local sections
5. Call for Papers in C&EN		$ 720.00	$ -	
6. Promotional Items		$ 5,000.00	$ 3,375.00	Promotional Give-Aways, etc
7. Miscellaneous		$ 2,000.00	$ -	Miscellaneous
C. Meeting Site Expenses				
1. Space Rental/Facility Charge		$ 21,600.00	$ 16,738.44	see contract (+ 23% service charge, then sales tax 10% on total)
2. Audiovisual Services - basics		$ 40,000.00	$ 45,840.05	PSAV contract with ACS, 20% discount
3. Audiovisual Services - special		$ -	$ -	Allowance for possible special requests from guest speakers and/or LCDs
4. Signage		$ 1,250.00	$ -	
5. Facility liability insurance		$ -	$ -	included in ACS umbrella package
6. Poster Sessions		$ 2,000.00	$ 930.55	Posterboard rental (need to check on cost)
7. Hospitality Suite*		$ 500.00	$ -	Room provided in contract; stock with water; soft drinks, and snacks
8. Internet Access		$ -	$ 1,253.70	Internet access in Meeting Rooms ?
9. Miscellaneous		$ 2,000.00	$ 349.30	

D. Program				
1. Symposia Grants	$ 25,000.00	$ 38,583.78	50 session max @ $500	
2. Complimentary registrations				
2a. LOC	$ 1,850.00	$ -	10 at $185	
2b. Volunteers	$ 3,850.00	$ 900.32	10 at $185 , 10 at $80, 20 at $60	
2c. Symposium Chairs	$ 8,325.00	$ -	45 invited get one registration at $185	
3. Plenary Speakers	$ 4,000.00	$ 8,854.32		
4. Awards Expenses	$ 1,000.00	$ -	Plaques/Cash Awards	
5. Postage for mailing plaques	$ 200.00	$ -		
E. Registration				
1 Telephone lines	$ -	$ -	Local Access and 800 # Only for use at registration area	
2. ACS -on-line registration processsing fee	$ 4,800.00	$ -	$4 fee/registration	
3. Credit card fees	$ 1,700.00	$ -		
F. Return of loan	$ 5,000.00	$ 5,500.00	Equals item A and/or B under revenues.	
Subtotal - non-discretionary expenses	**$ 140,795.00**	**$ 122,899.75**		
G. Exposition			Offset by revenues	
1. Decoration	$ 3,500.00	$ 2,865.50		
2. Exhibitor Prospectus Brochure	$ -	$ -	SERMACS Website	
3. Postage, phone expense	$ 300.00	$ -		
4. Space Rental	$ -	$ -	see C. 1.	
5. Security	$ 500.00	$ -		
6. Prizes/Contests	$ 1,000.00	$ -		
7. Miscellaneous	$ 1,000.00	$ -		

71				
72	**H. Special Events/Activities**			$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 @ $10
84				
85	**TOTAL EXPENSES**	**$ 200,195.00**	**$ 167,425.80**	
86				
87	**NET**	**$ 16,899.00**	**$ 65,924.85**	
88				
89	* count towards contracted food and beverage minimum of $34,000			minimum $34,000 + 33% tax and charges = $45220
90				
91	**Distribution**			
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	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

Booth	University	Booth	University
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*]

	1st choice	2nd choice	3rd choice
Booth reservation number			

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 Patkowski
Graduate Fair Chairman, SERMACS 2021
Department of Chemistry and Biochemistry
Auburn University
179 Chemistry Building
Auburn, AL 36849

kip0013@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.

	Send Booth Confirmation and additional information to:	**Person Responsible for Booth Set-up on Saturday Nov. 13:**
Company		
Contact Person		
Address		
Phone/FAX		
email		

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 Birmigham, 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,*

	1st choice	2nd choice	3rd choice
Booth reservation number			

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 Payment Information To:

Cindy Willingham
Exposition Chair, SERMACS 2021
UAB AMSTI
1720 2nd Ave South
Birmingham, Alabama 35294

205-934-4011 cwilling@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.