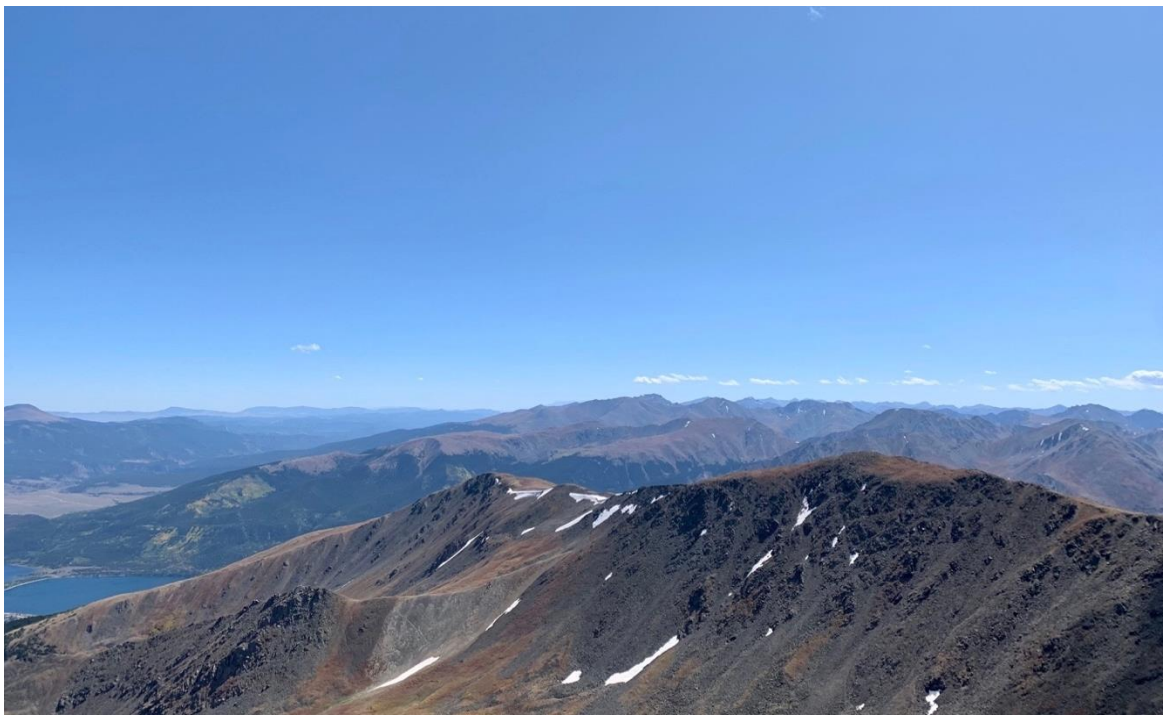
Colorado ACS Local Section Presents:

2020 Rocky Mountain Regional Virtual Meeting Book of Abstracts

Celebrating 100 Years of Chemistry in the Rockies

November 10, 12 – 13, 2020

By Kateryna Kostenkova and Debbie C. Crans



The summit of Mt Elbert near Leadville, CO

Colorado State University

Important Links and Contact Information

- Website:
  https://www.rmrm2020.com/

- Twitter:
  @ACS_RMRM_2020 (use the **#RMRM2020** to tag your posts)

- Virtual Platform
  https://premc.org/rmrm2020/

- Contact technical support:
  rmrm2020@premc.org

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Letter from the RMRM Chairs

Colorado State University
Knowledge to Go Places

Dear Participant,

We are delighted to welcome you to the 2020 Rocky Mountain Regional American Chemical Society (ACS) Meeting and help celebrate the 100-year anniversary of the Colorado Section of ACS (COACS). This meeting grew out of the mini meeting that was planned to take place at Colorado State University and also celebrate its 150-year anniversary. However, when it became clear that COVID-19 would prevent an in-person meeting, we converted to a virtual meeting. To develop a Zoom based platform we involved PremC, a French company, to manage our virtual platform and run the meeting for us.

To this end we are virtually presenting you a program which includes "Safety Programming", Programming by Women Chemist Committee, four symposia, and activities that demonstrate what chemists in the Rocky Mountain Region do. The two symposia, "Young Talent in the Rocky Mountains" and "Celebrating Senior Contributions in the Rocky Mountain Region", were specifically selected to be able to present all areas of chemistry. The additional two Symposia "Sustainability" and "Medicinal and Biological Chemistry" were selected to cover several interdisciplinary areas of chemistry.

Have a great meeting. We hope you enjoy it!

Carlos Olivo-Delgardo
Associate Professor
Colorado state University

Debbie C. Crans
Professor
Colorado State University

Ph +1-970-491-1300
Fax +1-970-491-6639
e.mail janice.nerger@colostate.edu

Colorado State University
Knowledge to Go Places

November 10, 2020

Dear 2020 RMRM Participants,

On behalf of Colorado State University, it is my pleasure to welcome you to the 2020 Rocky Mountain Regional ACS Meeting – A Century of Chemistry in the Rockies. This year's meeting brings together scientists from not only the Rocky Mountain region, but from across the U.S. and globe. While I wish you could join us in person here in beautiful Fort Collins, Colorado, I'm confident you will enjoy this year's virtual conference. The organizing committee has put together an exciting agenda with sessions and symposia covering a range of engaging topics. This year's meeting continues the unique tradition of featuring presentations from young talent as well as from senior scholars and providing opportunities for networking with fellow scientists. I hope you will find the meeting enjoyable and productive and that new collaborations are established. Here's to a Century of Chemistry in the Rockies!

Sincerely,

Jan Nerger

Janice L. Nerger, Dean
College of Natural Sciences
117 Statistics Building
Colorado State University

Abbreviate Meeting Program

American Chemical Society 2020 Rocky Mountain Regional Meeting

Nov. 12 -13, 2020

Debbie Crans, Program Chair

Kateryna Kostenkova, Assistant Program Chair

TUESDAY MORNING

Ice-breaker Mixer, Virtual Meeting, 2:00-3:00 pm

THURSDAY MORNING

Young Talent in the Rocky Mountain Region
D. C. Crans, Organizer; D. C. Crans, Presiding; C. J. Olivo-Delgado, Presiding; G. G. Stanley, Presiding Papers 1-6

THURSDAY AFTERNOON

Lunch Plenary
D. C. Crans, Organizer; D. C. Crans, Presiding; Papers 7-9

Sustainability Symposium
G. G. Stanley, Organizer; G. G. Stanley, Presiding; E. Y. Chen, Presiding; Papers 10-17

Senior Chemists Symposium
D. C. Crans, Organizer; R. Noriega, Presiding; H. Zhao, Presiding; M. B. Jacobs, Presiding; Papers 18-33

Young Talent in the Rocky Mountain Region
D. C. Crans, Organizer; C. J. Burrows, Presiding; J. A. Latham, Presiding; C. C. Aldrich, Presiding; J. E. Sabol, Presiding; Papers 34-64

THURDAY EVENING

Thursday Evening RMRM2020 Mixer

FRIDAY MORNING

Senior Chemists Symposium
D. C. Crans, Organizer; M. H. Rakowsky, Presiding; E. L. Clennan, Presiding; Papers 65-70

Medicinal Chemistry Symposium
D. C. Crans, Organizer; A. C. Smith, Presiding; K. Bowman-James, Presiding; A. J. Wiemer, Presiding; M. B. Jacobs, Presiding; Papers 71-93

Young Talent in the Rocky Mountain Region
D. C. Crans, Organizer; G. G. Stanley, Presiding; A. M. Morey, Presiding; S. S. Rocks, Presiding; A. K. Van Orden, Presiding; Papers 94-113

FRIDAY AFTERNOON

Lunch Plenary
D. C. Crans, Organizer; D. C. Crans, Presiding; J. K. Chung, Presiding; M. Braasch-Turi, Presiding; B. A. Hernandez-Sanchez, Presiding; Papers 114-115

Medicinal Chemistry Symposium
D. C. Crans, Organizer; D. C. Crans, Presiding; C. C. Aldrich, Presiding; Papers 117-123

General Papers

D. C. Crans, Organizer; M. Weinrich, Presiding; C. J. Olivo-Delgado, Presiding; K. Kitzmiller, Presiding; N. E. Levinger, Presiding; Papers 124-143

General Papers
D. C. Crans, Organizer; H. Zhao, Presiding; G. G. Stanley, Presiding; J. Carsella, Presiding; R. Noriega, Presiding; Papers 144-169

FRIDAY EVENING

Friday Evening RMRM2020 Award Banquet Mixer

Symposia

Young Chemists in the Rocky Mountain Region

Speakers: Prof. Rodrigo Noriega, University of Utah
Prof. Joseph Zadrozny, Colorado State University
Prof. Dylan Domaille, Colorado School of Mines
Prof. Jean K. Chung, Colorado State University
Prof. Aaron Apawu, University of Northern Colorado
Prof. Jim Carsella, Colorado State University (Pueblo, CO)
Peof. Jeffrew Bandar, Colorado State University
Prof. Melissa Weinrich, University of Northern Colorado (Greeley, CO)
Prof. Naomy Lee, Northern Arizona University (Flagstaff, AZ)

Sustainability Symposium

Speakers: Prof. Eugene Chen, Colorado State University
Prof. George Stanley, Louisiana State University
Dr. Andrew Sutton, Los Alamos National Lab

Senior Chemists Symposium

Speakers: Prof. Gareth Eaton, University of Denver
Prof. James Bamburg, Colorado State University
Prof. B. George Barisas, Colorado State University
Prof. Josef Michl, University of Colorado
Prof. Ellen Fisher, Colorado State University
Prof. Edward L. Clennan, University of Wyoming
Prof. Branka Ladanyi (Nancy Levinger) Colorado State University
Prof. Veronica Vaida, University of Colorado
Prof. John Enemark, University of Arizona
Prof. Ariel Anbar, Arizona State University
Prof. Bruce Parkinson, University of Wyoming

Medicinal Chemistry Symposium

Speakers: Prof. Courtney Aldrich, University of Minnesota
Prof. Gunda Georg, University of Minnesota
Prof. Andrew Wiemer, University of Connecticut
Prof. David Weimer, University of Iowa
Prof. Mark Brown, Colorado State University
Prof. Cynthia Burrows, University of Utah
Dr. Aaron C. Smith, Pfizer Global Research and Development, Groton

Safety Programming

Prof. Peter Dorhout, Kansas State University
Dr. Kim Johnson, Shell Chemicals, Houston
Amy K. Doane and Robin I. Livingston, Corden Pharma Inc., Colorado

Iota Sigma Pi and ACS Women Chemists Committee Programming

Prof. Nancy Levinger, Colorado State University
Prof. Gunda Georg, University of Minnesota

Organizing Committee

The organizing committee is shown from left to right of the Rocky Mountain Regional Meeting 2020:

Connie Gabel – Regional Consultant
Cameron Van Cleave -Treasurer
Carlos Olivo-Delgado – General Chair
Debbie Crans – General and Program Chair
Kateryna Kostenkova – Social Media and Program Assistant Chair
George Stanley – Awards Chair

Letter from the RMRM Organizing Committee

Dear RMRM2020 Participant,

We hope that you will enjoy the activities we have planned for the 2020 Rocky Mountain Regional American Chemical Society Meeting. The program is diverse and although it is intended to highlight the accomplishments of the Rocky Mountain Region, participants are included presentations from individuals from 25 different states as well as South America, Europe, and Australia.

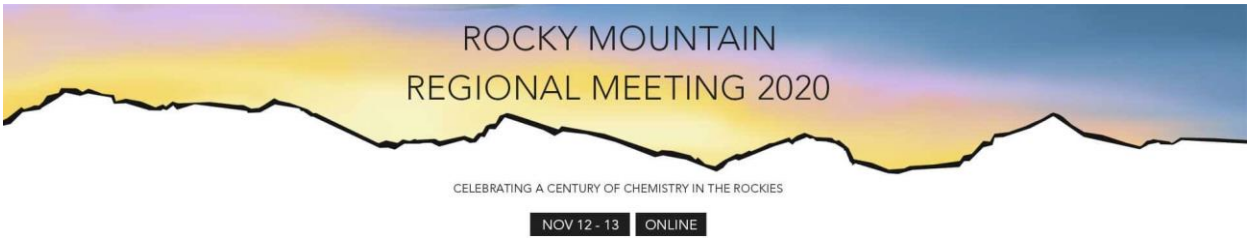
Considering the virtual format, where poster presentations can be really challenging, and that we wanted to give our youngest members a chance to get some live time in front of an audience, we choose to convert the format of posters to “pre-recorded flash presentations” managed by PremC. In this manner, our student presenters will have their questions and answers in real time. In addition to the opportunity to present their work, the flash presentations will be judged and there will be about 25 flash presentation awards. These monetary awards have been funded by the Divisions of Organic, Inorganic, Medicinal Chemistry, Sustainability, Women Chemist Committee, Senior Chemists, and Division of Business for Small Chemicals in addition to the Elsevier Publishers among others.

We also host some non-technical events involving the ACS Regional and National Board, the National Science Foundation, and other activities listed in the final program.

RMRM2020 Organization Committee

Carlos Olivo-Delgado – General Chair
Debbie Crans – General and Program Chair
George Stanley – Awards Chair
Cameron Van Cleave -Treasurer
Kateryna Kostenkova – Social Media and Program Assistant Chair
Connie Gabel – Regional Consultant

Instructions for Participants



Conference Dashboard Conference Rooms 3 Program Instructions for Participants

INSTRUCTIONS FOR PARTICIPANTS

The following information is provided to assist all authors and presenters with the preparation of their presentation and all the attendees in order to ensure smooth participation in this meeting.

Once you are registered, you will be able to access the participants list by using the conference app, no need to set up anything, just click on this link. You have also the opportunity to check the program in your own timezone and build your customized version by selecting the sessions that you are interested in.

For all attendees

☐ Please note that ZOOM will be used during this meeting, we have made a tutorial to explain how to use ZOOM. If you are not familiar with this tool, we highly recommend to test it before the meeting, our team is available to help and schedule a live test with you. Just send us an email to rmrm2020@premc.org.

☐ Please note that all the participants are muted automatically when joining the meeting. To ask a question during the Q&A time, you just have to raise your hand in ZOOM (click here to learn how) and wait for the session chair to unmute you. If you are facing a technical issue, use the chat to get help from the technical chair.

☐ You shall plug in your laptop charger and have your headphones with microphone near you if needed. We highly recommend to use them as a speaker, when you ask a question or in a networking room to ensure the audience hears you well.

☐ You shall set your camera: the best angle for the camera to capture your face is from the eye-level or a little above. If needed, add some books under your computer to reach the appropriate height.

☐ You shall get close to the camera but not too close. The camera should frame your face, neck, and shoulders. Also, you shall be at the center of the frame.

☐ You shall light your face, and darken the space behind you: The light source should come from in front of you. Natural light is highly advised.

☐ You shall pay attention to your background if you are at home and minimize background distractions for the audience. You can also use a virtual background customized to the conference, to do so, you have to go to the "Settings" of your ZOOM App then click on the "Virtual Background" section and add one of these pictures.

☐ You shall modulate your voice, being too slow or too monotone will disengage people. Eye contact with the audience is essential, imagine your audience, and look directly into your computer's camera.

☐ You shall make sure that you are in a quiet environment: check your room acoustics, ensure there is no background noise, dogs barking, people walking by, and more.

☐ You shall make your environment very simple and avoid any distracting object that you could be tempted to play with or touch while you are speaking to the audience like pens, pencils, etc.

☐ If you share your internet connection with others, you shall ask if they can limit their data consumption. You shall make sure the audience is not looking at a blurry or pixelated image.

☐ You shall put your preferred first and last name (as well as pronouns if you are inclined to) as username on ZOOM. A tutorial is available to explain how to rename yourself.

For live presentation
Purple Plenary, Award, & Invited Speakers

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☐ We shall do a test session before you go live to make basic checks (sound, video, and slides). Using the same set-up and being in the same area during the test and live sessions are highly recommended. We kindly invite you to schedule a test session at your convenience here, the test session should last about 5 minut

☐ You shall be connected 15 minutes prior to the first presentation in your session to ensure your connection is working, as well as your device.

☐ Your presentation shall last 45 minutes for the plenary, 25 minutes for the awards and invited speakers, followed by a Questions &Answers sessions of 5 minutes for all speakers. In the interest of fairness, please make sure that your whole session does not exceed 50 minutes for the plenary, 30 minutes for the award and invited speakers. You shall have a timer near you: you either have it on your cellphone or you have one on your computer.

☐ Each live presentation is recorded, if for any reason you would like us to turn off the recording during your presentation then please send your request to this address: rmrm2020@premc.org.

For recorded presentation
Brown Guest Speakers, Red Postdoctoral, Blue Graduate & Green Undergraduate Poster

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☐ You shall follow the tutorial on how to record your presentation and send it to us before **November 6th**. Another tutorial is available toexplain how to transfer your video presentation to us once recorded, please use this email address: rmrm2020@premc.org.

☐ Your presentation shall last 9 minutes for the postdoctoral, 6 minutes for the graduate, and 3 minutes for the undergraduate. The presentation duration is variable for the guest speakers, please check the program in order to get your limit of time. A live Questions & Answers sessions will be held after each cluster of 3-5 presentations, so all the presenters must be present in the room to answer the audience questions. In the interest of fairness, please note that all recorded presentations exceeding these limits will be cut.

☐ You shall keep your slides open and ready to be shared with the audience via ZOOM during the Questions & Answers session following your presentation, just in case a question is related to a specific slide that needs to be displayed for a better discussion.

☐ You shall be connected 15 minutes prior to the first presentation in your session to ensure your connection is working, as well as your device. Even if your presentation is recorded, the Questions & Answers sessions are live so basic checks (sound, video) will be made for y

Meeting Rooms

Pikes Peak Room

Listen to the talks and ask questions.
Open from 8 am to 4 pm (MST) on November 12-13, 2020.

Estes Room

Listen to the talks and ask questions.
Open from 8 am to 4 pm (MST) on November 12-13, 2020.

Horsetooth Room

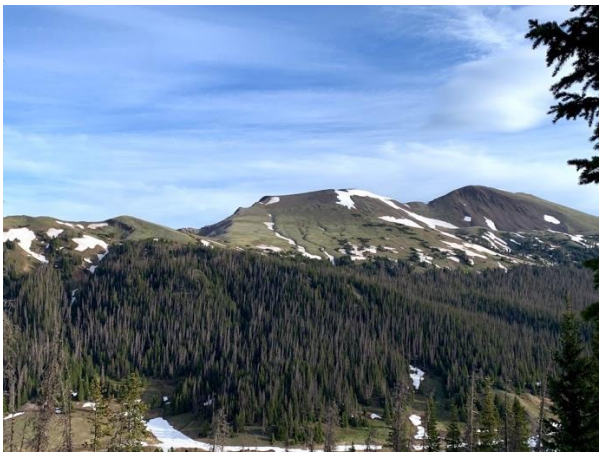
Listen to the talks and ask questions.
Open from 8 am to 4 pm (MST) on November 12-13, 2020.

Durango Room

Attend the ACS Workshops.
Open 30 min before the workshops on November 12-13, 2020.

Devil's Backbone Room

Attend the ACS Workshops.
Open 30 min before the workshops on November 12-13, 2020.



Red Rocks Room

Attend the ACS Workshops.
Open 30 min before the workshops on November 12-13, 2020.

Networking and Break Area

Network in small groups.
Open during breaks and networking sessions on November 12-13, 2020.

Welcome Desk

We would be happy to help you out!
Open from 7:30 am to 4 pm (MST) on November 12-13, 2020.

ACS Career Workshops

Fostering Innovations

Today, keeping pace in an environment of constant change requires continuous innovation. Whether you are in a non-profit, business or academic environment, the ability to contribute to the creation of new ideas, new processes, and new approaches is an important key to personal and organizational success. Yet coming up with new ideas is challenging and few of us have the tools and skills to do this effectively. Fostering Innovation teaches a proven, systematic process to generate ideas. You will gain understanding and tools to help you tap into your own innovation style and learn how to stimulate innovative thinking among team members and colleagues.

ACS Career PATHWAYS: Opportunities for Chemists in the Federal Government

Opportunities for Chemists in the Federal Government provides an overview of the demographics of employment for the federal government. Participants will also learn about the General Schedule (GS) as well as the three types of positions in the federal government. The course will also determine federal coding for chemists and chemical engineers as well provide data about employment by geography, discipline, department, and agency to help participants match job opportunities with their experience, strengths, and values.

ACS Career PATHWAYS: Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value

Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain offers an overview of the job market and job types for industrial chemistry. Participants will also learn how the industrial value chain can be used as a tool to help refine your job search in alignment with your strengths and values. The course will also help uncover key components of job descriptions and participants will learn how to break down job descriptions to best match job opportunities with their experience, strengths, and values.

Laboratory Safety Programming

Empowering Academic Researchers to Strengthen Safety Culture: Thursday, November 12th at 1 – 4 pm MST

A safety workshop organized by Jessica Martin (University of Connecticut) for graduate students. The American Chemical Society is sponsoring a program to help educate graduate students about lab safety culture and opportunities for promoting safety. The participants will be awarded a certificate for completion of the course (can be added on resumes). This three-hour workshop will be led by Sarah Zim (University of Chicago) and Jessica DeYoung (University of Iowa). The purpose of this workshop is to help develop individualized plans for the creation or improvement of student safety programs. You can read more about the results of previous workshops in this Journal of Chemical Health and Safety (K. A. Miller and K. I. Tyler, Journal of Chemical Health and Safety, 2019, 18715532; https://pubs.acs.org/doi/10.1021/acs.chas.8b26309). Other key topics include hazard assessment, risk management, safety management practices, and complementary top-down approaches. This workshop is primarily directed at graduate student issues, but faculty and staff are encouraged to participate.

How to convince others (that safety is important and that you're serious about it): Friday, November 13th at 5:28 pm MST

A safety workshop organized by James Kaufman (Laboratory Safety Institute, LSI) that covers the 33 critical safety program elements. Participants learn how to convince others by creating a more effective lab safety program (without a purchase order or requisition). You don't want to miss this opportunity for a highly informative, worthwhile and enjoyable learning experience!

The Laboratory Safety Institute is an international, non-profit center for safety in science and science education. LSI's lectures and courses, AV-lending library, Mini-Grants, Internet discussion list, and publications help both academic and non-academic institutions in 30 countries and 135 types of labs throughout the world. Over 100,000 scientists and science educators have attended these courses and presentations.

LSI conducts seminars, short courses, webinars, audits and inspections for schools, colleges, and companies. They also provide advice on regulatory compliance, safety program development, facilities inspections with written reports, facilities design, editorial commentary on laboratory texts, and expert witness testimony.

Non-Technical Events: Mixers

Thursday Mixer programming 6:00 pm – 8:00 pm

Hosts Carlos Olivo-Delgado (IT) & Debbie C. Crans (introductions)

6:00-6:30 pm mixer
6:30 pm
ACS President Elect H. N. Chen, Welcome
ACS National Board Chair John Adams, Historial Highlights
ACS Regional Past Chair Donivan Porterfield, Regional Highlights
Past ACS President, Bonnie Charpentier, Safety in Chemistry
ChemClub Colorado State University Chair, Benjamin Reynolds

7:10 pm Distribution into Specialty Rooms

1. Meet the ACS National Board Members
2. Meet the ACS Regional Board Members
3. Colorado ACS Future Communications - Interactive Discussion (Helen Gerhard and Michael Jacobs)
4. NSF – Program officer Mike Adams and Shing Ho
5. Do you want to improve your presentation skills? Susan Morris
6. Ensuring laboratory Safety. James Kaufman

Friday Award Banquet 6:00 pm – 8:00 pm

Hosts: Carlos Olivo-Delgado and Debbie C. Crans

6:00-6:30 pm Pre-Mixer
6:30 pm Brief presentations by:

- ACS National Board Chair, John Adams
- ACS Regional Board Chair, Michael Mosher
- COACS Senior Chemists Committee Chair, Margaret Rakowsky

Award Presentation hosts: Connie Gabel and Michael Mosher

George Stanley RMRM2020 Award Chair introducing Presenters of **Regional Awards**

• **Bonnie Charpentier**, ACS Past President: ***E. Ann Nalley Award for Volunteer Service***

This award was established in 2006 by ACS Past President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism.

• **Matt Jones,** CHED RMR Representative & **Connie Gabel,** RMR Board Awards Chair Presenting ***Regional Award for Excellence in High School Teaching***

The Division of Chemical Education (DivCHED) established an endowment to support Regional Awards for Excellence in High School Teaching in each of the ACS Regions.

• **Connie Gabel & Michael Mosher** presenting the award to ***Partners for Progress and Prosperity (P3) Award*** This award recognizes partnerships among industry, academia, government, small businesses and/or other organizations that result in impactful outcomes.

• **H. N. Cheng,** President-Elect ***ACS Stanley C. Israel Regional Award for Advancing Diversity in Chemical Sciences.*** The Stanley C. Israel Regional Award recognizes individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the ACS Regions.

George Stanley presenter of Conference Awards: Flash Presentations
3 ACS Division of Organic Chemistry Awards
1 ACS Award in Sustainability Award

Carlos Olivo-Delgado
1 Colorado State Chemistry Award
3 ACS awards

Bonnie Charpentier,
1 Helen Gerhard's LLC Company Award
2 ACS Division of Small Chemical Businesses Awards

Margaret Rakowsky
1 ACS Senior Chemists Committee Award

H. N. Chen
3 The Royal Society of Chemistry, New J. Chemistry Awards

Sandra Bonetti
3 ACS Division of Medicinal Chemistry Awards
1 COACS award in memory of John Conolly
1 COACS award in memory of Kim Pacheco

John Adams
3 ACS Division of Inorganic Chemistry Awards
3 Elsevier Coordination Chemistry Awards

Mary Singleton
3 Women Chemists Committee Awards

Michael Mosher and/or Connie Gabel
Innovative Project Grant Awards
COACS awards

Debbie Crans
Chair of COACS's Awards

Michael Mosher will introduction the next team to run the RMRM2021
Closing Comments **Debbie Crans** or **Carlos Olivo-Delgado**

Coaching by Susan Morris

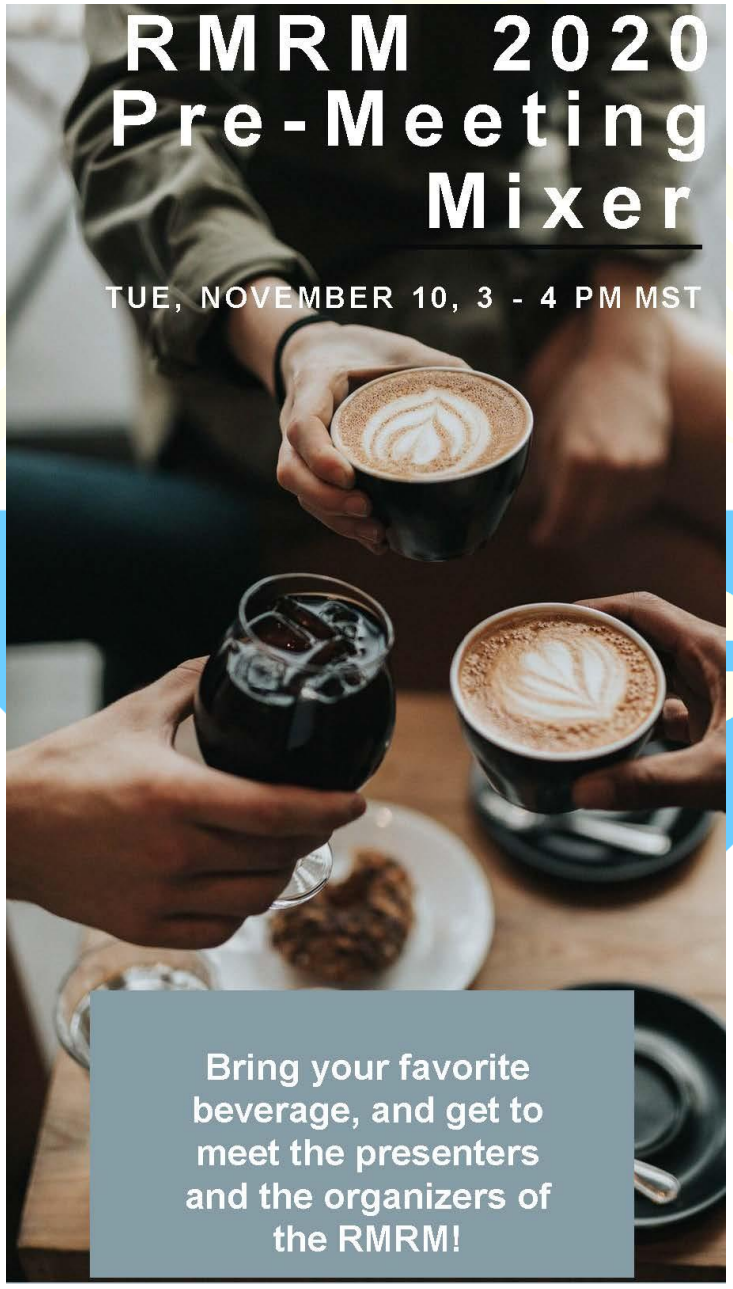
Stand up to stand out: Self-advocacy for the reluctant:
Friday, November 13th at 4:58 pm MST

Susan Morris has been a leadership consultant and professional coach for more than three decades. She has partnered with individuals and teams in the US and globally in the life sciences. Susan's passion is to help STEM professionals fulfill their career potential.

The purpose of her workshop is to uncover the benefits of advocating for oneself and explore alternative behaviors to bragging and boasting. Participants will learn to teach and educate others about their accomplishments, tell their story of triumph and most importantly, practice asking for a deserved promotion or getting recognition of a job well done.

Pre-Mixer

Ice-Breaker Mixer on Tuesday, November 10th 3-4 pm MST
Contact Kate Kostenkova at kostenk@rams.colostate.edu to sign up



Poster (pre-recorded Student Presentations) Prizes

Flash Presentation Awards with no topic target/restrictions

1 Colorado State Chemistry Award
2 COACS Program SEED Awards
1 Helen Gerhard's LLC Company
2 ACS Division of Small Chemical Businesses Award
4 ACS awards – sponsored by several sources
1 ACS Senior Chemists Committee Award
3 Innovative Project Awards
COACS awards (Specific amounts to de determined)
Chair of COAS's Awards

Flash Presentations Awards given to specific topics targets/restrictions

1 ACS Award in Sustainability Award
3 ACS Division of Inorganic Chemistry Awards
3 ACS Division of Organic Chemistry Awards
3 ACS Division of Medicinal Chemistry Awards
3 Elsevier Coordination Chemistry Awards
3 Royal Society of Chemistry Awards, New J. Chemistry
3 Women Chemists Committee award – Female Students – one each of Undergraduate and, Graduate and Post-Graduate Students

Plenary Presentations (by Iota Sigma Pi and Women Chemists Committee)

Biographical Sketches for Career Panel Members

Nancy Levinger, Colorado State University.

Dr. Nancy Levinger is this year's recipient of the COACS Award. She is a professor and a University Distinguished Teaching Scholar (2007) at Colorado State University. She is a fellow of the American Physical Society (APS, 2005), American Association for the Advancement of Science (AAAS, 2010), and American Chemical Society (ACS, 2014). She has received several honors from Colorado State University, especially for her role in education, mentoring, and service.

She earned B.A. degrees from Northwestern University in Integrated Science and Physics (1983), the Ph.D. in Chemical Physics from the University of Colorado (1990), and performed postdoctoral research as a National Science Foundation postdoctoral fellow in the Department of Chemistry at the University of Minnesota (1990-1992). Dr. Levinger joined the faculty at Colorado State University in 1992. Since joining the faculty at Colorado State University in 1992, her work has focused on dynamics of molecules in the condensed phase, especially water in molecular assemblies, molecules at liquid interfaces and in confined environments structure. Her research focus has recently expanded to investigate fundamental processes governing cell cryopreservation with a focus on exploring the fundamental mechanisms of permeating cryoprotectants in cells and model systems.

In addition to her passion for research, Dr. Levinger has a strong interest in educational issues; she has actively incorporated innovative teaching ideas to her courses and the curriculum in the chemistry department at Colorado State University. During her time at CSU, she was the director for the NSF REU program (dates) for the chemistry department for 6 years, renewing the funding for the program twice. For 8 years, she organized and led the Celebrate Undergraduate Research and Creativity showcase poster session (2003-2010) and continues to serve on its organizing committee. In 2015, an endowment to CSU by her first undergraduate research student honored her with the establishment of the Nancy E. Levinger Undergraduate Research Fellowship.

Levinger has also demonstrated significant professional leadership and service over her career. She founded and chaired the NSF Chemistry REU Leadership Group (2001-2004) She served in the executive leadership of the ACS Division of Physical Chemistry (2012-2016) as well as several national task forces and national award selection committees. She served the APS in the executive leadership of Division of Chemical Physics leadership (2001-2004) including as a councilor (2009-2012) and member of the executive board (2011-2012), as well as a representative and chair to several other

national committees. She has served as chair of two different Gordon Research Conferences (Water and Aqueous Solutions, 2014-2016; Chemistry and Physics of Liquids, 2019-2021). Currently, she leads the Telluride Science Research Center as its president.

Gunda I. Georg, University of Minnesota

Dr. Georg is Regents Professor and Head of the Department of Medicinal Chemistry and the founding Director of the Institute for Therapeutics Discovery and Development (ITDD) at the University of Minnesota College of Pharmacy. She holds the Robert Vince Endowed Chair and the McKnight Presidential Chair in Medicinal Chemistry. She is Editor-in-Chief for the Journal of Medicinal Chemistry, the most cited journal in the medicinal chemistry field. In 2020 she won the Alfred Burger Award in Medicinal Chemistry of the American Chemical Society and she was elected to the American Chemical Society Medicinal Chemistry Hall of Fame in 2017. She is an AAAS Fellow, a Fellow of the American Chemical Society, and has received the Ernest H. Volwiler Research Achievement Award of the American Association of Colleges of Pharmacy, the Sato Memorial International Award of the Pharmaceutical Society of Japan, the University of Minnesota Academy for Excellence in Health Research, and others.

Dr. Georg received a BS in pharmacy (1975) and a PhD degree in medicinal chemistry (1980) from Philipps University in Marburg, Germany. She was a postdoctoral fellow in the Department of Chemistry at the University of Ottawa in Canada. She started her independent career at the University of Kanas in 1984 and joined the University of Minnesota in 2007. Her research focuses on the design, synthesis, and evaluation of biologically active agents. Current major therapeutic areas are focused on cancer and male contraception.

She is co-inventor of Minnelide™, a prodrug of the natural product triptolide, which has completed a Phase I clinical trial for GI cancers, and has entered a Phase II clinical trial for refractory pancreatic cancer treatment and a Phase I trial for oral treatment of advanced solid tumors in 2017. She is the co-inventor of the marketed anesthetic Lusedra® (Eisai Pharma). She has led major research programs as the PI of a 10-year NIH-funded COBRE Center for Cancer for Experimental Therapeutics at the University of Kansas that supported the careers of junior faculty in the state of Kansas. She currently is the PI of a NIH-supported U54 Contraceptive Discovery, Development and Behavioral Research Center (2017-2021) that involves five research groups from Columbia University, Harvard University, University of Michigan, University of Massachusetts Amherst, and the Moffitt Cancer Center.

Dr. Georg's work is described in 250 publications. She has trained more than 100 PhD and post-doctoral students, most of whom have pursued careers in the pharmaceutical industry. She is actively involved in professional organizations including the American

Chemical Society and the AAAS. She has served for many years as grant reviewer on NIH study sections, for the NSF, AAAS, foundations and universities. She is a member of advisory boards for several scientific journals and universities.

Sandra S. Eaton, University of Denver

Sandra S. Eaton received her bachelor's degree at Wellesley College and obtained her Ph.D. in inorganic chemistry at MIT 1972. She joined the faculty of the University of Colorado at Denver in 1973. In 1990 she moved to the Department of Chemistry and Biochemistry at the University of Denver. In 1997 she received the John Evans Professorship at the University of Denver.

She teaches undergraduate and graduate level classes in analytical, physical, and inorganic chemistry. Since 2008 she has been chair of the Department of Chemistry and Biochemistry. Her research program involves continuous wave, rapid-scan, and pulsed EPR applied to the study of relaxation times, interspin distance measurements, metal ions in biological systems, and EPR imaging. She and her husband, Professor Gareth R. Eaton, have jointly authored over 400 research papers and book chapters. Professor Sandra Eaton and her husband Gareth have previously received the COACS award jointly. In 2002, they jointly received the Bruker prize and in 2008 they became Fellows of the International EPR/ESR Society.

Jaqueline Kiplinger, Los Alamos National Laboratories

Dr. Jaqueline L. Kiplinger is currently a Laboratory Fellow & Senior Scientist at Los Alamos National Laboratory (LANL) as part of the Inorganic, Isotope and Actinide Chemistry (C-IIAC) group. She is also a fellow of the American Chemical Society, the American Association for the Advancement of Science, the Royal Society of Chemistry, and the American Institute of Chemists. She received a B.Sc. in chemistry in 1990 from the University of Colorado, and a Ph.D. in organometallic fluorocarbon chemistry in 1996 from the University of Utah. She spent two years as a Presidential PD Fellow at the University of California, Berkeley before joining LANL as the Lab's first Frederick Reines Distinguished PD Fellow in 1999. She joined LANL as a Technical Staff Member in Chemistry Division in July 2002.

At LANL, she has been a pioneer in the development of inexpensive, simple and safe techniques to make rare earth and actinide halide starting materials, which has been critical to advancing the synthetic and mechanistic chemistry of these important elements and for understanding their behavior in a variety of applications.

She has authored over 100 publications in refereed journals and has 5 issued patents. Her chemistry research has been recognized by numerous LANL, NNSA, and R&D 100 awards. In 2015, she was selected as the first woman to receive the American Chemical Society (ACS) F. Albert Cotton Award in Synthetic Inorganic Chemistry. More recently,

she was honored and named a recipient of the University of Utah Distinguished Chemistry Alumni Award (2016), the Iota Sigma Pi Violet Diller National Award for Professional Excellence in Chemistry (2017), and IUPAC International Distinguished Women in Chemistry Award (2017). Her excellence in mentoring students and postdocs has been recognized by several LANL Student (2010) and Postdoctoral (2007, 2013) Distinguished Mentoring Awards.

Jennifer Maclachlan

As a co-owner of her family owned and operated small chemical business, PID Analyzers, LLC, Jennifer Maclachlan is responsible for managing relationships with distributors and key clients as well as the web-based marketing, social, and digital media initiatives, of which she was an early adopter.

In 2018, Maclachlan completed three years of service to the ACS as Chair of the American Chemical Society (ACS) National Committee on Public Relations and Communications (CPRC) and is currently serving as an Associate to the Committee on Chemical Safety as well as Public Relations Chair for the ACS Division of Small Chemical Businesses. She is a founder of the Cape Cod Science Café, which she started in 2011, with support from the Northeastern Section of the ACS (NESACS) and an International Year of Chemistry (IYC2011) mini-grant. STEM Journey, of which she is a founding member and organizer, is an award-winning K–12 annual public outreach, day-long event with collaborative efforts from the ACS Local Section (NESACS), the Cape & Islands Boy Scouts, Sandwich STEM Academy, and PID Analyzers, LLC.

Helen Gerhard, Helen B Gerhard, LLC.

Helen Gerhard is an Alternate Councilor for the Colorado section of the American Chemical Society and is the chair of the Communication Committee for the section. For the past year she has worked to develop a better web-site for the Colorado Section that will help in communication is a large state as Colorado. Helen received her B.S. in Chemistry from the University of Colorado, Colorado Springs.

Her first job out of university was with ManTech Environmental working on a project for the Department of Energy to test alternatively fueled vehicles at altitude for a project to predict the results of moving toward an alternative fuel infrastructure. After this project came to an end, she began working in the Medical Device Industry as a Quality professional, which she continues to do. She holds a M.B.A. in Technology Management from the University of Phoenix, a graduate certificate in Government Contracting from Webster University, and is certified through the American Society for Quality (ASQ) as a Manager of Quality/Organizational Excellence and through both ASQ and Exemplar

Global a Lead Quality Auditor. Since 2011, she has been self-employed through her company, Helen B Gerhard, LLC.

Full RMRM2020 Program (updated Oct. 26th)

Color codes: Invited speaker; Guest speaker; Post Doc; Grad; Undergraduate

1. Noon purple Plenary and award speakers, one is 45 min with 5 min Live Q&A follow the presentations; others are 25 min live presentations – 5 min Live Q&A follow the presentations

2. Purple session: invited speakers, most are 25 min live presentations – 5 min Live Q&A follows the presentations

3. Brown: guest speakers with variable times of recorded talks – these presentations are spread around the program and Live Q&A follows the cluster of presentations (3-5 talks)

4. Red: Postdoctoral pre-recorded presentations, 9 min recorded talk – Live Q&A follows the cluster of presentations (3-5 talks)

5. Blue: Graduate pre-recorded presentations, 6 min recorded talk – Live Q&A follows the cluster of presentations (3-5 talks)

6. Green Undergraduate pre-recorded presentations, 3 min recorded talk – Live Q&A follows the cluster of presentations (3-5 talks)

RMRM2020 Nov. 10, 12 and 13

Debbie Crans, *Program Chair*

Kateryna Kostenkova, *Assistant Program Chair*

TUESDAY AFTERNOON

Pre-meeting Icebreaker Mixer

3:00-4:00 pm Information on meeting details and getting to know your co-attendees

THURSDAY MORNING

Welcome Room

8:00 -9:00 am Information and welcome bag

(1) Pikes Peak

Opening Ceremony

8:45 Welcoming Words and Information on Symposium

Debbie C. Crans, Carlos Oligo Delgado and Dean Janice Nerger, Colorado State University

(1) Pike's Peak

Young Talent in the Rocky Mountain Region

Young Investigator Symposium

D. C. Crans, *Organizer, Presiding*
C. J. Olivo-Delgado, G. G. Stanley, *Presiding*

9:00 Introduction to Young Talent in Rocky Mountain Region.

9:01 1. Effects of a dynamic local environment on the properties of chemical systems. **R. Noriega**

9:31 2. Toward noninvasive biomedical thermometry with cobalt-59 molecular NMR thermometers. **J. Zadrozny**

10:01 3. Manipulating flux in living cells with biocompatible catalysis. **D. Domaille**

10:31 4. Coupled lipid miscibility and phosphotyrosine-driven protein condensation on membranes. **J.K. Chung**, W. Huang, C. Carbone, L.M. Nocka, A.N. Parikh, R.D. Vale, J.T. Groves

11:01 5. Elucidating the action of abused volatile organic solvent, toluene on the central reward pathway. **A. Apawu**, S.P. Callan, T.A. Mathews, S.E. Bowen

11:31 6. Partitioning of lead in plants, birds and arthropods found on the Colorado Smelter superfund site in Pueblo, Colorado. **J. Carsella**, E.K. Petersen, T. Schiffer, S. Staples, C. Varian-Ramos, M. Diawara

Durango

ACS Workshops

8:00 am Opportunities for Chemists in the Federal Government
10:00 am Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain

Devils Backbone

ACS Workshop

8:00 am Leadership: Fostering Innovation

THURSDAY AFTERNOON

(1) Pike's Peak

Lunch Plenary

Safety in the Rockies

D. C. Crans, *Organizer, Presiding*

12:00 Introduction

12:05 7. Creating a culture of safety in academic laboratories. **P.K. Dorhout**

12:50 8. Standardizing risk management in laboratory and pilot plant facilities: A model. **K. Johnson**

1:25 9. Critical aspects of a robust potent compound containment program. **A.K. Doane**, R.I. Livingston

(1) Pike's Peak

Sustainability Symposium

In Rocky Mountains Region and Beyond

G. G. Stanley, *Organizer, Presiding*
E. Y. Chen, *Presiding*

2:00 10. Towards a circular plastics economy: Design principles and synthetic methodologies for sustainable plastics with tunable properties and chemical circularity. **E.Y. Chen**

2:30 11. Strong Lewis acids slow heterogeneous electron transfer to heterobimetallic ruanyl complexes. **J.D. Blakemore**

2:50 12. Replacing non-renewable carbon with bio-derived alternatives. **A.D. Sutton**

3:20 13. Systematic investigation of graft copolymers as compatibilizers in a poly(styrene)-poly(lactic acid) model system. **O.N. Manahan**, G. Miyake

3:40 14. Plastics upcycling – benefits in manufacturing. **N. Rorrer**

4:10 15. Bifunctional nickel and copper electrocatalysts for CO_2 reduction and the oxygen evolution reaction. **H. Pan**, C. Barile

~~**4:30 16.** Extrinsic atom effects on the anodic properties of one-dimensional TiS2-xSex solid solutions. **R. Weeks**, E.J. Miller, L. Whittaker-Brooks~~
Canceled

4:30 17. Highly active cationic Co(II) bisphosphine hydroformylation catalysts. **G.G. Stanley**

(2) Estes

Senior Chemists Symposium

Celebrating Senior Chemists in the Rocky Mountains and Flash Presentations

D. C. Crans, *Organizer*
M. B. Jacobs, R. Noriega, H. Zhao, *Presiding*

2:00 Introduction of Session.

2:02 18. Reflections on a career built on the foundations of chemistry: From polysaccharides to dementia. **J.R. Bamburg**

2:32 19. Consensus structures of the Mo(V) sites of sulfite-oxidizing enzymes derived from variable frequency pulsed EPR spectroscopy, isotopic labelling and DFT calculations. **J. Enemark**

3:02 20. Porphene: A heterocyclic analog of graphene. T. Magnera, P. Dron, M. Jovanovic, J. Bozzone, E. Miller, W. Bu, **J. Michl**

3:32 21. New two-dimensional organic frameworks for membrane separations. **B.A. Parkinson**, J.O. Hoberg, K. Li

4:02 22. Dynamics and structure of molecular fluids - a tribute to Branka M. Ladanyi. **N.E. Levinger**

4:32 Introduction to Flash Presentations.

4:33 23. Demonstration of the use of NMR spectroscopy for the measurement of vapor−liquid equilibria. **J. Widegren**, C. Suiter, V. Malavé, E. Garboczi, M. McLinden

4:39 24. Rapid vapor collection method for vapor pressure measurements of low-volatility compounds. M. Harries, **C.N. Beuning**, B.L. Johnston, T.M. Lovestead, J. Widegren

4:48 25. Investigation of plasma modified zeolite catalyst on hydrothermal liquefaction of chlorella powder. B. Jang, **T.M. Haque**, M.P. Jaimes, E. Cardenas, K. Largent

4:54 26. Spatio-temporal super-resolution microscopy. **M. Dunlap**, D.P. Ryan, P.M. Goodwin, P. Bourdin, J.A. Hollingsworth, J.H. Werner, M.P. Gelfand, A.K. Van Orden

5:00 Discussion.

5:07 27. Investigating the shape of aerosol-OT reverse micelles and the impact of force field. **C. Gale**, M.D. Molayousefi, N.E. Levinger

5:13 28. Aerogels doped with nanomaterials show improved mechanical strength and potential for expanded application integration with printed structures. **C.J. Hanson**, S.L. Edwards, M.F. Beaux, D.R. Vodnik, C.E. Hamilton

5:19 29. Effect of molecular structure on the properties of self-assembled reverse bilayer vesicles. **O. Villanueva**, A.F. Cozzolino, S. Moaven

5:25 Discussion.

5:32 30. Modeling of unimolecular dissociation constants and reaction energies of ionic liquids: Applications in electrospray propulsion. **J. Deyanova**, B.D. Prince

5:38 31. Bond dissociation energies of transition metal borides. **D. Merriles**, C. Nielson, E. Tieu, M.D. Morse

5:44 32. Can infrared laser break the chemical bonds in viruses?. **C. Yu**

5:47 33. Nature of formal hydride transfer reactivity in mo-dependent formate dehydrogenase. **J. Lepluart**, M.L. Kirk

5:53 Discussion.

(3) Horsetooth

Young Talent in the Rocky Mountain Region

Young Talent in Rocky Mountains and Flash Presentations

D. C. Crans, *Organizer*
C. C. Aldrich, C. J. Burrows, J. A. Latham, J. E. Sabol, *Presiding*

2:00 Introduction to Biomedical, Nanoscinece, Bioanalytical Science and Protein Modifications.

2:01 34. Synthesis, characterization, biological activity against *Trypanosoma cruzi* and metallomics of novel heteroleptic oxidovanadium(V) compounds. **G. Scalese**, I. Machado, L. Perez, D. Gambino

2:10 35. Investigation of decomposition kinetics and anti-cancer activities and of mixed-ligand vanadium complexes. **C. Yigit**, H. Murakami, A. Levina, P.A. Lay, D.C. Crans

2:19 36. Multinuclear NMR studies of anticancerous Non-Innocent Vanadium Schiff Base Complexes showing isomer formation. **A.C. Bates**, H. Murakami, D.C. Crans

2:25 37. In-silico evaluation of DNAJB1-PRKACA fusion proteins binding site. **S. Cabrera**

2:31 38. Automated construction of fragment-based pharmacophores to elucidate novel GPCR ligands. **G.L. Szwabowski**, A.L. Parrill-Baker, D.L. Baker

2:37 Discussion; Nanoscience.

2:47 39. Synthesis and characterization of gold nanoparticles prepared with the flavonoid quercetin. **A. Holm**, M. Watzky

2:50 40. Preparation of gold nanoparticles in novel thioether-functionalized ionic liquids. **E. Kulesus**, **H. Leloup**, M. Watzky, H. Zhao

2:53 41. STM and XPS studies of co nanoparticles on reducible CeO_2(111) thin films. **L. Du**, D.L. Braedt, J. Miao, J. Zhou

2:59 Discussion: Nanoscience and Bioanalytical studies continued.

3:05 42. Nanoconfinement raises the barrier to hydrogen atom exchange between water and glucose. **S.L. Miller**

3:11 43. Direct carbon-carbon bond formation between single-wall carbon nanotubes: Fact or artifact?. **P.S. Senanayake**, M. Talipov

3:17 44. Development of chemical strategies prepare synthetic lasso peptides and their isomers. **L. Digal**, A. Ghorai, M. Mifflin, A.G. Roberts

3:23 Discussion: Bioanalytical Methods continued.

3:31 45. Preparation of apolipoprotein C III peptide antigens for display on virus like particles to combat cardiovascular disease. **N.R. Lopez**, N. Lee

3:34 46. Mapping electrostatic protein-membrane interactions of Slp-4 C2 domains using molecular phylogenetic analysis and structure prediction. **N. Chon**, S. Tran, C. Miller, H. Lin, J.D. Knight

3:43 47. Electroanalytical tools and molecular-based assays to measure the impact of noise on dopamine neurotransmission in the central auditory pathway. **P. Wilson**, A. Apawu

3:49 48. Detection of intracellular HNO delivery via a thiol-functionalized indicator with capillary zone electrophoresis. **A.N. Amarakoon**, D. Plewa, M. Han, N. Ke, C. Janczak, K.M. Miranda, C.A. Aspinwall

3:55 49. Statistical analysis of protein-protein comparison methods. **C. Dyer**, A.L. Parrill-Baker, D.L. Baker

4:01 Discussion: Bioanalytical Studies Continued.

4:10 50. Light-activated quantum dot potentiation of antibiotics to treat drug-resistant biofilms. **D.F. Stamo**, A. Chatterjee

4:16 51. Optimization of the attachment of a base labile fluorescence quencher in designing a triazabutadiene probe to image mosquito larval gut proteins. **W.N. Wijetunge**, L.E. Guzman, J.C. Jewett

4:22 52. Direct visualization of dimethyl sulfoxide permeation in live rice callus cells by coherent anti-Stokes Raman scattering (CARS) microscopy. **F.M. Samuels**, N.E. Levinger, G. Volk

4:28 53. Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: analysis of ligand type and receptor activation state. **B. Thomas**, A.L. Parrill-Baker, D.L. Baker

4:34 54. Investigating the relationship between receptor aggregation and signaling by luteinizing hormone receptor, a G protein-coupled receptor. D. Althumairy, **X. Zhang**, N. Baez, B. Barisas, D. Roess, G.R. Bousfield, D.C. Crans

4:40 Discussion: Bioanalytical Studies and Protein modification.

4:49 55. Towards de novo sequencing of the human milk glycome: High-resolution cyclic ion mobility separations. **G. Nagy**

4:55 56. Analysis of *Cannabinoids* in natural and synthetic samples. J. Chavez, **D. Spurlin**, R.M. Hyslop, C.E. Brown

4:58 57. Redox potentials of truncated menaquinone analogues in soybean phosphatidylcholine liposomes are sensitive to odd- or even-length of isoprene chain. **K. Doucette**, B. Heritage, C. Beuning, D.C. Crans

5:04 58. Improving enzymatic transesterification activity in functionalized ionic liquid. **C. Toe**, H. Zhao

5:07 59. Substituted decavanadate (V_9Mo) inhibits the growth of *Mycobacterium Smegmatis*. **Z. Arhouma**, K. Kostenkova, D.C. Crick, D.C. Crans

5:13 Discussion: Protein Modification and Processing.

5:21 60. Elucidating the role of the axial cysteine residue in NHase catalysis and the enzyme maturation. **I. Ogutu**

5:30 61. Determining co-modification of 5hmC-DNA and protein structure through mammalian evolution. **R.S. Czarny**

5:36 62. Non-enzymatic post-translational modification of lysine clusters in C2 domains. **C.C. Beauchamp-Perez**, C. Michel, R. Reisdorph, N. Reisdorph, K. Fritz, C. Shearn, J.D. Knight

5:42 63. Efficiency and selectivity of RNAse A cleaving RNA containing 8-oxo-7, 8-dihydroguanosine. **C. Phillips**

5:45 64. Evaluating changes in reactive oxygen species (ROS) as a plausible mechanism underlying the effect of noise on dopamine system in the hub for central auditory processes. **B. Doe**

5:51 Discussion.

(4) Red Rocks

Workshop: Empowering Academic Researchers to Strengthen Safety Culture

1:00 – 4:00 pm Safety workshop organized by Jessica Martin (University of Connecticut) for graduate students. The American Chemical Society is sponsoring a program to help educate graduate students about lab safety culture and opportunities for promoting safety. The participants will be awarded a certificate for completion of the course (can be added on resumes). This three-hour workshop will be led by Sarah Zim (University of Chicago) and Jessica DeYoung (University of Iowa). The purpose of this workshop is to help develop individualized plans for the creation or improvement of student safety

programs. You can read more about the results of previous workshops in this Journal of Chemical Health and Safety (K. A. Miller and K. I. Tyler, Journal of Chemical Health and Safety, 2019, 1871-5532; https://pubs.acs.org/doi/10.1021/acs.chas.8b26309). Other key topics include hazard assessment, risk management, safety management practices, and complementary top-down approaches. This workshop is primarily directed at graduate student issues, but faculty and staff are encouraged to participate.

Thursday Mixer programming 6:00 pm – 8:00 pm

Hosts Carlos Olivo-Delgado (IT) & Debbie C. Crans (introductions)

6:00-6:30 pm mixer
6:30 pm
ACS President Elect H. N. Chen, Welcome
ACS National Board Chair John Adams, Historial Highlights
ACS Regional Past Chair Donivan Porterfield, Regional Highlights
Past ACS President, Bonnie Charpentier, Safety in Chemistry
ChemClub Colorado State University Chair, Benjamin Reynolds

7:10 pm Distribution into Specialty Rooms

7. Meet the ACS National Board Members
8. Meet the ACS Regional Board Members
9. Colorado ACS Future Communications - Interactive Discussion (Helen Gerhard and Michael Jacobs)
10. NSF – Program officer Mike Adams and Shing Ho
11. Do you want to improve your presentation skills? Susan Morris
12. Ensuring laboratory Safety. James Kaufman

FRIDAY MORNING

(1) Pike's Peak

Senior Chemists Symposium

Celebrating the Contributions of Senior Chemists in the Rocky Mountains Region

D. C. Crans, *Organizer*
E. L. Clennan, M. H. Rakowsky, H.Gerhard *Presiding*

9:00 Introduction.

9:02 65. Chemistry at the environmental water-air interfaces. **V. Vaida**

9:32 66. Redox revolutions on Earth and beyond. **A. Anbar**

10:02 67. Plasma assisted catalysis: New approaches focused on fundamental chemistry. **E.R. Fisher**

10:32 68. Effects of luteinizing hormone receptor expression level on receptor aggregation and function. D. Althumairy, J.M. Pace, D.A. Roess, **B. Barisas**

11:01 69. From boron hydrides to lanthanides and nuclear reactors to in vivo imaging. **G.R. Eaton**

11:30 70. Heli-acenes as templates for a torque-lock-propagate approach for the synthesis of configurationally-pure twisted-acenes. **E.L. Clennan**, J. Weber, S. Tannir

(2) Estes

Medicinal Chemistry Symposium

Medicinal and Biological Chemistry: Oral and Flash Presentations

D. C. Crans, *Organizer*
M. B. Jacobs, A. C. Smith, A. J. Wiemer, *Presiding*

9:00 Introduction to the Biomedical and Biological Symposium.

9:03 71. "Water-mimicking" ionic liquids for lipase activation and enzymatic polymerization. **H. Zhao**

9:28 72. Directly observing cell-nanoparticle interactions by 3D localization microscopy in live flowing cells. **L.E. Weiss**, Y. Shalev Ezra, S. Goldberg, B. Ferdman, O. Adir, A. Schroeder, O. Alalouf, Y. Shechtman

9:37 73. Development of novel spiroligomer carbohydrate binding molecules. **S. Chepyshev**, C.E. Schafmeister

9:43 74. Inhibition of an iron-sulfur cluster biogenesis pathway towards development of novel antibiotics. **A. Boncella**, E. Sabo, C. Gladfelter, C. Morrison

9:49 75. Open questions on the biological roles of first-row transition metals. **K. Kostenkova**, D.C. Crans

9:55 Discussion.

10:04 76. Modular synthesis and characterization of diffusible signal factor analogs for the study of structure activity relationships and mechanism of action. **R. Wiley**, D.L. Baker

10:10 77. ^{1}H NMR study of menaquinone-2 interactions in a phosphatidylcholine liposome membrane model. **G. Bublitz**, K. Doucette, D.C. Crans

10:16 78. Bacterial inhibition with liposoluble extracts of *Padina gymnospora*. **P.N. Gines Velez**, **P.A. Balbuena**, G. Peña Hurtado

10:19 79. Stimuli-activated quantum dots clear *Salmonella* intracellular infections in preosteoblast cells. **K. Eller**, C. McCollum, M. Levy, P. Nagpal, A. Chatterjee

10:25 Discussion.

10:36 80. Synthesis and characterization of novel non-innocent vanadium Schiff base complexes with anti-cancer properties superior to cisplatin. **H. Murakami**, C. Yigit, J.T. Koehn, D.J. Gaebler, A. Bates, A. Levina, P.A. Lay, D.C. Crans

~~**10:42 81.** Evaluation of N-(9'-acridinyl)-O-phenylhydroxylamines. **J. Forster**, M.D. Mosher Canceled~~

10:42 82. Transcriptome-based design of PNA inhibitors re-sensitizes CRE E. coli to carbapenems. **T. Aunins**, K. Erickson, A. Chatterjee

10:48 83. Elucidating the neurochemical basis for the effect of chronic toluene inhalation on accumbal dopamine release. **K. Reiser**, A. Apawu

10:54 Discussion.

11:04 84. Discovery of novel fadd32 inhibitor of mycobacterium tuberculosis with improved drug properties. **J. Sethiya**, R. Scott, G. Majeres, L. Dieckman, E. North

11:10 85. Ligand binding site location comparison across class A GPCR complexes. **M. Griffing**, A.L. Parrill-Baker, D.L. Baker

~~**11:16 86.** Stereoselective synthesis of the potential 5-HT_{2A} agonist (2*S*,7*S*)-2-(4-bromo-2,5-dimethoxybenzyl)-7-(2-methoxyphenyl)azepane. **J. Talbert**~~

11:19 Discussion.

11:25 87. Receptor pharmacophore benchmarking: The role of ligand function in model development. **P. Castleman**, G.L. Szwabowski, D. Bowman, J. Cole, A.L. Parrill-Baker, D.L. Baker

11:31 88. Finding small molecule inhibitors that target DUSP5 using virtual screening: Applications in computational chemistry. **J. Grajeda**, M. Talipov

11:34 89. Bacterial inhibition with liposoluble extracts of *Mentha pulegium*. P.N. Gines Velez, **N. Cabrera**, **L. Rivera**, G. Peña

11:37 Discussion.

11:42 90. Synthesis and evaluation of the rhodamine- and biotin- probes for detection of cysteine containing proteins. **S.H. Nguyen**, **K.M. Okin**, **J.E. Ward**

11:45 91. Study of near infrared DNA damage and photo-cytotoxicity by a brominated 4-quinolinium dicarbocyanine dye (ESS2-2-4). **Y. Waku Kouomou**, E. Ahoulou, K.B. Grant, M. Henary, O. Taratula

11:48 92. Virus-like particles (VLPs) as a vaccine platform. **E. Sohn**, N. Lee

11:51 93. Synthesis and duplex stability of N2-Alkyl 8-Oxo-2'-deoxyguanosine oligonucleotides for use as substrate analogs for DNA repair protein MutY. **M. Bright**, R.P. Van Ostrand, S.S. David

11:54 Discussion.

(3) Horsetooth

Young Talent in the Rocky Mountain Region

Young Investigator and Flash Presentations

D. C. Crans, *Organizer*
A. M. Morey, S. S. Rocks, G. G. Stanley, A. K. Van Orden, *Presiding*

9:00 Introduction by session chair.

9:02 94. New synthetic methodology enabled by base-promoted proton, electron and halogen transfer processes. **J. Bandar**

9:32 95. Synthesis, characterization and reactivity of N-alkylated organic photocatalysts. **N.A. Swisher**, D. Corbin, G. Miyake

9:41 96. Total synthesis of indolizidine and quinolizidine alkaloids. **J. Renner**

9:47 97. "On water" synthesis of fluorosulfonyl 1,2,3-Triazoles. **A.L. Nazarova**, J. Thomas, V.V. Fokin

9:56 98. One-pot alkylation via traceless dearomatized pyridyl phosphonium ylides. **P. Fricke**, A. McNally

10:02 Questions for 3 presentations:Introduction of Flash Presentations.

~~**This presenation should be removed 10:11 99.** Synthesis of configurationally twisted acenes by the torque, lock, and propagate approach: The mallory and dione routes. **M. McConnell**, J. Weber, S. Tannir, E.L. Clennan~~ - **Canceled**

10:14 100. Exploratory syntheses of truncated, partially saturated menaquinone derivatives. **M. Braasch-Turi**, D.C. Crans

10:20 101. Synthesis of 2,4'-bipyridines via a unique radical coupling of cyanopyridines and heteroaryl phosphonium salts. **J. Greenwood**, J. Koniarczyk, J. Alegre-Requena, R.S. Paton, A. McNally

10:26 102. Synthesis of functionalized ionic liquids for coal dissolution and pretreatment. **M. Franklin**, H. Zhao

10:32 103. Synthesis of novel ionic liquids towards enzymatic ring-opening polymerization to polyesters. **C. Martin**, H. Zhao

10:35 Discussion and Questions.

10:43 104. Multivariate approach in designing chiral metal organic frameworks. **T. Ericson**, B. Tahmouresilerd, A.F. Cozzolino

10:49 105. Core-extended *N,N*-diaryl dihydrophenazine photoredox catalysts: Structure-property relationships and advantages in organocatalyzed atom transfer radical polymerization. **M. Price**, G. Miyake

10:55 106. Mechanistic insights into organocatalyzed birch reduction driven by visible light. **M. Kudisch**, J. Cole, D. Chen, R.M. Pearson, C. Lim, G. Miyake

11:01 107. Understanding the reactivity of tertiary amines and in situ generated ammoniums under reductive metal catalysis. **C.I. Nwachukwu**, T.P. McFadden, A.G. Roberts

11:07 108. Computational study of the torque, lock, and propagate approach to make configurationally stable twisted heli-thiopentacenes and heli-dithiopentacenes. **S. Tannir**, E.L. Clennan

11:16 Discussion and Questions.

11:25 109. Architectural analysis of branched polymers via soret contraction factor. **M. Toney**, K.R. Williams

11:31 110. Total THM-NOW: A low-cost online analyzer for total trihalomethanes in drinking water. **M. Alfonso**, N. Boppana, M.A. Brown, P.S. Simone, G.L. Emmert

11:37 111. Modeling pollutant levels. P. Johnson, **K. Johnson**, L. Huang

11:40 112. Measuring arsenic levels in the Fountain Creek watershed based on uptake by the bryophyte *Hygrohypnum ochraceum*. **A. Chavez**, **N. Gasparovic**, D.C. Crans, J. Carsella

11:46 113. Infrared spectrum and atmospheric chemistry of 1,1,2,3,3,4,4 heptafluorobut-1-ene. **R. Sapkota**, G. Rawling, P. Marshall

11:52 Discussion of papers.

FRIDAY AFTERNOON

(1) Pike's Peak

Lunch Plenary

Iota Sigma Pi - Meitnerium Chapter and WCC Session

D. C. Crans, *Organizer, Presiding*
M. Braasch-Turi, J. K. Chung, B. A. Hernandez-Sanchez, *Presiding*

12:00 Session Introduction by Debbie Crans.

12:05 114. Reflections in water: Musings on my favorite molecule. **N.E. Levinger**

12:40 115. Vignettes from a career in medicinal chemistry. **G.I. Georg**

1:10 116. ~~Anion coordination: Size, charge, and nexus with water. S. Pramanik, S. Kaur, S. Brunclik, V.W. Day, **K. Bowman-James**~~ Monitoring motion with electron spins. T. Ngendahimana, W. Moore, L. Woodcock. G. R. Eaton, and **S. S. Eaton**

1:40 Panel Introduction by Maggi Braasch-Turi and Bernadette Hernandez-Sanchez.

1:45 Iota Sigma Pi and WCC Panel. Academia: Nancy Levinger, Gunda Georg and Sandra S. Eaton; Industry Helen Gerhard and Jennifer McLauchlan and National Lab: Jaqueline Kiplinger

(1) Pike's Peak

Medicinal Chemistry Symposium

Medicinal and Bioinorganic Chemistry

D. C. Crans, *Organizer, Presiding*
C. C. Aldrich, *Presiding*
C. I. Georg, *Presiding*

2:30 Introduction.

2:32 117. Design of antibiotics to overcome resistance in mycobacteria. **C.C. Aldrich**

3:02 118. Inhibition of geranylgeranyl diphosphate synthesis by triazole bisphosphonates. A. Fairweather, D.B. Goetz, C.M. Schroeder, N.H. Bhuiyan, M.L. Varney, S.L. Haney, S.A. Holstein, **D.F. Wiemer**

3:32 119. Cellular kinetics of phosphoantigen prodrug forms. C.C. Hsiao, X. Huang, M. Schladetsch, N.A. Lentini, D.F. Wiemer, **A.J. Wiemer**

4:02 120. Inhibition of methyl transferases: The present and future. **M.A. Brown**, D.C. Crans

4:30 121. Small-molecule modulation of gene expression via DNA quadruplex structures. **C.J. Burrows**, A.M. Fleming

5:00 122. Optimization of the leads and synthesis of a ketohexokinase inhibitor clinical candidate. **A.C. Smith**

5:30 123. Discovery and development of BET bromodomain inhibitors for male non-hormonal contraception. **G.I. Georg**

(2) Estes

General Papers

Oral and Flash Presentations

D. C. Crans, *Organizer*
K. Kitzmiller, N. E. Levinger, C. J. Olivo-Delgado, M. Weinrich, *Presiding*

2:30 Chemical Education.

2:33 124. Artificial intelligence tool for accessible chemistry education. J. Watters, F. Jiang, A.A. Hill, **M. Weinrich**

3:03 125. Designing a culturally inclusive STEM and health research training program for Native American students. **N. Lee**, J. Lee

3:33 126. Tracking information literacy in science students: A longitudinal study of skills retention through the chemistry curriculum. **J.D. Knight**, M. Bruehl, D. Pan

3:53 127. Can students learn chemistry without midterm exams?. **D.J. Weiss**, P. McGuire, W. Clouse, R. Wrobel

3:59 128. Multiple ways to virtually engage students in chemistry labs. **A.S. Smeltzer Schwab**

4:05 Introduction to Flash Presentations.

4:10 129. Analysis of the impacts of student sense of social belonging on student outcomes in STEM. **J.D. Edwards**, R. Frey, R. Barthelemy

4:16 130. Comparison of online content homework with metacognitive training homework in general chemistry courses. N. Ellis, H. Wiegreffe, A. Hefzalla, **E. Heider**

4:19 131. Task analysis of undergraduate biology and chemistry laboratory activities. **A. Reid**, J. Heath, J. Velasco

4:22 132. Instructional behaviors in undergraduate biology and chemistry laboratory courses. **J. Heath**, A. Reid, M. Painter, J. Velasco

4:25 133. Chemistry of indigenous peoples. **M. Gomes da Silva**

4:28 Questions to 4 papers: Introduction to Session:General Papers.

4:37 134. Encapsulating metal-organic framweorks (MOFs) within mesoporous silica for use in heterogenous catalysis. **S.E. Massimi**, B.G. Trewyn

4:43 135. Visible-light-promoted reactions via intermolecular charge transfer using (thiol)phenols as electron donors. **B. Liu**, C. Lim, G. Miyake

4:52 136. Intra- and inter-ligand charge transfers in a new donor-acceptor complex. **S. Gao**, **J. yang**, **M.L. Kirk**

4:58 Cancelled #~~**137. Shining a new light on catalysis: Light responsive molecular dyads for direct control of redox switchable catalysts. C. J. Aviles Martin. E. Pinkhassik.**~~ **170.** "Exploring environmentally sensitive bezothiadiazole and their uses" **C. Warner**, S. Norris, B Lampkn, P. Bouc, A. Thooft, J lukesh, S. I, Suarez,H. Brown-Harding, B. VanWeller

5:04 138. Visible light driven synthesis of remdesivir precursor. **A. Green**, C. Lim, G. Miyake

5:10 Discussion; after that Electrochemical papers.

5:20 139. Photoredox catalyst design for proton coupled electron transfer. **C. Chrisman**, G. Miyake

5:26 140. Improved photoelectrochemical water oxidation catalysis via atomic layer deposition of alumina: Passivating surface trap states on a tin-oxide, phosphonate-functionalized perylene diimide plus CoO_x system. **C. Jewell**, R. Finke

5:32 141. Impacts of performing electrolysis during organocatalyzed atom transfer radical polymerization. **D. Corbin**, B. McCarthy, G. Miyake

5:38 142. Altering non-innocent anti-cancer compounds: How the addition of Cl to VO[HSHED] catecholates can change their electrochemistry. **A. Haase**, J. Hagan, H. Murakami, C.N. Beuning, P.A. Lay, D.C. Crans

5:44 143. Multimodal spectroscopic investigation of the conformation and local environment of biomolecules at an electrified interface. **S. Moonitz**, N. Shepard, R. Noriega

5:50 Discussion.

(3) Horsetooth

General Papers

Oral, Flash, and Safety Presentations

D. C. Crans, *Organizer*
J. Carsella, R. Noriega, G. G. Stanley, H. Zhao, *Presiding*

2:30 Flash Presentations in Inorganic, Physical and Analytical Chemistry;Career enhancement strategies.

2:32 144. Quantitative analysis of diffusible signaling factors using negative ion liquid chromatography electrospray ionization mass spectrometry (HPLC-ESI-MS). **B. Hoffman**, D.L. Baker

2:38 145. Complementary pairs from clashing forces throughout chemistry: Visualizing the pauli exclusion principle and its far-reaching implications. **J.P. Joyce**, A.K. Rappe, M.P. Shores

2:44 146. Frustrated Lewis pairs with applications in hydrogen storage. **G. Russell-Parks**, B.G. Trewyn, T. Gennett

2:50 ~~**147.** Chromophoric photonic crystals. **L. Garcia Alzate**~~ **- Canceled**

2:50 Physical-Inorganic Chemistry - General papers Questions.

3:00 148. Studies of the formation and infrared spectrum of formyl fluoride. **G. Rawling**, R. Sapkota, P. Marshall

3:06 149. Entropy and enthalpy of the hemoglobin-fluoride complex redox reactions (Fe^{3+}/Fe^{2+}) at pH 5 reveal significant heme-pocket structural changes with temperature. **K.G. Flanders**, T. Mada, J. Cerda

3:09 150. Earth abundant transtion metal effects on methane concerted metalation-deprotonation, a DFT study. **W.M. Grumbles**, K. Melancon, T.R. Cundari

3:15 151. Crystallographcially observed mechanistic conversion of lanthanide nitrates by hexamethylenetetramine (HMTA) to ceramic oxide materials. **P.C. Reuel**, T.J. Boyle, R.E. Cramer

3:18 Discussion; Inorganic and Organometallic Chemistry.

3:28 152. C-H activation of toluene by diruthenium nitride: DFT study. **W. Alharbi**, T.R. Cundari

3:37 153. Density functional study of methane activation by frustrated Lewis pairs with Group 13 trihalides and Group 15 pentahalides and a machine learning analysis of their barrier heights. **I. Migliaro**, T.R. Cundari

3:43 154. Supported palladium catalysts for selective hydrogenation of ethyl phenylpropiolate. **D. Knight**, **B. Santoyo**, J. Whelchel, S. Hussaini, B. Jang

3:46 155. Olefin polymerization by zirconium boratabenzene catalysts. **C. Carter**, T.R. Cundari, G. Rodriguez

3:52 156. Opening the $Co^{III,IV}_2(m\text{-}O)_2$ diamond core by Lewis bases leads to enhanced C–H bond cleaving reactivity. Y. Li, **S. Handunneththige**, J. Xiong, Y. Guo, M. Talipov, W. Dong

3:58 Discussion; Analytical Flash Presentations.

4:07 157. Utility of cyanophenylalanine derviates as spectroscopic probes. A.J. Haider, L. Metzroth, A.M. Zerwekh, R.J. Martinez, **J.P. Martin**

4:13 158. Hybrid additive manufacturing of poly(caprolactone)-modified bone-ligament composite scaffolds for interface tissue engineering. **O. Sanchez**, L. Mottishaw, C. Salas, C. Buska, M. Rush

4:16 159. Indium phosphide quantum dots activated by near-infrared light: A novel treatment for drug-resistant bacterial infection. **C. McCollum**, J. Bertram, P. Nagpal, A. Chatterjee

4:22 160. Utilizing multi-angle light scattering to count biological particles. **C. Plavchak**, A.Z. Werner, G. Beckham, K.R. Williams

4:28 Discussion: Analytical Flash Presentations.

4:34 161. Effects on membrane oxygen permeability due to lipid changes in breast cancer. **Q. Wang**, S. Pias

4:40 162. Design and construction of a Brewster angle microscope. **S. Croslow** , K.G. McLaughlin, A. Goach

4:43 163. Effects of pH, conformation, and metal cations on insulin aggregation. **K.G. McLaughlin**, S. Croslow , S.P. Distin, C. VanCleave, D.C. Crans, A. Goach

4:46 164. Investigating morphology of mixed monolayers containing short-chain menaquinones with brewster angle microscopy. **C. Van Cleave**, A. Haase, B.J. Peters, J.T. Koehn, D.C. Crick, D.C. Crans

4:52 Introduction to Session: Career Advancement, Safety and ACS assistance.

4:58 165. Stand up to stand out: Self-advocacy for the reluctant. **S. Morris**

5:28 166. How to convince others (that safety is important and that you're serious about it). **J.A. Kaufman**

5:40 167. Spotlight on the laboratory safety team workshops. **J.A. Martin**

5:52 168. Chemical business networking with SCHB. **J.E. Sabol**, G.W. Ruger, J. Skinner, A. Kantak, D.J. Deutsch, J.L. Maclachlan

5:55 169. South Dakota mines ACS student chapter: Promoting green chemistry concepts through outreach demonstrations and hands-on activities. **K. Ly**, **L.C. Cutler**, K.D. Barz

5:58 Discussion.

6**:00- 8:00** Award Presentation Mixer; Reginal Awards and "Video talk awards". There will be opportunities for mixing and activities (Details TBA).

Friday Award Banquet 6:00 pm – 8:00 pm

Hosts: Carlos Olivo-Delgado and Debbie C. Crans

6:00-6:30 pm Pre-Mixer
6:30 pm Brief presentations by:

- ACS National Board Chair, John Adams
- ACS Regional Board Chair, Michael Mosher
- COACS Senior Chemists Committee Chair, Margaret Rakowsky

Award Presentation hosts: Connie Gabel and Michael Mosher

George Stanley RMRM2020 Award Chair introducing Presenters of **Regional Awards**

• **Bonnie Charpentier**, ACS Past President: ***E. Ann Nalley Award for Volunteer Service***

This award was established in 2006 by ACS Past President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism.

• **Matt Jones,** CHED RMR Representative & **Connie Gabel,** RMR Board Awards Chair Presenting ***Regional Award for Excellence in High School Teaching***

The Division of Chemical Education (DivCHED) established an endowment to support Regional Awards for Excellence in High School Teaching in each of the ACS Regions.

• **Connie Gabel & Michael Mosher** presenting the award to ***Partners for Progress and Prosperity (P3) Award*** This award recognizes partnerships among industry, academia, government, small businesses and/or other organizations that result in impactful outcomes.

• **H. N. Cheng,** President-Elect ***ACS Stanley C. Israel Regional Award for Advancing Diversity in Chemical Sciences.*** The Stanley C. Israel Regional Award recognizes individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the ACS Regions.

George Stanley presenter of Conference Awards: Flash Presentations
3 ACS Division of Organic Chemistry Awards
1 ACS Award in Sustainability Award

Carlos Olivo-Delgado
1 Colorado State Chemistry Award

3 ACS awards

Bonnie Charpentier,
1 Helen Gerhard's LLC Company Award
2 ACS Division of Small Chemical Businesses Awards

Margaret Rakowsky
1 ACS Senior Chemists Committee Award

H. N. Chen
3 The Royal Society of Chemistry, New J. Chemistry Awards

Sandra Bonetti
3 ACS Division of Medicinal Chemistry Awards
1 COACS award in memory of John Conolly
1 COACS award in memory of Kim Pacheco

John Adams
3 ACS Division of Inorganic Chemistry Awards
3 Elsevier Coordination Chemistry Awards

Mary Singleton
3 Women Chemists Committee Awards

Michael Mosher and/or Connie Gabel
Innovative Project Grant Awards
COACS awards

Debbie Crans
Chair of COACS's Awards

Michael Mosher will introduction the next team to run the RMRM2021
Closing Comments **Debbie Crans** or **Carlos Olivo-Delgado**

List of RMRM2020 Abstracts

RMRM 1

Effects of a dynamic local environment on the properties of chemical systems

***Rodrigo Noriega**, noriega@chem.utah.edu. Chemistry, University of Utah, Salt Lake City, Utah, United States*

Most functional materials operate in the condensed phase and thus experience the presence of nearby molecules. As such, a molecule's local environment is an important determinant of its chemical properties - from relaxation and reactivity pathways, to dynamic fluctuations and molecular motions. Dynamic molecular environments span a large range of complexity, and active projects in our group investigate a variety of chemical systems with ultrafast spectroscopic tools that cover the UV to mid-infrared spectral range. At the simpler end of the chemical complexity scale, we are interested in bi-molecular reactive species in solution and the effect that solvent molecules have on their equilibration and reactivity dynamics. Beyond homogeneous solutions, we are interested in probing electrochemical processes that occur within a complex environment involving electrode surfaces, solvent molecules, ions, and free and surface-bound species. In this talk, I will describe our work using the photoexcitation of bimolecular charge transfer complexes in solution to generate reactive radical ions in their solvent-equilibrated electronic ground state, and their ensuing ultrafast reactive pathways. Additionally, these photogenerated radical pairs can tae part in photoelectrochemical reactions at a solid/liquid interface. I will show how a combinatoin of surface sensitive spectroscopic probes can monitor this buried electrochemically active interface, whose properties can be modulated by an applied surface potential. Our findings show that the local environment is an active participant in a variety of chemical transformations.

RMRM 2

Toward noninvasive biomedical thermometry with cobalt-59 molecular NMR thermometers

***Joseph Zadrozny**, joe.zadrozny@colostate.edu. Department of Chemistry, Colorado State University, Fort Collins, Colorado, United States*

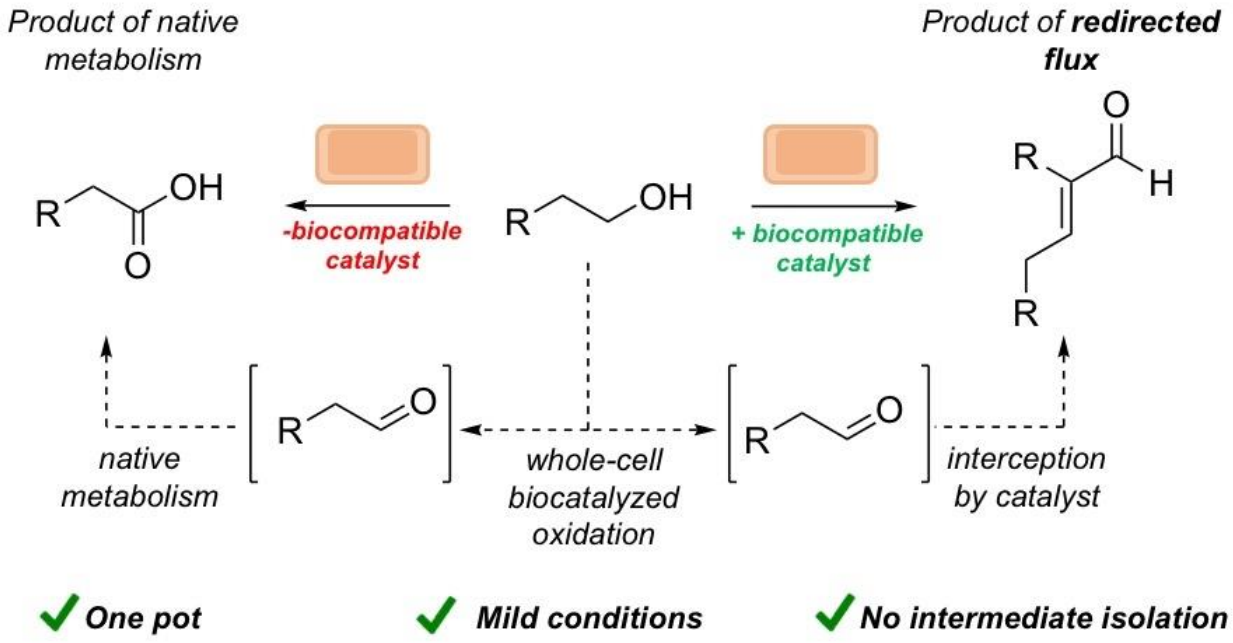
Noninvasive detection of temperature will provide transformative capabilities for thermal ablation of tumors and monitoring of physiology. Our approach to developing these capabilities is by targeting molecules with temperature-dependent properties that can be translated into measurable magnetic resonance signals. We focus on Cobalt-59 nuclear magnetic resonance for this purpose. Cobalt-59 was recognized decades ago for an exceptionally temperature sensitive magnetic resonance signature (two orders of magnitude greater than what is possible with 1H!). This sensitivity ultimately stems from temperature-dependent electronic structure, which is governed by the dynamic ligand field of complexes that contain this nucleus. Yet, the knowledge to understand and control the sensitivity by molecular design is lacking. I will present recent and ongoing efforts provide that insight.

RMRM 3

Manipulating flux in living cells with biocompatible catalysis

***Dylan Domaille**, ddomaille@mines.edu. Chemistry, Colorado School of Mines, Golden, Colorado, United States*

Biosynthetic methods have the potential to deliver value-added chemicals from renewable feedstocks. However, despite major advances in metabolic engineering and synthetic biology, the rapid engineering of microbes to deliver high yields and titers of target compounds remains as a challenge. This talk will discuss our new chemical catalysis-based strategy for expanding the types of products available from unmodified microorganisms. By combining *Gluconobacter oxidans* as a whole cell biocatalyst with a lysine organocatalyst in a single pot, we demonstrate that aqueous solutions of C_n n-aliphatic alcohols are converted to C_{2n} α,β-unsaturated aldehydes in a single pot in mild conditions. This carbon-doubling reaction works with a range of C_2–C_6 alcohol substrates. In the absence of the lysine organocatalyst, only n-aliphatic carboxylic acids are observed. Taken together, this is the first example of a chemical catalyst capable of redirecting flux to products that would be challenging to synthesize through biosynthetic means alone.



RMRM 4

Coupled lipid miscibility and phosphotyrosine-driven protein condensation on membranes

Jean K. Chung[1], *jkchung@colostate.edu, William Huang*[2], *Catherine Carbone*[3], *Laura M. Nocka*[4], *Atul N. Parikh*[5], *Ronald D. Vale*[3], *Jay T. Groves*[4]. *(1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Stanford University, Stanford, California, United States (3) University of California San Francisco, San Francisco, California, United States (4) University of California Berkeley, Berkeley, California, United States (5) University of California Davis, Davis, California, United States*

The lipid raft theory postulates that microdomains composed of specific lipids give rise to membrane protein platforms, such as the T-cell receptor cluster. The origin of this preferential lipid associations is thought to be the lipid phase separation of coexisting liquid phases, seen in vesicles with certain compositions. However, the theory has many shortcomings, one of which is that it cannot explain how lipid rafts can be triggered by cellular signals. In this work, we reconstituted the macroscopic assembly of LAT:Grb2:SOS in the early T-cell signaling on vesicles capable of undergoing phase separations. Our results indicate that the formation of protein assemblies through multivalent

interactions, also a type of phase transition, can produce lipid phase transition in a phosphorylation-dependent manner. Furthermore, this lipid reorganization propagates to compartmentalization of a downstream protein, K-Ras, into the LAT:Grb2:SOS assemblies. These results suggest that interactions between signaling proteins play the principal role in the lateral organization of the cellular membrane, with respect to lipids as well as proteins.

RMRM 5

Elucidating the action of abused volatile organic solvent, toluene on the central reward pathway

Aaron Apawu[1]*, aaron.apawu@unco.edu, Sean P. Callan*[2]*, Tiffany A. Mathews*[3]*, Scott E. Bowen*[2]*. (1) Department of Chemistry and Biochemistry, University of Northern Colorado, Greeley, Colorado, United States (2) Department of Psychology, Wayne State University, Detroit, Michigan, United States (3) Department of Chemistry, Wayne State University, Detroit, Michigan, United States*

The brain chemistry can be disrupted by environmental factors including illicit drugs, industrial solvents, and loud noise. Toluene, a readily available industrial solvent is a major component of substances frequently abuse as inhalant and can also be encountered through incidental or occupational exposures. Because inhalation of volatile organic solvents has debilitating effects on mental health, understanding their impact on the brain chemistry is crucial to develop effective interventions and therapies for inhalant abusers. Although existing data have implicated dopamine in toluene's action in the brain, the exact adaptations in the dopamine system leading to dependence experienced by inhalant users remain equivocal. In the present work, an electroanalytical technique, fast scan cyclic voltammetry (FSCV) was coupled with homemade carbon fiber microelectrode and optimized to achieve the selectivity, sensitivity, spatial and temporal resolution necessary to elucidate the neural mechanism underlying toluene's effect on the dopamine system in the nucleus accumbens, a region integral in addiction. Herein, brain slices were harvested from mice following acute (30 minutes) or chronic (30 minutes each day for 7 days) exposure to behaviorally relevant concentrations of toluene (2000 or 4000 ppm) and their air controls (n= 4-5 mice/group). FSCV was used to examine the dopamine dynamics in the experimental groups. Furthermore, *in vivo* microdialysis coupled to HPLC (with electrochemical detection) was employed to gain a complementary understanding of how toluene inhalation impact on the dopamine neurotransmission. The results reveal that both acute and repeated inhalation of organic solvent, toluene elicits spatiotemporal

changes in dopamine dynamics in the brain reward pathway and suggest that the dysregulation instigated by repeated toluene abuse may be the neuroadaptation underlining its compulsive and repetitive use.

RMRM 6

Partitioning of lead in plants, birds and arthropods found on the Colorado Smelter superfund site in Pueblo, Colorado

Jim Carsella[1]*, jim.carsella@csupueblo.edu, Elizabeth K. Petersen*[2]*, Teyah Schiffer*[3]*, Sean Staples*[2]*, Claire Varian-Ramos*[2]*, Moussa Diawara*[2]*. (1) Chemistry, Colorado State University - Pueblo, Pueblo, Colorado, United States (2) Biology, Colorado State University - Pueblo, Pueblo, Colorado, United States*

The latest investigation in a series of investigations on the Colorado Smelter superfund site examines the dynamics of the partitioning of Pb. The hypothesis is Pb increases significantly as we proceed up the food web from plant to arthropod to birds on the superfund site. A past study of geochemical hazards to identify potential problems from intensive industrial and agricultural uses conducted in the Pueblo, Colorado vicinity helped identify the contamination left behind from the Colorado Smelter. The contamination was significant enough for subsequent Environmental Protection Agency work to identify the Colorado Smelter site as a superfund site. Subsequent investigations have examined lead levels in human blood and hair. Current samples were gathered from the superfund site, a site across the river from the site and from two control sites west of the city of Pueblo. The samples were cataloged and digested according to EPA method 3052 and analyzed by EPA ICPMS method 6020a. The soil Pb levels are statistically significantly ($P<0.002$) different between the superfund and control sites. ANOVA and Nested General Linear models were constructed in Minitab 19 for Pb as a response and the variables of site, taxa (Plant, Arthropod, and Bird), diet (omnivore, carnivore, and herbivore). The results indicate statistically significant ($P<0.003$) increases in levels of Pb in carnivorous and omnivorous birds and arthropods, which supports the hypothesis. The plants on the superfund sites also exhibit a significant increase in Pb, which also supports the hypothesis. Oddly enough the herbivores in arthropods and birds did not exhibit a statistically significant difference in Pb levels and do not support the hypothesis. The results of this investigation show that the partitioning of Pb across the food web is complex involves many factors including diet selection. The evidence for this is lack of Pb partitioning in herbivores even though the plants accumulate the Pb but the increased

presence in the omnivores and carnivores. The lower Pb levels in birds are evidence of their larger home ranges as compared to arthropods.

RMRM 7

Creating a culture of safety in academic laboratories

***Peter K. Dorhout**, dorhout@ksu.edu. Department of Chemistry, Kansas State University College of Arts and Sciences, Manhattan, Kansas, United States*

ACS has undertaken an effort to respond to the call from the National Academies of Science and the Association of Public and Land-grant Universities for professional societies to take the lead in improving laboratory safety, particularly in academic chemistry laboratories, by encouraging a culture of safety. Safety culture refers to an organization's shared values, assumptions, and beliefs specific to workplace safety or, more simply, the importance of safety within the organization relative to other priorities. Consequently, ACS has made safety one of its core values and has taken action to change how its members approach safety as practitioners and educators. These actions include convening stakeholders at three Summits since 2018, developing an ACS journal on safety, and ensuring that safety is foremost in the culture of our acdemic, industry, and national laboratory settings. This presentation will share my perspectives on the steps that ACS has taken over the past few years to address this call and solicit your input on how we can help change the culture of safety in academic laboratories.

RMRM 8

Standardizing risk management in laboratory and pilot plant facilities: A model

***Kim Johnson**, kim.k.johnson@shell.com. Global Solutions, Shell Chemicals, Houston, Texas, United States*

By its very nature, a research and development site is in constant change. We try things that have not been done before. We create and test new processes, new chemical formulae, new products and new production techniques. Is it possible to find common ground for managing risk in such a diverse environment? The answer is yes…. But. With careful assessment of the risks and acknowledgement when the risks are truly unknown, a standard for the minimum level and types of acceptable controls and barriers can be established. But, that is a minimum. There is still some work to do to reduce

your risk to as low as reasonably practicable. See how the Shell Technology Center Houston has used a risk assessment matrix and model BowTies to develop a process to standardize the minimum requirements needed to manage health, safety and environmental risks.

RMRM 9

Critical aspects of a robust potent compound containment program

***Amy K. Doane**, Amy.VanAntwerp@cordenpharma.com, Robin I. Livingston. Corden Pharma Colorado Inc, Boulder, Colorado, United States*

Corden Pharma's Colorado API manufacturing facility has a long history of successfully implementing innovative solutions to ensure containment of Hightly Potent Active Pharmaceutical ingredients (HPAP), designed to protect workers from the unique hazards presented by potent compound handling. While the success of CordenPharma's programs requires effective Engineering Controls, the critical aspect to a robust containment program is the strength of the softer elements, including a Containment Culture, Process Development, Occupational Health Pre-Planning, and an ongoing Containment Execution Cycle. Without these supporting elements, even state-of-the-art containment equipment will not consistently and reliably contain HPAPI.

RMRM 10

Towards a circular plastics economy: Design principles and synthetic methodologies for sustainable plastics with tunable properties and chemical circularity

***Eugene Y. Chen**, eugene.chen@colostate.edu. Colorado State University, Fort Collins, Colorado, United States*

The worldwide distribution of vast quantities of synthetic polymers, especially lightweight, inexpensive, long-lasting, and high-performance plastics, has fueled modern economies, becoming indispensable for modern life and the global economy. However, the current manufacturing, consumption, and disposal schemes of fossil-based polymers follow an unsustainable linear 'mine, make, use, dispose' framework. The majority of today's polymers were designed and developed for cost, performance, durability, and disposability, rather than for reuse, repurposing, and recovery. The failure of this linear model to address the end-of-life issues of today's plastics has thus accelerated

depletion of finite natural resources, caused severe worldwide plastics pollution problems, and resulted in enormous energy and materials value loss to the economy. Thus, the design of next-generation polymers has to consider their afterlife issues and establish closed-loop lifecycles towards a circular economy. In addition, synthetic methodologies and catalytic routes have to be developed to effectively and expediently deconstruct post-consumer polymers with high selectivity for clean monomer recovery and polymer reproduction. Centering on addressing the above identified challenges, this presentation will first introduce fundamental principles for designing circular polymers with not only intrinsic chemical recyclability but also tunable thermal and mechanical properties. Next, the development of catalytic routes will be described for both the synthesis of designer monomers and polymers and the deconstruction of the circular polymers back to the monomers in pure state and quantitative selectivity under energy-efficient, cost-effective (de)polymerization conditions. Overall, the design and realization of such circular polymers must address: energy cost, depolymerization selectivity, and depolymerizability/performance tradeoffs.

RMRM 11

Strong Lewis acids slow heterogeneous electron transfer to heterobimetallic ruanyl complexes

***James D. Blakemore**, blakemore@ku.edu. Chemistry, University of Kansas, Lawrence, Kansas, United States*

The redox chemistry of uranium underlies the reprocessing of used nuclear fuels, but few methods are available for modulating the electrochemical properties of this challenging element. Efforts from diverse areas have shown that Lewis acids can reliably tune the reduction potential and chemical reactivity of heterobimetallic systems. On the other hand, understanding of the roles of Lewis acids in tuning the kinetics of electron transfer to heterobimetallic systems remains a frontier area. In this talk, I will discuss our group's recent observations regarding electron transfer and reactivity encountered with a family of compounds containing the redox-active uranyl moiety. We find that the Lewis acidity of associated redox-inactive metal cations (as judged by the pKa values of the corresponding metal aqua complexes) is a reliable descriptor for modulated ET kinetics. These results will be compared to those from other multimetallic systems, including other heterobimetallic species under investigation in our group.

RMRM 12

Replacing non-renewable carbon with bio-derived alternatives

***Andrew D. Sutton**, adsutton@lanl.gov. C-IIAC (Inorganic, Isotope, & Actinide Chemistry), Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

In attempts to “replace the whole barrel” and drastically reduce our petroleum dependency, it’s important to consider what a barrel of oil is used for. In the US, 76 % is used to make fuel and 16 % is used for chemicals, but with both markets having similar economic value a typical initial focus is typically the small volume, higher profit chemicals market. However, in order to have the most effect on environmental impacts (such as reducing CO2 emissions), the larger fuel market must not be neglected as a long-term focus. Our approach is to rationally design molecules and use group contribution methods to identify fuel candidates prior to actual cetane and octane testing. To that end we have been developing strategies to use small bio-derived molecules to construct more complicated carbon skeletons with varying degrees of functionalization and we can convert between the functional groups using simple catalytic approaches to produce molecules with promising fuel propeties. While a large proportion of biomass to chemicals/fuels work concentrates on producing hydrocarbons, there are numerous instances where over-defunctionalizing is not necessary and in fact is detrimental to the final properties and in the process consumes more energy and raw materials. By understanding this structure-function relationship we hope to synthesis molecules and molecule classes that have the optimum properties for specific applications.

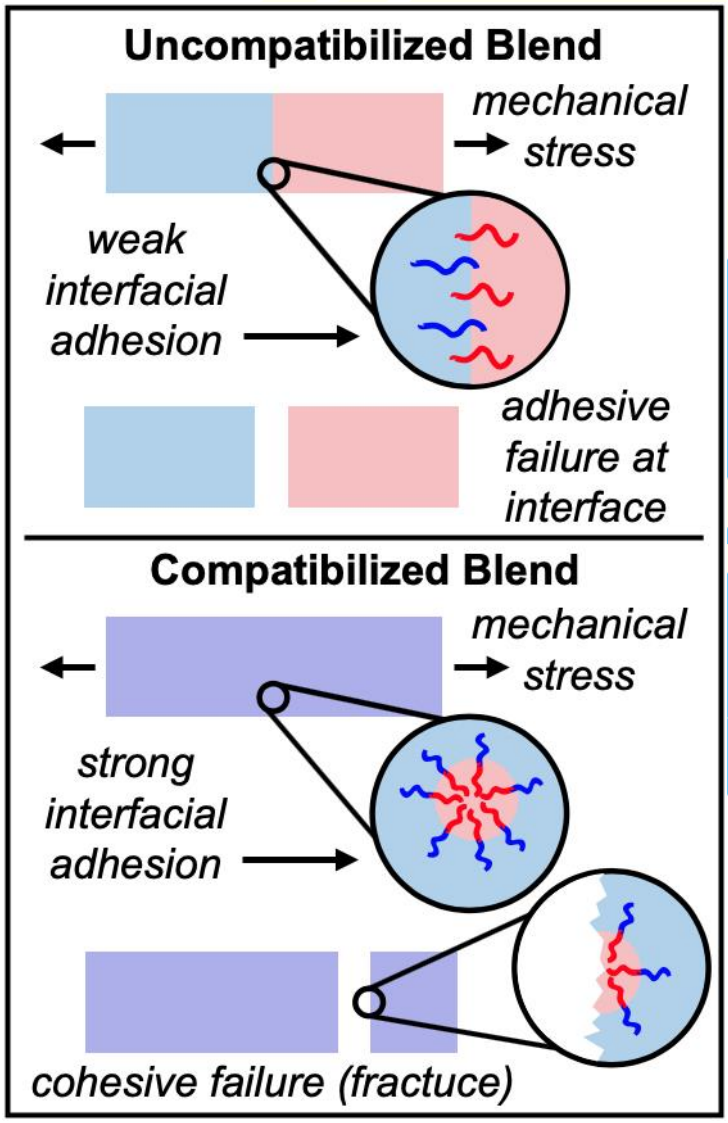
RMRM 13

Systematic investigation of graft copolymers as compatibilizers in a poly(styrene)-poly(lactic acid) model system

***Olivia N. Manahan**, onmanahan@gmail.com, Garret Miyake. Chemistry, Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States*

Current recycling systems mechanically break down plastic waste which, by consequence, will principally be down-cycled into low-value products such as plastic bags or carpeting. This in part drives the production of new plastic materials to replace those which have just been downcycled, diminishing the

impact that recycling would otherwise have. Combining several types of plastic into one homogenous blend through the addition of compatibilizers offers a potential path for upcycling mixtures of plastic waste into value-added materials, greatly improving recycling capabilities. Most examples of plastic compatibilizers are linear copolymers, but other polymer architectures have greater compositional variability. Graft copolymers, for instance, possess several parameters that could easily be tuned to improve compatibility of the plastic blend to which it is added. This presentation will discuss how varying parameters of graft copolymers affects the compatibility of poly(styrene)/poly(lactic acid) blends, an immiscible model system.



Addition of compatibilizer to otherwise immiscible polymer blends improves bulk mechanical properties.

RMRM 14

Plastics upcycling – benefits in manufacturing

***Nicholas Rorrer**, Nicholas.Rorrer@nrel.gov. National Renewable Energy Laboratory, Golden, Colorado, United States*

Plastics have become near ubiquitous with modern life due to their ideal properties and ease of manufacturing. Despite this, plastics represent a growing use of petroleum and have limited end-of-life options, which leads to plastics pollution globally. In order to combat these issues, it is fundamental to develop new technologies that either leverage natural or recycled feedstocks and evaluate their manufacturing relative to current petrochemical production. To these ends, we have leveraged the Materials Flow the Industry (MFI) tool to evaluate all plastics consumed a greater than 1 MMT/year. This study represents 18 different polymer chemistries, in which their United States consumption accounts for over 100 MMT of GHG emissions a year while requiring 3.2 Quads of energy in their manufacture. This work is further presented as three case-studies (i.e. polyolefins, polyesters, and thermosets) to elucidate areas for improvement for different polymer types. In addition to leveraging the MFI tool for commodity plastics, the MFI tool was also applied to a process from NREL in which reclaimed PET is combined with monomers that can be sourced from biomass to produce an unsaturated polyester (UPE) resin. The UPE resin possess a higher selling price than reclaimed PET and superior thermomechanical properties to the standard incumbent UPE resin. Importantly, analysis via the MFI tool elucidates that the implementation of biomass and recycled feedstocks can lead to a 57% reduction in supply chain energy and a 44% reduction in GHG emissions.

RMRM 15

Bifunctional nickel and copper electrocatalysts for CO_2 reduction and the oxygen evolution reaction

***Hanqing Pan**, schizokangaroo@hotmail.com, Christopher Barile. Chemistry, University of Nevada Reno, Reno, Nevada, United States*

In this study, a bifunctional electrocatalyst for CO_2 reduction and the O_2 evolution reaction (OER) was constructed from the electrodeposition of cuprous oxide (Cu_2O) and Ni on a carbon substrate. Different Ni thicknesses on Cu_2O were achieved by varying the time of chronopotentiometric deposition

of Ni. Electrochemical CO_2 reduction was carried out at -0.89 V and -1.89 V vs. RHE, and it was found that formate and CO were the two major products. Cu_2O modified with a Ni overlayer with a thickness of ~700 nm resulted in the highest formate Faradaic efficiency of 18%, and Cu_2O resulted in highest CO Faradaic efficiency of 7.9%. The enhanced Faradaic efficiency for formate is attributed to the synergistic effect between Ni and Cu_2O due to maximized amounts of exposed bimetallic sites that facilitate CO_2 reduction. The electrocatalyst also produces ~9 times more current density than previous studies using Ni-Cu_2O electrocatalysts for the OER. The ability of the Ni-Cu_2O thin films to catalyze both the OER and CO_2 reduction allows them to be incorporated in the first demonstration of a two-electrode CO_2 conversion device with a bifunctional catalyst.

RMRM 16 **CANCELED**

Extrinsic atom effects on the anodic properties of one-dimensional TiS2-xSex solid solutions

***Rory Weeks**, u0662093@utah.edu, Edwin J. Miller, Luisa Whittaker-Brooks. Chemistry, University of Utah, Salt Lake City, Utah, United States*

The transition-metal dichalcogenide TiS2 has been extensively studied in the context of advancing energy storage applications, particularly through its use as a cathode material in Li-ion and beyond Li-ion batteries due to its high electrical conductivity (≈ 104 S m-1), a higher theoretical specific capacity (239 mAh g-1) than that of LiCoO2 (130 mAh g-1), and a low discharge voltage (2.1 V vs. Li/Li+). Its use as an anode, however, has thus far been less studied. Recently, we reported the systematic control of sulfur vacancies in TiS2-x and the enhanced electrochemical properties arising from controlling defects. Here, we utilize selenium as an extrinsic atom in sulfur deficient TiS2-x nanoribbons to fill those vacancies (x) and subsequently investigate the anodic properties of TiS2-xSex compounds resulting from the formation of 1D solid solutions. The incorporation of Se within the TiS2-x lattice reduces the voltage window (< 2.1 V) with respect to Li/Li+ when compared to pristine TiS2, thus making TiS2-xSex a more suited anode material. In this presentation, I will describe our efforts towards the synthesis and characterization of TiS2-xSex solid solutions with a controlled 1D morphology, as well as preliminary electrochemical studies investigating their anodic characteristics as promising materials for energy storage.

RMRM 17

Highly active cationic Co(II) bisphosphine hydroformylation catalysts

***George G. Stanley**, gstanley@lsu.edu. Chemistry, Louisiana State University System, Baton Rouge, Louisiana, United States*

A new class of highly active cationic cobalt(II) bisphosphine hydroformylation catalysts will be discussed. They are at least a hundred times more active than the known industrial cobalt catalysts: $HCo(CO)_4$ and $HCo(CO)_3(PR_3)$. These catalysts have the general form: $[HCo(CO)_x(P_2)](BF_4)$, where x = 1-3, and P_2 = chelating bisphosphine. Unlike all other hydroformylation catalysts this new class has higher activity with electron-donating alkylated phosphine ligands. Unlike rhodium hydroformylation catalysts, these catalysts are remarkably resistant to metal-induced phosphine ligand degradation reactions and are capable of extremely high turnover numbers (e.g., > one million). The high activity of these catalysts allow them to operate under far lower temperatures and pressures relative to $HCo(CO)_4$ and $HCo(CO)_3(PR_3)$. These cationic Co(II) catalysts are very active at alkene isomerization, similar to neutral cobalt(I) hydroformylation catalysts and $HRh(CO)_4$. They are especially effective at hydroformylating internal branched alkenes to produce linear aldehydes. Comparisons with rhodium phosphine/phosphite catalysts and $HCo(CO)_4$ will be presented.

RMRM 18

Reflections on a career built on the foundations of chemistry: From polysaccharides to dementia

***James R. Bamburg**, james.bamburg@colostate.edu. Biochemistry and Molecular Biology, Colorado State University, Fort Collins, Colorado, United States*

With memberships in the Society for Neuroscience, the International Society for Neurochemistry, and American Society for Cell Biology, I would be described by most fellow academics as a cellular neurobiologist. However, my roots are in chemistry and for over 50 years I have been a member of the American Chemical Society. Today I want to share a few stories on my research career, which started doing carbohydrate chemistry in the Department of Chemistry at the University of Illinois, progressed through natural products research in Biochemistry at the University of Wisconsin, and then to studies at Stanford University working on nerve growth factor. This latter work led me into protein

chemistry and the neuronal cytoskeleton, and ultimately to pursue questions in neuroscience. The directions of my research program were strongly influenced by my chemistry background and reshaped from new knowledge gained from each of my five sabbaticals during my 49 years at CSU. The fantastic colleagues I have worked with along the way have allowed me to acquire new skills and keep up with the challenges of doing relevant research for the benefit of society. During the past 20 years, we have focused our efforts in defining a common target causing synapse loss in several major forms of dementia, including Alzheimer's disease, Parkinson's disease with Lewy Body dementia and HIV-associated neurocognitive disorder. Together, these diseases account for a large majority of all age-related dementias. We hope to bring this work to a successful conclusion in 2021 with the characterization of a possible oral therapeutic that can block and perhaps reverse the pathological feature these multiple dementias have in common.

RMRM 19

Consensus structures of the Mo(V) sites of sulfite-oxidizing enzymes derived from variable frequency pulsed EPR spectroscopy, isotopic labelling and DFT calculations

***John Enemark**, jenemark@arizona.edu. Chemistry and Biochemistry, University of Arizona, Tucson, Arizona, United States*

Sulfite-oxidizing enzymes (SOEs) from eukaryotes and prokaryotes have five-coordinate distorted square-pyramidal coordination about the molybdenum atom (Figure). The paramagnetic Mo(V) state is easily generated, and over the years four distinct CW EPR spectra have been identified, depending upon enzyme source and the reaction conditions, namely high and low pH (*hpH* and *lpH*), phosphate inhibited (P_i) and sulfite (or blocked). Extensive studies of these paramagnetic forms of SOEs using variable frequency pulsed electron spin echo (ESE) spectroscopy, isotopic labeling and density functional theory (DFT) calculations have led to consensus structures for each form. Errors in some of the previously proposed structures will be corrected.

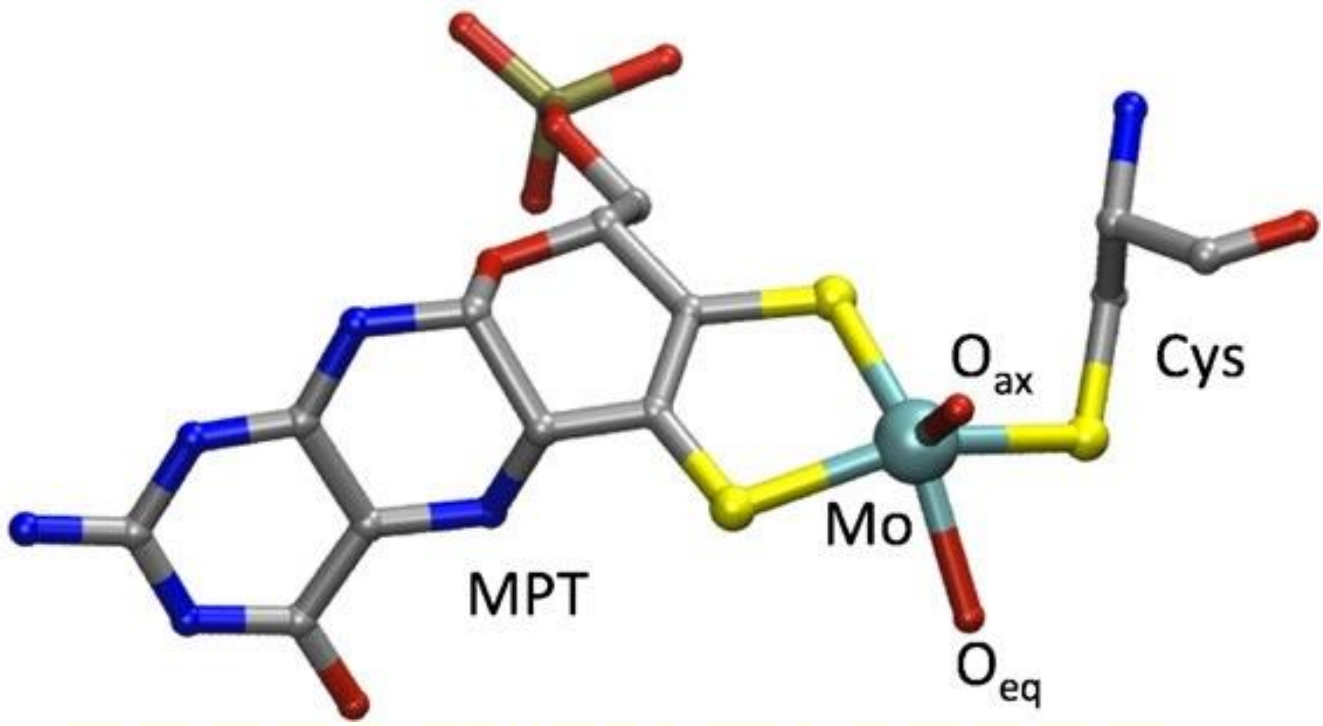


Figure Ball-and-stick representation of the fully oxidized molybdenum center of SOEs, showing the dithiolene coordination of the MPT unit and the conserved equatorial Cys residue. The identity of O_{eq}, which is solvent-exposed, varies for the different Mo(V) forms.

RMRM 20

Porphene: A heterocyclic analog of graphene

*Thomas Magnera[1], Paul Dron[1], Milena Jovanovic[1], Jared Bozzone[1], Elisa Miller[2], Wei Bu[3], **Josef Michl**[1,4], Josef.Michl@colorado.edu. (1) University of Colorado Boulder, Boulder, Colorado, United States (2) National Renewable Energy Laboratory, Golden, Colorado, United States (3) ChemMatCARS, The University of Chicago, Chicago, Illinois, United States (4) Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Praha, Czechia*

We report a structural characterization of bilayer zinc porphene, a periodic 2-D polymer formed upon oxidative polymerization of zinc porphyrin on water-air interface, using grazing incidence X-ray diffraction (GIXD), X-ray reflectivity, atomic force microscopy (AFM), scanning tunneling microscopy (STM), X-ray

photoelectron spectroscopy (XPS), UV-visible spectroscopy, and most important, mid-IR spectroscopy by attenuated total reflection (ATR) on a germanium multiple reflection plate. IR showed a gradual disappearance of CH vibrations of zinc porphyrin during the oxidation process and their complete absence at its completion, proving that the coupling is of the desired meso-meso and beta-beta type. Treatment with Fe(2+) at the air-water interface under acidic conditions caused a replacement of Zn(2+) with Fe(+2) and Fe(+3) ions. Very similar results were obtained by oxidative polymerization of free-base porphyrin, except that now NH vibrations were also present (and transformed into ND vibrations upon treatment with D2O). Oxidative polymerization of platinum porphyrin under identical conditions produces a monolayer of a periodic 2-D polymer (GIXD and X-ray reflectivity). The original CH vibrations again disappear in the IR but are replaced by new weak ones that persist even after complete coupling, suggesting that some or all of the oxidative coupling is of the meso-beta type. STM and TEM confirm the periodic pattern; one of the two likely structures is apparently formed. These experiments were accompanied by PBE0/POB-TZVP calculations using periodic boundary condition methods that so far yielded optimized geometries, band structures and predictions of STM images for three highly symmetric tautomers of free-base porphene and for one of the other two expected 2-D periodic structures.

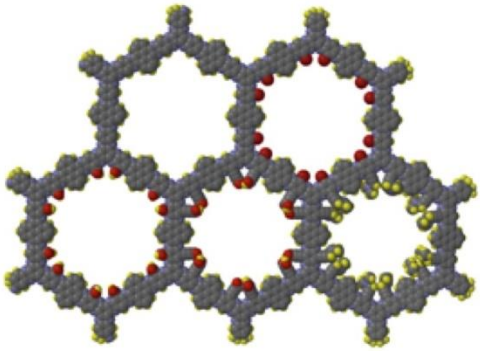
RMRM 21

New two-dimensional organic frameworks for membrane separations

Bruce A. Parkinson[1]*, bparkin1@uwyo.edu, John O. Hoberg*[1]*, Katie Li*[2]*. (1) Chemistry, University of Wyoming, Laramie, Wyoming, United States (2) Chemical Engineering, University of Wyoming, Laramie, Wyoming, United States*

Two dimensional materials, such as graphene and transition metal dichalcogenides, have recently been intensely investigated due to their unique properties. However, these materials are not easily modified to optimize their performance for a given application since this usually degrades their unique intrinsic properties. This lack of adaptability presents significant barriers to technological implementation and broad use. In this presentation, we present new highly ordered two-dimensional covalent organic frameworks (COFs) with a very stable semiconducting aromatic backbone and nanometer sized pores that can be functionalized, either pre or post synthesis, with almost any desired functional group (figure 1). Examples will be presented where a highly ordered COFs are synthesized with ionizable carboxylate groups in 2.8 nm diameter pores. Membranes fabricated with this material demonstrate both high solvent

throughput (>300x faster than graphene oxide membranes) and high selectivity to conduct only cations smaller than a precise size threshold. Pores with functional groups to either increase or reduce pore size or make anion selective membranes are also easily constructed. Examples of self-assembling, two-pore COFs with single metal binding sites will also be presented.



2D-COF Showing Pore Functionalization

RMRM 22

Dynamics and structure of molecular fluids - a tribute to Branka M. Ladanyi

Nancy E. Levinger, *nancy.levinger@colostate.edu. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

When the general public thinks of chemistry, they envision reactions occurring in beakers and flasks filled with liquid solutions. Chemistry often focuses on the solutes in these chemical systems but what of the fluids that support those reactions? These systems formed the basis of the far-reaching and important contributions from the late Branka Ladanyi, whose scientific contributions added profoundly to the theory and modeling of molecular fluids, and stimulated significant collaborations between theorists and experimentalists. In addition to her spectacular science, Ladanyi was a trailblazer for women scientists. This presentation will highlight some of the research and activities that comprise the hallmark left by this impressive scientist.

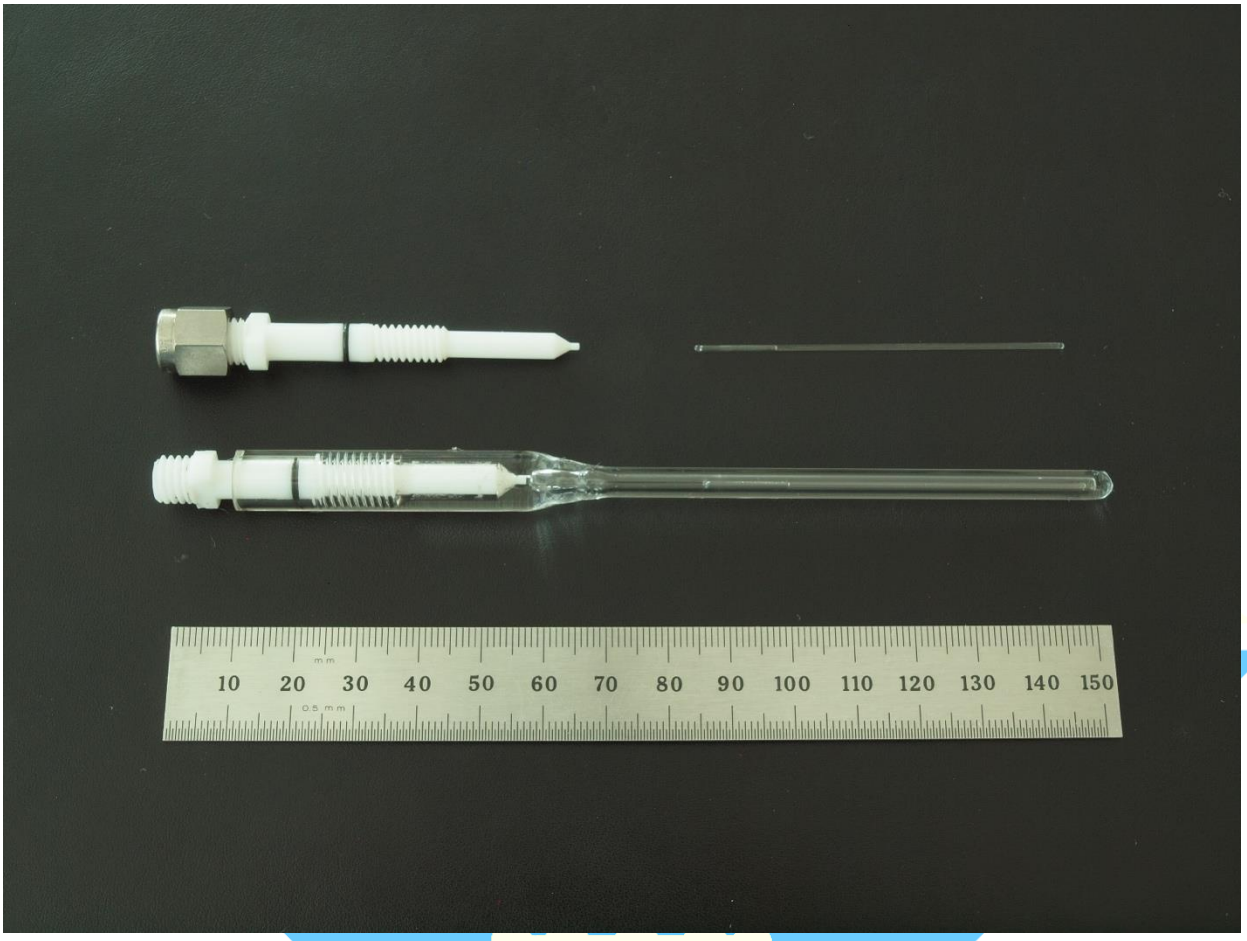
RMRM 23

Demonstration of the use of NMR spectroscopy for the measurement of vapor−liquid equilibria

***Jason Widegren**, jason.widegren@nist.gov, Christopher Suiter, Veruska Malavé, Edward Garboczi, Mark McLinden. Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, Colorado, United States*

Vapor-liquid equilibrium (VLE) data (T, p, x, y) are vital for the development of mixture thermodynamic models. Herein, we demonstrate the use of nuclear magnetic resonance (NMR) spectroscopy as an in-situ method for VLE measurements. The experiment is carried out entirely inside the NMR sample tube. The simultaneous measurement of liquid- and vapor-phase composition was achieved by the addition of a sealed glass capillary to the NMR sample tube. In this way, a small amount of the liquid phase wicks into the wedge-shaped gap between the capillary and the inner wall of the NMR tube. The presence of a suspended liquid meniscus was confirmed by X-ray computed tomography, and its behavior was examined by computational fluid dynamics. The components of the two phases are observed as distinct signals in the NMR spectra. The temperature-dependent spectrum of methanol, contained in a

sealed capillary, was used to measure setpoint temperature. Vapor density was measured instead of pressure. This was accomplished by calibration with gas-phase ethane at known densities. With this approach, we provide proof-of-concept results at 291.2 K on binary mixtures of (R32 + R125), (R125 + R143a), (ethane + neopentane), and (ethane + benzene).



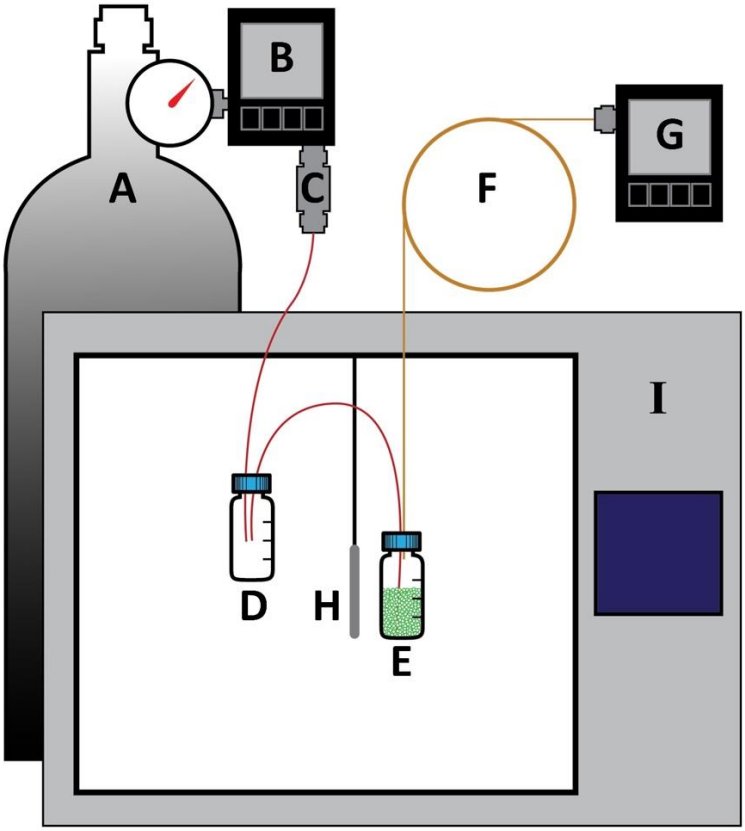
Sample tube and capillary used for the measurement of vapor-liquid equilibria.

RMRM 24

Rapid vapor collection method for vapor pressure measurements of low-volatility compounds

*Megan Harries, **Cheryle N. Beuning**, cheryle.beuning@nist.gov, Bridger L. Johnston, Tara M. Lovestead, Jason Widegren. Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, Colorado, United States*

Dynamic vapor microextraction (DVME) is a new method developed at NIST that enables high-quality vapor pressure measurements for large molecules with unprecedented state-of-the-art measurement uncertainties. Three key features of DVME allow for the rapid collection of vapor samples under thermodynamic conditions, including the use of a miniature vapor-equilibration vessel (the “saturator”) to minimize temperature gradients and internal volume, the use of a capillary vapor trap to minimize internal volume, the use of helium carrier gas to minimize nonideal mixture behavior, and the direct measurement of pressure inside the saturator to accurately account for overpressure caused by viscous flow. The performance of DVME was validated with vapor pressure measurements of *n*-eicosane ($C_{20}H_{42}$) at temperatures from 344 K to 374 K. A thorough uncertainty analysis indicated a relative standard uncertainty of 1.98 % to 2.79 % for measurements in this temperature range. The measurements were compared to a reference correlation with a relative standard uncertainty of 2.0 % for the vapor pressures of *n*-eicosane; the deviation of the measurements from the correlation was ≤ 2.85 %. The enthalpy of vaporization of *n*-eicosane at 359 K was calculated to be $\Delta_{vap}H$ = 91. 27 ± 0.28 kJ/mol, compared to $\Delta_{vap}H(corr)$ = 91.44 kJ/mol for the reference correlation. Total measurement periods as short as 15 min (3 min of thermal equilibration plus 12 min of carrier gas flow) were shown to be sufficient for high-quality vapor pressure measurements at 364 K.



A schematic of the DVME apparatus (not to scale) with a helium supply cylinder (A), a precision mass flow controller (B), an adsorbent tube (C), a transfer vial (empty 2-mL autosampler vial) (D), the saturator 2-mL vial containing 1-mm glass beads (E), a capillary vapor trap (F), a precision mass flow meter (G), a 100 Ω platinum resistance thermometer (H), and a GC oven (I).

RMRM 25

Investigation of plasma modified zeolite catalyst on hydrothermal liquefaction of chlorella powder

*Ben Jang, **Tarek M. Haque**, thaque1@leomail.tamuc.edu, Martin P. Jaimes, Erika Cardenas, Kevin Largent. Chemistry, Texas A and M University-Commerce, Commerce, Texas, United States*

The development of third generation biofuels from microalgae has seen extensive research over the last few years. The hydrothermal liquefaction (HTL) is the promising route for the production of bio-oils. The major drawback in HTL

is the high temperature and high pressure which result in high capital cost of equipment. To make HTL an economical process for bio-oil production, the temperature and pressure should be reduced and can be achieved adding alcohol to water during HTL. The efficiency of the HTL process can also be improved by using a suitable catalyst.
In this project, we investigated the effect of dielectric barrier discharge (DBD) plasma modified zeolites (Zeolite Y and ZSM-5) as catalysts on the yield and quality of bio-oils produced at different temperatures and times. The mixture of solvents (50 vol. % water & 50 vol. % ethanol) were used in HTL to increase the yield of bio-oils. Chlorella powder was successfully converted into bio-oils with/without catalysts at 250 ^{0}C and reaction time of 30 min, 45 min, and 60 min. The introduction of DBD plasma modified zeolites in HTL process improved the bio-oil quality and increased the percentage of yield. The highest percentage (56.69 %) of bio-oil obtained at 250 ^{0}C for 60 min reaction time. Hydrothermal liquefaction uses dichloromethane (DCM) to extract bio-oil from aqueous phase. There were two extractions of bio-oils from HTL products using dichloromethane. The bio-oils of the 1st extraction contained higher percentages of C and H and the 2nd extraction contained higher percentages of N and O. Different analytical techniques; elemental analysis, high heat value (HHV), thermogravimetric analysis, and gas chromatography-mass spectrometry were used to analyze the physiochemical properties of the bio-oils.

RMRM 26

Spatio-temporal super-resolution microscopy

Megan Dunlap[1]*, mdunlap@rams.colostate.edu, Duncan P. Ryan*[2]*, Peter M. Goodwin*[2]*, Paul Bourdin*[2]*, Jennifer A. Hollingsworth*[2]*, James H. Werner*[2]*, Martin P. Gelfand*[3]*, Alan K. Van Orden*[1]*. (1) Chemistry, Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States (2) Center for Integrated Nanotechnology, Los Alamos National Laboratory, Los Alamos, New Mexico, United States (3) Physics, Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States*

Temporal and spatial information that is acquired by a super-resolution microscope equipped with time-correlated single photon counting detectors may be combined to get a higher resolution image. Furthermore, the combined information can be used to resolve multiple non-blinking emitters spaced closer than the diffraction limit of light. In this talk, we report the results of using this new analysis method to study semiconductor quantum dot-in-rod structures and other nanomaterials. LA-UR-20-26165

RMRM 27

Investigating the shape of aerosol-OT reverse micelles and the impact of force field

***Christopher Gale**, cgale@colostate.edu, Mortaza D. Molayousefi, Nancy E. Levinger. Chemistry, Colorado State University, Colorado State University, Fort Collins, CO, US, academic, Fort Collins, Colorado, United States*

Aerosol-OT (AOT) reverse micelles are ideal systems for the study of nanoconfinement with molecular dynamics (MD) simulations often serving as a useful way to gain molecular level understanding of the system. In the present study, we examine the impact of the force field on the behavior of the simulated AOT reverse micelles and benchmark the results. We simulated $w_0 = 5$ reverse micelles using the CHARMM force field and three variations on the OPLS-AA force field. We benchmark the system against experimental values for the dipole moment, the relaxation constant of the complex permittivity, and the quasi-elastic neutron scattering spectrum. We evaluate the eccentricity and convexity as well as local curvature of the reverse micelle to assess how the force field impacts various values, e.g., the radial distribution function. We find that the force field has a large impact on the eccentricity of the micelle despite all force fields tested recreating the experimental dipole moment well. Our eccentricity results also report a surprisingly high abundance of oblate ellipsoidal shaped micelles not reported in previous literature. A likely explanation for the apparent oblate shape of the micelles is the appearance of kinks into an otherwise prolate micelle. These results highlight the importance of testing the force fields for accuracy in order to obtain correct molecular level insight into the system.

RMRM 28

Aerogels doped with nanomaterials show improved mechanical strength and potential for expanded application integration with printed structures

***Christina J. Hanson**, cjh@lanl.gov, Stephanie L. Edwards, Miles F. Beaux, Douglas R. Vodnik, Christopher E. Hamilton. Los Alamos National Laboratory, Los Alamos, New Mexico, United States*

Polyimide (PI) aerogels, due to their mechanical strength, low density, flexibility, and high thermal conductivity, have been of interest to a variety of applications, including commercial aviation, communication infrastructures, and everyday consumer products. However, for very thin samples, or samples under vacuum, it will be important to develop easy synthetic methods to finely tune the strength of these materials further. One potential solution to this is to introduce a dopant material at variable concentrations to control slight changes to a material property of interest. At LANL, we have experience synthesizing and growing a variety of different types of nanomaterials, and have been researching the integration of helical nanofibers and nanowires into PI aerogels to test the impact on mechanical properties. Helical nanofibers have been used in the past to reinforce dental and orthopedic implants [1], so we expect that the integration of these materials into PI aerogels will improve mechanical properties for a variety of new applications. Towards that end, we will present the results from our research on doped PI aerogels with nanomaterials. Additionally, we have developed a way to additively manufacture PI aerogels of various sizes and shapes consistently, and expect to be able to integrate nanomaterials into the ink used for printing. We are confident that these advances will further expand the potential applications of these materials.

[1] Hass, J.L., Garrison, E.M., Wicher, S.A. *et. al. Journal of Nanobiotechnology* **2012** 10 6

RMRM 29

Effect of molecular structure on the properties of self-assembled reverse bilayer vesicles

***Olivia Villanueva**, olivia.villanueva@ttu.edu, Anthony F. Cozzolino, Shiva Moaven. Texas Tech University, Lubbock, Texas, United States*

Carefully designed materials for the encapsulation and transportation of compounds for medicinal and research utilization are paramount. We have constructed pnictogen alkoxides and thiolates that form vesicles in non-aqueous environments. Notably, these molecules self-assemble through pnictogen bonds to form reversed bilayers. This study investigates the impact of molecular features (such as the pnictogen atom, the chalcogen atoms, and length and shape of the alkyl tail), preparation conditions and solvent environment on the macroscopic properties of the vesicles. Properties such as size, stability, and ability to encapsulate and affect a cargo are proposed with an eye on potential applications that rely on diffusion, transportation, and delivery of a cargo. Single crystal diffraction, dynamic light scattering, infrared

spectroscopy, and microscopy are used to characterize and examine the nature of the structure/property relationships between these molecules and the resulting self-assembled reverse bilayer vesicles.

RMRM 30

Modeling of unimolecular dissociation constants and reaction energies of ionic liquids: Applications in electrospray propulsion

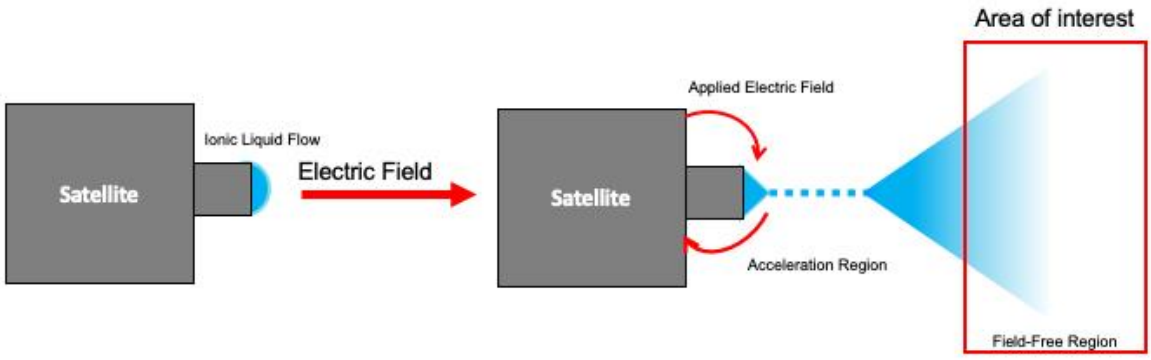
Julia Deyanova[1,2,3]*, Julia.deyanova@ucdenver.edu, Benjamin D. Prince*[1]*. (1) Space Vehicles, AFRL, Air Force Research Laboratory, Kirtland AFB, NM, US, academic/govt, Albuquerque, New Mexico, United States (2) Integrated Sciences, University of Colorado Denver, Denver, Colorado, United States (3) Universities Space Research Association, Columbia, Maryland, United States*

Electrospray thrusters are next-generation electric propulsion systems designed for space-vehicle applications such as cube satellites due to their unique high thrust density and maneuverability. Understanding the fundamental physics associated with the electrospray plume is crucial for the performance and lifetime of vehicles utilizing these propulsion systems. Experimental results have demonstrated that emitted clusters break apart over time. Studying the mechanism through which these clusters dissociate will provide insight as to the viability of novel electrospray propellants, allowing for a maximization of their performance. Development of computational models to describe and predict these behaviors is instrumental to electrospray propellent advancement.

The unimolecular dissociation rates of the 1-ethyl-3-methylimidazolium tetrafluoroborate (EMIM-BF_4) and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMIM-Tf_2N) ionic liquid clusters in the field-free region were investigated using classical molecular dynamics (MD) and quantum mechanical (QM) simulation techniques. Their temperature dependent dissociation constants were modeled using Eyring-Polanyi (EP) and Arrhenius equations and applied in corroboration to recent literature experimental measurements.

An *ab initio* QM approach was utilized to verify the MD force field presented in the literature associated with the EMIM-BF_4 clusters. Simulations were performed on various clusters and the resulting 0K and 300K binding energies were calculated and compared against the predicted *ab initio* values. In the absence of initial EMIM-BF_4 experimental rate constant data, the QM approach provided the benchmark through which MD results were compared. Thus, the literature force field was verified for MD simulation.

The developed simulation method was utilized to predict the dissociation constants for the EMIM-BF_4 (n=1c) and EMIM-Tf_2N (n=1a) ionic liquids using a thermal distribution ranging from (350 – 1000)K. Current work focuses on utilizing EP and Arrhenius thermodynamic values to reproduce threshold collision-induced dissociation experimental results.



Simple electrospray thruster

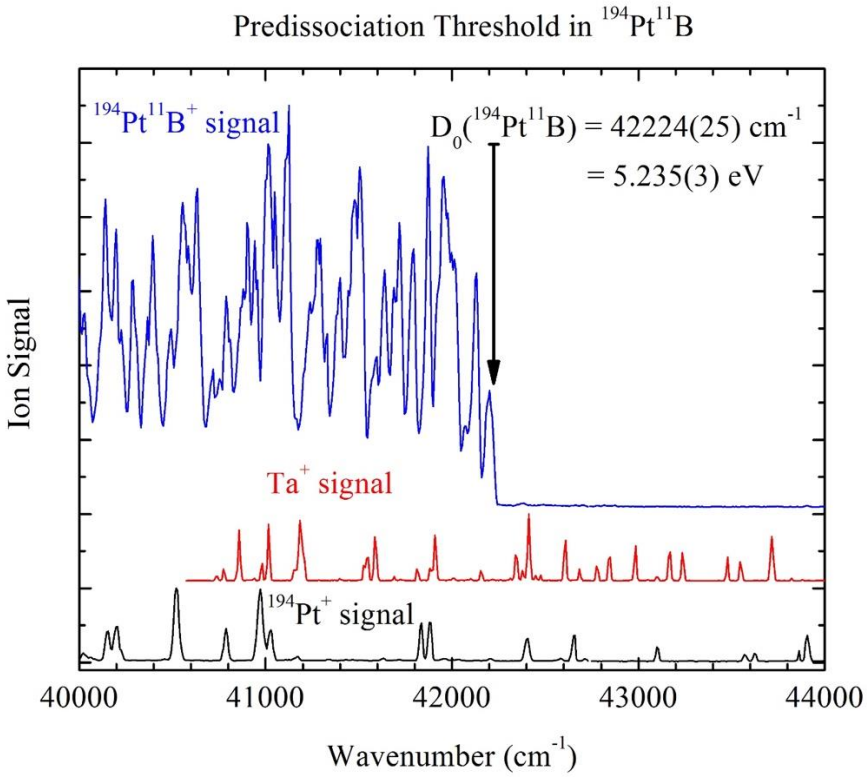
RMRM 31

Bond dissociation energies of transition metal borides

Dakota Merriles, *u1130765@utah.edu, Christopher Nielson, Erick Tieu, Michael D. Morse. Chemistry, University of Utah, Salt Lake City, Utah, United States*

Transition metal boride compounds have unique properties that make them as chemically interesting as they are relevant in a multitude of disciplines. As more applications are discovered for metal boride species, improved chemical models are needed to accurately predict the behavior of these species. To assist in this effort, we have developed a method for the precise and accurate

measurement of bond dissociation energies (BDEs) and have applied it to the diatomic transition metal borides (MB). The method relies on the fact that in the open d-subshell MB molecules, there is a large density of electronic states present at energies near the dissociation limit. Spin-orbit and adiabatic couplings among the large number of potential energy curves in this region enable the molecules to hop from curve to curve, finding their way to dissociation as soon as sufficient energy is available for this process. In our resonant two-photon ionization experiments, the high density of states in this region leads to a quasi-continuous spectrum below the dissociation energy, followed by a sharp drop to baseline when the molecules are excited above the dissociation limit. The sharp drop in signal occurs at a wavelength that corresponds to the BDE of the molecule. Using this method, the BDEs of 18 MB molecules have been measured to high accuracy. These data provide important benchmarks for the development and testing of improved computational methods for these species which will be helpful for modeling larger metal boride clusters and nanoscopic materials.



R2PI spectrum of PtB (upper trace) with its predissociation threshold showing the bond dissociation energy of PtB at 42 224(25) cm−1. The atomic spectra

of Ta (middle trace) and Pt (lower trace) were used for laser calibration.

RMRM 32

Can infrared laser break the chemical bonds in viruses?

***Chung-Hsun Yu**, chung-hsunyu@hotmail.com. Chemistry, Fort Hays State University, Hays, Kansas, United States*

This article is to explore the possibility of breaking the chemical bonds of viruses by the infrared laser. The frequency from the energy is expressed as a function of amplitude and the physical nature that the amplitudes can shatter and break the materials suggests that amplitudes are cumulated in quantity to reach a fracture point. Hypothetically the mechanism of the chemical bond breaking can be portrayed as a process forming a transition state. The infrared spectroscopy for a chemical bond describes the characteristics of the vibration modes and indicates the locations of radiations being absorbed. Corresponding to the characteristic band, a monochromatic and coherent infrared laser is suggested to apply to perform the task of breaking the chemical bond. An example of the virus with an amide functional group is discussed.

RMRM 33

Nature of formal hydride transfer reactivity in mo-dependent formate dehydrogenase

***Jesse Lepluart**, lepluart@unm.edu, Martin L. Kirk. University of New Mexico, Albuquerque, New Mexico, United States*

Formate dehydrogenases (FDHs) are type III DMSO reductase family mononuclear molybdenum enzymes that function to catalyze the interconversion of formate and carbon dioxide. Research efforts over the past two decades has elucidated the active site structures of these enzymes and determined a general mechanism for formate oxidation. Using this information, we have performed a computational study that reveals geometric and electronic structural contributions to the reactivity of these enzymes. Natural Bond Order (NBO) computations show that the early stages of the formate reduction reaction involve C-H bond activation of the substrate with subsequent formal hydride transfer to the Mo≡S sulfur of the enzyme active site. Here, we show reaction coordinate, relaxed surface, and DFT computations that reveal the unique ability of FDHs – and possibly of all DMSO reductase family enzymes –

to lock the enzyme active site in a high energy conformation, or entatic state, that optimizes orbital contributions to reactivity.

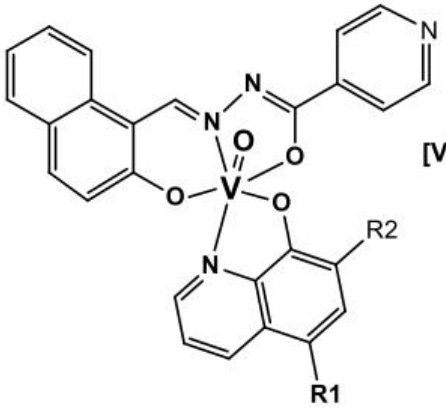
RMRM 34

Synthesis, characterization, biological activity against *Trypanosoma cruzi* and metallomics of novel heteroleptic oxidovanadium(V) compounds

Gonzalo Scalese[1,2]*, gscalese@fq.edu.uy, Ignacio Machado*[3]*, Leticia Perez*[4]*, Dinorah Gambino*[1]*. (1) Inorganic Chemistry Area, Universidad de la Republica Facultad de Quimica, Montevideo, Montevideo, Uruguay (2) Graduate in Chemistry Program, Universidad de la Republica Facultad de Quimica, Montevideo, Montevideo, Uruguay (3) Analytical Chemistry Area, Universidad de la Republica Facultad de Quimica, Montevideo, Montevideo, Uruguay (4) Molecular Interactions Laboratory, Universidad de la Republica Uruguay Facultad de Ciencias, Montevideo, Montevideo, Uruguay*

Chagas' disease is a potential lethal zoonosis caused by the trypanosomatid parasite *Trypanosoma cruzi*, which presents a life cycle that involves a biological vector (Triatominae insect) and the mammalian host, showing infective and non-infective forms. Available drugs are decades old and/or suffer from limited efficacy, undesirable collateral effects and development of resistance. Our group mainly focuses research efforts on the rational design of new metal-based drugs for the treatment of diseases by trypanosomatids. Searching for prospective vanadium-based drugs, in the current work we studied five structurally-related compounds, [$V^{V}O$(IN-2H)(L-H)], where IN is a tridentate ligand obtained by condensation of isoniazid and 2-hydroxinaftaldehyde and L are 8-hydroxyquinoline derivatives, a series of bioactive ligands that has shown good antiparasitic activity (see Figure). Compounds were synthesized and fully characterized in the solid state and in solution.
Complexes *showed in vitro* activity on both, non-infective and infective forms of *Trypanosoma cruzi*, with IC_{50} values in the micromolar and submicromolar range. Unspecific cytotoxicity was tested on VERO cells as mammalian cell model. The selectivity towards the parasites increased in respect to the free ligands. Trypomastigotes (infective form) are more sensitive than epimastigotes (non-infective form). Vanadium uptaken by the parasites and subcellular distribution was determined in the trypomastigote form. These are the first metallomics results reported in trypomastigotes of *T. cruzi*. These complexes show good activity against *T. cruzi* infective form and selectivity, deserving [$V^{V}O$(IN–2H)(L2–H)] to perform further studies in the

search for a new prospective drug for the treatment of Chagas disease. The whole set of results of these promising compounds will be presented and comparatively discussed.



$[V^{V}O(IN\text{-}2H)(L\text{-}H)]$

L = L0-L4

R1	R2	
H	H	**L0**
Cl	Cl	**L1**
Cl	I	**L2**
I	I	**L3**
NO_2	H	**L4**

RMRM 35

Investigation of decomposition kinetics and anti-cancer activities and of mixed-ligand vanadium complexes

Canan Yigit[1], *canan.uslanyigit@sydney.edu.au, Heide Murakami*[2], *Aviva Levina*[1], *Peter A. Lay*[3], *Debbie C. Crans*[2,4]. *(1) School of Chemistry, University of Sydney, Sydney, New South Wales, Australia (2) Chemistry, Colorado State University, Fort Collins, Colorado, United States (3) School of Chemistry and Sydney Analytical, University of Sydney, Sydney, New South Wales, Australia (4) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States*

Amongst the metal-containing compounds, vanadium complexes have recently stood out of non-platinum anticancer agents. Three vanadium Schiff base complexes were halogenated and compared to their non-halogenated counterparts and bound to different catacholate ligands. All of these compounds were examined for their anti-cancer activities against human brain cancer (T98g) cells. Conditions for determining the cytotoxicity of the V(V) complexes in T98g cells were designed based on the decomposition kinetics of the compounds in cell culture media. Decomposition reactions of all compounds were found to be the first-order process. The duration of the decomposition for the compounds was based on the time-dependent changes in the UV-vis

spectra of the most stable compound in the series 310K. Concentration-dependent changes in T98g cell viability and the corresponding IC_{50} values were established. 3,5-di(tert-butyl)catechol substituted compound showed the highest activity among the non-chloro analogous. It was observed that chloro substitution in the Schiff base ligand increased the cytotoxic activity of the complexes.

RMRM 36

Multinuclear NMR studies of anticancerous Non-Innocent Vanadium Schiff Base Complexes showing isomer formation

Andew C. Bates[1]*, Andrew.Bates@rams.colostate.edu, Heide Murakami*[1]*, Debbie C. Crans*[1,2]*. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States*

A hydrophobic Schiff base/catecholate non-innocent vanadium complex has recently been reported to have anti-cancer properties suited for chemotherapy of platinum resistant cell lines. Their desirable properties arise from the combination of high reactivity and hydrophobicity making them well suited for intratumoral injections regardless of their limited lifespan in a biological system. The most active complex V(V) di-t-butyl substituted catecholate [[VO(HSHED)(DTB)] is found to form isomers in solution using 51V NMR spectroscopy. The isomer destribution for the V(V) di-t-butyl substituted catecholate is compared to that of the parent catecholate complex[[VO(HSHED)(cat)], (HSHED = N-(salicylideneaminato)-N'- (2-hydroxyethyl)-1,2-ethanediamine, cat = pyrocatechol, DTB = 3,5- di(tert-butyl)catechol). We find that several isomers form for both compounds and their solution structures are investigated using 2D NMR spectroscopy and compared.

RMRM 37

In-silico evaluation of DNAJB1-PRKACA fusion proteins binding site

Sergio Cabrera*, secabrer@nmsu.edu. Chemistry & Biochemistry, New Mexico State University, Las Cruces, New Mexico, United States*

Fibrolamellar hepatocellular carcinoma (FHC) is a rare cancer that affects the liver of adolescents, having a median age of 20 years. The only known treatment, usually ineffective, is invasive and involves rigorous removal of the tumors. Being comparatively new research, there are many unknowns related

to docking with the FHC fusion protein DNAJB1-PRKACA. A literature search for binding studies on the fusion reveals little information about protein-ligand interactions, making it difficult to identify a docking site. Aimed at the identification of the protein binding site, computational studies were performed using unoptimized and computed optimized structures of our chosen chalcone derivatives. Preliminary results expose a proposed site of interaction with the J-domain on the DNAJB1-PRKACA protein surface. This result was accomplished by taking the best pose from many ligand interactions using YASARA and other computational evaluation software. Discoveries are presented through tabulated values of binding energies, dissociation constants, hydrophobic interactions, hydrogen bonds, pi-pi interactions, and cation-ligand interactions. Using the tabulated results a proposed docking site for the fusion protein DNAJB1-PRKACA is identified. Through exhibition of the binding results will be offered in the fourth coming presentation.

RMRM 38

Automated construction of fragment-based pharmacophores to elucidate novel GPCR ligands

Gregory L. Szwabowski*, gszwbwsk@memphis.edu, Abby L. Parrill-Baker, Daniel L. Baker. Chemistry, The University of Memphis, Memphis, Tennessee, United States*

Pharmacophores represent three-dimensional arrangements of molecular features required to elicit a specific biological activity. G protein-coupled receptors (GPCR) are integral membrane proteins of considerable interest as targets for drug development. Pharmacophore models can be used in virtual screening efforts to identify ligands that are likely to interact with biological targets. Ligand-based pharmacophore models are traditionally constructed to identify structural commonalities between known bioactive ligands. However, structure-based pharmacophores have gained more attention as the number of high-resolution GPCR structures has increased (67 unique receptors as of July 15, 2020). Thus, work discussed herein describes a structure-based pharmacophore approach using functional group fragments energetically optimized within the active sites of 8 class A GPCR structures. Pharmacophores were created via automated feature annotation of 5 randomly selected functional group fragments in an attempt to sample effective combinations of diverse pharmacophore features. Each of 5000 generated pharmacophores was then used to search a database of active compounds and was scored using enrichment factor and goodness-of-hit scores as metrics. This approach samples pharmacophores possessing the theoretical maximum

enrichment factor for each receptor studied. Work is ongoing to apply the pharmacophores generated as a means to prioritize small molecules for screening as novel GPCR ligands. As one proof-of-principle example, pharmacophores have been generated for the dopamine (D2) receptor D2, followed by in silico screening of the Zinc database. This work resulted in the identification of a prioritized set of novel ligands for subsequent in vitro analysis. Additional progress will be discussed.

RMRM 39

Synthesis and characterization of gold nanoparticles prepared with the flavonoid quercetin

***Annika Holm**, holm9680@bears.unco.edu, Murielle Watzky. Chemistry and Biochemistry, University of Northern Colorado, Greeley, Colorado, United States*

Metal nanoparticles offer a large surface-to-volume ratio that leads to differences in both chemical and physical properties compared to bulk metal. Gold metal nanoparticles are of interest to researchers because of their potential applications as biosensors and/or in drug delivery. The goal of this project is to synthesize gold nanoparticles that can be biocompatible, via a 'green synthesis' method. This project will look at the ability of a common flavonoid compound, quercetin, to synthesize gold nanoparticles from gold metal ions using modifications of a literature procedure. The formation of nanoparticles is achieved by reacting hydrogen tetrachloroaurate with quercetin in basic aqueous solution, wherein quercetin acts as both a reducing and stabilizing agent. UV-visible spectroscopy is utilized in this project to follow the reaction and reaction kinetics by monitoring changes in surface plasmon resonance for the gold nanoparticles. Other methods such as scanning electron microscopy with energy-dispersive X-ray will be utilized to characterize the nanoparticles.

RMRM 40

Preparation of gold nanoparticles in novel thioether-functionalized ionic liquids

***Elisabeth Kulesus**, kule2770@bears.unco.edu, **Hannah Leloup**, lelo8955@bears.unco.edu, Murielle Watzky, Hua Zhao. Chemistry and Biochemistry, University of Northern Colorado, Greeley, Colorado, United States*

Gold nanoparticles have found a range of applications in the biomedical field as chemical and biochemical sensors, which take advantage of the nanoparticles' plasmonic properties, as well as of the relative chemical inertness of gold metal. In this project, novel phosphonium and imidazolium ionic liquids functionalized with thioether groups are used as stabilizing agents in "bottom up" syntheses of gold nanoparticles. The project will look at optimizing the synthesis, synthetic reproducibility, and isolation of the gold nanoparticles prepared with these novel thioether-functionalized ionic liquids. The reaction with be followed with UV-visible spectroscopy, and the nanoparticles will be characterized using scanning electron microscopy with energy-dispersive X-ray.

RMRM 41

STM and XPS studies of co nanoparticles on reducible CeO_2(111) thin films

***Linze Du**, lduhill@outlook.com, Daniel L. Braedt, Jintao Miao, Jing Zhou. University of Wyoming, Laramie, Wyoming, United States*

Cobalt metal catalysts have been of great interest as economical and promising catalysts for ethanol reforming and dry reforming of methane reactions. Ceria can be a suitable choice as the catalytic support for Co since unique redox properties and oxygen storage capacities of ceria can influence the size, structure, chemical state, and thus the catalytic performance of Co. To elucidate the nature of the reactivity, it is of significance to gain a fundamental understanding of the structure and electronic properties of Co particles on ceria supports. Here we report our studies of Co deposited on fully oxidized CeO_2(111) and reduced CeO_x(111) thin films using scanning tunneling microscopy and X-ray photoelectron spectroscopy. Ceria thin films were grown in situ on Ru(0001) under ultrahigh vacuum conditions. The growth of Co particles was investigated as a function of Co coverages, deposition temperatures, post-deposition annealing temperatures, as well as degrees of Ce reduction. At 300 K, oxidation of Co to Co^{2+} occurs on fully oxidized CeO_2. At low Co coverages (<0.2 ML), Co^{2+} is the predominant species. With the increase of the Co coverage, both metallic and Co^{2+} species can be present on CeO_2. Metallic Co is the major species formed on partially reduced ceria. Co forms two-dimensional small particles on ceria at room temperature. With further heating to 1000 K, the particles can agglomerate into three-dimensional structures. However, they are on average less than 1 nm high at 1000 K. A comparison of the growth of Co on CeO_2(111) with our previous studies of Au, Ni, Pt, and Rh at the same coverage demonstrates that Co forms the smallest clusters, which suggests a stronger Co-ceria interaction. Our study presents

model Co-ceria catalytic systems for further investigation of the chemistry in the reforming process related with particle sizes, chemical states and support effects.

RMRM 42

Nanoconfinement raises the barrier to hydrogen atom exchange between water and glucose

***Sam L. Miller**, sam.miller@colostate.edu. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Using 1D Exchange Spectroscopy (EXSY) NMR experiments, we employ a direct method for measuring the proton exchange between water and glucose while nanoconfined within reverse micelles. EXSY NMR selectively spin labels the water nuclei and uses an arrayed mixing time to subsequently sample the location of the spin labelled protons that have exchanged from water onto the target molecule. Carried out at a range of different temperatures, this experiment produced a series of rate constants that were subsequently used to construct an Arrhenius plot to calculate the energy barrier constraining this process.

When studied in bulk, this exchange process occurs on a time scale so fast that the resultant line broadening in NMR spectrum prevents observation of the necessary hydroxyl peaks of glucose. However, confinement in a nanoscale pocket of water dramatically slows the process. These reverse micelles make a particularly ideal model system because of extensive prior characterization and ease of preparation. Our research results may have significant impact on applications in biotechnology or pharmacology, as important processes can occur in similarly nanoscale environments.

RMRM 43

Direct carbon-carbon bond formation between single-wall carbon nanotubes: Fact or artifact?

***Punhasa S. Senanayake**, punhasa@nmsu.edu, Marat Talipov. Department of Chemistry & Biochemistry, New Mexico State University, Las Cruces, New Mexico, United States*

Single-walled carbon nanotubes (SWNTs) are being considered for use in nanoelectronic devices, hydrogen storage, and numerous other applications

due to their extraordinary material properties. SWNTs have large elastic moduli, which would make them perfect for low-density high-modulus fibers. However, bundling of nanotubes leads to worse performance, which is attributed mostly to the weak interaction between tubes. Many structural modifications were conducted to improve the intra SWCNT interactions which leads to the enhancement of the properties of nanotubes.

Studying of the properties of SWCNTs can be approached by observing the properties of acene and graphene sheets. The optimized structures for bilayer acenes and graphene sheets showed a covalent bond at the zig-zag edges but absent in armchair edges regardless of the dimensions. Hence, the covalent bond formation is a morphological factor. Similar observation can be obtained with SWCNT dimers, where the covalent bond is formed independently from the metallic nature and the length of the SWCNTs. Interestingly, there was a tendency for the formation of a covalent bond when a zig-zag edge was facing each other in the SWCNT dimers. In SWCNTs with higher number of zig-zag edges, the covalently linked dimer was stable; while the Van der Waals dimer was more stable in SWCNTs with arm-chair edges.

This unusual observation of the covalent linking of acenes, graphene dimer, and SWCNT dimers can be explained using the Clar's aromaticity theory. According to this theory, the most stable structure is achieved for a system with the highest possible number of disjoint aromatic sextets. In agreement with the Clar's theory, the most stable system for SWCNT is the CNT with the arm-chair edges. Since the driving factor for the covalent linking between SWCNTs is thermodynamic, the stability of the arm-chair edged SWCNT can be further justified by calculating the enthalpies of formation at 0K. When analyzing the SWCNT dimer with arm-chair edges, the stabilization when forming the Van der Waals dimer is higher than the covalent dimer regardless of the chirality of the SWCNT.

In conclusion, the formation of the covalent bond between SWCNTs should be uncommon because it requires that both SWCNTs should be thermodynamically unstable. However, it could be expected that such covalently bonded factionalized CNTs can be formed during an artifact of SWCNTs that leads to the zig-zag edge nanotube formation.

RMRM 44

Development of chemical strategies prepare synthetic lasso peptides and their isomers

***Lori Digal**, lori_digal@yahoo.com, Abhijit Ghorai, Marcus Mifflin, Andrew G. Roberts. Chemistry, University of Utah, Salt Lake City, Utah, United States*

Lasso peptides are a class of biologically active natural products with intriguing tertiary structures despite their short sequences. The knot-like feature common to all lasso peptides is formed by the cyclization of the N-terminus (*e.g.*, Gly) with an internal Asp or Glu side-chain carboxylate, which wraps around a C-terminal 'tail' to generate a peptide rotaxane. In many cases, the lasso motif imparts excellent stabilities toward proteases and is linked to the observed biological properties. Accordingly, our primary interest is in the development of synthetic strategies to access lasso structures. Sungsanpin and ulleungdin were identified as exemplary lasso targets to better understand their unique ability to inhibit cellular invasion, a critical step in cancer metastasis. We predict the lasso topology imparts bioactivity, and therefore plan to conduct structure-activity relationship studies by comparing the effects of the natural lassos with isomeric topologies. The *de novo* chemical synthesis of the native lasso structure presents a considerable challenge, and sequence-independent strategies capable of achieving this undertaking are unknown. Indeed, efforts addressing the limitations encountered by methods for heterologous expression would allow for more robust protocols to evaluate the efficacy of novel lassos. We hypothesize that a guided amide bond equilibration process will enable the selective formation of the isopeptide linkage at Gly1–Asp8, providing a thermodynamic distribution of the folded and unfolded isomers. Here we report on the systematic evaluation of an auxiliary-mediated, acyl transfer system based on reversible native chemical ligation as a prospective strategy to attain these fascinating natural products.

RMRM 45

Preparation of apolipoprotein C III peptide antigens for display on virus like particles to combat cardiovascular disease

***Nicholas R. Lopez**, nicholas.lopez7714@gmail.com, Naomi Lee. Chemistry and Biochemistry, Northern Arizona University College of Engineering Forestry and Natural Sciences, Flagstaff, Arizona, United States*

Cardiovascular disease (CVD) is the leading cause of death for men, women, and people of most racial and ethnic groups in the world. Common risk factors for CVD include elevated serum levels of low-density lipoprotein cholesterol (LDL-C) and triglycerides (TG). Research has shown that Apolipoprotein C III (ApoC3) plays an important role in the metabolism of TGs by inhibiting both the hepatic clearance of TGs and the enzyme lipoprotein lipase which hydrolyzes

TGs into free fatty acids for uptake by muscular tissue. Changes in gene expression of ApoC3 can drastically affect TG levels as seen in ApoC3 knockout mice that are hypotriglyceridemic and overexpression of ApoC3 that leads to hypertriglyceridemia. This makes therapeutics that reduce ApoC3 levels a potential target for vaccine development. We will synthesize potential ApoC3 peptide antigens using solid phase peptide synthesis and characterization of the peptides will be conducted using MALDI-TOF MS, HPLC, and Circular Dichroism spectroscopy. Using chemical biology tools, we will increase the alpha helical content of ApoC3 peptide antigens to best mimic the alpha helical character of human ApoC3. Eventually the ApoC3 peptide antigens will be conjugated to virus like particle vaccine platforms and mice will be challenged to better understand the role of immunization on the murine antibody response and the effects on serum levels of LDL-C and TGs.

RMRM 46

Mapping electrostatic protein-membrane interactions of Slp-4 C2 domains using molecular phylogenetic analysis and structure prediction

Nara Chon[1], *nara.chon@ucdenver.edu, Sherleen Tran*[2], *Christopher Miller*[3], *Hai Lin*[1], *Jefferson D. Knight*[1]. *(1) Department of Chemistry, University of Colorado Denver, Denver, Colorado, United States (2) University of Colorado School of Dental Medicine, Aurora, Colorado, United States (3) Department of Integrative Biology, University of Colorado Denver, Denver, Colorado, United States*

Many cytosolic proteins bind to anionic lipids on secretory organelles and the plasma membrane during cell signaling and membrane trafficking. Synaptotagmin-like proteins (Slp) attach to phosphatidylinositol-(4,5)-bisphosphate (PIP2) and phosphatidylserine (PS) lipids via tandem C2 domains (C2A and C2B) and contribute to secretory vesicle plasma membrane docking in a Ca^{2+}-independent manner. In our previous study, we have found that the C2A domain of Slp-4 (also called granuphilin) binds to physiological membranes containing PIP2 and PS with very high affinity. Furthermore, molecular dynamics simulations revealed that the interaction involves residues comprising a broad positive electrostatic surface. Particularly, a three-Lys cluster located in the beta3-beta4 region forms the center of a conserved PIP2-binding site, while the positively charged residues near the cluster interact with nearby PS molecules. We hypothesize that this surface provides a nonspecific electrostatic anchor to PS and therefore the net charge on the protein surface is likely to be more strongly evolutionarily conserved than the individual residues. To test this hypothesis, the sequences of Slp-4 C2A domains and

C2AB tandems in vertebrates were compared to assess the evolution of charged residues using a molecular phylogenetic approach. The consensus sequences were found per clade, and the net charges of individual and consensus sequences were calculated. The crystal structure of Slp-4 C2A was used to generate homology models, from which Poisson-Boltzmann calculations were carried out in order to quantify the positive electrostatic surfaces. This approach may help characterize nonspecific yet potentially strong electrostatic interactions between proteins and charged surfaces.

RMRM 47

Electroanalytical tools and molecular-based assays to measure the impact of noise on dopamine neurotransmission in the central auditory pathway

***Patrick Wilson**, patrick.wilson@unco.edu, Aaron Apawu. University of Northern Colorado, Greeley, Colorado, United States*

In the United States, loss of hearing impacts approximately 48.1 million people. The cumulative effects of noise are experienced in every area of society whether occupational, environmental, or through aging. Previous work has reported changes in dopamine receptor gene expression following acoustic trauma, suggesting a possible role of dopamine in auditory processing. This conclusion is supported by recent data that showed patients suffering from Parkinson's disease (a condition associated with dopamine depletion) exhibit deficits in auditory processing. Thus, the present work focuses on the role of dopamine neurotransmission within the central auditory pathway and how it's impacted by noise exposure. Characterizing the complexities of neurotransmission requires elegant methods of inquiry, regarding both the neurotransmitter and neuron physiology. Fast scan cyclic voltammetry (FSCV) with carbon fiber microelectrodes is uniquely well-suited for real time neurochemical measurement because it has the speed, selectivity, sensitivity, and the spatial resolution needed for such measurements. Immunoassays on the other hand provides information about the neural protein receptors distribution and levels. In this work, dopamine neurotransmission release and uptakes events are measured and characterized using FSCV in the inferior colliculus in vivo and in vitro by both electrical and sound stimulation. Then, Western blot and immunocytochemistry are utilized to demonstrate the impact of noise on dopamine receptors of the inferior colliculus. The combination of FSCV with immunoassays allows for a more comprehensive examination of dopamine's role in the central auditory pathway.

RMRM 48

Detection of intracellular HNO delivery via a thiol-functionalized indicator with capillary zone electrophoresis

Amarakoon Appuhamilage Thilini N. Amarakoon,
navodiamarakoon@email.arizona.edu, Daniel Plewa, Minhui Han, Neng Ke, Colleen Janczak, Katrina M. Miranda, Craig A. Aspinwall. Chemistry and Biochemistry, University of Arizona, Tucson, Arizona, United States

Nitroxyl (HNO) has been recognized as a potential therapeutic agent in a number of conditions, including cardiovascular ailments and cancers. Due to its high reactivity and short half-life direct intracellular quantification can only be achieved using trapping agents that react quickly. HNO reaction with thiols yields sulfinamide derivatives that can be easily separated and identified using capillary zone electrophoresis (CZE) with laser induced fluorescence (LIF) detection. Here, mercaptoethylamine derivatized carboxyfluorescein (CFS) was utilized as a cell-permeable, fluorescent, thiol-functionalized trapping agent which can directly load into cells and forms sulfinamide. HNO-generated sulfinamide was stable for over 4 h and was detectable at levels as low as 3±0.5 nM *in-vitro* with baseline resolution from CFS. Potential interference from reactive nitrogen and oxygen species, including GSNO (an endogenous *S*-nitrosothiol), hydrogen peroxide (H_2O_2) and diethylamine dinitric oxide adduct (DEA/NO) was also assessed. The results show that CFS can detect HNO *in-vitro* even in the excess of large cellular pools of natural and pharmacological reactive nitrogen and oxygen species, including GSNO, DEA/NO and H_2O_2. The intracellular reactivity of CFS demonstrated preference for HNO without interference from other cellular components. The sulfinamide was detectable upon exposure to different extracellular HNO donor concentrations and was formed in a dose-dependent manner, with as little as 18±1.7 nM resolvable which correlates to 530±50 nM total intracellular concentration. These results show that CFS can be used as a promising trapping agent to quantitatively determine HNO *in-vivo* thus understanding its reactivity in cellular redox signaling so that this model can be used to test other donors/prodrugs in different cell types.

RMRM 49

Statistical analysis of protein-protein comparison methods

***Christy Dyer**, cldyer@memphis.edu, Abby L. Parrill-Baker, Daniel L. Baker. Chemistry, The University of Memphis College of Arts and Sciences, Memphis, Tennessee, United States*

Nicotinamide adenine dinucleotide cofactors (NADC) are critical cofactors for proteins facilitating biological metabolism and energy production. Thus, a thorough understanding of proteins that bind NAD^+, NADH, $NADP^+$, and NADPH is of broad scientific interest. NipSnap homolog 1 (NipSnap) is a mitochondrial protein associated with Alzheimer's disease. Preliminary data for NipSnap supports nicotinamide cofactor binding giving a point of commonality to one of the largest classes of mitochondrial proteins, dehydrogenases. Many dehydrogenases contain a conserved secondary structural motif called a Rossmann fold, which often includes a NADC binding site. Due to the nature of proteins, knowing their structure is at the base of understanding their functions. Computational homology modeling allows structural predictions for proteins with unresolved structures. Traditionally, structural models are built for target proteins by homology to template proteins using an amino acid alignment that optimizes sequence identity. Homology model quality depends on the template selected. Proteins with high sequence similarity and similar function are expected to have common evolutionary origin, thus conserved structure. While this classic approach works for many proteins, it fails for many others (including NipSnap) due to the lack of a suitable template. The goal of this work is to develop and apply a novel approach to homology modeling template identification using secondary structure propensity measures, rather than primary sequence identity, to drive sequence alignments. Statistical analysis using sequence identity driven alignments for protein-protein comparisons showed poor intracluster cohesion and intercluster separation, i.e. the results were not meaningful. Clustering proteins based on sequence identity driven alignments does not identify the structural similarities identified using structurally driven alignments, which do produce meaningful clusters. The current aim is to develop a predicted secondary structural propensity replacement for sequence identity in protein alignments to determine if structural correspondence can be reproduced without the need for resolved protein structures.

RMRM 50

Light-activated quantum dot potentiation of antibiotics to treat drug-resistant biofilms

***dana f. stamo**, dana.stamo@colorado.edu, Anushree Chatterjee. Chemical and Biological Engineering, University of Colorado Boulder, Boulder, Colorado, United States*

Antimicrobial resistance is one of the biggest threats to global health and demands alternative therapies for multi-drug resistant (MDR) infections. Light-activated quantum dots (QDs) are a versatile candidate for treating MDR bacteria without harming mammalian cells. Furthermore, their ease of diffusion and ability to photo-potentiate allows for precise, localized treatment and their dynamic tunability keeps them in pace with bacterial evolution. While QDs are shown to be a viable alternative therapy for planktonic cultures, they have not been applied in treating bacterial biofilms (a common growth form that affords bacterial strains more resistance and persistence to immune and traditional drug attack). Additionally, the mechanism of QD attack—production of reactive oxygen species—and sub-breakpoint antibiotic treatments have been shown to stimulate biofilm formation, especially in clinical isolates. Herein, I demonstrate the previously-observed monotherapeutic stimulation of biofilm formation and apply QD-antibiotic combination therapies overcome and nearly eradicate 48-hour, early-stage, static biofilms. These results lay the groundwork for QD-antibiotic combination treatments for late-stage clinical and industrial biofilms, contributing to the development of QD nanotherapeutics for combating MDR superbugs.

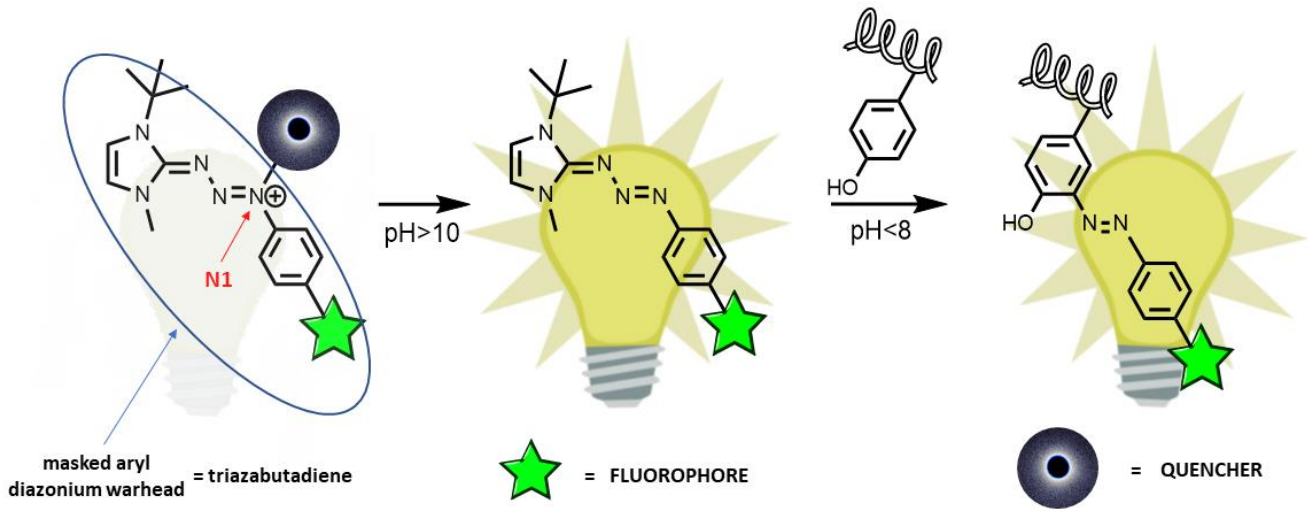
RMRM 51

Optimization of the attachment of a base labile fluorescence quencher in designing a triazabutadiene probe to image mosquito larval gut proteins

***W Mudiyanselage Anjalee N. Wijetunge**, anjaleewijetunge@email.arizona.edu, Lindsay E. Guzman, John C. Jewett. Chemistry and Biochemistry, University of Arizona, Tucson, Arizona, United States*

Delivery of a chemical probe to a specific target is often challenging, given the complexities of the environment of the biological milieu. Therefore, stable dormant probes were made to be activated only in particular environments. The unique gut pH of a mosquito larva (pH 7 - 11) is the targeted environment for

the chemical probe discussed herein. Determining possible target proteins of mosquito larval gut will facilitate the development of better larvicides. A masked aryl diazonium warhead known as triazabutadiene (TBD) has been used in labeling electron-rich aryl residues in proteins such as tyrosine and histidine. Protection of the nitrogen at the N1 position with chloroformates renders the TBD stable to protic degradation but is readily deprotected under basic conditions. This two-step process enables targeted delivery in basic environments. By careful selection of a chloroformate containing a fluorescence quencher as an N1 protecting group, targeted delivery of a fluorophore with reduced background fluorescence is enabled. A vital feature of the design of the chemical probe is the use of secondary handles to attach the fluorophore and the quencher to the triazabutadiene scaffold, which provides modularity to the scaffold. Several strategies for the compound design were explored and will be discussed.



Expected behaviour of triazabutadiene probe inside the mosquito larval gut

RMRM 52

Direct visualization of dimethyl sulfoxide permeation in live rice callus cells by coherent anti-Stokes Raman scattering (CARS) microscopy

Fionna M. Samuels[1], *fionna.drozda@gmail.com, Nancy E. Levinger*[1], *Gayle Volk*[2]. *(1) Chemistry, Colorado State University, Fort Collins, Colorado, United*

States (2) USDA ARS, USDA Agricultural Research Service, Fort Collins, CO, US, academic/govt, Fort Collins, Colorado, United States

Cryopreservation, or the freezing of biological material, of plant tissue is vital to ensure the preservation of important agricultural crops and endangered plant species into the future. Prior to freezing, cells are exposed to mixtures of small molecules called cryoprotecting agents (CPAs) to maximize post-freeze viability. It is well known that without CPAs the viability of plant materials after cryopreservation is severely limited. Unfortunately, exactly how these molecules work to protect cells against the extreme temperatures of cryopreservation is not completely understood. This work aims to fill part of this knowledge gap through the direct visualization of CPAs entering and interacting with live plant cells. Bright field microscopy indicates that common CPAs, e.g., glycerol, ethylene glycol, and dimethyl sulfoxide, used at concentrations relevant to cryoprotection, induce different levels of plasmolysis and deplasmolysis in living rice callus cells. This result suggests differing interactions of the CPA with the cells, though CPA-cell interactions are not directly observable with bright field microscopy. Recent advances in vibrational microscopy give the opportunity to directly image these CPA-cell interactions. In this work, coherent anti-Stokes Raman scattering (CARS) microscopy is used to image deuterated dimethyl sulfoxide (d_6-DMSO) inside living rice callus cells. Our preliminary results demonstrate that d_6-DMSO pools in organelles and that measuring kinetics of CPA permeation is possible with additional equipment. Understanding these fundamental differences in CPA-cell interactions will inform improvements to current CPA formulations to maximize cell viability post-freezing, improving the outlook of frozen cells used in an exceptionally wide variety of fields, from fundamental plant research to the preservation of critically endangered species.

RMRM 53

Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: analysis of ligand type and receptor activation state

***Brittany Thomas**, bnthmas1@memphis.edu, Abby L. Parrill-Baker, Daniel L. Baker. Chemistry, University of Memphis, Memphis, Tennessee, United States*

G protein-coupled receptors (GPCR) are the largest family of cell surface receptors in vertebrates, with over 800 examples encoded in the human genome. Both their abundance and role in nearly all physiological systems

make GPCR targets for pharmaceutical therapies. Drug discovery is aided by molecular docking simulations that allow critical analysis of the interactions between small molecules and proteins in the resulting docked complexes. Crystallized GPCR in complex with known ligand(s) serve as reference complexes for molecular docking. However, many GPCR lack currently available crystallized structures and therefore lack a reference complex. It is pivotal to have methods that provide accurate docking results to facilitate ligand discovery when reference complexes are unavailable. The central question of this work was – are there performance differences in cross docking simulations based on differences in 1) ligand function (agonist, inverse agonist, antagonist) or 2) receptor activation state (active, intermediate, inactive)? Simulations were performed on 13 Class A GPCR crystallized in multiple activation states (a total of 41 complexes were included, with 41 self-docking and 72 cross docking simulations). The goal of this work was to create a workflow for future cross-docking approaches necessary for ligand discovery targeting GPCR lacking currently available crystal structures. Docking poses selected by lowest ligand root mean squared deviation (RMSD), hydrogen bonding complementation score, and highest ranked automated docking scores were compared. As expected, average ligand RMSD values were lower for self-docking than cross-docking by ~2Å. Cross-docking simulations were subdivided into four categories based on whether the receptor activation state and ligand function were matched between docking pairs. When activation state and ligand function were matched, docking performance was most similar to that of self-docking with an average ligand RMSD difference of ~1Å. Additional progress will be discussed, as will impact these data have on future GPCR ligand discovery workflows.

RMRM 54

Investigating the relationship between receptor aggregation and signaling by luteinizing hormone receptor, a G protein-coupled receptor

*Duaa Althumairy[2,6], **Xiaoping Zhang**[5], Zxpchinadh@gmail.com, Nicholas Baez[1], B. George Barisas[2,5], Deborah Roess[3], George R. Bousfield[4], Debbie C. Crans[2,5]. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States (3) Department of Biomedical Sciences, Colorado State University, Fort Collins, Colorado, United States (4) Department of Biological Sciences, Wichita State University, Wichita, Kansas, United States (5) Department of Chemistry, Colorado State University, Fort*

Collins, Colorado, United States (6) Department of Biological Sciences, Imam Abdulrahman Bin Faisal University, Dammam, Saudi Arabia

Luteinizing hormone receptors (LHR) is a member of a subset of G-protein coupled receptors (GPCRs) described as the glycoprotein hormone receptors. It's ligands, luteinizing hormone (LH) is an extensively glycosylated large protein hormone. Although the primary physiologic functions of these receptors are in ovarian function and maintenance of pregnancy in human females and spermatogenesis in males, there are reports of LHR involvement in disease processes both in the reproductive system and elsewhere. To find advantageous treatment on diseases relating to LHR function and GPCRs signaling in general, various methods have been used to study the activation and aggregation process of LHR. In this presentation, I will briefly summarize the historical development on those methods to study LHR activities and demonstrate a current experimental strategy using small molecules for either increasing or reducing the activity of the LHR.

RMRM 55

Towards de novo sequencing of the human milk glycome: High-resolution cyclic ion mobility separations

***Gabe Nagy**, gavril.nagy@pnnl.gov. The University of Utah Department of Chemistry, Salt Lake City, Utah, United States*

Human milk oligosaccharides (HMOs), the highly diverse class of unconjugated glycans, have been implicated for promoting the healthy development of the brain, immune system, and gut microbiome of an infant, but are not readily incorporated into infant formula. Interestingly, HMOs are indigestible by humans; instead, they have been shown to have prebiotic function and mimic the natural attachment sites of harmful bacteria, thus protecting the gut microbiome and immune system of the neonate. As compared to other biomolecules, such as DNA and proteins, HMO synthesis occurs in a non-template driven fashion, where biological responses drive their syntheses and thus dictate their final structures. While the potential monosaccharide constituents in HMOs are known, their arrangement order, fucosylation/sialylation pattern, glycosidic linkage position, α/β anomericity, and numerous isomeric species, make their accurate characterization very challenging. To gain a better understanding of how the brain and gut microbiome are linked together in the production of infant-specific HMOs, better, and faster, analytical methods are needed. Ion mobility spectrometry-based approaches, especially when coupled to mass spectrometry (IMS-MS),

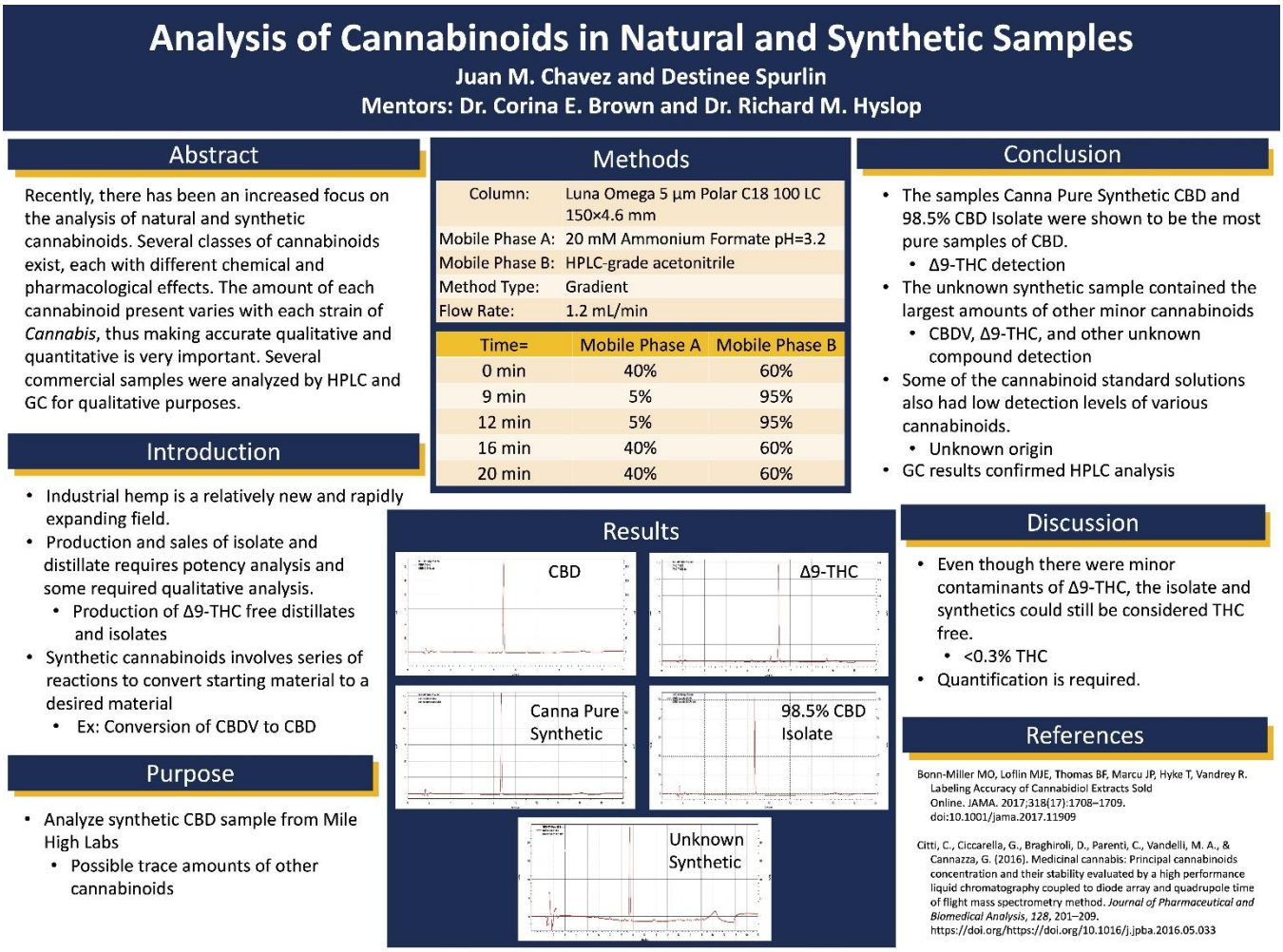
provide an attractive, and higher-throughput, alternative to solution-phase separations, such as liquid chromatography. In IMS, ions are separated in the gas phase on the order of milliseconds based on their size/shape (i.e., mobilities). Unfortunately, conventional IMS-MS platforms suffer from limited resolution, thus precluding their ability to resolve all potential isomeric HMOs. Herein we describe the use of high-resolution cyclic ion mobility separations, in conjunction with isomer-specific fragmentation, to resolve core disaccharide and trisaccharide isomer HMO building blocks. We anticipate this methodology will be readily coupled to front-end liquid chromatographic separations thus extending its applicability to larger, and more complex, oligosaccharides.

RMRM 56

Analysis of *Cannabinoids* in natural and synthetic samples

*Juan Chavez, **Destinee Spurlin**, spur5139@bears.unco.edu, Richard M. Hyslop, Corina E. Brown. Chemistry and Biochemistry, University of Northern Colorado, Greeley, Colorado, United States*

Recently there has been an increased focus on the analysis of natural and synthetic cannabinoids. Several classes of cannabinoids exist, each with different chemical and pharmacological effects. The amount of each cannabinoid present varies with each strain of *Cannabis*, thus making accurate quantitation very important. We analyzed through HPLC and GC the CBD content of several commercial samples. CBD content variations were found and there were some unidentified compounds in the synthetic samples. We will discuss the analytical methods used and the results.



RMRM 57

Redox potentials of truncated menaquinone analogues in soybean phosphatidylcholine liposomes are sensitive to odd- or even-length of isoprene chain

Kaitlin Doucette[2], *kdou14@colostate.edu, Brian Heritage*[1], *Cheryle Beuning*[1], *Debbie C. Crans*[1]. *(1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology, Colorado State University, Fort Collins, Colorado, United States*

A number of bacteria, particularly gram-positive and gram-negative obligate anaerobes, produce menaquinone (MK) as their sole electron transporter in their electron transport system (ETS). Examples of gram-positive bacteria which use MK in their ETS include *Listeria monocytogenes, Staphylococcus*

aureus, and *Mycobacterium tuberculosis* (Mtb), which are pathogens that have a significant impact on human disease, as well as potential impact on bioterrorism worldwide. For some of these bacteria which produce MK, a specific MK derivative has been identified; for example, Mtb produces primarily MK9(II-H_2), while others produce MK analogues with different lengths of isoprene chain and degree of saturation. Despite the importance of its function as an electron transporter, little is known about how these changes affect the redox properties of MK. This work examines the redox potentials of truncated menaquinones in phosphatidylcholine liposomes to determine what effect chain length and saturation may have on their redox abilities in a biologically relevant environment. Half-wave potentials ($E_{1/2}$) were found to have a distinct odd-even effect with respect to chain length and saturation, in which increasing the number of saturations in even-length isoprene chains resulted in more positive $E_{1/2}$ potentials, and an increase in saturations of odd-length resulted in more negative $E_{1/2}$ potentials, with fully unsaturated analogues showing an average $E_{1/2}$ vs. Fc/Fc of -0.51 V. Reversibility (ip_a/ip_c) studies showed a similar odd-even effect, in which MK-*n* analogues with odd-length isoprene chains are inherently more reversible than even-length; however, increasing the number of saturations in the isoprene tail reverses this trend. In contrast, even-length chains are inherently less reversible but an increase in saturations of the chain reverses this effect. Diffusion coefficient analysis showed that shorter analogue MK1 is likely not fully confined by the bilayer of the liposome but longer and more hydrophobic MK-*n* analogues reside completely within the bilayer. This work characterizes the redox properties of short truncated MKs and may lead to insights about the advantages that may exist in bacterial species producing specific MK analogues for electron transport.

RMRM 58

Improving enzymatic transesterification activity in functionalized ionic liquid

***Christopher Toe**, toe6574@bears.unco.edu, Hua Zhao. Chemistry and Biochemistry, University of Northern Colorado, Greeley, CO, US, academic, Greeley, Colorado, United States*

Typically, enzymes are much less active in nonaqueous solvents (e.g. organic solvents, ionic liquids, and supercritical fluids) than in aqueous media. To improve enzyme's activity in nonaqueous environment, we hypothesized that water-mimicking solvent structures would enable a high enzyme activity in nonaqueous media. In this study, we synthesized a dual-functionalized ammonium-based ionic liquid to mimic the water structure, and conducted the

lipase-catalyzed transesterification of ethyl sorbate with 1-propanol in this solvent. We observed a higher transesterification activity in this new ionic solvent than in *tert*-butanol and conventional ionic liquids. With further optimization of ionic liquid structures, we envision much higher enzyme activities could be achieved in nonaqueous solvents.

RMRM 59

Substituted decavanadate (V_9Mo) inhibits the growth of *Mycobacterium Smegmatis*

Zeyad Arhouma[1,2]*, zkrahuma@rams.colostate.edu, Kateryna Kostenkova*[1]*, Dean C. Crick*[2,3]*, Debbie C. Crans*[1,2]*. (1) Department of Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States (3) Microbiology, Immunology, and Pathology Department, Colorado State University, Fort Collins, Colorado, United States*

Decavanadate ($[V_{10}O_{28}]^{6-}$, abbreviated V_{10}) is an isopolyoxometalate that has been found to be a more potent inhibitor of *Mycobacterium smegmatis* (*M.smeg*)than monovanadate (VO_4^{3-}, abbreviated V_1), and, as such, the growth inhibitory effects of substituted decavanadates are of interest.[1] In this study, we investigated the inhibitory activity of one of the monosubstituted decavanadates, monomolybdo(VI)nonavanadate(V) ($[V_9Mo^{VI}O_{28}]^{5-}$,[2] abbreviated V_9Mo) against the growth of *M.smeg*. Since polyoxometalates have different effects, depending on their structures and properties, it is important to carefully monitor their stabilities and the potential formation of oxometalates under the conditions of the biological study by using of spectroscopic techniques. Nuclear Magnetic Resonance (^{51}V NMR) was carried out at different time points (0, 1, 5, 24hr) for V_9Mo in aqueous solution, 7H9 medium, supernatant and heated supernatant to evaluate their stability in their respective media and to determine what species exist when *M. smeg* growth is inhibited . The results have shown that V_9Mo is growth inhibitor of *M.smeg* in their respective media; however, V_9Mo (IC_{50}=54.6µM) is not as effective growth inhibitor as the V_{10} (IC_{50}=6.9µM). This is surprising because V_9Mo is more stable in biological medium compared to the V_{10}. The fact that the V_{10} is a more potent inhibitor than V_9Mo is particularly interesting, considering that it is present in the biological medium for a much shorter time, and may have mechanistic consequences.[3]

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D. C. Decavanadate Inhibits Mycobacterial Growth More Potently Than Other Oxovanadates. *Front. Chem*. **2018**, *6*, 519.
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3. Kostenkova, K.; Arhouma, Z. *et. al*. In preparation.

RMRM 60

Elucidating the role of the axial cysteine residue in NHase catalysis and the enzyme maturation

***Irene Ogutu**, iogutu@mines.edu. Chemistry, Colorado School of Mines, Colorado School of Mines, Golden, CO, US, academic, Golden, Colorado, United States*

Nitrile hydratases are metalloenzymes with trivalent Fe/or Co in the active site coordinated in N_2S_3 ligand environment, the sulfur atoms have three different oxidation states(Cys, Cys-SOH and Cys-SOO^-) while the nitrogen atoms are deprotonated. The axial unmodified cysteine residue has been proposed to push electrons, therefore assisting the metal ion in substrate binding and activation during catalysis. However, the NHase cysteine residue thiolate character is likely modulated through hydrogen bonding interactions. Herein we utilized site-directed mutagenesis to examine the role of the axial thiolate ligand by mutating it to alanine, methionine, serine, and histidine in the Co-type NHase. We further explored the effect of the hydrogen bonding between the axial cysteine and αS162A in *Pt*NHase or αT162A in *Re*NHase. Analysis of the mutants with ICP-MS demonstrated reduced metal ion content to <5% (αC108A), ~44% (αC108M), ~50% (αC108S) and ~55%(αC108H) and the enzyme catalytic activity also decreased to ~0.3%, ~0.8%, ~1.6%, and ~6.7% respectively towards acrylonitrile. The reduced metal ion content and catalytic activity is likely due to reduced electron push by the axial ligand to the metal ion. The X-ray crystal structure of the αC108A further revealed lack of metal ion in the active site. The *Pt*NHase αS162A mutant eluted as two different peaks retaining ~0.2% and ~3.5% of enzyme activity towards acrylonitrile; the αT162A in *Re*NHase similarly had decreased protein turnover of ~76%(acrylonitrile), ~91%(methacrylonitrile), and ~50% (acetonitirile). ICP-MS and X-ray crystallography revealed reduced metal ion content for the first peak of the αS162A mutant while the second peak had 100% metal ion content. EPR of the ReNHase revealed the presence of~65% of inactive high spin Fe(III) form of the enzyme. The hydrogen bonding to the axial cysteine therefore is necessary for active site maturation and modulation of the electron donating ability of the axial thiolate ligand.

RMRM 61

Determining co-modification of 5hmC-DNA and protein structure through mammalian evolution

Ryan S. Czarny, *rczarny@colostate.edu. BMB, Colorado State University, Fort Collins, Colorado, United States*

Endonuclease G is a mitochondrial localized protein involved in cleaving DNA both in duplex and Holliday Junction forms. It has also been shown to be involved with recognizing the 5-hydroxymethylcytosine epigenetic marker. In this work, we look at how the protein-DNA interaction occurs and determine what within the protein is responsible for localizing to 5hmC. Additionally, we use two model, mice and C elegans. Lower eukaryotes lack 5hmC so they provide an interesting model to determine what has occurred with this highly conserved protein throughout evolution. New work in the lab has been able to determine the affinity of the protein-DNA interaction as well as the catalytic rate in order to show how the 5hmC marker plays a role in the cellular interactions. Furthermore, we show how the rates of the protein changes with respect to the species and ultimately leads to a loss in differentiation between Holliday Junction and 5hmC modified Holliday Junction. This differentiation is believed to be a result of a Hydrogen Bond forming between a conserved cysteine and the hydroxyl group of the 5hmC modification which positions the DNA in order for it to be cleaved at certain sites.

RMRM 62

Non-enzymatic post-translational modification of lysine clusters in C2 domains

Cisloynny C. Beauchamp-Perez[1], *cisloynny.beauchampperez@ucdenver.edu, Cole Michel*[2], *Richard Reisdorph*[2], *Nichole Reisdorph*[2], *Kristofer Fritz*[2], *Colin Shearn*[3], *Jefferson D. Knight*[1]. *(1) Chemistry, University of Colorado, Denver, Colorado, United States (2) Pharmaceutical Sciences, University of Colorado Denver School of Medicine, Aurora, Colorado, United States (3) Medicine, University of Colorado Denver School of Medicine, Aurora, Colorado, United States*

C2 domains are membrane-binding motifs found in a wide range of proteins involved in signal transduction and membrane trafficking, including key proteins in neurotransmitter and hormone secretion. A large subset of C2 domains bind membranes containing the signaling lipid, phosphatidylinositol-(4,5)-

bisphosphate (PIP2), via a conserved cluster of lysine residues. Because lysine residues can be non-enzymatically modified by reactive compounds such as lipid aldehydes formed during oxidative stress, we are investigating the susceptibility of C2 domain lysine clusters to modification by carbonyl-containing compounds. Previous research has shown that synaptotagmin-like protein 4 (Slp-4), a C2 domain protein, becomes carbonylated in alcoholic liver disease. Our *in vitro* results using the purified protein domain indicate that the lysine cluster is among several sites that react with the lipid aldehyde 4-hydroxynonenone, a major byproduct of cellular oxidative stress. Furthermore, when expressed in *E. coli*, some of the expressed Slp-4 C2A domain becomes phosphogluconoylated at the lysine cluster, a nonenzymatic modification that is normally found only at the low-pKa amino termini of His-tagged proteins. Using mass spectrometry, Western blotting, and cation exchange chromatography, we are now seeking to determine if other C2 domains and lysine cluster-containing proteins are similarly susceptible to modification. The pKa values of lysine residues in several lysine cluster-containing proteins were predicted using the program H++ to be lower than average for lysine residues. Further investigation will include the study of other highly reactive metabolites and their reactivity toward a variety of membrane-binding proteins that contain lysine clusters. Nonenzymatic damage to secretory proteins as a result of oxidative stress represents an underexplored possible mechanism for deterioration of secretory pathways in diseases of exocytotic cells.

RMRM 63

Efficiency and selectivity of RNAse A cleaving RNA containing 8-oxo-7, 8-dihydroguanosine

***Cheyenne Phillips**, cheyenne.n.phillips@ucdenver.edu. University of Colorado, University of Colorado, Denver, CO, US, academic/system, Denver, Colorado, United States*

Oxidation of RNA has been linked to the development/progression of neurodegenerative diseases and other muscular atrophies. However their exact relationship in a biochemical context is not known, i.e., intracellular handling. Guanosine may lead to 8-oxo-7, 8-dihydroguanosine (8-oxo-G) under oxidative stress and this lesion is, arguably, one of the most abundant/important outcomes of such oxidation reactions. We are interested in studying the effect of ribonuclease activity on oxidized RNA in order to gain a better understanding on the impact that this lesion has on biological systems. Specifically, this research focuses on the activity of bovine pancreatic ribonuclease, RNase A, towards strands of RNA containing 8-oxo-G. Previous work from our lab has

shown that RNase A recognizes and cleaves single strands containing 8-oxo-G, while it does not recognize guanosine. It was determined that RNase A cleaves with the following selectivity C > 8-oxo-G > U. This research will determine the efficiency to which RNase A cleaves at these positions. Dodecamers (AGA AGG XAG AAG; X=C, U, and 8-oxo-G) of RNA are being used as models to explore the reactivity in single stranded RNA. Steady-state kinetics were obtained by plotting Hanes-Woolf relationships carried out by measuring the cleavage efficiency as a function of RNase A concentration. The second stage focuses on RNAse A's efficiency toward C, U, and 8-oxo-G in other structural contexts, i.e., bulges, hairpin loops, and internal loops. The goal is to use RNAse A to probe for the structural impact that 8-oxo-G has on secondary and tertiary structures of RNA.

RMRM 64

Evaluating changes in reactive oxygen species (ROS) as a plausible mechanism underlying the effect of noise on dopamine system in the hub for central auditory processes

***Bridget Doe**, bridget.doe@unco.edu. Chemistry and Biochemistry, University of Northern Colorado College of Natural and Health Sciences, Greeley, Colorado, United States*

Excessive exposure to noise has been implicated in hearing loss but the mechanism by which this happens remains unknown. The central auditory system requires that several major players maintain their modes of action while at the same time achieving integration in order to achieve the complex sensory action of hearing. At the center of the auditory pathway lies dopamine, an important neurotransmitter which is part of the central reward system. It is found in the pockets of the inferior colliculus region of the brain where it modulates auditory neurons by altering how they respond to sound. The enzyme which synthesizes dopamine from the precursor tyrosine is tyrosine hydroxylase. Recent research has shown that excessive noise exposure decreases tyrosine hydroxylase which leads to diminished dopamine levels. Another independent study demonstrated that excessive noise exposure leads to the production of excessive reactive oxygen species (ROS). Current data from our research laboratory has also demonstrated that loud noise leads to decreased dopamine release in the IC of adult Sprague Dawley rats. Thus, we hypothesize that loud noise would trigger the overproduction of ROS, specifically hydrogen peroxide (H_2O_2), and downregulate ATP production. These two phenomena, in sound exposed rats, working in tandem to attenuate dopamine release in the IC.

Using horse radish peroxidase and glycerol kinase, we assay H_2O_2 and ATP levels (respectively) in both 4-hour sound-exposed and control rats. This work will shed light on the neural mechanisms of ROS that may ultimately lead to hearing loss via the dopamine modulation in the inferior colliculus. Understanding the mechanisms of normal dopaminergic modulation will help guide novel diagnostic and therapeutic approaches for disorders associated with abnormal dopamine signaling, including hearing loss.

RMRM 65

Chemistry at the environmental water-air interfaces

Veronica Vaida[1,2]*, VAIDA@COLORADO.EDU. (1) Chemistry, University of Colorado Boulder, Boulder, Colorado, United States (2) Cooperative Institute for Research in Environmental Sciences, University of Colorado at Boulder, University of Colorado Boulder, Boulder, CO, US, academic, Boulder, Colorado, United States*

Inspired by atmospheric measurements, which have established that atmospheric aerosols have a large organic content, my collaborators and I proposed that they likely consist of an aqueous core with an organic surface, with profound consequences to their chemical properties. In this presentation, the special morphological and chemical properties of organic films on aqueous solutions will be discussed. Langmuir trough experiments have contributed to making the case that the surface of water in aqueous drops (models for atmospheric aerosols) and at the sea surface provides a special and unique reaction environment with qualitatively different thermodynamic and kinetic properties from bulk aqueous solutions. Examples from our lab of chemistry initiated at the water surface leading to oligomers and polymers thus increasing the chemical complexity of the organic molecules involved. The generation of such oligomeric organic molecules from smaller precursors is of interest to planetary atmospheric chemistry. The relevance of this chemistry to reactions in aqueous microdroplets, aerosols, at the sea surface, and to chemistry in the contemporary atmosphere as well as chemistry that may have occurred prebiotically, in the absence of enzymes on ancient Earth.

RMRM 66

Redox revolutions on Earth and beyond

Ariel Anbar[1,2]*, anbar@asu.edu. (1) School of Earth & Space Exploration, Arizona State University, Tempe, Arizona, United States (2) School of Molecular Sciences, Arizona State University, Tempe, Arizona, United States*

The molecule O_2 looms large in the search for life on extrasolar planets, because Earth's O_2-rich atmosphere is a consequence of biology. Commonly, it is assumed that an Earth-like planet on which oxygenic photosynthesis evolves will inevitably accumulate O_2 in its atmosphere and pervasively alter the surface environment – that biological redox innovations inexorably lead to environmental redox revolutions. However, close examination of Earth's environmental redox history challenges this assumption.

Increasingly, it appears that evolution of the solid Earth played a key role in modulating the oxygenation of Earth's surface environment. Multiple lines of evidence now suggest that O_2 was being produced biologically hundreds of millions of years before its accumulation in the atmosphere during the Great Oxidation Event (GOE), ca. 2.4 Ga, and hence that Earth's surface redox revolution was substantially delayed. This delay can be accounted for by interactions between the atmosphere and the solid planet, because the biological production of O_2 is ultimately balanced by consumption through reaction with reductants derived from Earth's interior. In particular, recent examinations of oxygen fugacity during the formation of Precambrian basalts and komatiites suggest that large volumes of the mantle underwent a secular increase of oxygen fugacity through the Archean and early Proterozoic. The cause(s) of this secular shift remain unclear, but when translated into a secular evolution of the redox state of volcanic gases, the observed mantle trend can account for a shift from net O_2 consumption to net O_2 production at about 2.4 Ga.

This emerging understanding of Earth's redox revolution raises important questions about the likelihood of similar revolutions on other worlds even in the presence of large biospheres powered by oxygenic photosynthesis. Even modest differences in mantle compositions or tectonics might substantially alter the timing of surface oxygenation. On some worlds, atmospheric O_2 accumulation might be impossible. This realization highlights the need for far better understanding of solid Earth processes - and how these processes might operate on other nominally "Earth-like" worlds.

RMRM 67

Plasma assisted catalysis: New approaches focused on fundamental chemistry

***Ellen R. Fisher**, ellen.fisher@colostate.edu. Chemistry, Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States*

Plasma processing represents a powerful approach to modification of a range of substrates utilizing an array of chemistries and morphologies. New applications for plasma deposited thin films continue to be developed and they are employed in a vast array of industries to produce high impact, high value products. One strategy for increasing the robustness of plasma surface modification and deposition processes lies in increasing our understanding of the fundamental chemistry of the gas phase chemistry in plasmas, the resulting film chemistry and perhaps most importantly, the gas-surface interface. This talk will focus on recent work in our laboratory that explores not only the impact of the plasma on the surface, but also the effect of the substrate on the plasma chemistry. Data on systems used for plasma assisted catalysis (PAC) and plasma production of low D carbon materials will be presented. As one example, we have combined a range of spectroscopy techniques, materials characterization tools, and plasma-surface interface studies to reveal that the presence of a catalytic substrate in the plasma system results in significant changes in the plasma chemistry, most notably affecting the internal temperatures (vibrational, rotational) of various plasma species. Results from NO_x and CH_4-containing systems will be presented. Changes in plasma composition as well as substrate surface chemistry and morphology were also observed. Connections between these results and other trends we observe at the plasma-surface interface will be discussed.

RMRM 68

Effects of luteinizing hormone receptor expression level on receptor aggregation and function

*Duaa Althumairy[2], Jason M. Pace[3], Deborah A. Roess[1], **B. George Barisas**[3], george.barisas@colostate.edu. (1) Department of Biomedical Sciences, Colorado State University, Fort Collins, Colorado, United States (2) Department of Biological Sciences, King Faisal University, Riyadh, Saudi Arabia (3) Department of Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Luteinizing hormone receptors (LHRs) are G protein-coupled receptors which play a critical role in reproductive processes. The oligomerization state of LHRs has been suggested to regulate receptor signaling, desensitization and internalization after hormone binding. We examined the effect of LHR expression levels on receptor oligomerization using polarized homo-transfer FRET (homo-FRET). CHO cell lines stably expressing averages of 10 000, 32 000, 123 000 and 560 000 LHR-YFP per cell were prepared. Receptor expression was determined by flow cytometry using fluorescent bead standards and in turn related to YFP fluorescence observable microscopically. LHR-YFP fluorescence intensity and anisotropy were measured as individual cells were photobleached. Initial anisotropy of LHR-YFP decreased with increasing initial receptor expression. LHR-YFP fluorescence anisotropy also decreased during bleaching. Anisotropy depended almost exclusively on the number of intact, i.e. unbleached, receptor chromophores, whether this number appeared on an unbleached cell or arose when a more strongly-expressing cell was partially photobleached. We examined models for homo-FRET among aggregates, including those allowing for energy transfer among multiple receptors. Experimental data were not consistent with LHRs existing only in dimers or larger aggregates; models indicate that monomers and oligomers must coexist on the cell surface even when LHRs are weakly expressed. The simplest such system involved a monomer-dimer equilibrium. A single dissociation constant of ~30 receptors/μm^2 fit the dependence of anisotropy both on initial LHR expression level and on levels remaining during photobleaching over a 30-fold range. We thus hypothesize that, in the absence of hormone, LHRs exist as an equilibrium mix of monomers and dimers. After binding hormone, receptors undergo varying degrees of additional aggregation depending on LHR expression levels. The relationships between LHR expression, distributions of monomers and oligomers and intracellular cAMP levels are also discussed.

RMRM 69

From boron hydrides to lanthanides and nuclear reactors to in vivo imaging

Gareth R. Eaton*, geaton@du.edu. Chemistry and Biochemistry, University of Denver, Denver, Colorado, United States*

At about 30 seconds per year of my career in chemistry, I will illustrate how seemingly disparate inputs contribute to problem solving, and how we have taken advantage of technology developed for other applications to create new capability in electron paramagnetic resonance (EPR). There are spins everywhere. New methods and new instruments provide new perspectives.

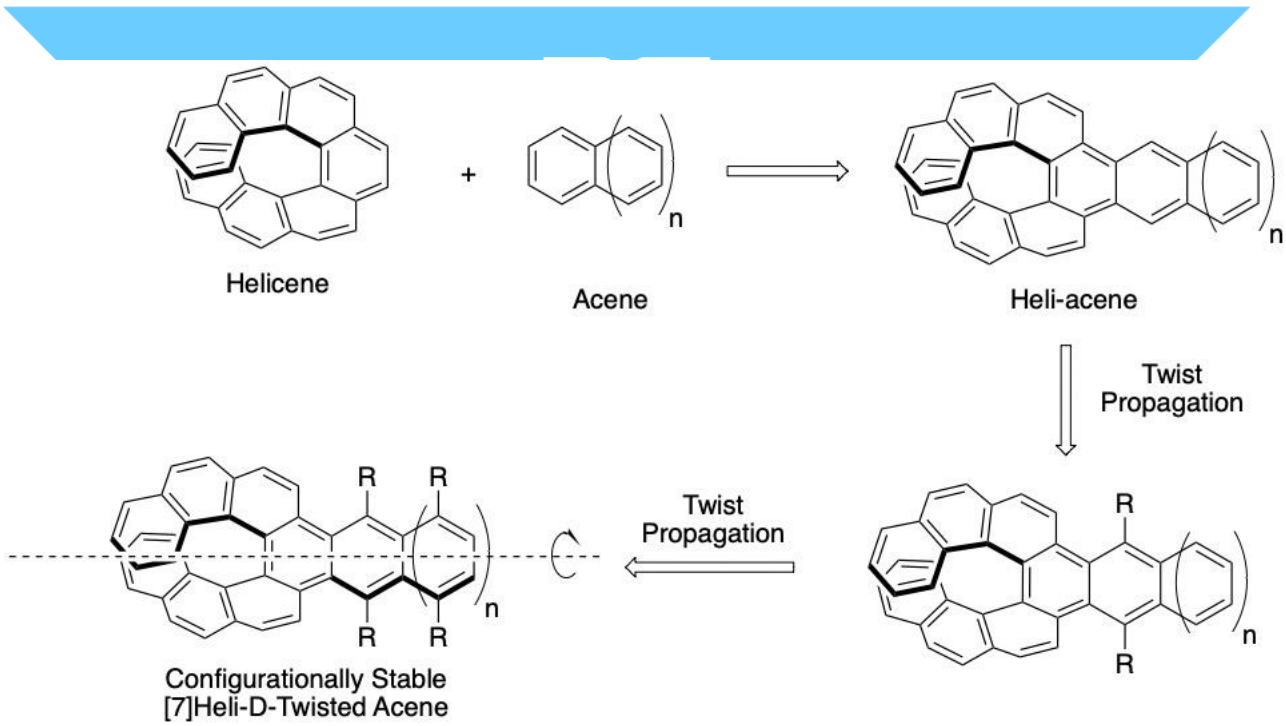
Exciting new applications of EPR emerge, so our future research will not just continue our past.

RMRM 70

Heli-acenes as templates for a torque-lock-propagate approach for the synthesis of configurationally-pure twisted-acenes

***Edward L. Clennan**, clennane@uwyo.edu, Jacob Weber, Shambhavi Tannir. Chemistry, University of Wyoming, Laramie, Wyoming, United States*

Hybrid polyaromatic hydrocarbons (PAHs) consisting of helicene and acene domains, referred to as heli-acenes, are introduced as scaffolds to generate entiopure twisted acenes by a torque, lock, and propagate approach. Computational methods were used to explore the structural and electronic features of these hybrid PAHs and to serve as the basis for the choice of the optimal heli-acene platform series. The feasibility of this new method will be demonstrated with the synthesis of 19, 24-dicyano-[7]heli-D-anthracene. Its X-ray structure, absorption, fluorescence, phosphorescence, and CD spectrum will be discussed.



RMRM 71

"Water-mimicking" ionic liquids for lipase activation and enzymatic polymerization

***Hua Zhao**, hua.zhao@unco.edu. Chemistry and Biochemistry, University of Northern Colorado, Greeley, CO, US, academic, Greeley, Colorado, United States*

Enzyme activity in nonaqueous media is typically lower than in water by several orders of magnitude. We hypothesize nonaqueous solvents with "water-mimicking" structural features would provide enzyme-activating environment. As a proof-of-concept study, we designed dual-functionalized ionic liquids following two harmonic properties of water: hydrogen-bond acceptor (via carrying an ether group) and hydrogen-bond donor (via carrying a *tert*-alcohol group). After synthesizing several dual-functionalized imidazolium and ammonium-based ionic liquids, we carried out lipase-catalyzed transesterification reaction in these "water-like" ionic solvents, and observed up to 2-4 times higher activities than in non-functionalized ionic liquids (e.g. [BMIM][Tf_2N]), and up to 40-100% higher activities than in diisopropyl ether and *tert*-butanol. In addition, the lipase showed higher thermal stability in these "water-mimicking" solvents than in conventional media. We further applied these unique ionic solvents in enzymatic ring-opening polymerization (ROP) of ε-caprolactone, producing polyesters with high molecular mass M_w (up to 18,000 Da) and high yields (up to 74%).

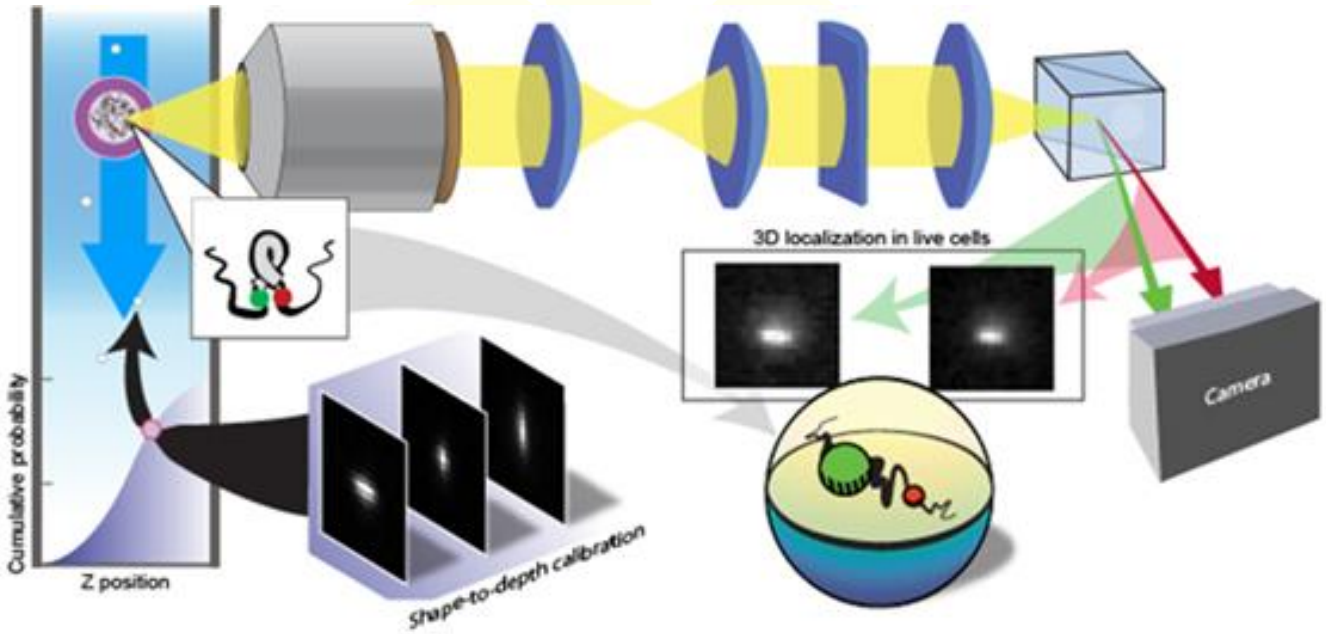
RMRM 72

Directly observing cell-nanoparticle interactions by 3D localization microscopy in live flowing cells

***Lucien E. Weiss**[1,3], fromlab@gmail.com, Yael Shalev Ezra[1,3], Sarah Goldberg[1,3], Boris Ferdman[1,3,4], Omer Adir[2,4], Avi Schroeder[2], Onit Alalouf[1,3], Yoav Shechtman[1,3]. (1) Biomedical Engineering, Technion Israel Institute of Technology, Haifa, Haifa, Israel (2) Chemical Engineering, Technion Israel Institute of Technology, Haifa, Haifa, Israel (3) Lorry I, Lokey Interdisciplinary Centre for Life Sciences and Engineering, Technion Israel Institute of Technology, Haifa, Haifa, Israel (4) Russell Berrie Nanotechnology Institute, Technion Israel Institute of Technology, Haifa, Haifa, Israel*

Attaining three-dimensional data at high throughput is a grand challenge in microscopy. We demonstrate a new method that extends the capabilities of

flow-based imaging to 3D localization microscopy using point-spread-function engineering. Our method uses an additional optical element placed in the imaging system and fluorescent nanospheres to perform a novel calibration procedure that utilizes the distributions of these beads within the flow cell to recover 3D positions in the sample with tens of nanometer precision. Importantly, this approach is compatible with existing commercial systems. We demonstrate the applicability of our approach to biology and medicine by imaging the 3D positions of fluorescently tagged DNA loci in yeast at >1000 cells each minute, and by characterizing the uptake of nanoparticles in human cancer cells.



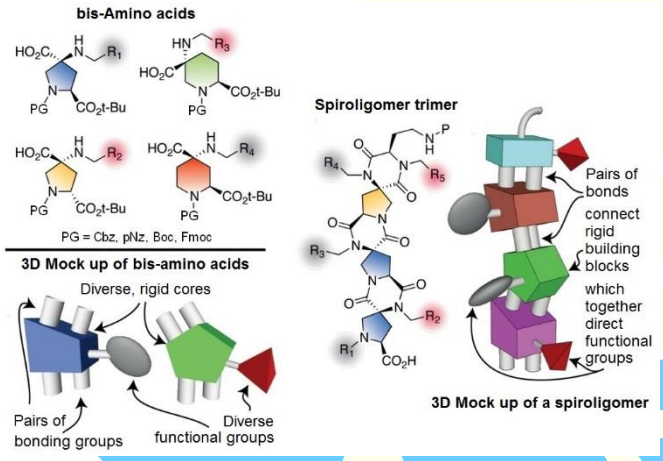
3D localization microscopy in live flowing cells.

RMRM 73

Development of novel spiroligomer carbohydrate binding molecules

Sergiy Chepyshev[1], *tuj51954@temple.edu, Christian E. Schafmeister*[1,2]*. (1) Department of Chemistry, Temple University, Philadelphia, Pennsylvania, United States (2) ThirdLaw Molecular LLC, Blue Bell, Pennsylvania, United States*

Spiroligomers are shape programmable synthetic oligomers with highly functionalized spiro-fused ring system made by coupling pairs of stereochemically pure, cyclic bis-amino acids. The rigidity of the fused ring system and diversity of functional groups allow the prediction of the 3D-shape of a spiroligomer that can be used for molecular modeling and dynamics. Recent advances in Dr. Schafmeister's laboratory make spiroligomers particularly useful for the development of new asymmetric catalysts, metal, protein and carbohydrate binding molecules, and membranes. The presentation describes improvements in the solid phase synthesis of spiroligomers from pNz-protected bis-amino acid pentafluorophenyl esters. Further development in the synthesis of amino acid building blocks with orthogonal protecting groups and spiroligomers derivatization will be discussed.



Spiroligomer scaffolds

RMRM 74

Inhibition of an iron-sulfur cluster biogenesis pathway towards development of novel antibiotics

***Amy Boncella**, aboncella@gmail.com, Emily Sabo, Cierra Gladfelter, Christine Morrison. Chemistry, Colorado School of Mines, Golden, Colorado, United States*

Antibiotic resistance is a significant threat to human health in today's society and, as such, new therapeutic strategies are required to effectively address this problem. In response to this issue, we aim to utilize a fragment-based drug

discovery approach to target an essential pathway in bacteria, iron-sulfur cluster biogenesis. Iron-sulfur (Fe-S) clusters are composed of iron and inorganic sulfur atoms, usually coordinated by cysteine residues. These clusters are prevalent in all forms of life and participate in essential processes such as cellular respiration, catalysis, and electron transport. Gram-positive bacteria, including the pathogens *Mycobacterium tuberculosis*, *Staphylococcus aureus*, *Enterococcus faecalis*, and *Streptococcus pneumoniae*, as well as the malaria-causing parasite *Plasmodium falciparum*, utilize only one pathway to synthesize iron-sulfur clusters, termed the sulfur utilization factor (SUF) pathway. The SUF pathway is essential for survival of these organisms and is not conserved in humans, thus reducing the risk of off-target effects of any drugs developed to inhibit this pathway. To begin to probe the therapeutic potential of the SUF pathway, we are targeting the cysteine desulfurase step of the SUF pathway. Cysteine desulfurase activity is performed by SufS and SufU at the first stage in the biogenesis of Fe-S cluster formation. We are utilizing a fragment-based and structure-based drug discovery approach to identify classes of small molecules that inhibit cysteine desulfurase activity in the Gram-positive model bacteria *Bacillus subtilis*.

RMRM 75

Open questions on the biological roles of first-row transition metals

Kateryna Kostenkova[1]*, kostenkova.kateryna@gmail.com, Debbie C. Crans*[1,2]*. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States*

First-row transition metals have a variety of applications, and play several roles in biological processes and medicine. Many roles of these elements have been investigated; however, there are many questions regarding the toxicity and the biological properties of these elements that are yet to be answered and which speciation chemistry may be able to solve. This talk will cover the biomedical applications and the toxicity of first-row transition metals, and then focus on two classes of vanadium coordination compounds that can potentially be used for the treatment of disease. Vanadium salts have been used for more than a decade; however, the complexation of the vanadium has been found to lead to more efficacious and less toxic compounds. The first class of vanadium coordination compounds, vanadium(V) dipicolinates, was found to enhance the oncolytic viruses and, as a result, be used as a more potent combination therapy against cancer. This led the Crans group to explore other vanadium compounds in combination with the oncolytic viruses, as well as different forms

of cancer. The second class of vanadium compounds to be discussed here is polyoxovanadates which were found to inhibit the growth of *Mycobacterium smegmatis*. The growth inhibitory effects and the speciation chemistry of the decavanadate ($[V_{10}O_{28}]^{6-}$ or V_{10}) and two monosubstituted polyoxovanadates, monomolybdo(VI)nonavanadate(V) ($[V_9Mo^{VI}O_{28}]^{5-}$ or V_9Mo) and monoplatino(IV)nonavanadate(V) ($[H_2Pt^{IV}V_9O_{28}]^{5-}$ or V_9Pt), were determined and are compared in context of the biological effects of the compounds. Finally, these studies are put in the broader context of some of the open questions about the biological roles of first-row transition metals.

RMRM 76

Modular synthesis and characterization of diffusible signal factor analogs for the study of structure activity relationships and mechanism of action

***Rachel Wiley**, erwiley@memphis.edu, Daniel L. Baker. Chemistry, The University of Memphis, Memphis, Tennessee, United States*

Biofilms are a compilation of bacteria and bacterial-derived biomolecules that contribute to microbial antibiotic resistance. According to the Centers for Disease Control and Prevention, at least 2.8 million people are affected by antibiotic-resistant infections yearly. Likewise, biofilms pose a significant problem for large scale societal needs including drinking water and food production hygiene. Biofilms can form in drinking water distribution systems and both protect pathogenic microbes from normal disinfection treatmentsand release bacteria into drinking water. Biofilms can also form on food manufacturing surfaces which can cause public health issues and food waste. Biofilm formation/ dispersal is regulated, in part, by fatty acid analogs termed diffusible signal factors (DSF). The mechanism of action behind DSF remains poorly understood. One highly studied DSF is cis-2-decenoic acid (C2DA) which we have successfully synthesized on a gram scale. C2DA has been shown to disperse biofilms in several gram-negative and gram-positive biofilms and is also capable of preventing the formation of biofilms. We have previously synthesized (one gram scale) a more potent C2DA analog-heptylcyclopropane-1-carboxylic acid (2CP) which stabilizes the bioactive cis conformation through replacement with a cyclopropyl group. Herein we describe a modular synthetic approach to create a library (>100 examples) of DSF based on the 2CP lead to be used to examine the structure activity relationship (varying head groups and alkyl chain length) and mechanism of action (photoaffinity analogs) that define DSF-mediated antibiofilm actions. Progress toward this goal will be discussed.

RMRM 77

^{1}H NMR study of menaquinone-2 interactions in a phosphatidylcholine liposome membrane model

Gaia Bublitz[1,3], *gaia.rachel.bublitz@colostate.edu, Kaitlin Doucette*[2,3], *Debbie C. Crans*[3,2]*. (1) Department of Biochemistry and Molecular Biology, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States (3) Department of Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Menaquinones (MK) are electron carriers composed of a naphthoquinone moiety and an isoprenyl side chain of variable length and saturation. These molecules are the quinone derivatives present in the electron transport systems of all gram-positive bacteria and some gram-negative anaerobes. Subsequently, MK plays a critical role in respiration for pathogens such as Staphylococcus aureus and Mycobacterium tuberculosis. Although the physiological function and relevance of MK as a redox cofactor have been established, its chemical interactions within the plasma membrane and the effects of these properties on MK-mediated electron transport are still obscure. These unknowns are reflected in existing literature, as MK is commonly depicted in an extended conformation. In this study, we implemented ^{1}H NMR spectroscopy and dynamic light scattering techniques to characterize the location and 3D conformation of MK-2 within a L-α-phosphatidylcholine liposome model. MK-2, a truncated menaquinone analog, was selected due to its conserved base structure, limited rotational variability and previous characterization in a simple monolayer lipid system. Our data suggests that MK-2 is largely incorporated into the phospholipid bilayer, with an aqueous subspecies residing at the polar membrane interface in a concentration-dependent manner. 2D NOESY and ROESY spectroscopic analysis support the interpretation that both the aqueous and membrane-associated forms of MK-2 adopt a folded conformation.

RMRM 78

Bacterial inhibition with liposoluble extracts of *Padina gymnospora*

Paola N. Gines Velez*, paola.gines@upr.edu,* ***Pedro A. Balbuena****, pedro.balbuena@upr.edu, Guido Peña Hurtado. Chemistry & Physics, University of Puerto Rico, Arecibo, PR, Arecibo, United States, Puerto Rico*

Since the past, seaweeds have been utilized as foods and medicine for its curative properties. Given the biological activities of seaweeds, numerous studies have been executed particularly in macro algae, but still are far away of its pharmacological application. Seaweeds samples were collected in the reef areas of “La Parguera” (Lajas, Puerto Rico), after washing and grinding them we proceeded to the extraction using organic solvents in a proportional mix 2:1 of chloroform and methanol. Employing roto-evaporation, the organic solvents were eliminated from the liposoluble extracts of the algae. The liposoluble extracts were maculated in bacterial cultures, for algae: two Gram (+): *Bacillus subtilis* and *Staphylococcus aureus* and two Gram (-): *Pseudomona aeruginosa* and *Echerichia coli,* to compare its bacterial inhibition with penicillin, novobiocin, bacitracin and gentamicin. It was proved that the seaweed extract succeeded effectively inhibiting all the bacteria to which it was exposed; yet, with Gram (-) bacteria it worked even better than commercial antibiotics. The results demonstrate that the inhibition varies depending of the type seaweed and bacteria. It has been noted that there is also a stationary effect with the inhibition that is probably related with the seaweed’s reproduction cycle.

RMRM 79

Stimuli-activated quantum dots clear *Salmonella* intracellular infections in preosteoblast cells

Kristen Eller[1], *kristen.eller@colorado.edu, Colleen McCollum*[1], *Max Levy*[1], *Prashant Nagpal*[1,2,3], *Anushree Chatterjee*[1,4]. *(1) Chemical Engineering, University of Colorado Boulder, Boulder, Colorado, United States (2) Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, Colorado, United States (3) Materials Science and Engineering Program, University of Colorado Boulder, Boulder, Colorado, United States (4) Biofrontiers Institute, University of Colorado Boulder, Boulder, Colorado, United States*

Antibiotic resistance combined with pathogen internalization, causing decreased treatment transport and immune system evasion, leads to persistent and debilitating infections. Here we develop a new type of antibiotic: superoxide producing, stimuli-activated quantum dots (QDs). These cadmium telluride (CdTe) quantum dots are precisely tuned so that when stimulated (e.g., light) they create an electron-hole pair at the precise energy to reduce dissolved oxygen to superoxide and kill bacteria. The small size of the QDs, ~3 nm in diameter, make them effective treatments for intracellular infections as they can penetrate bacteria and mammalian cells. We test this in an intracellular infection

of *Salmonella enterica* serovar Typhimurium in an osteoblast precursor cell line. We show QDs provide tunable clearance and limited host cell toxicity by modulating their concentration and stimuli intensity. We show clearance at various multiplicities of infection, dosing, and potentiation of traditional antibiotic treatment. Our established model proves the efficacy of superoxide producing QDs for intracellular infection treatment and establishes a framework for further testing for different infection models.

RMRM 80

Synthesis and characterization of novel non-innocent vanadium Schiff base complexes with anti-cancer properties superior to cisplatin

Heide Murakami[1]*, heideam@gmail.com, Canan Yigit*[2]*, Jordan T. Koehn*[1]*, D. J. Gaebler*[1]*, Andrew Bates*[1]*, Aviva Levina*[2]*, Peter A. Lay*[2]*, Debbie C. Crans*[1]*. (1) Chemistry, Colorado State Unversity, Fort Collins, Colorado, United States (2) University of Sydney, Sydney, New South Wales, Australia*

Hydrophobic Schiff base/catecholate non-innocent vanadium complexes have recently been reported to have anti-cancer properties suited for chemotherapy of platinum resistant cell lines. Their desirable properties arise from the combination of high reactivity and hydrophobicity making them well suited for intratumoral injections regardless of their limited lifespan in a biological system. Three V(V) chloro-catecholate substituted analogues, [VO(Cl-HSHED)(cat)], [VO(Cl-HSHED)(3-Me)], and [VO(Cl-HSHED)(DTB)], (HSHED = N-(salicylideneaminato)-N'-(2-hydroxyethyl)-1,2-ethanediamine, cat = pyrocatechol, 3-Me = 3-methylcatechol, DTB = 3,5-di(tert-butyl)catechol) and the vanadium(V) precursor [VO_2(Cl-HSHED)] were synthesized and tested for anti-cancer properties. These non-innocent Schiff base complexes form two or three isomers in solution and the nature of the major isomer was elucidated using 1D ^{51}V and ^{1}H NMR and 2D NMR spectroscopy. The anti-cancer properties of these complexes were compared to cis-platin in T98g glioblastoma multiforme cells and found to be superior when the complex was intact and, in some cases, when the complex was degraded.

RMRM 81 **CANCELED**

Evaluation of N-(9'-acridinyl)-O-phenylhydroxylamines

Jana Forster*, jana.forster@unco.edu, Michael D. Mosher. University of Northern Colorado College of Natural and Health Sciences, Greeley, Colorado, United States*

Targeting the DNA replication mechanism within a cell is one way to combat cell growth. Aminoacridines are a class of compounds that are known to intercalate DNA. The acridine-DNA complex then forms a ternary complex with Topoisomerase II. This results in antagonism of the reannealing process during supercoiling and cellular apoptosis due to numerous lethal strand scissions. N-(9'-Acridinyl)-O-phenylhydroxylamines can be made in three steps starting from commercially available aryl bromides. Catalytic palladium is used form the O-Ar bond from an N-protected hydroxylamine. The protecting group is then hydrolyzed to make the O-arylhydroxylamine. This is then coupled to an aminoacridine in molten phenol. Substituents (i.e. OCH_3, CH_3, H, Cl, and NO_2) were selected to explore the effect of electronics on the intercalation of DNA. Viscosity measurements using calf thymus DNA were used to determine the intercalation and potential effectiveness of these compounds as anti-cancer agents.

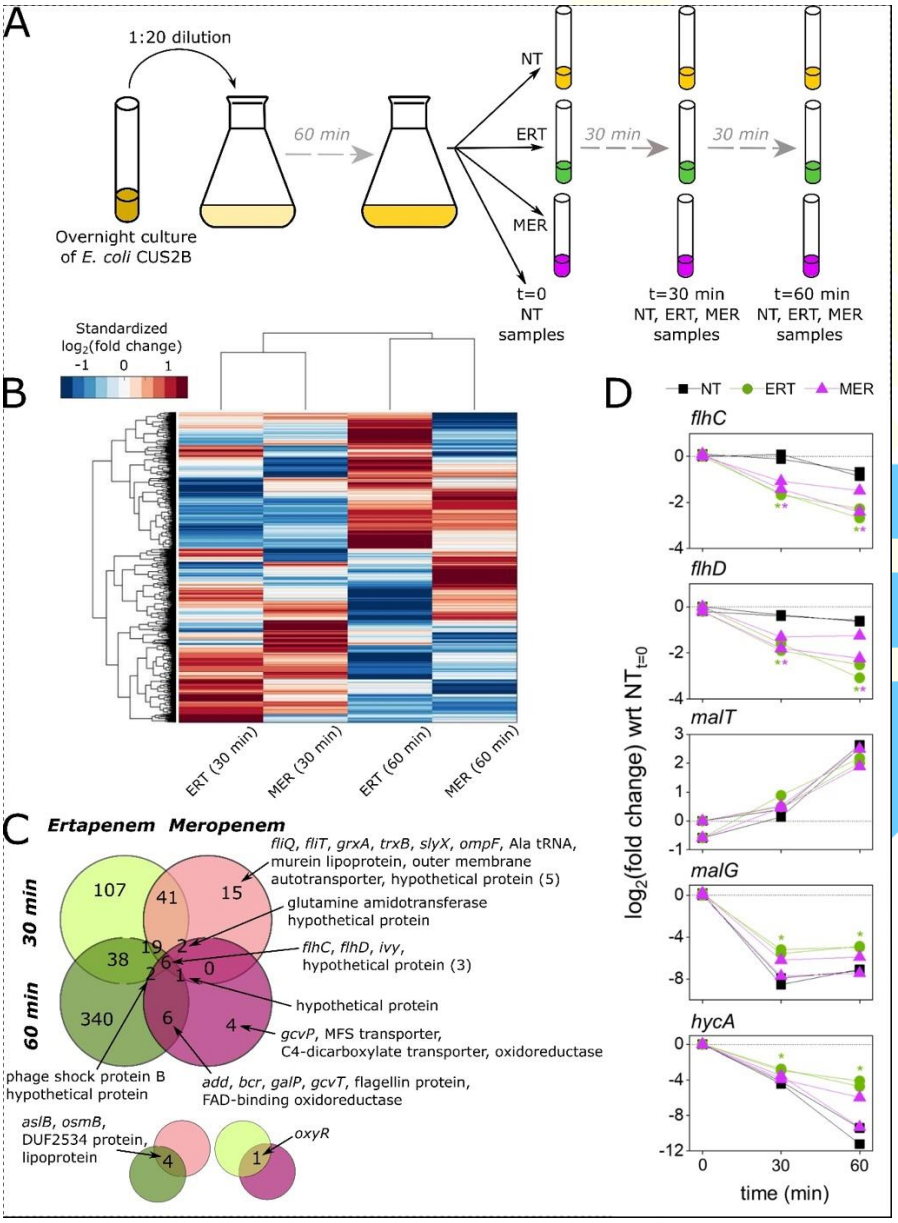
RMRM 82

Transcriptome-based design of PNA inhibitors re-sensitizes CRE E. coli to carbapenems

***Thomas Aunins**, thau4793@colorado.edu, Keesha Erickson, Anushree Chatterjee. Chemical and Biological Engineering, University of Colorado, Boulder, Boulder, Colorado, United States*

Carbapenems are a powerful class of antibiotics, often used as a last-resort treatment to eradicate multidrug-resistant infections. In recent years, however, the incidence of carbapenem-resistant *Enterobacteriaceae* (CRE) has risen substantially, and the study of bacterial resistance mechanisms has become increasingly important for antibiotic development. In this research, we use transcriptomics and antisense gene inhibitors both to explore the resistance profile of a CRE *Escherichia coli* clinical isolate and to engineer carbapenem re-sensitization. The clinical isolate demonstrates resistance to the carbapenem ertapenem but sensitivity to meropenem, and, though genomic analysis identified thirteen antibiotic resistance genes (including four β-lactamases), no dedicated carbapenemases were found. Transcriptomic analysis of total and small RNA was performed to examine the strain's short-term (<1 hr) gene expression changes in response to ertapenem or meropenem. While we did not observe differential expression of any resistance gene, significant expression changes were found in genes related to motility, maltodextrin metabolism, the formate hydrogenlyase complex, and the general stress response. Using our lab's Facile Accelerated Specific Therapeutics (FAST) platform, we designed sequence-specific antisense peptide nucleic

acids (PNA) to inhibit the translation of genes that were identified by our transcriptomic analysis. These PNA were tested in combination with each carbapenem, either to assess their ability to re-sensitize the isolate to ertapenem or their ability to alter the minimum inhibitory concentration of meropenem. We observed significant interaction between PNA and carbapenem treatments with five different PNA. These results identify gene expression-based resistance factors, and confirm the utility of transcriptomic analysis in engineering antibiotic re-sensitization.



RMRM 83

Elucidating the neurochemical basis for the effect of chronic toluene inhalation on accumbal dopamine release

***Kris Reiser**, treiser@gustavus.edu, Aaron Apawu. University of Northern Colorado, Greeley, Colorado, United States*

Inhalants as environmental contaminants or recreational drugs pose a considerable health concern but little is known about their mode of action. In 2011, a study from the National Institute for Drug Addiction revealed that an estimate of 21.7 million people aged 12 or older have used inhalants that contain high concentrations of volatile organic compounds, primarily toluene. These compounds can have debilitating impact on brain chemistry. While toluene's impact on the central dopamine reward pathway has been already reported, the exact mechanism underlining toluene's effect is still obscure. Towards this goal, the present work seeks to combine both electroanalytical and molecular-based tools to unravel how toluene affects the dopamine system in the nucleus accumbens, a region implicated in addiction. Following exposing mice to 30 minutes toluene inhalation each day for seven consecutive days, slice fast scan cyclic voltammetry (FSCV) with carbon fiber microelectrodes were combined with pharmacological assay to delineate the mechanism behind toluene induced dopamine release. The impact of toluene on the dopamine neurotransmission was further assessed by examining D2 receptor levels, localization and distribution using immunoassays. The combination of the electroanalytical and immunoassays revealed toluene induced dysregulation in dopamine neurotransmission that could be the neuroadaptation underlining compulsive and repetitive use of toluene.

RMRM 84

Discovery of novel fadd32 inhibitor of mycobacterium tuberculosis with improved drug properties

***Jigar Sethiya**[1], jse67396@creighton.edu, Robyn Scott[1,2], Grace Majeres[2], Lynne Dieckman[2], Elton Jeffrey North[1]. (1) Department of Pharmacy Sciences, Creighton University School of Pharmacy and Health Professions, Omaha, Nebraska, United States (2) Department of Chemistry, Creighton University College of Arts and Sciences, Omaha, Nebraska, United States*

Tuberculosis (TB), caused by *Mycobacterium tuberculosis* caused 1.5 million deaths worldwide in 2018. Drug shortages, treatment mismanagement, and

adverse side-effects resulting reduced patient compliance have helped increase multidrug-resistant (MDR) and extensively drug-resistance (XDR) strains that remain a major public threat. Mycolic acids, the outer lipid-layer of the mycobacterial cell wall, are the long chain fatty acids which are responsible for cell wall integrity, permeability, and virulence. FadD32 is an essential fatty acyl-AMP ligase involved in the mycolic acid biosynthesis. FadD32 activates and transfers the meromycolyl chain to the condensing enzyme, Pks13. Recently identified coumarin derivatives are potent FadD32 inhibitors, however, they show a poor metabolic profile, with lead compounds having a half-life of ~8.63 minutes in the presence of mouse liver microsomes. In this study, we employed scaffold hopping and rational drug design principles to design three mini-series of FadD32 inhibitors that increased the metabolic stability. The three mini-series comprised of 5,7-dihalogenated 2-quinolones, 5,7-dihalogenated coumarins, and 5,7-dimethyl-8-halogenated coumarins. Synthesis of the coumarin/quinolone derivatives involve four-step reaction, Steglich esterification or amidation with propiolic acid and phenol/aniline, followed by methylation of amide using methyl iodide. Ring closure was catalyzed in the presence of palladium (II) acetate resulting in coumarins or 2-quinolones. Lastly, Suzuki-Miyaura coupling was utilized to produce final products. The metabolic stability of the compounds was assessed in human and mouse S9 fractions. Assays to determine the kinetics of both the FadD32-mediated ligase and synthetase reactions have been developed. Products were isolated in 30-80% yields. All the compounds were characterized by the ^{1}H NMR, ^{13}C NMR, and mass spectroscopy. FadD32 inhibitors showed high purity as assessed by melting point determination. Lead inhibitors showed improved metabolic stability over coumarin-based FadD32 inhibitors. Scaffold hopping and rational drug design approaches were successful in improving metabolic stability of FadD32 inhibitors. Our future studies include compound evaluation to determine whole cell *M. tb* growth inhibition, FadD32 inhibition, full ADMETox evaluation with subsequent lead compounds undergoing *in vivo* pharmacokinetic and efficacy studies.

RMRM 85

Ligand binding site location comparison across class A GPCR complexes

Makenzie Griffing, *robo.pooka@yahoo.com, Abby L. Parrill-Baker, Daniel L. Baker. The University of Memphis, The University of Memphis, Memphis, TN, US, academic, Memphis, Tennessee, United States*

G-protein coupled receptors (GPCR) are integral membrane proteins that are common drug targets due to their role in the cellular signaling pathways that regulate numerous physiological processes such as blood pressure, immune system activity, and mood regulation. Low cost computational studies of these proteins have become popular due, in part, to the high cost of drug development which is driven largely by low success rates at all stages. A list of ligand interactions for every published class A GPCR crystal structure was obtained and analyzed to obtain a list of landmark interactions. The structures were also analyzed to observe the difference in binding location between agonists, antagonists, and inverse agonists, showing how the physical location of the ligand differs within the protein based on the effect it has on the receptor. Locating ligand binding sites and identifying features common across GPCR-ligand complexes will help focus and direct future computational studies used to select drug candidates for screening. The common interaction sites can be used as a starting binding site in a docking simulation or as a filter for selection of docking poses when performing modeling, drug design, or drug selection studies. These applications could improve docking accuracy, allowing for better selection of candidate drugs for experimental studies.

RMRM 86

Stereoselective synthesis of the potential 5-HT$_{2A}$ agonist (2*S*,7*S*)-2-(4-bromo-2,5-dimethoxybenzyl)-7-(2-methoxyphenyl)azepane

***Julie Talbert**, jtalbert1@gulls.salisbury.edu. Salisbury University, Salisbury, Maryland, United States*

Serotonin, or 5-hydroxytryptamine (5-HT), is a neurotransmitter predominantly active within the peripheral and central nervous systems of mammals and plays a significant role in many biological functions. There are seven different subfamilies of the 5-HT receptors, 5-HT$_1$ through 5-HT$_7$. The 5-HT$_2$ subfamily, which consists of the 5-HT$_{2A}$, 5-HT$_{2B}$, and 5-HT$_{2C}$ receptors, has unique signaling properties, yet selective agonists for them, especially for 5-HT$_{2A}$, are lacking. Specifically, the 5-HT$_{2A}$ receptor is thought to be the primary target of psychedelics, while also mediating the action of atypical antipsychotics and being involved in learning processes. Since the intricacies of the binding between the 5-HT$_{2A}$ receptor and agonists remain poorly known, this research proposes to slightly vary the angles between two critical groups within the known selective agonist (2S,6S)-2-(4-bromo-2,5-dimethoxybenzyl)-6-(2-methoxyphenyl)piperidine to determine the optimal configuration for potency and selectivity for the 5-HT$_{2A}$ receptor. This piperidine-based molecule has

good selectivity (124-fold) for the 5-HT_{2A} receptor over the very similar 5-HT_{2C} receptor, but its affinity is 10-fold worse than its predecessor. We believe that by decreasing two bond angles around the central nitrogenated ring, the new molecule, (2*S*,7*S*)-2-(4-bromo-2,5-dimethoxybenzyl)-7-(2-methoxyphenyl)azepane, could regain the lost potency while at least maintaining the selectivity for the 5-HT_{2A} receptor over the 5-HT_{2C} receptor. Through this presentation, we report our progress on the synthesis of the aforementioned azepane-based compound. If our product is as potent and selective as expected, it would allow for a more in-depth understanding of the conformational requirements and interactions between the agonists and 5-HT_{2A} receptor, and possibly lead to the development of new treatments for PTSD and learning disabilities.

RMRM 87

Receptor pharmacophore benchmarking: The role of ligand function in model development

Paige Castleman[1]*, pncastleman@gmail.com, Gregory L. Szwabowski*[1]*, Dale Bowman*[2]*, Judy Cole*[3]*, Abby L. Parrill-Baker*[1]*, Daniel L. Baker*[1]*. (1) Chemistry, The University of Memphis College of Arts and Sciences, Memphis, Tennessee, United States (2) Mathematical Sciences, The University of Memphis College of Arts and Sciences, Memphis, Tennessee, United States (3) Biological Sciences, The University of Memphis College of Arts and Sciences, Memphis, Tennessee, United States*

G Protein-Coupled Receptors (GPCR) are integral membrane, cell signaling receptors that are attractive targets for drug development due to their roles in many and varied physiological pathways. Due to the high cost associated with targeted drug development, computational ligand identification methods continue to play an increasingly important role in the prioritization of candidates for experimental screening. Ligand-based pharmacophore modeling is an *in silico* method that uses comparisons of known ligand structures to generate models relating positions of common functional groups in three dimensions, pharmacophores. The development of and use of pharmacophores in database mining is frequently used to identify candidate ligands for subsequent *in vitro* and *in vivo* validation. This *in silico* benchmark study examined the potential to develop functionally-biased pharmacophores using current datasets and methods, determined whether or not successful pharmacophores could be constructed using ligands of mixed (or the same) function and established a pharmacophore development protocol for the identification of novel GPCR ligands. GPCR included in this study are the adrenergic alpha-1A receptor,

adrenergic alpha-2A receptor, adrenergic alpha-1D receptor, adrenergic beta 2 receptor, adrenergic beta 3 receptor, kappa opioid receptor, delta opioid receptor, mu opioid receptor, serotonin receptor 1A, serotonin receptor 2A, muscarinic 1 receptor and muscarinic 2 receptor. Pharmacophores were developed with multiple training set selection methods and evaluated using percent failure to generate a pharmacophore, Güner-Henry enrichment scores and Güner-Henry goodness-of-hit scores. The seven annotation schemes evaluated in MOE 2018.0101 were narrowed to three, Unified, PCHD, and CHD, by comparing the percent failure to generate a pharmacophore and the enrichment score. Pharmacophore elucidations performed with these schemes these schemes had the lowest failure rates, below 34% compared to 100% for other annotation schemes. Enrichment and GH scores were used to determine the optimal construction protocol for pharmacophores of varying purposes—general ligand identification or functionally specific ligand identification (agonist or antagonist).

RMRM 88

Finding small molecule inhibitors that target DUSP5 using virtual screening: Applications in computational chemistry

***Josue Grajeda**, jag123@nmsu.edu, Marat Talipov. Chemistry and Biochemistry, New Mexico State University, Las Cruces, New Mexico, United States*

The Mitogen-activated protein kinases (MAPK's) pathways regulate cellular signaling by relaying signals outside the cell to the interior of the cell. The dual-specificity phosphatases (DUSP's) plays a significant role in the cellular signaling process. They do this by regulating the MAPK pathway. DUSP's are cysteine-based protein tyrosine phosphatases that dephosphorylate phosphotyrosine, phosphothreonine, and phosphoserine residues. DUSPs contribute to brain function, cell growth and immune activation. It has been observed that diseases like diabetes, cardiovascular disease, and cancer have all been attributed to overexpression of the DUSP enzyme. DUSP5 a member of the DUSP family has been shown to play a vital role in vascular disease. Hyperactivity of DUSP5 has been shown to be the cause of vascular disease. Previous studies have shown that DUSP5 plays an important role in vascular development. More importantly mutations in DUSP5 have been identified in the tissue of vascular anomalies. This suggest a relationship between DUSP5 and vascular disease. Inhibition of DUSP5 has been shown to be a viable treatment for vascular disease. If we can find small molecule inhibitors that bind efficiently to DUSP5 it will be possible to develop new

treatments for cardiovascular disease. A library of FDA approved ligands was screened to find suitable candidates that could bind to DUSP5. All compounds were ranked in terms of affinity in kcal/mol. Out of the screened candidate's prednisone, sorafenib, and cefazedone were found to be some of the highest scoring candidates. Screening will also be performed on other members of the DUSP family. This includes DUSP3, DUSP6, DUSP10, DUSP13, DUSP14, and DUSP15. This will be done to see if any of these molecules are DUSP5 selective. Upon completion of the virtual screening process the best candidates will be tested. This will be done by using in vitro assays to test the best possible candidates.

RMRM 89

Bacterial inhibition with liposoluble extracts of *Mentha pulegium*

*Paola N. Gines Velez[1], **Natalia Cabrera**[2], natalia.cabrera2@upr.edu, **Leslie Rivera**[1], 129eslie.rivera10@upr.edu, Guido Peña[1]. (1) Chemistry and Physics, University of Puerto Rico, Universidad de Puerto Rico, Arecibo, PR,, Arecibo, United States, Puerto Rico (2) Biology, Universidad de Puerto Rico, Universidad de Puerto Rico, Arecibo, PR,, Arecibo, United States, Puerto Rico*

Since the past, mint plants have been utilized as foods and medicine for its curative properties. Given the biological activities of mint plants, numerous studies have been executed particularly in macro pennyroyal, but still are far away of its pharmacological application. Pennyroyal samples were collected in Lares, Puerto Rico, after washing and grinding them we proceeded to the extraction using organic solvents in a proportional mix 2:1 of chloroform and methanol. Employing roto-evaporation, the organic solvents were eliminated from the liposoluble extracts of the pennyroyal. The liposoluble extracts were maculated in bacterial cultures, for pennyroyal: two Gram (+): *Bacillus cereus* and *Staphylococcus aureus* and two Gram (-): *Poteus vulgaris* and *Echerichia coli* to compare its bacterial inhibition with penicillin, novobiocin, bacitracin and gentamicin. It was proved that the extract of pennyroyal succeeded effectively inhibiting all the bacteria to which it was exposed; yet, with Gram (+) bacteria worked even better than commercial antibiotics. The results demonstrate that the inhibition varies depending of the mint plants and bacteria. It has been noted that there is also a stationary effect with the inhibition that is probably related with the mint plants reproduction cycle.

RMRM 90

Synthesis and evaluation of the rhodamine- and biotin- probes for detection of cysteine containing proteins

***Son H. Nguyen**, nguyensh@hollins.edu, **Kaitlyn M. Okin**, okinkm@hollins.edu, **Jaclyn E. Ward**, wardje@hollins.edu. Chemistry Department, Hollins University, Roanoke, Virginia, United States*

Along with glutathione, biological thiol cysteine (Cys) plays important roles in many biological processes such as cellular detoxification and metabolism in living organisms. Changes in intracellular Cys concentration have a profound effect on these biological processes. Given the critical importance of Cys homeostasis in biological systems, a strong interest has emerged in developing effective probes to detect and image Cysrich proteins. In this presentation, the synthesis and evaluation of probes which are hoped to make and use to label Cys-rich proteins in biological systems, especially in redox systems, will be presented.

RMRM 91

Study of near infrared DNA damage and photo-cytotoxicity by a brominated 4-quinolinium dicarbocyanine dye (ESS2-2-4)

***Yewouemoe Lynda Waku Kouomou**[1], ywakukouomou1@student.gsu.edu, Effibe Ahoulou[1], Kathryn B. Grant[1], Maged Henary[1], Oleh Taratula[2]. (1) Chemistry, Georgia State University College of Arts and Sciences, Atlanta, Georgia, United States (2) Pharmaceutical Sciences, College of Pharmacy, Oregon State University, Portland, Oregon, United States*

In photodynamic therapy (PDT), the light of known wavelength is used to activate a photosensitizing agent, which generates reactive oxygen species (ROS) in cancerous tissue. The ROS damages DNA and other nearby macromolecules, causing targeted cells to die. As a result of its clinical success, PDT is considered a viable alternative solution to treat localized cancers for which surgery may not be an option. Most PDT agents absorb red light. However, a dye that is best suited for PDT should absorb 700 nm to 900 nm near-infrared light. This wavelength window allows the maximum transmission of the light deeply into targeted tissues. In this presentation, we report on a symmetrical carbocyanine dye with two 4-quinolinium rings that are attached by a central pentamethine bridge meso-substituted with bromine (ESS-2-4). UV-Visible spectra show that the dye not only absorbs near-infrared light but that it

avidly interacts with DNA in aqueous solutions. Agarose gel electrophoresis demonstrates that the dye cleaves DNA when irradiated with 830 nm near-infrared light (pH 7.0, 10 degrees C). ESS-2-4 is additionally taken up by ES2 ovarian cancer cells, where it causes substantial levels of near-infrared photo-toxicity. Therefore, the preliminary data presented here, suggest that 4-quinolinium-based carbocyanine dyes may one day be useful in photodynamic cancer therapy.

RMRM 92

Virus-like particles (VLPs) as a vaccine platform

***Erich Sohn**, es2298@nau.edu, Naomi Lee. Northern Arizona University, Flagstaff, Arizona, United States*

Virus-like particles (VLPs) are composed of self-assembling viral structural proteins that resemble viruses but do not contain a viral genome. Therefore, VLPs are non-infectious themselves and may provide an efficient platform for vaccine development. VLPs increase the efficacy of poorly immunogenetic antigens, increase vaccine stability, and allow for a more versatile display of antigens. In this project, we produced VLPs from the MS2 bacteriophage in E. Coli. W used standard molecular biology techniques to transform MS2 single-chain dimer plasmid (pDSP62) through electroporation of electrocompetent C41 cells. Transformed cells containing an antibiotic resistant for kanamycin grew colonies on an agar plate. Addition of IPTG induced cells to synthesize VLPs. We then lysed the cells to isolate and confirm VLP formation using agarose gel electrophoresis by detecting the presence of RNA encased in the VLPs, indicating successful VLP production. Unfortunately, agarose gels did not indicate successful VLP formation, at this time. However, Sodium Dodecyl Sulfate–polyacrylamide (SDS) gel electrophoresis confirmed expression of the MS2 coat protein. Therefore, next steps are to continue troubleshooting VLP synthesis then purify crude VLP samples via gravity column. Upon successful VLP synthesis, qualitative VLP concentration will be determined using SDS gel electrophoresis. Future studies will focus on chemical conjugation of nucleoside adjuvants via the tyrosine side chain using Diels-Alder chemistry. In conclusion, VLPs could serve as an effective vaccine platform due to their non-infectious nature and their ability to increase antigen immunogenicity.

RMRM 93

Synthesis and duplex stability of N2-Alkyl 8-Oxo-2'-deoxyguanosine oligonucleotides for use as substrate analogs for DNA repair protein MutY

***Madeline Bright**, mmbright@ucdavis.edu, Robert P. Van Ostrand, Sheila S. David. Chemistry, University of California Davis, Davis, California, United States*

Oxygen, required by aerobic organisms to sustain life, also yields reactive oxygen species (ROS) which cause oxidative damage to nucleobases in DNA. This oxidative damage results in 8-Oxoguanine (8-OG), a common oxidative product which mispairs with adenine due to its thymine-resembling Hoogsteen base pair face. Such 8-OG:A mispairs cause G:C→T:A transversions upon DNA replication, a build-up of which is destructive to the cell. MutY, a base excision repair (BER) enzyme, combats oxidative damage to guanine nucleobases in DNA by cleaving the mispaired adenine nucleobase. This cleavage results in an abasic site across from 8-OG, which is later repaired by downstream BER enzymes. Inherited variants of MUTYH, the human homolog, have been linked to the initiation and development of carcinogenesis. How MutY is able to differentiate the mispaired adenine from correct T:A pairs is the focus of my research in the David Lab. Discovering critical structural features, like which amino acids are primarily responsible for MutY recognition, will aid in the development of inhibitor or activator molecules with therapeutic applications. Prior work by the David Lab showed the N2-exocyclic amino of 8-OG in DNA is critical for repair by MutY. This work will determine the effect of steric bulk and hydrogen bonding imparted by the exocyclic amino of 8-OG on the target recognition mechanism of MutY via 8-Oxo-2'-dG analogs modified at the 2-position, and will analyze the duplex stability of produced oligonucleotides. The use of our synthetic analogs as substrates of MutY will reveal the structural features dominant in MutY's target recognition of the 8-OG:A mispair.

Previously unreported N2-Ethyl-, N2,N2-Diethyl-, and N2,N2-Dimethyl-8-Oxo-2'-dG phosphoramidite analogs have been synthesized and confirmed. Numerous DNA sequences of the N2-Ethyl-, N2,N2-Dimethyl-, and N2,N2-Diethyl-8-Oxo-2'-dG oligonucleotides have been purified and confirmed. Furthermore, the results of the herein reported duplex stability studies support the viability of produced oligonucleotides for use as substrates in enzymatic assays; future work will involve EMSA-based and cellular-based assays using

MutY and reported oligonucleotides, and further examination of duplex stability will be conducted.

RMRM 94

New synthetic methodology enabled by base-promoted proton, electron and halogen transfer processes

***Jeffrey Bandar**, jeff.bandar@colostate.edu. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Strong bases are widely used reagents for promoting many of the most used reactions in organic chemistry. Brønsted and Lewis bases typically activate compounds via simple deprotonation and coordination mechanisms, respectively. This seminar will cover our work on the discovery, utility and generalization of unconventional base-promoted mechanistic pathways. First, organic superbases are used to catalyze challenging anti-Markovnikov addition reactions to alkenes as a replacement for traditional hydroboration/oxidation protocols. Second, base-catalyzed aryl halide isomerization will be presented as a strategy for achieving new selectivities in nucleophilic aromatic substitution reactions. Third, electron transfer from base-activated organosilanes will be shown to enable substitution reactions of extremely strong C–F bonds. Mechanistic studies on these new base-promoted processes will be included to highlight their generality and future applications.

RMRM 95

Synthesis, characterization and reactivity of N-alkylated organic photocatalysts

***Nicholas A. Swisher**, nicholas.swish@gmail.com, Daniel Corbin, Garret Miyake. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Organic photocatalysts with highly reducing excited states have successfully been applied to a variety of macromolecular and small molecule transformations. Specifically, N-aryl core-extended phenoxazines have been shown to be effective catalysts for the controlled radical polymerization of methacrylates. Mechanistic studies of these photocatalysts have elucidated how the presence of certain N-aryl groups facilitate intersystem crossing to form long lived triplet excited states, which are belived to play a key role in successful polymerization catalysis. Replacement of N-aryl groups in phenoxazine

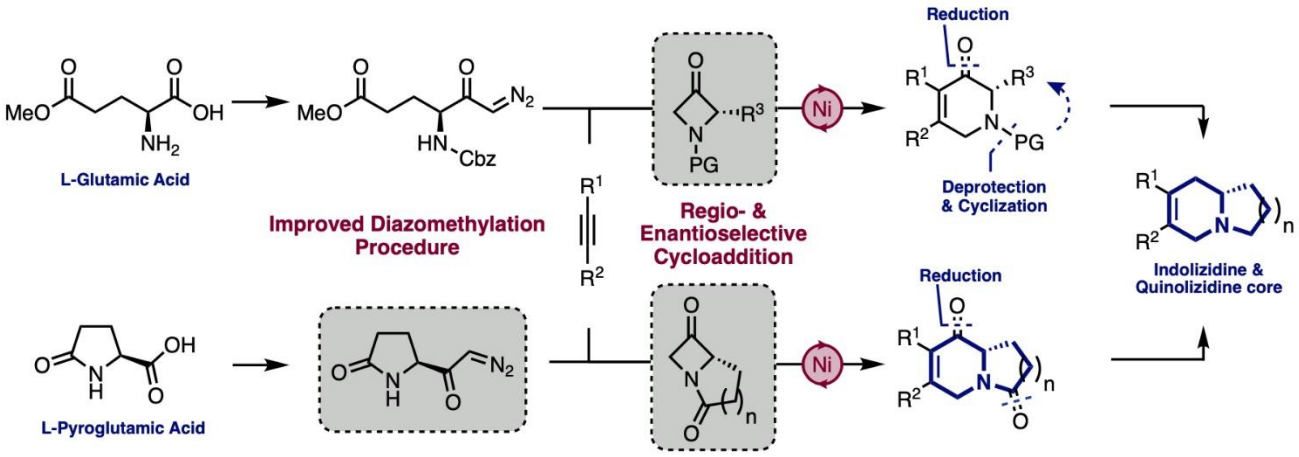
photocatalysts with alkyl substituents should promote excited state reactivity from singlet manifolds. Such behavior is attractive from the perspective of enabling reactivity with known triplet quencher substrates like styrene. In this presentation the synthesis and characterization of core-extended N-alkyl phenoxazines and their reactivity in polymerization photocatalysis will be discussed.

RMRM 96

Total synthesis of indolizidine and quinolizidine alkaloids

***Jonas Renner**, jonas.renner@utah.edu. Chemistry, University of Utah, Salt Lake City, Utah, United States*

One of the many challenges of treatments in cancer therapy is the occurrence of resistances. Currently used small molecule drugs, e.g. tyrosine kinase inhibitors, induce dramatic clinical responses, unfortunately, acquired resistances seem to be an inevitable consequence of this treatment approach. This fact raised immense interest in indolizidine and quinolizidine alkaloids, which have shown remarkable activities against multidrug resistant cancers and have since led to many different synthetic routes to these natural products. Aforesaid alkaloids additionally exert novel anti- coronaviral activities against SARS-CoV and MERS-CoV, through a significant reduction of cytopathic effects.
We have extended our previously developed nickel-catalyzed (4+2) cycloaddition of azetidinones and alkynes as general approach towards indolizidine alkaloids. Our approach offers a novel and orthogonal pathway to current syntheses and commences from cheap starting materials, such as glutamic acid. In addition, we showed that the employed azetidinone serves as advance intermediate and that our nickel-catalyzed reaction can utilize different alkynes with high regiocontrol. Moreover, we have developed an improved diazomethylation procedure to access bicyclic azetidinones from amides, such as pyroglutamic acid, which enables an even more condense route to indolizidine and quinolizidine alkaloids.



Condensed Total Synthesis of Indolizidine and Quinolizidine Alkaloids

RMRM 97

"On water" synthesis of fluorosulfonyl 1,2,3-Triazoles

Antonina L. Nazarova[1,2]*, nazarova@usc.edu, Joice Thomas*[1,2]*, Valery V. Fokin*[1,2]*. (1) University of Southern California Loker Hydrocarbon Research Institute, Los Angeles, California, United States (2) The Bridge at USC, Los Angeles, California, United States*

"On water" reactions can be identified as those transformations that occur between water-insoluble reactants in the water solvent, driven by hydrogen bonding on the water-organic interface. We report a novel, metal-free, environmentally sustainable synthesis of fluorosulfonyl-substituted heterocycles in the presence of phase-transfer agent in water. Mechanistic studies were performed to elucidate the observed reactivity in some insights. The reaction time for the fluorosulfonyl-functionalized triazoles was drastically reduced from 42 hours (when performed in organic solvents) to 8 hours for the "on water" mediated protocol.

The developed on-water and phase transfer catalyst-assisted regioselective protocol employing bromoethenylsulfonyl fluoride (BESF) and ethenesulfonyl fluoride (ESF) was extended to various 1,3-dipoles and resulted in the formation of fluorosulfonylated and non-substituted heterocyclic azoles, such as 1H-pyrazoles, 5-(fluorosulfonyl)-1H-pyrazoles, and Diels-Alder reaction adducts.

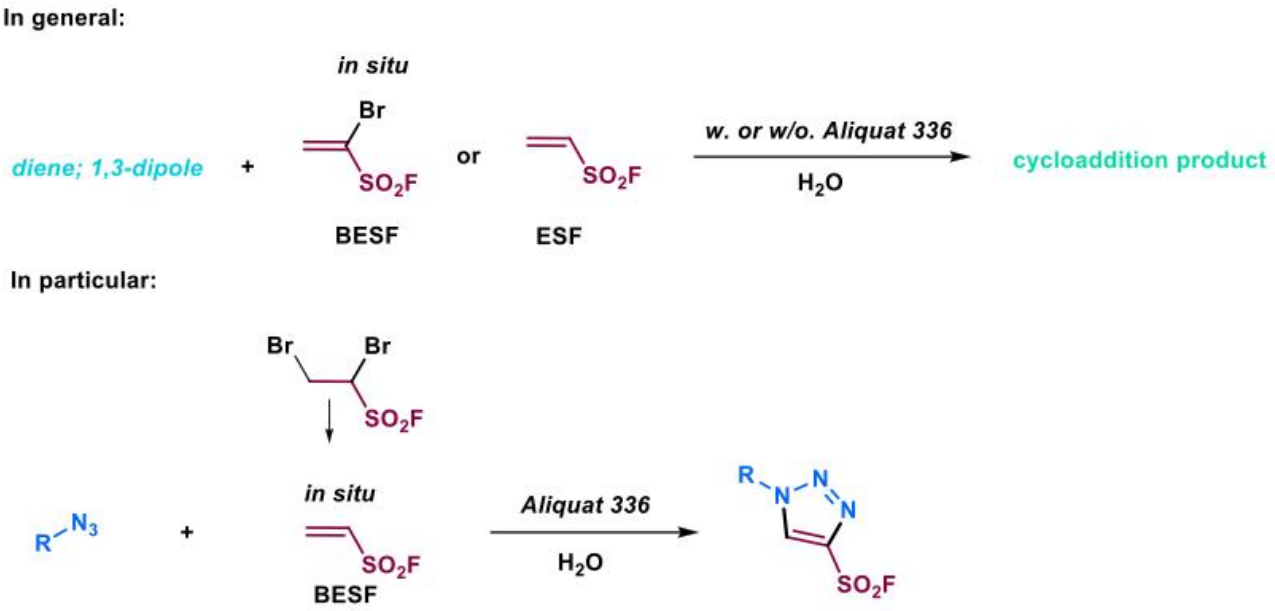


Figure 1. Schematic procedure of formation of sulfonyl triazoles, fluorosulfonyl and 5-bromo-functionalized pyrazoles, non-substituted pyrazoles and various derivatives of Diels-Alder additions from ESF, DBESF and organic azides.

RMRM 98

One-pot alkylation via traceless dearomatized pyridyl phosphonium ylides

***Patrick Fricke**, frickep2016@gmail.com, Andrew McNally. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

4-position alkylated pyridines can be found in several pharmaceuticals, and are common in natural products, materials, and ligands. Due to how frequent these scaffolds are found, methods for synthesizing them directly from the pyridyl C-H bond are highly desired. Several methods already exist to alkylate pyridines directly, including Minisci-type reactions and C-H functionalization using transition metal-catalysis with alkenes. Although these methods have made significant progress, further developments in this field are still needed. Here, we report an alternative, one-pot method that goes through a traceless dearomatized pyridyl phosphonium salts. Sequential addition of a triazinyl chloride, *n*-tributylphosphine, and methyl lithium selectively yields a 4-position

phosphonium ylide within the pyridine scaffold as a single isomer, in near quantitative yield. Upon addition of an aldehyde, Wittig olefination occurs with the ylide, resulting in a pyridine anhydrobase, which can be converted to the alkylated pyridine by acidic workup. Additionally, we found that in the absence of an acidic workup, this pyridine anhydrobase could serve as a versatile intermediate for further derivatization. We demonstrate that a range of substituted pyridines can be alkylated from either alkyl or aryl aldehydes. Since our method relies on the well-established Wittig olefination reaction, various complex aldehydes are amenable, providing an extensive drug-fragment coupling scope. Finally, we demonstrate that under a similar set of conditions, methylation of pyridines and pharmaceuticals can be achieved.

RMRM 99 **CANCELED**

Synthesis of configurationally twisted acenes by the torque, lock, and propagate approach: The mallory and dione routes

***Madison McConnell**, madrose4550@gmail.com, Jacob Weber, Shambhavi Tannir, Edward L. Clennan. Chemistry, University of Wyoming, Laramie, Wyoming, United States*

Twisted heli-acenes are attractive replacements for acenes as semiconductors for the construction of organic electronic devices. The substituents responsible for the twist also provide steric protection of the acene core from detrimental oxidation, dimerizations, and polymerizations. In this study, we will discuss the advantages and disadvantages of two different routes for the synthesis of these molecules. We will also describe a new mechanism for the Mallory photocyclization and illustrate its use in the synthesis of [7]heli-D-anthracene. We will also describe the synthesis of [5]helicene-7,8-dione and [7]helicene-9,10-dione and describe the use of the latter dione in the synthesis of 19, 24-di-cyano[7]heli-D-anthracene.

RMRM 100

Exploratory syntheses of truncated, partially saturated menaquinone derivatives

***Margaret Braasch-Turi**, maggi.braasch-turi@colostate.edu, Debbie C. Crans. Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States*

Oxidative phosphorylation is a vital part of cellular metabolism. Menaquinones are a critical component of the electron transport chain within oxidation in *Mycobacteria*. They consist of naphthoquinones with a C2 methyl group and C3 chain varying in length from 1-13 isoprene units. Most bacteria have at least one saturated isoprene unit within the chain, shifting position from species to species. Studies showed the first isoprene unit must have E stereochemistry to restore oxidative phosphorylation in *Mycobacterium phlei*. This vital process decouples upon manipulation of the first isoprene double bond. As of now, no structure-activity relationship studies have been done to understand why the first isoprene unit disrupts ATP synthesis, but not oxidation. To learn more about this disruption, we are synthesizing a library of truncated menaquinone derivatives to facilitate an SAR study in two bacterial strains with the saturated unit in different locations: *Halococcus morrhuae*, MK-8(II-H2), and *Rhodococcus fascians*, MK-8(VIII-H2). We will report on the synthesis of derivatives where the saturation and alkene stereochemistry are varied using a range of the synthetic strategies compiled in our recent review.

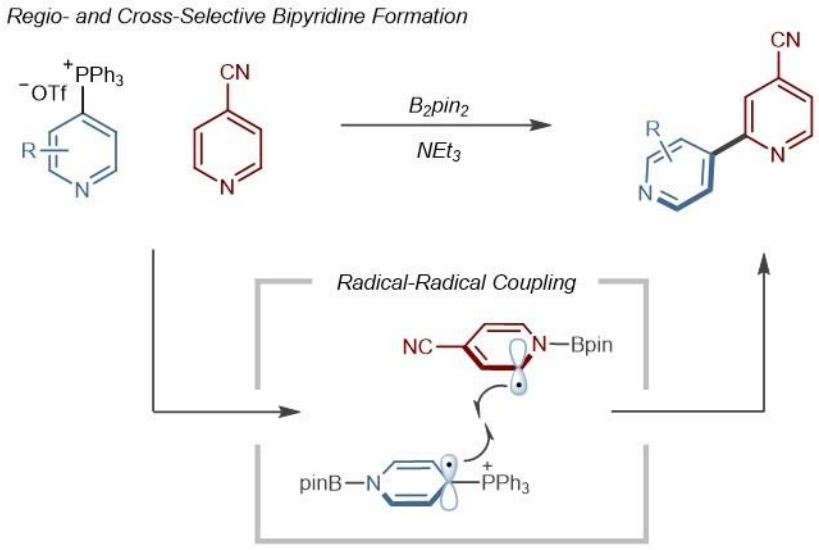
RMRM 101

Synthesis of 2,4'-bipyridines via a unique radical coupling of cyanopyridines and heteroaryl phosphonium salts

Jake Greenwood[1], *jakegreenwood1016@gmail.com, J. Luke Koniarczyk*[1], *Juan V. Alegre-Requena*[1], *Robert S. Paton*[1,2], *Andrew McNally*[1]. *(1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Chemistry, University of Oxford, Oxford, Oxfordshire, United Kingdom*

Bipyridines are commonly found in a range of chemical applications including pharmaceuticals, materials, and ligands for metal catalysis. Due to the ubiquity of bipyridines, methods for the synthesis of this scaffold are in high demand. Metal-catalyzed cross-couplings are an essential part of the organic chemist's toolbox for biaryl synthesis, but these methods are less effective when coupling heteroarenes or even fail completely. A practical and powerful method for pyridine functionalization is the Minisci reaction in which a carbon-centered radical adds to an activated heteroaromatic ring; however, a Minisci coupling between two pyridine partners has not been reported. This is likely due to an electronic incompatibility between the activated pyridine and the pyridyl radical coupling partner as well as a lack of control over selectivity for the correct pyridine acceptor. Our lab made an unexpected observation that led to the development of an alternative, metal-free pyridine-pyridine cross-coupling reaction that overcomes these deficiencies of the Minisci reaction. Cyanopyridines were successfully coupled with pyridyl phosphonium salts with

complete regio- and cross-selectivity to form a variety of 2,4'-bipyridines. Importantly, phosphonium salts were found to be the only effective radical precursors under the reaction conditions. After an extensive experimental and computational mechanistic investigation, the reaction was found to proceed through a unique coupling between two boryl-stabilized, dearomatized pyridyl radicals. This discovery provides a mild, mechanistically distinct method for the synthesis of valuable bipyridines.



RMRM 102

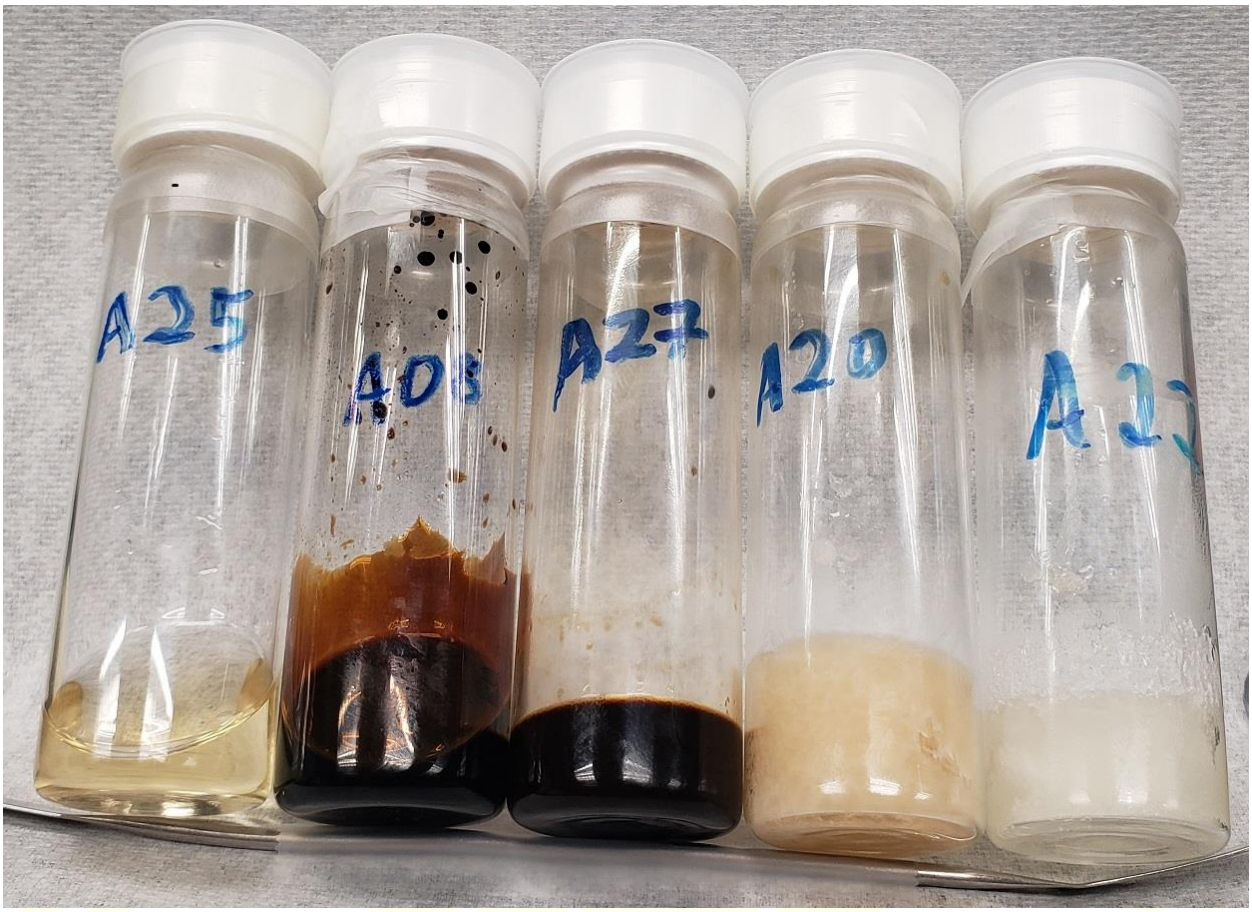
Synthesis of functionalized ionic liquids for coal dissolution and pretreatment

***Michael Franklin**, michael.franklin@unco.edu, Hua Zhao. Chemistry & Biochemistry, University of Northern Colorado, University of Northern Colorado, Greeley, CO, US, academic, Greeley, Colorado, United States*

Low-rank coal (such as brown coal, or known as lignite) accounts for ~45% of global coal reserves. However, brown coal is not favorable for energy production because of its lower calorific value, emission of NO_x/SO_x and ashes, as well as mining challenges. Brown coal contains complex polar networks of hydrogen bonds involving phenolic -OH groups, carboxylic acids, and other functional groups. To convert low-rank coal to valuable commodities, it is

essential to break down so called second bonding interactions in coal (such as hydrogen bonding, aromatic stacking, acid-base, and donor-acceptor) that hold stable three-dimensional structure of coal. As non-volatile solvents, ionic liquids (ILs) are becoming potential 'greener' substitutes of volatile organic solvents toward this application. In this study, we custom made a series of nitrogen- and phosphorus-based ILs that have high hydrogen-bond basicity. These ionic solvents were characterized by NMR, water content, TGA, viscosity, and their hydrogen-bond acidity, basicity, and polarity. We demonstrated the utilization of these ionic solvents for partial dissolution of brown coal, and the impact of such pretreatment on the coal structure and morphology changes.

Synthesis set-up and sample ILs



Sample of physical characteristics of ILs

RMRM 103

Synthesis of novel ionic liquids towards enzymatic ring-opening polymerization to polyesters

***Caden Martin**, mart3059@bears.unco.edu, Hua Zhao. Chemistry and Biochemistry, University of Northern Colorado, Greeley, CO, US, academic, Greeley, Colorado, United States*

Ionic liquids have displayed advantageous properties such as high thermal stability, high enzyme compatibility, and the ability to dissolve many diverse substrates. Ionic liquids have shown some potential as co-solvents for enzyme-catalyzed ring-opening polymerization (ROP) of lactones and lactides to produce biodegradable and biocompatible polyesters. To further develop lipase-compatible ionic solvents for high-temperature (70-130 °C) enzymatic ROPs, we incorporated both *tert*-butanol and ether groups into the ionic liquid

structure. We hypothesize the dual functionalization would lead to more biocompatible ionic liquids because just like water, *tert*-butanol acts as a hydrogen-bond donor while ether acts as a hydrogen-bond acceptor. We synthesized and characterized dual-functionalized ionic liquids and evaluated their biocompatibility by a transesterification reaction catalyzed by Novozym 435 (immobilized *Candida antarctica* lipase B). We found the lipase being more active in some dual-functionalized ionic liquids than in diisopropyl ether or *tert*-butanol. We further demonstrated the use these ionic solvents in enzymatic ROPs to polyesters.

RMRM 104

Multivariate approach in designing chiral metal organic frameworks

Thomas Ericson[2]*, Thomas.Ericson@ttu.edu, Babak Tahmouresilerd*[1,2]*, Anthony F. Cozzolino*[2]*. (1) University of Huston, Huston, Texas, United States (2) Texas Tech University, Lubbock, Texas, United States*

Chiral metal organic frameworks (MOF) have the ability to perform a variety of tasks. Such tasks include separation across membranes, separation in chromatography, enantioselective catalysis, and so on. Chirality in materials is a commonly observed feature, which has applications in many fields such as pharmacy and agriculture. With that goal in mind we have designed a multivariate homochiral metal organic framework that employs the use of inexpensive and readily available linkers. The combination of metal, amino acid and ditopic terephthalic acid linker into a ternary framework provides three independent variables that can fine tune the properties through the design of multivariate framework. Solvothermal synthesis yielded crystalline solids that were recovered and characterized with single crystal x-ray crystallography, PXRD, FTIR, TGA and surface area analysis. Properties and applications of these homochiral multivariate porous frameworks are discussed.

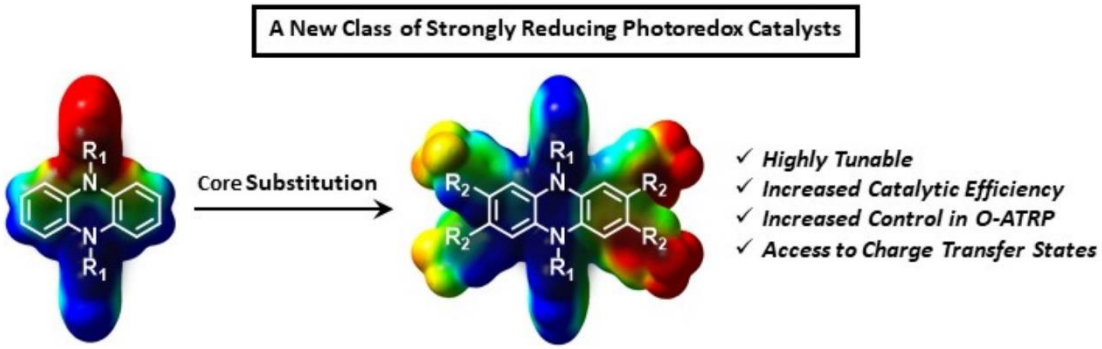
RMRM 105

Core-extended *N,N*-diaryl dihydrophenazine photoredox catalysts: Structure-property relationships and advantages in organocatalyzed atom transfer radical polymerization

Mariel Price*, mariel.price@colostate.edu, Garret Miyake. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Photoredox catalysis has gained increased traction over the last decade as a powerful method through which new and challenging chemical transformations can be accomplished under mild conditions. The Miyake group has done extensive work in developing strongly reducing organic photoredox catalysts (PCs), specifically for use in organocatalyzed-atom transfer radical polymerizations (O-ATRP). O-ATRP is a controlled radical polymerization that uses the combined power of light and PCs to synthesize well-defined polymers under mild and metal-free conditions. *N,N*-diaryl dihydrophenazine PCs possess the requisite electrochemical and photophysical properties for mediating control in O-ATRP, but they have a propensity to undergo radical addition side reactions. Radical addition side reactions can hinder the catalytic activity of the PC and alter its photophysical and electrochemical properties. We hypothesized that substitution of the *N,N*-diaryl dihydrophenazine core would limit radical addition side reactions and provides additional handles to tune PC properties enabling us to optimize their performance in O-ATRP.

The work described in this presentation will encompass the effects that core-extension has on the properties of *N,N*-diaryl dihydrophenazine PCs and on their performance in O-ATRP. Initial studies show that core-extension provides handles that allows for significant tuning of the photophysical and redox properties of these PCs. Additionally, when employed as catalysts in O-ATRP, these new PCs demonstrate exceptional control over the polymerization at catalyst loadings as low as 50 ppm. Ultimately, the PCs discussed in this presentation are more efficient in O-ATRP than previously reported systems and have significant potential for applications in other photoredox reactions that require tunable, stable, and strongly reducing PCs.

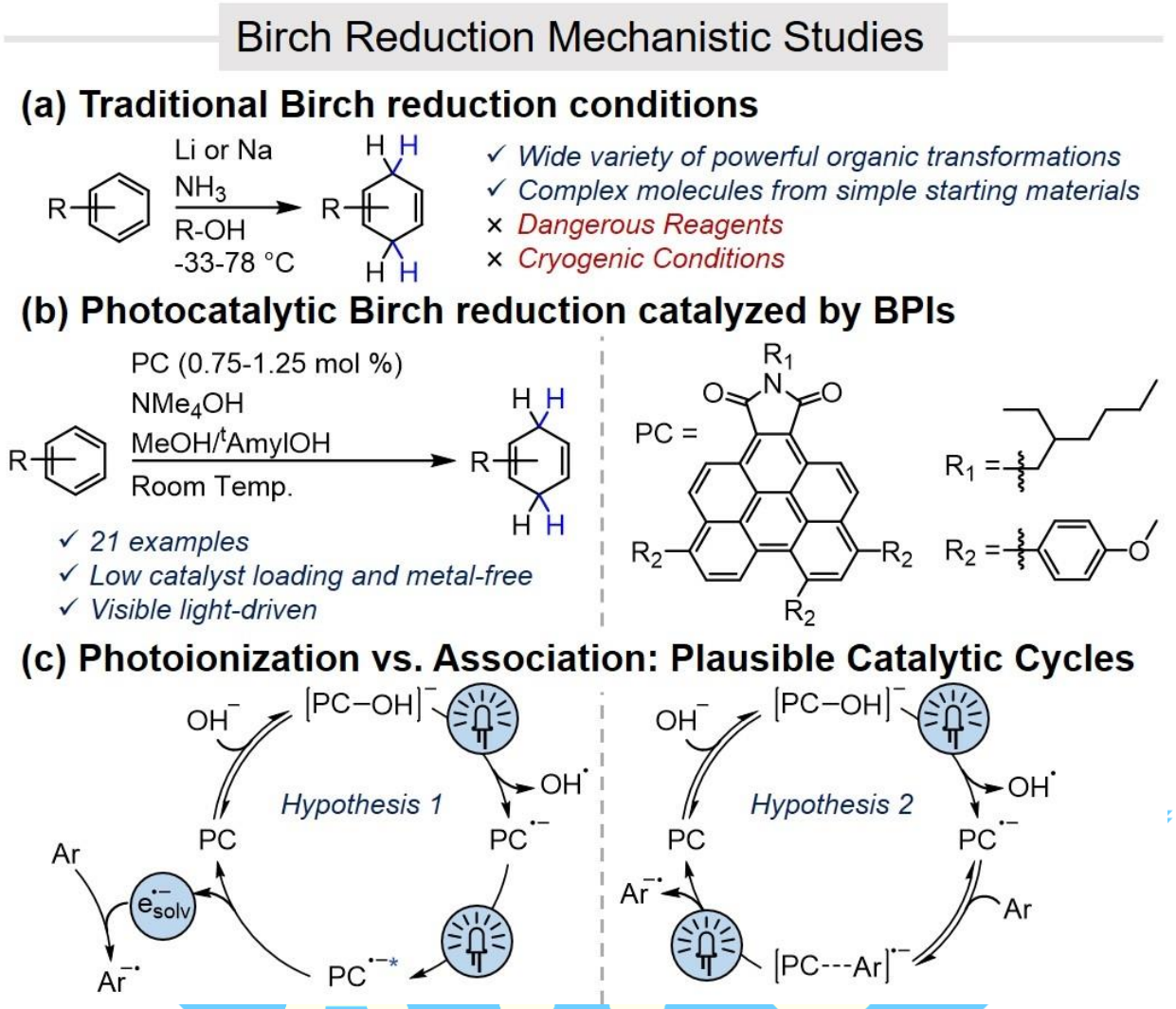


RMRM 106

Mechanistic insights into organocatalyzed birch reduction driven by visible light

Max Kudisch[1], *max.kudisch@colostate.edu, Justin Cole*[1,2], *Dian-Feng Chen*[1], *Ryan M. Pearson*[1,3], *Chern-Hooi Lim*[1,4], *Garret Miyake*[1]. *(1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Boulder Scientific Co, Longmont, Colorado, United States (3) Cypris Materials, Berkeley, California, United States (4) New Iridium, Fort Collins, Colorado, United States*

The Birch reduction reaction, of which the transformation of benzene to 1,4-cyclohexadiene is a prototypical example, constitutes an important synthetic method for building molecular complexity. Traditionally, use of an alkali metal in liquid ammonia at cryogenic temperatures leads to production of solvated electrons which reduce the substrate (Fig. 1a). These conditions motivate the development of a milder methodology. Many strategies have been developed, including ammonia-free, electrochemical, and photochemical variants of Birch reduction. However, despite the recent development of a handful of photocatalysts (PCs) with excited state reduction potentials more negative than –3 V vs. SCE, only benzo[ghi]perylene monoimides (BPIs) have been demonstrated to reduce benzene to 1,4-cyclohexadiene (Fig. 1b, *JACS* **2020** Just Accepted; DOI: 10.1021/jacs.0c05899). Benzene is challenging to engage due to its extremely low reduction potential of E_p = –3.42 V vs. SCE and high triplet energy (3.6 eV). Current studies are focused on elucidating the mechanism of light-driven Birch reduction. Initial experiments support that the PC imide moiety is attacked by hydroxide to produce a covalent adduct, $[PC–OH]^-$, which undergoes subsequent photolysis to produce the persistent radical anion, which is long-lived enough to be photoexcited to generate an extremely reducing excited state. However, the nature of the subsequent excited state reaction is currently unknown. The PC radical anion might reduce the solvent to liberate a solvated electron, or it may engage the substrate directly via single electron transfer (Fig. 1c). For the latter pathway to be viable, I hypothesize that ground or excited state association between PC radical anion and the arene is required due to the extremely short lifetimes of doublet excited states. Ongoing experiments aim to uncover which pathways are active and to elucidate the reasons for why the methoxyphenyl-substituted BPI performs best out of the BPI PCs explored.



RMRM 107

Understanding the reactivity of tertiary amines and in situ generated ammoniums under reductive metal catalysis

Chideraa I. Nwachukwu*, nwachukwu123@live.missouristate.edu, Timothy P. McFadden, Andrew G. Roberts. Chemistry, University of Utah, Salt lake, Utah, United States*

The construction of carbon–carbon (C–C) bonds via transition metal catalysis is a powerful tool—enabling the convergent assembly of complex molecular frameworks. A vast majority of cross-coupling protocols rely on the use of organohalides (C–X) as electrophilic coupling partners. Consequently, there are far fewer reports on the use of amine-derived electrophiles in such

reactions. Amines remain underutilized as electrophiles relative to organohalides in transition metal-catalyzed reactions due to both the relatively higher bond dissociation energy of C–N bonds and the oversight of tertiary amines as templates for C–C bond construction. Most methods that engage C–N bonds in catalysis rely on amine pre-activation by permethylation or diazotization. Activation weakens the C–N bond and precludes inhibitory amine chelation reactivity. This process also relegates amines to function as mere organohalide replacements. Our research program has focused on the development of methods to leverage amines as templates to facilitate multiple organometallic events in cascade sequences. Such processes require the development of a strategy to activate amines *in situ* by methylation, forming activated ammonium intermediates.
Herein, we report reductive metal-catalyzed methods for benzalkyl C–N bond cleavage with concomitant C–C bond formation. A Ni-catalyzed method, together with stoichiometric Mn and trimethylphosphate, allows for iterative benzyl transfer reactions from *in situ* generated ammonium substrates. The optimized application of this method to cyclic tertiary amine substrates enables deaminative ring-contraction reactions. These discoveries permit synthetic chemists to consider the use of tertiary amine templates as latent surrogates for C–C bond formation.

RMRM 108

Computational study of the torque, lock, and propagate approach to make configurationally stable twisted heli-thiopentacenes and heli-dithiopentacenes

***Shambhavi Tannir**, stannir@uwyo.edu, Edward L. Clennan. Chemistry, University of Wyoming, Laramie, Wyoming, United States*

Acenes like pentacene are well known organic semiconductors but suffer from stability issues associated with oxidations, dimerizations, and polymerizations. Their heteroatom analogues containing thiophene rings have also recently attracted attention as potential semiconductors. Twisted acenes, and thiophenes are promising surrogates for their more planar hydrocarbon and heteroatom analogues because they are not expected to have these stability problems. However, twisted thioacenes have received far less attention. We will present a computational study of chiral (twisted) thio-acenes using the B3LYP/6-31G(d) computational model. These sulfur containing compounds are expected to have the advantage of stability, easy of synthesis, and comparable charge transport and chiroptical properties to those of the acenes. We will describe the structures of unsubstituted and substituted [7]heli-D-

thiopentacenes in which the sulfur has been embedded in rings, D1, D2, D3, and D4 and “ortho” and “para” di-substituted analogues. We will also discuss how substituents propagate a twist down the longitudinal axis of the acene that was originally induced by a torque generated by the fused helicene. Finally, we will present a study of how the twist angle can influence the HOMO-LUMO gaps and other electronic properties of the heli-thioacenes.

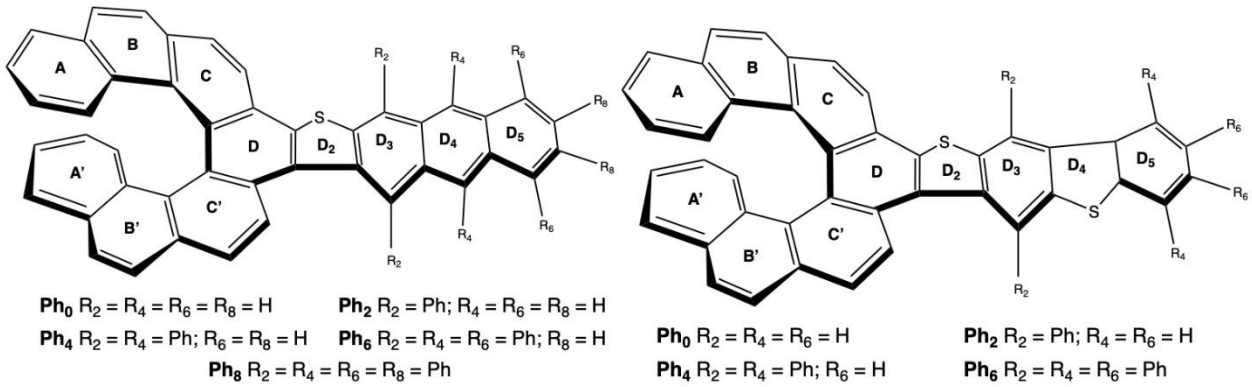


Fig 1. (left) [7]-Heli-D-2-Thienopentacene; (right) para-[7]-Helibenzothiopentacene

RMRM 109

Architectural analysis of branched polymers via soret contraction factor

***Michael Toney**, mtoney@mymail.mines.edu, Kim R. Williams. Colorado School of Mines, Golden, Colorado, United States*

Branched polymers are utilized in a broad range of applications and their properties depend on topology and molar mass. Polymer synthesis often yields broad distributions in molar mass and architecture. These polydispersities may obscure structure-function relationships and inhibit rational design of new materials. Current characterization methods are ensemble or separation techniques. The former is used to either directly monitor branching (e.g., NMR) or to calculate a contraction factor (e.g., viscometry and light scattering). Average values are obtained with no information about the distributions in size or architecture. A separation in conjunction with ensemble methods must be employed to determine distributions. The most common is size exclusion chromatography (SEC), where analytes are separated by their hydrodynamic size. Analysis of high molar mass (>10^6 Da) and branched polymers can suffer from non-ideal column interactions which result in chain anchoring or scissions. Thermal field flow fractionation is a technique that resolves some challenges presented by SEC and contraction factors. Separation is driven by differential transport of analytes in the presence of a temperature gradient. This is known as thermal diffusion and is described by the thermal diffusion coefficient (D_T). Furthermore, retention of analytes may be calculated if the Soret coefficient (S_T), a ratio of D_T to the translation diffusion coefficient, is known or can be approximated. In recent years the Soret contraction factor, a ratio of a branched S_T to a linear, was introduced to characterize star/pom-pom and hyperbranched topologies. In these studies, a linear analog, which is not always available, was used to approximate $S_{T,linear}$ at a given molar mass. Despite the lack of a well-developed theory for polymer thermophoresis, a predictive model has been identified which permits the estimation of S_T at different molar masses. This presentation introduces this model and its use to analyze bottlebrush with varied degrees of polymerization (DP) in backbone and sidechain. A linear relationship between S_T and the sidechain and backbone DP was observed, which allows for the approximation of sidechain DP if the backbone is known. Additionally, when compared to data from previous works, a plot of g” with respect to number of chain ends defines regions which are specific to stars/pom-poms (polystyrenes/polyacrylates), pseudo-dendrites (polyesters), and bottlebrushes (polyacrylates).

RMRM 110

TotalTHM-NOW: A low-cost online analyzer for total trihalomethanes in drinking water

***Melissa Alfonso**, mrlfonso@memphis.edu, Naga Boppana, Michael A. Brown, Paul S. Simone, Gary L. Emmert. Chemistry, The University of Memphis, The University of Memphis, Memphis, TN, US, academic, Memphis, Tennessee, United States*

Trihalomethanes (THMs) are one of the two classes of halogenated disinfection by-product (DBPs) that are regulated under the United States Environmental Protection Agency (USEPA). Chloroform, dichlorobromomethane, dibromochloromethane, and bromoform are collectively called total trihalomethanes (THM4). The USEPA has a set maximum contamination level (MCL) for THM4 at 0.060 mg/L. A 2007 survey by Environmental Working Group (EWG) shows that ~20% of all drinking water industry violations in the United States were THMs MCL possibly affecting millions of customers. The occurrence of THMs violation is widespread as thousands of utilities struggle each year to meet these regulations. A simple, low-cost analyzer was developed to provide THM4 data that can help operators comply with regulations and optimize their treatment process. Current research uses the capillary membrane sampling device to separate the THMs from the drinking water sample followed by reaction with nicotinamide to produce fluorescence signal. The TotalTHM-NOW has a method detection limit of 0.002 mg/L with accuracy measured as mean percent recovery of 108% and precision measured as percent relative standard deviation of 5%. An overview of TotalTHM-NOW and specific improvements will be discussed. Improvements addressed in the current research are reagent delivery, continuous to discontinuous reagent flow, continuous calibration, data acquisition, and 3D-printed detector. Results of comparison studies conducted at the Lebanon Tennessee water treatment plant will be presented on TotalTHM-NOW and THM-RR.

RMRM 111

Modeling pollutant levels

*Paul Johnson[1], **Kate Johnson**[2], kj864LTJ@gmail.com, Ling Huang[3]. (1) Clinical SAS Programmer, Davis, California, United States (2) University of California Davis, Davis, California, United States (3) Sacramento City College, Sacramento, California, United States*

The United States Environmental Protection Agency reports on how the protection of water resources are compromised by the inability to adequately determine ecological health risks posed for example by chemical contamination. Methods for detection are constantly being updated and to some extent changed. These methods are important and should be examined as changes and updates are made, since they significantly impact the health of water resources; especially stream and river water supply and conditions. One such focus of the EPA has been the development of methods to detect polyfluoroalkyl substances (PFAS) and cyanotoxins [see methods 536, 537, 545 and 546; Method 537.1 has been updated as recently as of March, 2020]. Pollutant levels are measured from streams and rivers; often means and percentiles are determined. This poster describes how to retrieve water monitoring data from the EPA (public domain data) where the user can retrieve local data pertinent to their own environment and impacts on health. We will consider the use of the delta-lognormal distribution to find the means and percentiles with the presence of non-detects, and make use of the Bootstrap to find percentiles of these estimates. Improved estimates incorporating any bias will be calculated. SAS® and SAS/STAT® will be used for the data analysis. Simulated pollutant data will be used to illustrate methodology. Their toxicity and health effects will be discussed.

RMRM 112

Measuring arsenic levels in the Fountain Creek watershed based on uptake by the bryophyte *Hygrohypnum ochraceum*

Alejandra Chavez[1]*, archavez5494@gmail.com,* ***Nathaniel Gasparovic***[1]*, ng3894@colostate.edu, Debbie C. Crans*[1]*, Jim Carsella*[2]*. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Chemistry, Colorado State University – Pueblo, Pueblo, Colorado, United States*

The leaching of arsenic from the abandoned smelter site located at Gold Hill, Colorado Springs, CO is a concern and therefore was investigated. Since the toxicity of arsenic changes with the different species, the levels of arsenic and its speciation in the Fountain Creek watershed was investigated. Water and bryophyte samples were collected at 4 upper Fountain (UFC), 5 lower Fountain (LFC) and 5 Monument Creek (MC) sites. They were harvested at the tenth day of exposure, washed, dried, and analyzed by inductively coupled plasma mass spectroscopy (ICP-MS). A dose response relationship between the bryophyte and the water were evaluated by statistical analysis and speciation diagrams were modeled using the HYSS program. Elevated levels of arsenic in the water

were present below Gold Hill, with levels exceeding the limits set by the EPA. Current results indicate statistically significant (P<0.025) bioaccumulation of arsenic in the bryophyte. In addition, the bioaccumulation of arsenic in the bryophyte follows a statistically significant seasonal pattern (P< .005). The spring contributed higher concentrations of arsenic at upper Fountain Creek while the fall contributed higher concentrations of arsenic at Monument Creek. Higher concentrations in the water at LFC combined with lower Kd values in LFC suggest that as we move further down LFC the uptake of arsenic by the bryophytes decreased.

RMRM 113

Infrared spectrum and atmospheric chemistry of 1,1,2,3,3,4,4 heptafluorobut-1-ene

***Ramesh Sapkota**, Rameshsapkota@my.unt.edu, George Rawling, Paul Marshall. Chemistry, University of North Texas, Denton, Texas, United States*

The recognition that photolysis of hydrochlorofluorocarbon (HCFC) compounds depletes stratospheric ozone has led to their substitution by hydrofluorocarbon (HFC) compounds. However, such species absorbs infrared radiation strongly and, if this is coupled to a long atmospheric lifetime, HFCs can exhibit high global warming potentials (GWP). Here we characterize a fluorinated alkene which, by virtue of the pi bond, offers the chance for high reactivity with atmospheric radicals and thus a small lifetime and GWP.
The relative rate method was used to determine the reaction rate of heptafluorobut-1-ene (CF_2=$CFCF_2CF_2H$) with chlorine atoms. A mercury UV lamp photolyzed Cl_2 and the reaction was monitored by FTIR spectroscopy. Ethane was the reference compound for relative rate studies. The rate constant was found to be (3.8 ± 0.4) 10^{-11} cm^3 $molecule^{-1}$ s^{-1} in 750 torr of argon diluent at 296 K. With 25% added O_2, oxidation of heptafluoro-but-1-ene initiated by a chlorine atom creates carbonyl difluoride (COF_2) with 95 ± 7 % yield and 2,2,3,3 tetrafluoro-propanoyl fluoride ($O=CFCF_2CF_2H$) as the only other product. The IR cross-sections of heptafluoro-but-1-ene yield a radiative efficiency of 0.29 W m^{-2} ppb^{-1} and its GWP was calculated to be 0.08 for 100 years' time horizon. Subtracting a reference COF_2 spectrum from the oxidative product spectrum we obtain the first IR spectrum of 2,2,3,3 tetrafluoropropanoyl fluoride. Its radiative efficiency is 0.18 W m^{-2} ppb^{-1} and its GWP is 0.05 for 100 years' time

horizon. Anharmonic frequency calculations for 1,1,2,3,3,4,4 heptafluorobut-1-ene and 2,2,3,3 tetrafluoropropanoyl fluoride based on density functional theory (B2PLYP/N07D) are in good accord with measurements, when all low-energy conformations are taken into account.

RMRM 114

Reflections in water: Musings on my favorite molecule

***Nancy E. Levinger**, nancy.levinger@colostate.edu. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

Over the course of my career, water has stayed as a constant theme. I am honored to review the ways that ACS has facilitated my ability to pursue exciting research and to contribute to the society through programming and leadership. Explorations of water in confining environments to our newest forays into cryopreservation, water has played a leading role. The ACS has also provided ample opportunity to develop my leadership in many different avenues from organizing symposia, through five years in the leadership of the Division of Physical Chemistry, to task forces and more. ACS has also served as an excellent venue to advance student careers. This presentation provides a lovely opportunity to reflect on the people and institutions that have enabled a long, productive career.

RMRM 115

Vignettes from a career in medicinal chemistry

***Gunda I. Georg**, georg@umn.edu. Medicinal Chemistry, University of Minnesota, Minneapolis, Minnesota, United States*

The lecture will provide a brief overview of my career that started with a degree in pharmacy and a doctorate in medicinal chemistry from the University of Marburg in Germany. After postdoctoral studies in synthetic organic chemistry at the University of Ottawa in Canada, I moved to the United States and spent 22 years as a faculty member at the University of Kansas in the Department of Medicinal Chemistry, before moving to the University of Minnesota Department of Medicinal Chemistry in 2007 as Department Head. I founded the Institute for Therapeutics Discovery and Development to provide infrastructure for probe and drug discovery at the University of Minnesota and for training of the next generation of drug discovery scientists.

RMRM 116 **CANCELED**

Anion coordination: Size, charge, and nexus with water

Subhamay Pramanik, Sandeep Kaur, Sam Brunclik, Victor W. Day, ***Kristin Bowman-James****, kbjames@ku.edu. Chemistry, University of Kansas, Lawrence, Kansas, United States*

Beyond the recognition and selective binding of simple single ions in supramolecular hosts, expanded hosts have the potential to target highly charged ions as well as multiple clusters of ions. Clusters of anions, as well as multiply-charged single anions, possess complexities above and beyond those of simple mono- or di-valent anions, as well as more complex and structured interactions with their solvent surroundings. In the synthesis of macrocyclic anion hosts we have isolated macrocycles with 36-membered ring systems and have begun exploring larger anion guests with multiple negative charges such as inositol hexaphosphates and multiple clusters of anions (Figure 1). This presentation will describe these findings and additionally the roles water can play.

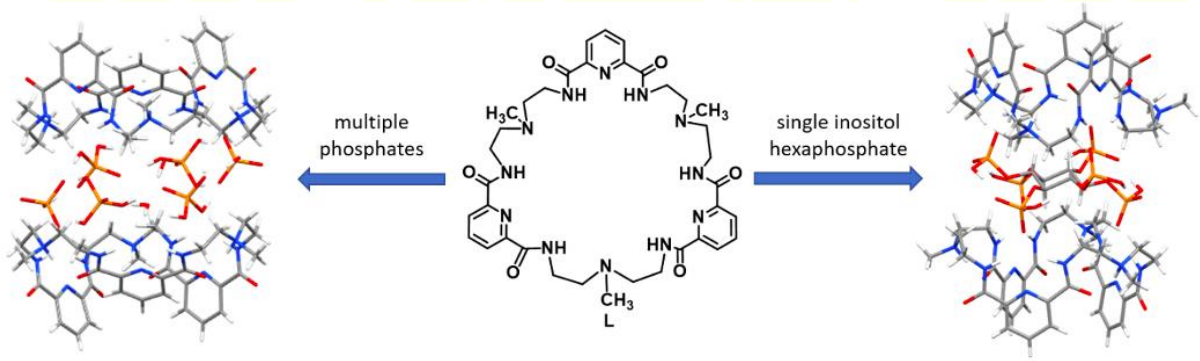


Figure 1. Clusters of phosphate anions (left) and a single multiply-charged inositol hexaphosphate anion (right) sandwiched between 36-membered ring macrocyclic hosts.

RMRM 117

Design of antibiotics to overcome resistance in mycobacteria

Courtney C. Aldrich*, aldri015@umn.edu. Medicinal Chemistry, University of Minnesota, Minneapolis, Minnesota, United States*

Mycobacterium tuberculosis remains the leading cause of death due to infection in humans. Although antibiotics are available to treat drug sensitive *M.*

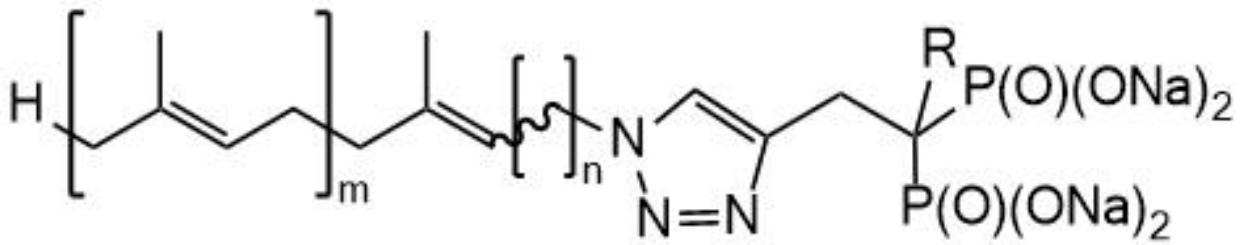
tuberculosis infections, the increasing incidence of drug resistant strains is threating our ability to gain hold of this pandemic. In addition, infections caused by non-tuberculous mycobacteria (NTM) are increasing globally. These infections are intrinsically resistant to most antibiotics. In this presentation, three short stories will be described of complimentary strategies to overcome drug resistance in mycobacteria including design of novel prodrugs for selective drug delivery with the mycobacterial periplasm, synthesis of rationally designed rifamycin analogs to overcome intrinsic drug resistance by NTMs, and design of antibiotics targeting biotin metabolism that prevent development of resistance.

RMRM 118

Inhibition of geranylgeranyl diphosphate synthesis by triazole bisphosphonates

Alisa Fairweather[1], Daniel B. Goetz[1], Chloe M. Schroeder[1], Nazmul H. Bhuiyan[1], Michelle L. Varney[2], Staci L. Haney[2], Sarah A. Holstein[2], ***David F. Wiemer****[1], david-wiemer@uiowa.edu. (1) Department of Chemistry, University of Iowa, Iowa City, Iowa, United States (2) Department of Internal Medicine, University of Nebraska Medical Center, Omaha, Nebraska, United States*

Multiple myeloma is an incurable cancer of the bone marrow that is characterized by production and release of excessive amounts of abnormal antibodies. We have explored a novel strategy for triggering apoptosis in malignant myeloma cells through inhibition of Rab-mediated protein trafficking, resulting in induction of the unfolded protein response and ultimately cell death. Because the Rab proteins must be geranylgeranylated for their proper activity, inhibition of geranylgeranyl diphosphate synthase results in diminished Rab function. Our efforts have focused on synthesis and bioassays of isoprenoid triazole bisphosphonates (e.g. **1**). Our structure-activity studies have determined that isoprenoid chain length (m and n), olefin stereochemistry, and the nature of the alpha substituent (R) impact inhibitor potency as well as *in vivo* biodistribution. In the best cases, effective concentrations as low as 20 nM have been observed in cellular assays.



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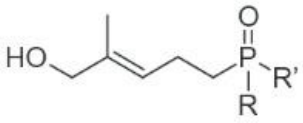
RMRM 119

Cellular kinetics of phosphoantigen prodrug forms

*Chia-Hung C. Hsiao[1], Xueting Huang[1], Megan Schladetsch[1], Nicholas A. Lentini[2], David F. Wiemer[3], **Andrew J. Wiemer**[1], andrew.wiemer@uconn.edu. (1) Pharmaceutical Sciences, University of Connecticut, Storrs, Connecticut, United States (2) Chemistry, University of Southern California, Los Angeles, California, United States (3) Chemistry, University of Iowa, Iowa City, Iowa, United States*

Butyrophilin 3A1 (BTN3A1) is an immune co-receptor that binds phosphoantigens such as (*E*)-4-hydroxy-3-methyl-but-2-enyl diphosphate (HMBPP). BTN3A1 binding stimulates an immune response coordinated by the Vgamma9Vdelta2 T cells. We have characterized novel butyrophilin ligands and various prodrug forms which improve the cellular uptake of these otherwise charged phosphorus compounds. The prodrugs stimulate T cell effector functions such as cytokine production with low nanomolar activity that requires expression of BTN3A1. Here, we have examined the dose- and time-dependency of varied prodrug forms that release the monophosphonate payload C-HMBP, including bis-POM (pivaloyloxymethyl), bis-amidate, aryl-POM, and aryl-amidate forms. We have explored the relative cellular efficacy of these prodrug forms for payload internalization into K562 leukemia cells through the ability of loaded K562 cells to stimulate interferon gamma production by Vgamma9Vdelta2 T cells. These results show that bis-ester C-HMBP prodrugs are internalized much faster relative to bis-amide forms and the rate of C-HMBP prodrug activation is the driving factor of their cellular potency.



R	R'
OH	OH
O-POM	O-POM
Gly-Et	Gly-Et
O-Ph	Gly-Et
O-Ph	O-POM

C-HMBP and some prodrug forms

RMRM 120

Inhibition of methyl transferases: The present and future

Mark A. Brown[2,3]*, Mark.Brown@colostate.edu, Debbie C. Crans*[1,2]*. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States (3) Clinical Sciences, Colorado State University, Fort Collins, Colorado, United States*

Methyl transferases are a class of enzyme that catalyze methyl transfer from the methyl donor S-adenosyl-l-methionine (SAM) to their DNA or RNA protein substrates. The SET and MYND domain-containing (SMYD) family of lysine methyltransferases are essential in several mammalian developmental pathways. Based on the broad expression pattern of SMYD2 in mammalian tissues, it is likely that it plays pivotal roles in a host of additional normal and pathological processes. SMYD3 is a lysine methyltransferase that is required for the uncontrolled proliferation of most breast, colorectal, and hepatocellular carcinomas. When aberrantly expressed, the SMYD3 lysine methyltransferase upregulates over 80 genes including oncogenes involved in cell cycle regulation and cell proliferation. Elimination of SMYD3 restores normal expression patterns of these genes and halts aberrant cell proliferation. The progress in both these areas and others will be described.

RMRM 121

Small-molecule modulation of gene expression via DNA quadruplex structures

***Cynthia J. Burrows**, burrows@chem.utah.edu, Aaron M. Fleming. Chemistry, University of Utah, Salt Lake City, Utah, United States*

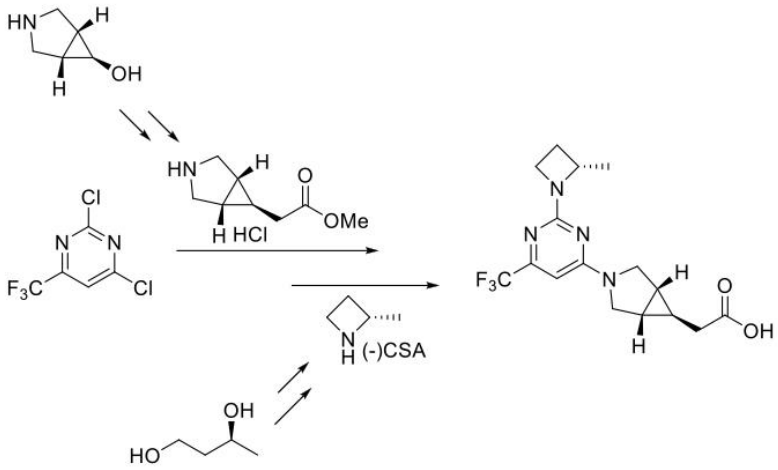
G-quadruplex (G4)-forming sequences are common in regulatory regions of mammalian genomes, notably within the first 300 nucleotides upstream of transcription start sites. In early studies, the prevailing dogma was that G4s inhibit transcription, and therefore small molecules were designed and synthesized to target G4s in oncogene promoters such as c-myc. Recent work in our laboratory has shown that the location of the G4 is critical to its impact on gene expression, wherein the presence of the G4 in the non-template (vs. template) strand of the promoter actually increases gene expression. Additionally, oxidative damage in the G-rich sequence can further enhance gene expression. We have developed a cell-based assay to examine the impact of small molecules on gene expression in order to understand targeting of either the G4 or the corresponding i-motif (a C-quadruplex) in the opposite strand as a function of oxidative stress.

RMRM 122

Optimization of the leads and synthesis of a ketohexokinase inhibitor clinical candidate

***Aaron C. Smith**, acsmith23@gmail.com. Pfizer Global Research and Development, Groton, Connecticut, United States*

Ketohexokinase (KHK) inhibition has shown potential as a treatment for non-alcoholic steatohepatitis (NASH) and non-alcohol fatty liver disease (NAFLD). As the KHKi program at Pfizer narrowed in on lead matter for clinical development, multiple compounds were profiled in parallel, and a robust plan was created to both allow time for data generation and for optimization of the synthesis of multiple leads on large scale without having to adjust timelines. Strategic planning to enable bulk delivery of multiple compounds along with the necessity for crisp decision making to balance long-term optimization with short term delivery goals allowed the team to position for efficient access to the clinical candidate. The triaging of lead matter and the synthesis of key compounds will be presented including the enablement of key monomers: 2-methyl azetidine and [3.1.0] amino ester which were used to access >300 g of the clinical candidate to support pre-clinical efficacy and safety studies.



RMRM 123

Discovery and development of BET bromodomain inhibitors for male non-hormonal contraception

Gunda I. Georg, *georg@umn.edu. Medicinal Chemistry, University of Minnesota, Minneapolis, Minnesota, United States*

The BET (bromodomain and extra-terminal) proteins are a sub-family of bromodomain-containing proteins consisting of BRD2, 3, 4, and T. BRD4 inhibitors are currently in clinical trial for cancer treatment. BRDT, which is selectively expressed in the testis plays a crucial role in spermatogenesis. BRDT-1 knock-out mice are infertile and therefore it has been hypothesized that a BRDT-selective inhibitor could become a male contraceptive agent. Progress towards the discovery and structure-activity relationships of bromodomain inhibitors will be discussed.

RMRM 124

Artificial intelligence tool for accessible chemistry education

Jacob Watters[2], Feng Jiang[2], April A. Hill[2], ***Melissa Weinrich[1]****, 158elissa.weinrich@unco.edu. (1) University of Northern Colorado, Greeley, Colorado, United States (2) Metropolitan State University of Denver, Denver, Colorado, United States*

A primary challenge in chemistry education is creating accessible laboratory

experiences for students with visual impairments (VI). A common approach is to rely on sighted lab partners to complete much of the hands-on work, forcing students with VI to be passive learners. In this session, we introduce an artificial intelligence (AI) tool developed using natural language processing (NLP) techniques and the Amazon Alexa Skills Kit (ASK). This AI tool is called the Virtual Laboratory Assistant (VLA). When launched by a smartphone or computer in the laboratory workspace, the VLA provides procedural details, chemical information, and other web-searchable content in response to voice queries. The VLA can also impart voice-control capabilities to electronic laboratory equipment, such as a Talking LabQuest, allowing the student with VI to fully control data collection. We believe this AI tool will promote the inclusion of learners with VI in laboratory courses while potentially benefiting all learners.

RMRM 125

Designing a culturally inclusive STEM and health research training program for Native American students

Naomi Lee[1,2], *naomi.lee@nau.edu, Joslynn Lee*[3]*. (1) Chemistry and Biochemistry, Northern Arizona University, Flagstaff, Arizona, United States (2) Center for Materials Interfaces in Research and Applications, Northern Arizona University, Northern Arizona University, Flagstaff, AZ, US, academic, Flagstaff, Arizona, United States (3) Chemistry and Biochemistry, Fort Lewis College, Durango, Colorado, United States*

The presentation is an informative session on the successes and obstacles in designing a culturally inclusive STEM and health research training program for Native American students. In 2019, the Department of Chemistry and Biochemistry at Northern Arizona University launched a new summer internship program for local high school students referred to as ACS-CARE (American Chemical Society - Cultural and Academic Research Experience). The ACS-CARE program aims to increase the diverse pool of academic and research professionals by engaging underrepresented, specifically Native American, and low-socioeconomic status (SES) high school students in STEM and medical-related fields through culturally relevant curriculum and summer research training. ACS-CARE was designed as a two-year program with students receiving 7-9-weeks of research experience and culturally relevant training in chemistry, biology, and healthcare fields in the months of June and July. In ACS-CARE's inaugural year (2019), the program included 10 high school students primarily from Flagstaff High School but also included Coconino HS

and Many Farms HS (located on the Navajo Nation). Due to the COVID-19 national emergency, the 2020 ACS-CARE program ran a 4-week virtual program in parallel to ACS Project SEED from July 6 – 31, 2020. Seven ACS-CARE students received online chemistry training through at-home kitchen experiments that focused on food chemistry and traditional knowledge. Students also participated in professional development sessions such as resume writing, public speaking, and designing a poster. In September 2020, ACS-CARE will expand to include a virtual academic year program for high school students (ages 14+) years in the southwest. Finally, to assess the overall impact of the program, we administered a pre- and post-program electronic survey along with regular feedback forms. The survey included subscales on mentoring, science identity, science self-efficacy, and intent to persist in science. Overall, students had a strong sense of cultural/ethnic identity and STEM identity.

RMRM 126

Tracking information literacy in science students: A longitudinal study of skills retention through the chemistry curriculum

Jefferson D. Knight[1]*, jefferson.knight@ucdenver.edu, Margaret Bruehl*[1]*, Denise Pan*[2]*. (1) Department of Chemistry, University of Colorado Denver, Denver, Colorado, United States (2) University Libraries, University of Washington, Seattle, Washington, United States*

Information literacy (IL) is a key skill for undergraduate students to develop, but is explicitly addressed in relatively few courses. For chemistry and other science students, IL skills include the ability to locate appropriate sources of information in the scientific literature, as well as to effectively construct scientific meaning from reading those sources. Here, we evaluate how well students retain these IL skills when they are taught and assessed in a first-year course (Honors General Chemistry) and then again in a course sequence popular among third-year students majoring in chemistry or biomedical sciences (Biochemistry I and II). Briefly, students in Biochemistry I and II worked in groups to write mini-review articles on chosen topics each semester, drawing from relevant primary and secondary scientific literature. Student performance on these assignments using a variety of metrics was compared between those who had previously taken Honors General Chemistry (in which IL skills were taught) versus those who had not. We find that students who had received prior IL instruction tended to perform better on the IL-based assignment in Biochemistry I. In contrast, the difference between scores on the IL-based assignment was insignificant in Biochemistry II, suggesting that the prior instruction and practice provided during Biochemistry I was sufficient to bring both cohorts of students up to the same standard. In this collaboration between a General Chemistry instructor, a Biochemistry instructor, and a University librarian, we assess the type and quality of journal articles cited by each group, as well as the IL search tools used by each individual student, in order to discern skills that improve upon prior IL instruction and impact student performance. The methods and results of this multi-year study will be useful for science faculty and departments who want to provide explicit IL instruction as part of their curriculum.

RMRM 127

Can students learn chemistry without midterm exams?

David J. Weiss[1]*, dweiss@uccs.edu, Patrick McGuire*[2]*, Wendi Clouse*[3]*, Robert Wrobel*[1]*. (1) Chemistry and Biochemistry, University of Colorado at*

Colorado Springs, Colorado Springs, Colorado, United States (2) Teaching and Learning, University of Colorado at Colorado Springs, Colorado Springs, Colorado, United States (3) Institutional Research, University of Colorado at Colorado Springs, Colorado Springs, Colorado, United States

Do we need a formal lecture in order for students to learn upper division analytical chemistry? How do we know they have learned the material without midterm exams? Changing our course to active learning, we wanted to know if students could learn chemistry and retain that knowledge without a traditional lecture course, and if they could demonstrate this using the national American Chemical Society exam. We also were interested to see if students liked an active learning approach more, and felt more engaged in an active learning course compared with traditional lecture. The professor's lecture was shortened with the expectation that students would prepare for lecture, and much of the lecture time was spent working on inquiry sets based upon the course material (like in-class homework based on the textbook and the current literature in the area), as well as learning the literature in the area. Students wrote a short literature review and a research proposal on analytical chemistry, and learned how to give a presentation on this work. They also gave short lectures on the course material themselves to the other students. Can they learn this material and increase their engagement without formal lecture and exams?

RMRM 128

Multiple ways to virtually engage students in chemistry labs

***Audrey S. Smeltzer Schwab**, bluetiger313@yahoo.com. Muhlenberg High School, Reading, Pennsylvania, United States*

During the pandemic it is difficult to have students participate in chemistry lab, regardless if they have virtual school, traditional school, or some version in between. However, it is important that students learn the skills from experimentation. Furthermore, students need the chemistry lab experience for their future studies. This presentation will provide you with multiple ways to have students engage in the chemistry laboratory experience but virtually. From this presentation, you will leave having chemistry labs you can implement right away Furthermore, it will give you ways to modify your labs, so you can still teach the standards and skills students need, but from the virtual platform.

RMRM 129

Analysis of the impacts of student sense of social belonging on student outcomes in STEM

Joshua D. Edwards[1]*, 122750edwards@chsbr.net, Regina Frey*[1]*, Ramón Barthelemy*[2]*. (1) Chemistry, University of Utah, Salt Lake City, Utah, United States (2) Physics and Astronomy, University of Utah, Salt Lake City, Utah, United States*

In introductory STEM courses, including general chemistry, students' course sense of belonging and their self-reported classroom inclusivity and the effect of those responses on their exam performances and persistence in course series were examined. These effects were examined across various subgroups, such as gender, race/ethnicity, and first-generation status. Additionally, open comments in surveys were qualitatively analyzed to better understand students' reported reasons for their level of course sense of belonging and classroom inclusivity.

RMRM 130

Comparison of online content homework with metacognitive training homework in general chemistry courses

Nakita Ellis[1]*, Holly Wiegreffe*[3]*, Andrew Hefzalla*[2]*,* ***Emily Heider***[1]*, eheider@uvu.edu. (1) Utah Valley University, Orem, Utah, United States (2) University of Central Florida, Orlando, Florida, United States (3) Chemistry, Florida State College, Jacksonville, Florida, United States*

Use of online homework for general chemistry courses is increasingly common, especially given recent transition to online course platforms due to the COVID-19 pandemic. There are many ways online homework assignments can be organized to exploit innovations in technology and cognitive research, such as adaptive, spaced, and massed. The aim of this study was to determine if graded metacognitive self-assessment assignments paired with ungraded assigned homework, could result in student content mastery relative to graded online assessments. Using four large-enrollment (>300 student) face-to-face general chemistry classes, an online homework platform was presented in delivery of three different organizational methods and compared to a course in which no online homework was used, but for which students completed weekly study inventory self-assessments with metacognition training. Homework times, scores, standardized final exam scores, course grades and survey results were

used to compare the various homework delivery methods. The results indicate that mean final exam scores improve with higher average homework scores, but that longer homework times negatively correlate with exam scores. Additionally, weekly student study self-assessments with metacognition training is as effective as any of the online homework delivery strategies, and results in fewer students withdrawing from the course.

RMRM 131

Task analysis of undergraduate biology and chemistry laboratory activities

***Abigail Reid**, ah.reid@pack.csupueblo.edu, Juliet Heath, Jonathan Velasco. Colorado State University - Pueblo, Pueblo, Colorado, United States*

Problem resolution allows students to engage in the process of inquiry and the scientific method by exploring new situations and coming up with solutions to real problems that we face. Students who engage in problem resolution during their laboratory exercises have shown an improved understanding of concepts over students in traditional laboratory courses. Laboratory manuals in introductory college classes tend to follow protocol developed by the instructor rather than using problem resolution. While it is necessary for introductory-level laboratory courses to provide structure to their students, problem resolution more accurately depicts authentic scientific practices. The analysis of undergraduate laboratory investigations utilizes the Laboratory Structure and Task Analysis Inventory (LAI). These analyses will be used to determine the extent of problem resolution that is present in laboratory experiments.

RMRM 132

Instructional behaviors in undergraduate biology and chemistry laboratory courses

***Juliet Heath**, jm.heath@pack.csupueblo.edu, Abigail Reid, Mariah Painter, Jonathan Velasco. Colorado State University - Pueblo, Pueblo, Colorado, United States*

It has been observed that teachers implement the same curriculum with different teaching styles, which may impact learning. This study analyzes the behaviors between teachers and students to better identify and understand teaching styles. Videos of chemistry and biology laboratory activities were

recorded to analyze teacher-student interactions using the Laboratory Observation Protocol for Undergraduate STEM (LOPUS) was used to analyze laboratory interactions through descriptions of student and teacher behaviors as well as conversational topics. Hierarchical cluster analyses were carried out to illustrate clusters of videos that are characterized by a certain set of behaviors. Further analysis was carried out to show which clusters were showing significant differences for each behavior.

RMRM 133

Chemistry of indigenous peoples

Marcos Aurelio Gomes da Silva,
marcosaureliojf@hotmail.com. Universidade federal de juíz de fora, Juiz de fora, Minas Gerais, Brazil

The chemistry of indigenuos peoples techniques pharmaceutical science important scientist research legacy of indigenuos peoples.

RMRM 134

Encapsulating metal-organic framweorks (MOFs) within mesoporous silica for use in heterogenous catalysis

Scott E. Massimi[1], *smassimi@mymail.mines.edu, Brian G. Trewyn*[1,2]*. (1) Chemistry, Colorado School of Mines, Golden, Colorado, United States (2) Materials Science, Colorado School of Mines, Golden, Colorado, United States*

Metal-organic frameworks (MOFs) are materials that have shown great promise in the field of heterogenous catalysis. They have often been likened to zeolites due to their microporosity and inorganic structure. However, a key benefit of MOFs is the use of organic linkers that allow for significant variation in the structures available and therefore the reactivity of metal sites. Where these materials struggle is in their robustness, the importance of zeolites in industrial catalysis is largely due to their stability at extreme conditions that MOF materials cannot withstand.
Herein, our aim is to increase the stability of MOFs by embedding them in the pores of mesoporous silica nanoparticles (MSNs). It is expected that MOFs grown inside the mesopores of MSN supports will have greater chemical and thermal stability because of non-covalent interactions within the pore framework while retaining excellent catalytic ability. Our objectives are to discuss

challenges that contribute to these synthetic approaches along with the difficulties encountered in conclusively characterizing these materials. Our synthetic approach of embedding specifically ZIF-8 within MSN-10 will be shared. We will also go into the nitrogen sorption, TGA, XRD, and microscopy data required to fully characterize this material. Future directions will be shared within the fundamental and applied catalysis fields.

RMRM 135

Visible-light-promoted reactions via intermolecular charge transfer using (thiol)phenols as electron donors

***Bin Liu**, liuchem315@gmail.com, Chern-Hooi Lim, Garret Miyake. chemistry, Colorado State University, Fort Collins, Colorado, United States*

This presentation will discuss visible-light promoted reactions using (thiol)phenols as electron donors. Aryl halides and ethynylbenziodoxol(on)es are used as electron acceptors respectively. The reaction is driven by the photochemical activity of in situ generated electron donor/acceptor complexes, formed by the aggregation of (thiolphenolates and electron acceptors.

RMRM 136

Intra- and inter-ligand charge transfers in a new donor-acceptor complex

***Shiyue Gao**, gaosy92@gmail.com, **Jing yang**, yangjing@unm.edu, **Martin L. Kirk**, mkirk@unm.edu. Chemistry and Chemical Biology, University of New Mexico, Albuquerque, New Mexico, United States*

We will present a combined spectroscopic and theoretical study of new Pt donor-acceptor complexes that possess thiophene elaborated bpy acceptors (thp-bpy). These new complexes provide deep insight into the role of the thiophene moiety in the thp-bpy acceptor ligand, and how tph elaboration contributes to an antenna effect by turning on an intense new charge transfer feature. This work explains how the electron donor properties of the thiophene lead to a dramatic electron density redistribution between thiophene and bipyridine moieties in the charge transfer state. The intense charge transfer transitions are observed at 22,000 cm^{-1} and 14000 cm^{-1}, which are assigned as

thp → bpy intraligand charge transfer (ILCT) and cat → thp-bpy ligand-to-ligand charge transfer (LL'CT or interligand CT), respectively. Laser excitation into the ILCT band yields resonance Raman enhancement of localized thiophene and bipyridine totally symmetric vibrational modes that we use to directly probe the nature of this ILCT. The observed vibrational fine structure in the ILCT absorption band is understood in the context of the ground state Raman data and the time-dependent wavepacket formulation of Heller. Additionally, the electron redistribution observed in the thp → bpy ILCT is highlighted by the results of S K-edge spectroscopy and electron density difference map (EDDM) computations, which are also are used to describe the nature of the lower energy ligand-to-ligand charge transfer (LL'CT) band.

RMRM 137 **CANCELED**

Shining a new light on catalysis: Light responsive molecular dyads for direct control of redox switchable catalysts

***Cristian J. Aviles Martin**, cristian.aviles_martin@uconn.edu, Eugene Pinkhassik. Department of Chemistry, University of Connecticut, Storrs, Connecticut, United States*

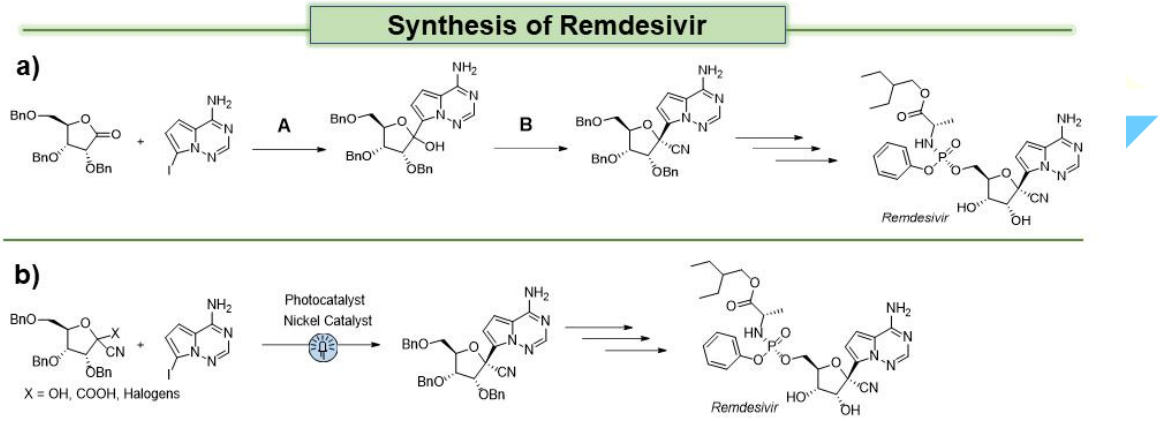
The use of redox-switchable catalysts in organic synthesis is an efficient and direct way of controlling reaction rates and selectivity. However, these catalysts are usually controlled by the addition of chemical redox agents into the reaction medium, meaning that redox sensitive substrates would be incompatible with these methodologies. This project focuses on the synthesis of light responsive ferrocene derived molecular dyads that undergo intramolecular electron transfer upon exposure to light. The stability, fluorescence lifetimes, and other optical properties of these dyad assemblies are studied through time-resolved spectroscopy. Furthermore, these dyads will then be connected to a redox-switchable catalyst using click chemistry to test the feasibility of using intramolecular electron transfer as a redox switching mechanism.

RMRM 138

Visible light driven synthesis of remdesivir precursor

***Alexander Green**[1], alexanderag8@gmail.com, Chern Lim[2], Garret Miyake[1]. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) New Iridium, Fort Collins, Colorado, United States*

Remdesivir is a promising treatment for COVID-19 and other SARs (Severe acute respiratory system) related diseases. COVID-19 is the disease caused by 2019-nCoV, a part of the Coronaviridea family of RNA viruses, and Remdesivir is a nucleoside analogue that interrupts the virus's RNA replication process. The COVID-19 pandemic has resulted in over 4 million cases and 150,000 deaths in the United States alone. Because of the rapid increase in cases and deaths, Remdesivir is in very high demand. However, in order to facilitate scaling the synthesis of Remdesivir effectively, we target improving key synthetic steps depicted in Figure 1a. To achieve effective scaling of Remdesivir we have begun investigating a metallaphotoredox approach using visible light to synthesize precursors to Remdesivir, (figure 1b). The traditional synthesis includes demanding conditions and cyrogenic temperatures (Grignard (A), cyanation (B)) which also have fairly low yields. This presentation will cover our efforts to devlop this drug synthesis using milder conditions using photoredox catalysis to overcome current bottlenecks.



RMRM 139

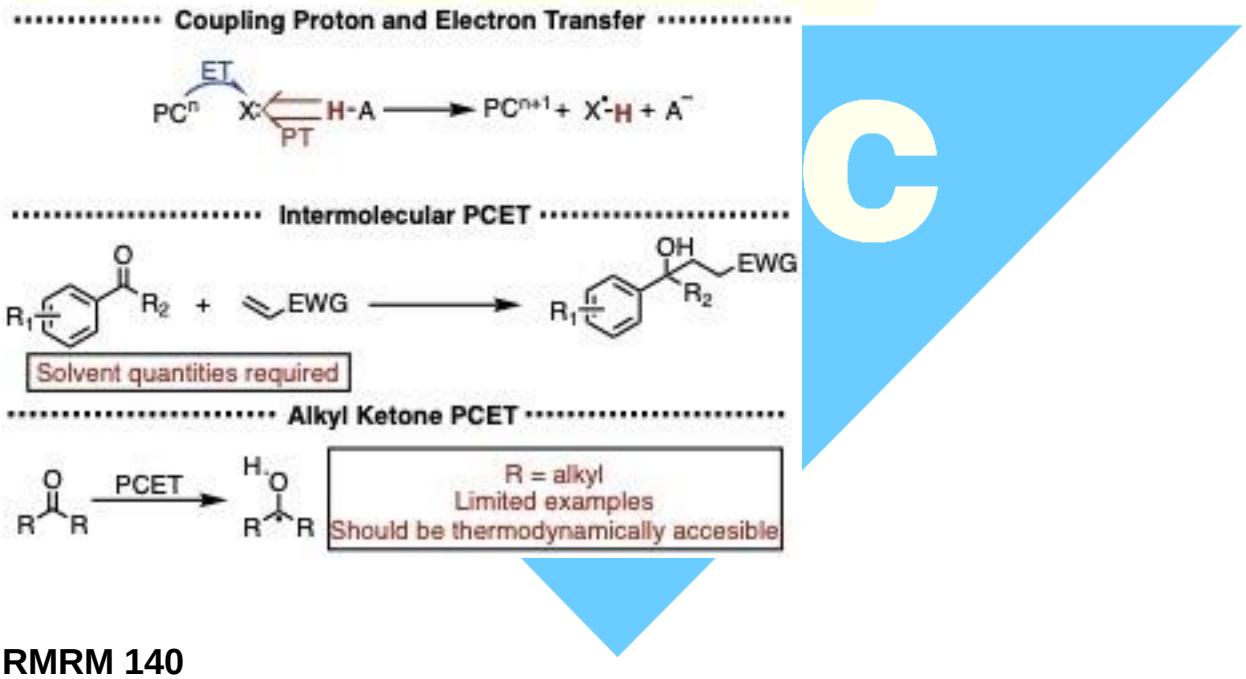
Photoredox catalyst design for proton coupled electron transfer

***Cameron Chrisman**, cchris@colostate.edu, Garret Miyake. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

The field of proton coupled electron transfer (PCET) has become an integral part of photoredox catalyzed organic methodology. PCET enables the activation of substrates beyond the reduction potential of common photocatalysts by coupling a reduction event to a protonation. For example, the

protonation or single electron reduction of ketones is challenging due to their weakly basic nature (pKa = -0.1 for acetophenone) and high reduction potentials (-2.48 V vs Fc for acetophenone), but a concerted protonation/reduction makes ketone activation more facile by lowering the energy barrier and eliminating high energy intermediates. Even though the field of PCET in organic synthesis has been expanding rapidly, many limitations still exist.

Two main limitations of PCET in organic methodology are the inability to engage alkyl ketone substrates and intermolecular couplings. Though alkyl ketones are more difficult to reduce than aryl ketones, many of the current acid/photocatalyst systems are thermodynamically capable of performing alkyl ketone PCET. However, there have been limited examples of alkyl ketone PCET, and no mechanistic studies have been performed to explain the difficulty of this reaction. Additionally, limited reports on intermolecular couplings have been published. Of the publications on intermolecular couplings, solvent level quantities of one of the reactants is typically required, limiting the applicability of these methodologies. This presentation will address work being done on the design and synthesis of organic photocatalysts to overcome the limitations of PCET.

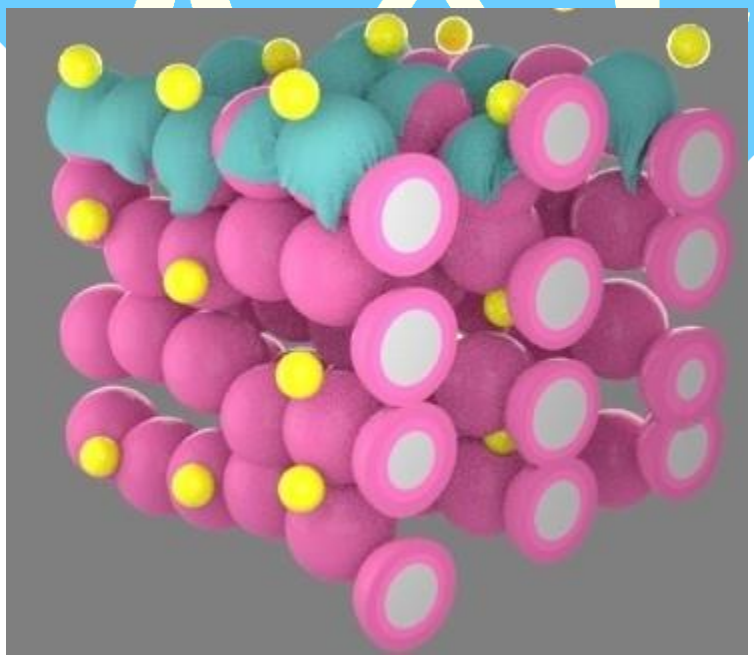


RMRM 140

Improved photoelectrochemical water oxidation catalysis via atomic layer deposition of alumina: Passivating surface trap states on a tin-oxide, phosphonate-functionalized perylene diimide plus CoO_x system

***Carly Jewell**, carly.jewell@colostate.edu, Richard Finke. Chemistry, Colorado State University, Fort Collins, Colorado, United States*

One of the challenges facing the world is the need to fulfill the growing demand for energy via renewable resources while minimizing CO_2 emissions. Photoelectrochemical water splitting into hydrogen and oxygen is one such system capable of renewable solar energy conversion. Previously, we developed a water-oxidation photoanode consisting of nanostructured SnO_2 coated with a perylene diimide dye derivative (N,N'-bis(phosphonomethyl)-3,4,9,10-perylenediimide, PMPDI) and a CoO_x water oxidation catalyst. Surprisingly, the addition of the CoO_x catalyst results in an approximately 50% *decrease* in photocurrent due, apparently, to limitations imposed by recombination and trap states at the CoO_x/SnO_2 interface. Here, we show the addition of an alumina overlayer deposited by atomic layer deposition (ALD) on the PMPDI dye designed to reduce recombination caused by the addition of CoO_x. Under optimized alumina deposition conditions, steady-state photocurrent was indeed improved approximately 3-fold over the SnO_2/PMPDI/CoO_x system without alumina as well as an increase in oxygen production. However, the addition of the CoO_x water-oxidation catalyst still results in a decrease of approximately a third in photocurrent in comparison to the SnO_2/PMPDI/AlO_x system without CoO_x. The improvements afforded by the alumina ALD, the negative impact of the catalyst addition, as well as the implications for future study of this and related systems will be discussed.



RMRM 141

Impacts of performing electrolysis during organocatalyzed atom transfer radical polymerization

Daniel Corbin[1]*, dnlcorbin2@gmail.com, Blaine McCarthy*[2,1]*, Garret Miyake*[1]*. (1) Department of Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Department of Chemistry, Stanford University, Stanford, California, United States*

Organocatalyzed atom transfer radical polymerization (O-ATRP) is a controlled radical polymerization method employing organic photoredox catalysts (PCs) for the synthesis of well-defined polymers. To achieve controlled polymer growth, the PC mediates a reversible activation/deactivation mechanism, wherein chain-end radicals are generated through activation by the photoexcited PC to enable chain propagation and then quickly deactivated by the PC radical cation (PC^+). The ultimate effect of deactivation is that radicals in the polymerization are generated in only small quantities, kinetically limiting radical-based side reactions that would otherwise hinder control over the polymer structure. Despite the importance of deactivation in O-ATRP, this key mechanistic step remains poorly understood. As such, investigations into the mechanism of this process and methods to manipulate it during a polymerization are necessary.

In this work, potentiostatic electrolysis was studied as a means to control the relative quantities of the PC and PC^+ during O-ATRP, with the ultimate goal of improving deactivation by increasing the concentration of PC^+ present in solution. During this work, side reactions arising as a result of electrolysis were investigated, the electrochemical apparatus was optimized, and evidence was found supporting the potential to improve polymerization control using this approach. Despite these achievements, this work revealed the complexity of performing electrolysis during O-ATRP and motivated several questions that are guiding current work in this area of research.

RMRM 142

Altering non-innocent anti-cancer compounds: How the addition of Cl to VO[HSHED] catecholates can change their electrochemistry

Allison Haase[1]*, allisonhaase@earthlink.net, John Hagan*[1]*, Heide Murakami*[1]*, Cheryle N. Beuning*[2]*, Peter A. Lay*[3]*, Debbie C. Crans*[1]*. (1) Chemistry, Colorado State University College of Natural Sciences, Fort Collins, Colorado, United States (2) Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, Colorado, United States (3) Chemistry, University of Sydney, Sydney, New South Wales, Australia*

Vanadium(V) Schiff base catecholate complexes have recently been found to be active anti-proliferation agents against certain types of brain cancer cells. In the following presentation, were will characterize new vanadium complexes in which the Schiff base ligand has been modified with a chlorine atom. These perturbations will have an impact on the compound's half-wave potentials, the compound's hydrophobicity, their stability, and their overall effectiveness in anti-cancer treatment. The complexes were studied using cyclic voltammetry and spectroelectrochemistry and other experimental techniques such as hysteresis of the complexes and time-based studies of decomposition in organic solvent. It was found that the chlorinated compounds were slightly easier to reduce than their parents, while substituted catechols that were more electron-donating will have more negative $E_{1/2}$ values. If reactive oxygen species were the mode of action for these anti-cancer compounds, one would expect that the most readily reduced compound is the most biology active anti-cancer agent. Since this observed trend indicates that the more challenging to reduce ligands are more effective, ROS is not likely to be the major mode of action of anti-cancer activity.

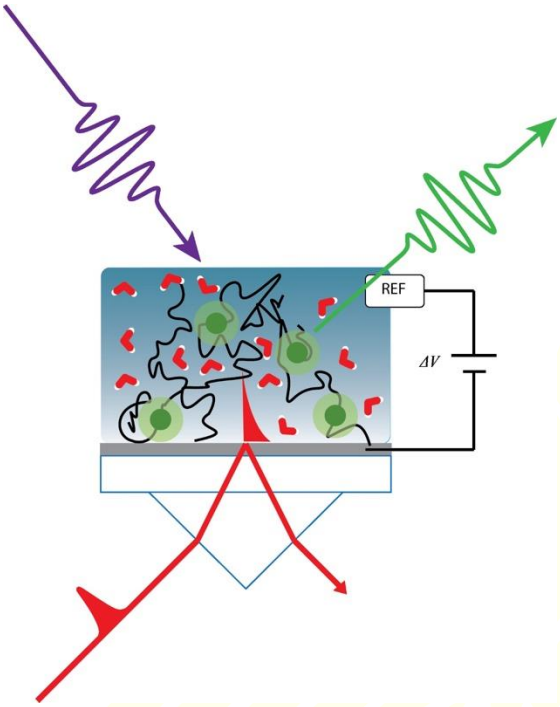
RMRM 143

Multimodal spectroscopic investigation of the conformation and local environment of biomolecules at an electrified interface

Sasha Moonitz*, sasha.moonitz@utah.edu, Noah Shepard, Rodrigo Noriega. Chemistry, University of Utah, Salt Lake City, Utah, United States*

Electrified interfaces are a complex and dynamic environment where the electrode surface, solvent molecules, ions, and both free and surface-bound biomolecules interact over multiple time scales. Complementary mid-infrared plasmonic resonances and time-resolved fluorescence detection in the visible range are employed to obtain detailed information on the molecular-scale changes in local environment and conformation of adsorbed poly-L-lysine chains on the electrode surface. Correlated changes in the reflectivity of surface plasmon resonances, time-resolved brightness, fluorescence lifetime, and fluorescence anisotropy dynamics reveal the interplay between solvent-

dependent hydration state, electric field-mediated ion concentration, and collective rearrangement of adsorbed polypeptides.



RMRM 144

Quantitative analysis of diffusible signaling factors using negative ion liquid chromatography electrospray ionization mass spectrometry (HPLC-ESI-MS)

***Brian Hoffman**, bhoffman@memphis.edu, Daniel L. Baker. Chemistry, The University of Memphis, Memphis, Tennessee, United States*

Biofilms are noted for their antibiotic resistance and are a prominent threat of infections within hospitals. Approximately 65% to 85% of all infections obtained in a hospital involve biofilms. These infections occur most often during the wound healing process (burn wounds, surgical wounds, etc.). Biofilms are a collection of bacteria that utilize a polysaccharide matrix, signaling molecules, and networking proteins to function in unison. This polysaccharide matrix increases the antibiotic resistance of bacteria within the biofilm. Diffusible signaling factors (DSF) are fatty acid analogs known for their ability to break up the extracellular matrix and function as antibiofilm agents. By utilizing DSF to disperse the extracellular matrix bacteria become more susceptible to

antibiotics. The DSF cis-2-decenoic acid (C2DA), has shown effectiveness against *biofilms including those generated by S. Aureus and P. aeruginosa*. The cis-double bond of C2DA is susceptible to isomerization and oxidation due to heat, light, or oxidative conditions. As the stability of C2DA is pivotal to its activity as an anti-biofilm agent, it is necessary to monitor and quantify the degradation of C2DA. Through the utilization of HPLC-ESI-MS, it is possible to resolve the cis and trans isomers of decenoic acid and quantify their presence in various samples. Method development of a quantitative assay for DSF analogs has been completed utilizing both normal phase and reverse phase HPLC-ESI-MS of the negative molecular ions. Calibration curves for C2DA and its trans-isomer (T2DA) were generated using decanoic acid as an internal standard. The normal phase calibration had a limit of detection (LOD) of 1.5 ng/mL, a limit of quantitation (LOQ) of 4.8 ng/mL, and an overall linear correlation coefficient (R^2) of 0.98. The reverse-phase calibration had a LOD of 0.1 ng/mL, an LOQ of 0.3 ng/mL, and an overall R^2 value of 0.99. Progress on the development and application of these methods will be discussed.

RMRM 145

Complementary pairs from clashing forces throughout chemistry: Visualizing the pauli exclusion principle and its far-reaching implications

Justin P. Joyce*, jpjoyce@colostate.edu, Anthony K. Rappe, Matthew P. Shores. Colorado State University, Fort Collins, Colorado, United States*

The Pauli Exclusion Principle derives from the concept of electronic spin, and forms the basis of chemical richness and molecular complexity. While foundational to quantum mechanics, the Pauli Exclusion Principle is routinely relegated to the role of strain, with the portrayal of exchange repulsion as antagonistic to molecular stability. We outline a kinetic energy-based model that establishes orthogonality of parallel electrons as the source of both chemical bonding and non-covalent interactions. We establish the complementarity between electronic exchange and attractive interactions, ranging from electrostatics, to charge transfer, to dispersion. We present a computational procedure that provides visual clarity and quantification of non-covalent interactions that are supported by experimental data. We consider the intra- and inter-molecular forces that lead to branched alkane stability and fluorocarbon hydrophobicity before further extending our perspective to the magnetic interactions of Cr^{3+} polypyridyl complexes.

RMRM 146

Frustrated Lewis pairs with applications in hydrogen storage

Glory Russell-Parks[1,2]*, grussellparks@mymail.mines.edu, Brian G. Trewyn*[1,2]*, Thomas Gennett*[1,2]*. (1) Colorado School of Mines Department of vChemistry, Golden, Colorado, United States (2) National Renewable Energy Laboratory, Golden, Colorado, United States*

The development of new materials that can harness renewable sources of energy such as hydrogen is in high demand due to the rise in environmental issues associated with current petroleum-based energy technologies. Due to its abundance and large gravimetric energy density, hydrogen is considered a potential source of energy; however, there are major challenges associated with utilizing hydrogen for energy specifically in safely and efficiently storing and transporting it. While there are many different materials that have been developed and tested to address these issues, we are still in search of a material that can meet the challenging Department of Energy's 2025 gravimetric and volumetric targets.
Frustrated Lewis pairs (FLPs) have recently proven their importance in hydrogen storage applications. In contrast to commonly known Lewis acid-base pairs, functionalizing the acid and base to contain bulky ligands prevents them from binding to their counterpart causing them to be in a "frustrated" state. The acid and base are held together by weak intermolecular forces without neutralization, which catalyzes the heterolytic cleavage of hydrogen molecules into a proton and hydride which electrostatically bond to the Lewis base and acid, respectively. In addition to potential liquid carriers, we are investigating solid state materials that can be hydrogenated upon cleavage of the hydrogen components. Utilizing FLPs as catalysts has become attractive due to their unique characteristics including compatibility with a wide range of donors and acceptors (metal and non-metal). As this field continues to develop there will be many challenges that will need to be addressed, our goals are to demonstrate that systems utilizing FLPs may assist with lowering the sorption temperature and pressure, reducing the activation energy barrier and potentially allowing for hydrogenation and dehydrogenation to occur. This work focuses on the novel synthesis and characterization of an FLP system.

RMRM 147 **CANCELED**

Chromophoric photonic crystals

Luis Garcia Alzate*, lfgarcia@colostate.edu. Chemistry, Colorado State University College of Natural Sciences, Colorado State University College of*

Natural Sciences, Fort Collins, CO, US, academic/gen, Fort Collins, Colorado, United States

Nature gives us amazing examples of color seen in Chameleons, Octopuses, Butterflies, and Opals. This color arises from the periodic nanostructure, coined photonic crystals, which can selectively reflect wavelengths of light because of their structure. These photonic crystals found in nature can be mimicked, through the synthesis of block copolymers and sequentially the self-assembly of these polymers. It has been shown that by changing the molecular weight of graft block copolymers, the wavelength of reflected light can be precisely tuned across the visible light spectrum and into the IR. In contrast, color from dyes and pigments arise from the emission of light from the chromophores in these molecules. This presentation will discuss the synthesis of photonic crystals with chromophores on the backbone of the polymer chain. The optical properties and the applications of this new class of polymeric photonic crystals will be presented.

RMRM 148

Studies of the formation and infrared spectrum of formyl fluoride

George Rawling[1,2]*, grawling@comcast.net, Ramesh Sapkota*[1,2]*, Paul Marshall*[1,2]*. (1) Chemistry, University of North Texas System, Denton, Texas, United States (2) Center for Advanced Scientific Computing and Modeling, University of North Texas, Denton, Texas, United States*

A common atmospheric degradation product of hydrofluorocarbon molecules is formyl fluoride, HC(O)F. Better characterization of HC(O)F clarifies its role in the environment and assists laboratory studies. Here we derive absolute cross sections for infrared absorption, and use them to estimate its GWP and to gain information about the chemistry of CH_2F. Mixtures of fluoromethane, molecular chlorine, and oxygen, made up to atmospheric pressure with argon, were subjected to continuous UV photolysis and monitored with Fourier Transform Infrared (FT-IR) spectroscopy. The major products are chlorofluoromethane (CH_2FCl), and HC(O)F, with each major product the result of a different chemical pathway for CH_2F radicals. The $[O_2]/[Cl_2]$ ratio determines which pathway dominates, with high $[O_2]$ favoring HC(O)F and low $[O_2]$ favoring CH_2FCl. The ratio of the rate constants for CH_2F with Cl_2 and O_2 is determined to be 1.43 ± 0.13. Infrared analysis confirms the cross section of HC(O)F at 1850 cm^{-1} as (9.78 ± 0.12) x 10^{-19} cm^2 $molecule^{-1}$ and yields the first measurement of its absolute band intensities, which for the carbonyl stretching mode at 1780-1880 cm^{-1} is (3.55 ± 0.15) x 10^{-17} cm

molecule^{-1}. Anharmonic vibrational calculations for HC(O)F have been performed with CCSD(T)/aug-pVTZ theory, and the results show a match with the frequencies to within 3% and the major band intensities to within 5%. Transition State Theory calculations for the CH_3F + Cl reaction have been initiated for comparison with the observed rate constant and kinetic isotope effect.

RMRM 149

Entropy and enthalpy of the hemoglobin-fluoride complex redox reactions (Fe^{3+}/Fe^{2+}) at pH 5 reveal significant heme-pocket structural changes with temperature

***Kayla G. Flanders**, kf716170@sju.edu, Tanaka Mada, Jose Cerda. Saint Joseph's University, Philadelphia, Pennsylvania, United States*

In our most recent study, we utilized fluoride binding in hemoglobin (Hb) to measure the thermodynamic values such as enthalpy (D*H*) and entropy (D*S*) for the Fe^{3+}/Fe^{2+} redox change in Hb-F complexes and determined the reduction potentials (E_m) of the heme-bound fluoride complex of adult hemoglobin (Hb-F) as a function of pH. The midpoint potentials of the reduction (Fe^{3+}/Fe^{2+}) of Hb-F were measured at room temperature by using UV/vis spectroelectrochemistry, from pH 4.5 to pH 7. Our results show that the E_m of the Hb-F complex is about 80 mV (vs SHE) between pH 5.5 and pH 7. However, below pH 5.5 the E_m drops to a value of 53 mV (vs SHE) at pH 4.5. The drop in E_m is indicative of the stabilization of the oxidized state (Hb-F) upon lowering the pH. To further understand the thermodynamics of the Hb-F redox reactions, we measured the enthalpy (D*H*) and entropy (D*S*) of the reduction (Fe^{3+}/Fe^{2+}) of Hb-F at pH 7 and pH 5. A detailed study of the thermodynamics of the reduction revealed that the D*S* and D*H* at pH 7 were -108 J K^{-1} mol^{-1} and -40.0 kJ mol^{-1}, respectively. These were measured in the 5 ^oC to 40 ^oC temperature interval. In this same temperature range at pH 5, there is a flip in the entropy and enthalpy of (Fe^{3+}/Fe^{2+}) reduction. In the “high” temperature range, 17 ^oC to 40 ^oC, the measured D*S* and D*H* at pH 5 were -120 J K^{-1} mol^{-1} and -43.0 kJ mol^{-1}, respectively. However, in the “low” temperature range, 5 ^oC to 17 ^oC, the measured D*S* and D*H* at pH 5 were +90 J K^{-1} mol^{-1} and +18.0 kJ mol^{-1}, respectively. The perpendicularity of the temperature dependency at pH 5 of the “low” temperature, relative to that of the “high” temperature range, is peculiar. The D*G* of the heme reduction (Fe^{3+}/Fe^{2+}) for the Hb-F complex is -7.5 and -5.7 kJ mol^{-1} at 5 and 40 ^oC, respectively. While the free energy change is less than 2 kJ mol^{-1} in this temperature range, the entropy and enthalpy changes of 210 J K^{-1} mol^{-1} and 60 kJ mol^{-1}, respectively, suggest significant

structural changes in the heme-pocket of the Hb-F complex below 17 ^{o}C. We are further investigating if the hydrogen bonding between the heme-bound fluoride and the distal His64 at pH 5, which is also responsible for effecting the reduction potential of the Hb-F complex, triggers this structural change. This study ultimately demonstrates that the use of fluoride binding in Hb has the potential of helping us understand the molecular mechanism of oxygen transport in Hb.

RMRM 150

Earth abundant transtion metal effects on methane concerted metalation-deprotonation, a DFT study

William M. Grumbles*, williamgrumbles@my.unt.edu, Kortney Melancon, Thomas R. Cundari. Department of Chemistry, University of North Texas, Denton, Texas, United States*

Methane activation and functionalization still poses a challenge to make this abundant alkane, the primary component of natural gas, into a more useful and economic resource. One possible method of methane activation is via the concerted metalation-deprotonation, CMD, pathway, which previously has been largely limited to heavy metals and functionalized substrates. In this DFT study, a CMD cycle is assessed by employing cheaper, more Earth-abundant transition metals, to see the effects of the metal and ligands on factors like C-H acidity and metal carbon bond strength and to understand how these impact the overall kinetics and thermodynamics of methane CMD.

RMRM 151

Crystallographcially observed mechanistic conversion of lanthanide nitrates by hexamethylenetetramine (HMTA) to ceramic oxide materials

Paris C. Reuel[1,2]*, reuelparis@gmail.com, Timothy J. Boyle*[1]*, Roger E. Cramer*[3]*. (1) Sandia National Laboratories, Albuquerque, New Mexico, United States (2) University of New Mexico, Albuquerque, New Mexico, United States (3) University of Hawai'i at Manoa, Honolulu, Hawaii, United States*

The ability to generate large scaled (>100 g) of nanomaterials is a continuing problem. We are interested in the production of lanthanide oxide nanomaterials in a silica matrix, as a potential electromagnetic performance enhancer in high temperature materials. As can be imagined, a large amount of nanomaterial in the silica will be necessary to coat devices. The reported reduction of cerium

nitrates using hexamethylenetetramine (HMTA) to its oxide appeared a reasonable route. Due to the unique nature of cerium having the 3+/4+ oxidation state, it was of interest to explore the remainder of the lanthanide series. As the mechanism is not reported, it was of interest to determine the various stages available to the lanthanide nitrates during this reaction. Therefore, a crystallographic study involving varied molar equivalencies of *n* HMTA to $Ln(NO_3)_3 \bullet 6H_2O$ (n = 1,2,3) revealed the denitrification mechanism of this reaction through the isolation and characterization of the various stable intermediates: $[La(k^2\text{-}NO_3)_2(k^1\text{-}NO_3)(H_2O)_4]$ ●HMTA, $[Ln(k^2\text{-}NO_3)_3(H_2O)_4]$ ●HMTA ●H_2O, $[Ho(k^2\text{-}NO_3)_2(H_2O)_5]$ ●NO_3 ●HMTA, $[Ln(k^2\text{-}NO_3)_2(H_2O)_6]$ ●NO_3 ●HMTA ●$3H_2O$, $[Ln(k^2\text{-}NO_3)_3(H_2O)_4]$ ●3HMTA ●$2H_2O$, (H3O)[Ln(H2O)8]2[Ln(H2O)7(OH)] ●9NO3 ●6HMTA ●9H2O. Additional processing and calcination of the full system indicated additional lanthanide oxide material could readily be generated by this methodology as well. Details of the synthesis, the crystal structures, the nanomaterials generated, and the potential mechanism for this conversion will be presented at the Rocky Mountain Regional Meeting. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

RMRM 152

C-H activation of toluene by diruthenium nitride: DFT study

***Waad Alharbi**, waadalharbi@my.unt.edu, Thomas R. Cundari. Chemistry, University of North Texas, Denton, Texas, United States*

Two diruthenium-azide species are modelled to investigate nitrogen insertion into a C-H bond of toluene. Model 1 has four formate bridging ligands; Model 2 is larger and has benzoate bridging ligands. For each of these, three different mechanisms were studied. The first two mechanisms – amination – are achieved via hydrogen atom abstraction (HAA) of either a benzylic (sp^3) C-H or an aromatic (sp^2) C-H bond of toluene, followed by radical rebound (RR), yielding a new Csp3-N (benzylamine) or Csp2-N bond (para-toluidine), respectively. The third route studied – nitrene addition – first forms an aziridine-like intermediate, which is followed by a hydrogen transfer to produce the same Csp2-N bond para-toluidine as the sp^2 C-H amination route. Toluene's reactivity with Ru_2N intermediates was accomplished from analysis of geometric features and free energy calculations and shows that a benzylic C-H amination via

HAA/RR route is the most favorable route kinetically among the three activation pathways studied.

RMRM 153

Density functional study of methane activation by frustrated Lewis pairs with Group 13 trihalides and Group 15 pentahalides and a machine learning analysis of their barrier heights

***Ignacio Migliaro**, ignaciomigliaro@my.unt.edu, Thomas R. Cundari. Chemistry, University of North Texas, Denton, Texas, United States*

Frustrated Lewis pairs (FLP) are an important advancement in metal-free catalysis. FLPs activate a variety of small molecules, notably dihydrogen. Methane activation, however, has not been reported despite it being an abundant chemical feedstock. DFT calculations were utilized to elucidate the reaction mechanism of methane activation by triel trihalide and pnictogen pentahalide-ammonia Lewis pairs. Two reaction mechanisms were modelled for methane activation: proton abstraction and hydride abstraction. In all cases, deprotonation was thermodynamically and kinetically favored versus hydride abstraction. The use of heavier pnictogens and bigger triels were calculated to be more favorable for the activation of methane. To discern factors affecting the activation energies, different descriptors were correlated – ground state thermodynamics, orbital energies, transition state strain energies, *etc*. - but no consistent patterns were identified. Thus, machine learning methods were used to correlate ground state parameters to barrier heights. A neural network was used to correlate ground state descriptors (global electrophilicity index, bond dissociation energies, reaction energies) to activation free energies (R^2 = 0.90).

RMRM 154

Supported palladium catalysts for selective hydrogenation of ethyl phenylpropiolate

***Dylan Knight**, dknight3@leomail.tamuc.edu, **Benjamin Santoyo**, bsantoyo@leomail.tamuc.edu, Jordan Whelchel, Syed Hussaini, Ben Jang. Chemistry, Texas A and M university-Commerce, Commerce, Texas, United States*

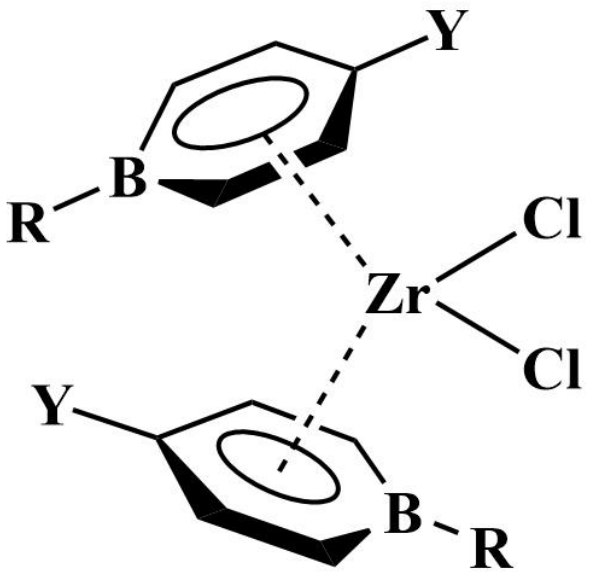
The semi-hydrogenation of alkynes to alkenes is an important transformation that is followed by both fine chemical and pharmaceutical industries, and thus the catalysts that specialize in such conversions are highly demanded. In this paper, the investigation focuses on the effects of pretreatments such as non-thermal DBD plasma and hydrogen reduction on supported palladium and palladium-ceria for liquid-phase semi-hydrogenation of ethyl phenylpropiolate in methanol at room temperature. The current results from different reduction temperatures show that the activity order is 400°C ~ 500°C > 300°C > 600°C while the selectivity order is 600°C > 500°C ~ 300°C > 400°C. Overall, with 500°C reduction, its yield of cis ethyl cinnamate is the highest of 90.9% at 30-min.
It is interesting that the reduction temperature has a very critical impact on the performance of the catalyst, likely due to the properties of the formed PdCeOx solid solution after reduction. The detailed surface and bulk properties of PdCeOx will be investigated with in-situ FTIR, pulse chemisorption and temperature programmed techniques.

RMRM 155

Olefin polymerization by zirconium boratabenzene catalysts

Carly Carter[1]*, carlycarter@my.unt.edu, Thomas R. Cundari*[1]*, George Rodriguez*[2]*. (1) University of North Texas, Denton, Texas, United States (2) ExxonMobil Baytown Technology and Engineering Complex, Baytown, Texas, United States*

In the present quantum chemical study, a-olefin dimerization and trimerization by zirconium boratabenzene catalysts has been studied as the single site reactivity of Group 4 metallocene catalysts has proven to be industrially important. The thermodynamics and kinetics of C=C insertion for ethylene, 1-butene, and 1-hexene as well as relevant b-H elimination barriers have been quantified using density functional theory, using methodology previously calibrated in earlier research by the UNT and EMCC team for bis-indenyl zirconium catalysts. The insertions of the alkenes are relevant to chain growth processes, while the b-H eliminations model chain termination. Various substituents on the boratabenzene rings were also compared to determine how these ligands change the behavior of the thermodynamics and kinetics of the insertion and chain termination steps.



Boratobenzene precatalysts ($Bt_2Zr^{IV}Cl_2$) modeled in this research. Y = H, ^{t}Bu; R= phenyl, N(^{i}Pr)$_2$. **1:** Y = H, R = phenyl; **2:** Y = H, R = N^{i}Pr$_2$; **3:** Y = ^{t}Bu, R = phenyl; **4** Y=^{t}Bu, R = N^{i}Pr$_2$. The active species is assumed to be a cationic mono-methyl complex.

RMRM 156

Opening the $Co^{III,IV}_2$(m-O)$_2$ diamond core by Lewis bases leads to enhanced C–H bond cleaving reactivity

*Yan Li[2], **Suhashini Handunneththige**[1], suhashi@nmsu.edu, Jin Xiong[3], Yisong Guo[3], Marat Talipov[1], Wang Dong[2]. (1) Chemistry and biochemistry, New Mexico State University, Las Cruces, New Mexico, United States (2) Chemistry and biochemistry, University of Montana System, Missoula, Montana, United States (3) Chemistry and biochemistry, Carnegie Mellon University, Pittsburgh, Pennsylvania, United States*

In many biological and synthetic processes, activation of strong sp^3 C–H bonds is a key step in functionalizing inert hydrocarbons. In nature these C-H bond activation reactions are carried out by metalloenzymes containing Fe or Cu metal centers. One such example is soluble methane monooxygenase (sMMO) enzyme containing a high-valent Fe^{IV}_2(m-O)$_2$ “diamond core” complex (intermediate **Q**). Recently there have been studies claiming this intermediate **Q** has an open-core structure. However, synthetic models mimicking C-H bond hydroxylation of sMMO-Q have displayed limited reactivity.

In a previous study we have described a high-valent Co diamond core complex, $Co^{III,IV}_2(m\text{-}O)_2$ (**1**) supported by tetradentate tris(2-pyridylmethyl)amine (TPA) ligand, showing remarkable C-H bond activation ability. Here we are improving the C-H bond activation reactivity of **1** by introducing a Lewis base X, which leads to the formation of open-core species $X–Co^{III}–O–Co^{IV}–O$ (**1-X**). Compared to **1**, this novel **1-X** complex demonstrates higher kinetic rate constants and has the ability to cleave stronger C-H bonds. Characterization of **1-X** is done using DFT calculations and EPR studies. According to DFT studies while **1** has a diamond core structure, **1-X** has an open-core configuration. DFT optimization provided stable low-spin ground states for both **1** and **1-X,** with two structural isomers (i.e. *cis* vs *trans*) where *trans* isomer is the most stable configuration. Spin density plots demonstrates complex **1** is a mixed valence delocalized system, while unpaired electron in **1-X** is delocalized on Co^{IV}–O unit with a partial radical character on terminal oxygen. Calculations show that **1-X** has a stronger oxidation ability compared to **1** both kinetically and thermodynamically, since **1-X** has a higher thermodynamic driving force and a lower activation barrier to carry out hydron atom transfer reactions. According to EPR studies**,** both **1** and **1-X** are EPR active species with $S = 1/2$ signals where EPR signal shown by **1-X** is clearly different from that of **1**. Remarkably, kinetics studies for ethylbenzene oxidation using **1-X** shows a million-fold rate enhancement compared to **1** with the ability to cleave stronger C–H bonds up to 96 kcal/mol. Furthermore, when compared with its diiron analogs, **1-X** is more reactive by about four orders of magnitude. These insights suggest that diamond core isomerization is a possible enzymatic strategy employed by sMMO-**Q** in order to activate highly C-H bonds in various substrates**.**

RMRM 157

Utility of cyanophenylalanine derviates as spectroscopic probes

*Austin J. Haider, Lucy Metzroth, Andrew M. Zerwekh, Roman J. Martinez, **Joshua P. Martin**, jmart490@msudenver.edu. Department of Chemistry and Biochemistry, Metropolitan State University of Denver, Denver, Colorado, United States*

We report photophysical studies of 2-cyanophenylalanine and 3-cyanophenylalanine used as both spectroscopic reporters of the local solvent environment and site-specific probes within peptides. Absorption of an ultraviolet photon by a cyanophenylalanine derivative results in a $\pi^* \leftarrow \pi$ transition with a molar absorptivity similar to common biological probes, such as tyrosine and tryptophan, and a factor four larger than phenylalanine. Due to

intermolecular interactions with the nitrile group on the chromophores, the local solvent environment can be monitored by changes in the quantum yield of the $S_1 \leftarrow S_0$ transition. Fluorescence quenching of the fluorophores with biologically relevant anions results in Stern-Volmer constants that depend on the position of the nitrile group on the phenylalanine ring. As a site-specific probe, 2-cyanophenylalanine can be paired with tryptophan to perform Forster Resonance Energy Transfer (FRET) experiments with an R_0 of 15 Å and only slight perturbation of the native geometries of peptides. Incorporation of 2-cyanophenylalanine at two locations in olfactory peptides where tryptophan occupies the N-terminus provides a model system for spectroscopic reporting of structural dynamics. Measurement of the FRET efficiency within various solvent environments that either promote or inhibit secondary structures of these peptides results in the determination of the distance between the intrinsic probes. Comparison of computational calculations of the electronic structure with experimental results further demonstrate the utility of cyanophenylalanine derivatives as spectroscopic reporters of peptide structure and dynamics in various solvent environments.

RMRM 158

Hybrid additive manufacturing of poly(caprolactone)-modified bone-ligament composite scaffolds for interface tissue engineering

***Orion Sanchez**, orionedward97@gmail.com, Lorraine Mottishaw, Christina Salas, Christopher Buska, Matthew Rush. University of New Mexico, Albuquerque, New Mexico, United States*

Ligament reconstruction due to damage currently results in a 26% incidence of re-injury as a result of a failure to recapitulate the complex biomechanical bone-ligament interface. To overcome these limitations, 3D bioprinting (3DBP) aims to replicate the bone-ligament interface using polymer-based solutions optimized to match the structural competency needed for bone and ligament tissue regeneration. Using near-field electrospinning (NFE) to produce highly aligned tensile resistant fibers for ligament regeneration, we have demonstrated the ability to fabricate complex composite scaffolds with fully integrated bone and ligament phases. This study focuses on the optimization of the biochemical and biomechanical properties of each distinct phase of the composite scaffolds. Printing parameters (extrusion rate, voltage, and print speed) as a function of viscosity and solvent evaporation were used to optimize scaffold features and mechanical strength to match the corresponding tissue phase. When compared, the tensile strength of a 0-45° biaxial fiber configurations (11.09 ± 3.10MPa) was better suited to match the strength of native ligament (20MPa)

over 0° uniaxial and 0-90° biaxial configurations. Furthermore, cell viability (LIVE/DEAD) on 3DBP 25 MPa and NFE scaffolds and immunocytoskeletal staining indicate biocompatibility of scaffolds with the ability to direct cell alignment and growth.

RMRM 159

Indium phosphide quantum dots activated by near-infrared light: A novel treatment for drug-resistant bacterial infection

Colleen McCollum[1]*, colleen.mccollum@colorado.edu, John Bertram*[3,2]*, Prashant Nagpal*[1,2]*, Anushree Chatterjee*[1]*. (1) Chemical and Biological Engineering, University of Colorado Boulder, University of Colorado Boulder, Boulder, CO, US, academic, Boulder, Colorado, United States (2) Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, Colorado, United States (3) Material Science and Engineering, University of Colorado Boulder, Boulder, Colorado, United States*

Drug-resistant bacterial infections are a growing cause of illness and death globally. Current methods of treatment are not only proving less effective, but also perpetuate evolution of new resistance. Here, we propose a new methodology to allow for the treatment of drug-resistant bacterial infection while limiting the occurrence of new resistance. We have developed semiconductor nanoparticles, called quantum dots (QDs), that can be activated by light to specifically and effectively kill drug-resistant bacteria isolated from clinical patient samples. Upon photoactivation, our QDs produce superoxide, without the generation of other reactive oxygen species. Superoxide targets iron-sulfur clusters in bacteria, depleting their store of iron, triggering DNA damage by iron atom release, and disrupting pathways necessary for survival. We have previously shown that this specific generation of superoxide allows for killing of bacterial cells without causing toxicity to surrounding mammalian cells *in vitro*. Our QDs show great promise as a novel antimicrobial therapy. Indium phosphide (InP) QDs injected subcutaneously into mice caused no measured toxicity to the host animal after six consecutive days of treatment. InP QDs are activated by near-infrared (NIR) light, which was provided to the injection site using high-intensity LEDs. NIR light also has the added benefit of being invisible to the murine eye, allowing for constant, high-intensity light exposure without affecting murine circadian rhythms. Toxicity was measured through body weight, organ histology, and inflammation and oxidative stress markers in serum, and no significant, dose-dependent effects were observed. We then used InP QDs to treat subcutaneous abscesses of human clinical isolate *Escherichia coli* in mice. As NIR light falls within the window of optical

transparency for skin and tissue, QDs injected under the skin were sufficiently activated for bacterial killing. We observed a trend of decreasing bacterial count by QD dosages of 2 and 4 μM compared to PBS treatment. A greater than 30-fold drop in average abscess colony-forming units was observed in mice treated with 4 μM QDs compared to PBS control. Unlike currently available antibiotic treatments, our quantum dots offer a completely novel approach that could revolutionize last-resort treatments of burn and wound infections, with the potential to be expanded to other infection types such as respiratory infection, sepsis, and urinary tract infection.

RMRM 160

Utilizing multi-angle light scattering to count biological particles

Christine Plavchak[1]*, plavchakcl@gmail.com, Allison Z. Werner*[2]*, Gregg Beckham*[2]*, Kim R. Williams*[1]*. (1) Chemistry, Colorado School of Mines, Golden, Colorado, United States (2) Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, Colorado, United States*

Biological nanoparticles include lipoproteins, liposomes, protein aggregates, viruses, and extracellular vesicles/outer membrane vesicles (OMVs). Ranging in size from 1-1000 nm, these particles have important roles in fields as diverse as health and sustainability. Quantitation of lipoprotein subclasses is used to diagnose heart disease while OMV enumeration is essential to understanding their efficacy and the impact of biochemical heterogeneity in biopolymer degradation. Bioparticle counting is still a developing field where current techniques such as flow cytometry, Coulter counter, or NTA lack either the sensitivity to count particles below 500 nm in diameter and/or cannot address polydisperse populations. To overcome this, we must look beyond approaches that provide only average values. Asymmetrical flow field-flow fractionation (AF4) is a sized-based separation technique that is utilized for particles that span 1 - 1000 nm in diameter when utilizing the normal mode separation mechanism. AF4 coupled to multi-angle light scattering (MALS) provides the separation needed to produce the more monodisperse size subpopulations required for accurate size and count distributions by MALS. Recent work with AF4-MALS has shown successful enumeration of virus particles and colloids in solution by measuring the amount of scattered light from the particles and known information on particle shape and refractive index to calculate a particle count. While promising, separation and enumeration using AF4-MALS for OMVs has yet to be extensively studied because compositional information of OMVs (i.e., starting masses and

refractive indices) is difficult to measure. This work utilizes liposome standards as OMV surrogates to better understand how light scattering intensity for particles of a known size and concentration translate into particle counts. Relative particle counts (10^9-10^{11} particles/mL) have been established for two AF4-separated OMV populations (50-150 and 200-500 nm) using calibration curves of surrogate particles. The method described here has the capability to examine not only other biological systems but also inorganic and polymeric systems where particle quantification is needed.

RMRM 161

Effects on membrane oxygen permeability due to lipid changes in breast cancer

***Qi Wang**, qi.wang@student.nmt.edu, Sally Pias. Chemistry, New Mexico Institute of Mining and Technology, Socorro, New Mexico, United States*

The proliferation of tumor cells relies on upregulated lipid biosynthesis and hypoxic conditions, resulting in abnormal levels of *de novo* (“new”) lipids and low levels of intracellular oxygen (O_2). Breast cancer cells have been observed to have high levels of 14:0 myristoyl (M) phospholipid tail, which is two carbons shorter than the predominant 16:0 palmitoyl (P) phospholipid tail, and 16:1 palmitoleoyl (Y) phospholipid tail, which is also two carbons shorter than the predominant 18:1 oleoyl (O) phospholipid tail. Y and O tails are the most common lipid tails in normal breast cells. We hypothesized that lipid bilayers rich in *de novo* lipids would show reduced oxygen (O_2) permeability, due to physical effects of the altered chain lengths, which might be related to breast tumor hypoxia. To investigate this effect, atomic resolution molecular dynamics simulations were used to test a variety of chain lengths. From the simulations, we have estimated the permeability of the *de novo* lipid biosynthesis product 1-palmitoyl,2-palmitoleoylphosphatidylcholine (PYPC) to be 9.7 ± 0.5 cm/s at 37°C, compared with a higher permeability of 16.5 ± 0.6 cm/s for the “normal” phospholipid 1-palmitoyl,2-oleoylphosphatidylcholine (POPC). However, we have estimated the permeability of the *de novo* lipid 1-myristoyl,2-oleoylphosphatidylcholine (MOPC) to be higher than POPC, at 18.1 ± 0.3 cm/s. The observed enhanced permeability of MOPC compared to POPC may be due to greater O_2 lipid solubility promoted by tail chain-length mismatch. We have yet to find a satisfactory explanation for the reduced permeability of PYPC, which also has chain-length mismatch. Lipid chain-length mismatch and lateral packing density may contribute to permeability changes. Investigation of chain-length effects in more complex membrane models will be required to understand the influence of *de novo* lipids on cellular oxygenation.

RMRM 162

Design and construction of a Brewster angle microscope

Seth Croslow *, croslowseth123@gmail.com, Kyle G. McLaughlin, Audra Goach. Chemistry, Monmouth College, Monmouth, Illinois, United States*

Brewster angle microscopy (BAM) is a valuable visualization technique, specifically when utilized with the Langmuir monolayer technique, which allows for the simplification of a 3D cellular membrane as a 2D monolayer. These two techniques allow for the study of the monolayer's interactions at the air-water interface and for the determination of properties of the monolayer including micro- and macroscopic phases and film thickness. Therefore, the addition of a BAM to a surface science group is very advantageous, though the high costs associated with its purchase may not be suitable for most small colleges. The solution to this problem is to create a BAM using commonly sourced optical and structural components and to build the BAM in-lab. Herein, the design and construction of a lab-built BAM is discussed.

RMRM 163

Effects of pH, conformation, and metal cations on insulin aggregation

Kyle G. McLaughlin[1]*, kmclaughlin@monmouthcollege.edu, Seth Croslow* [1]*, Steven P. Distin*[1]*, Cameron VanCleave*[2]*, Debbie C. Crans*[2]*, Audra Goach*[1]*. (1) Chemistry, Monmouth College, Monmouth, Illinois, United States (2) Chemistry, Colorado State University, Fort Collins, Colorado, United States*

The Langmuir monolayer technique was utilized to distinguish between the three different conformations of the insulin hexamer. In the presence of various divalent metal cations, insulin aggregates into a hexameric conformation. The effects of zinc, copper, and vanadium were tested with insulin at physiological pH and temperature. Each metal cation was studied with the three conformations of insulin, T6, T3R3, and R6, to assess their effects on the conformation, aggregation, and interactions among insulin hexamers. Additionally, the effect of pH on the T3R3 hexamer conformation was studied for the zinc, copper, and vanadium hexamers at pH of 3.3, 5.3, and 7.4.

RMRM 164

Investigating morphology of mixed monolayers containing short-chain menaquinones with brewster angle microscopy

Cameron Van Cleave[1]*, camvc@colostate.edu, Allison Haase*[1]*, Benjamin J. Peters*[1]*, Jordan T. Koehn*[1]*, Dean C. Crick*[3,2]*, Debbie C. Crans*[1,2]*. (1) Chemistry, Colorado State University, Fort Collins, Colorado, United States (2) Cell and Molecular Biology Program, Colorado State University, Fort Collins, Colorado, United States (3) Microbiology, Immunology, and Pathology, Colorado State University, Fort Collins, Colorado, United States*

Menaquinones (MK) are hydrophobic lipoquinones consisting of a naphthoquinone headgroup and an isoprenyl sidechain of varying length. MKs often function as electron transport molecules in some bacteria species. As such, they are affiliated with the cell membrane. Surprisingly, little is known about how these molecules affect the membrane itself and what role different structural components play. We have previously used Langmuir monolayers to investigate the effects MKs on the area and surface pressure of model membranes during compression, but this technique does not give clear information on morphology. In this study, we utilize Brewster angle microscopy to visualize Langmuir monolayers consisting of varying mol fractions of MKs and phospholipids. It was found that MKs can disrupt lipid packing at low surface pressures, which is in agreement with previous work.

RMRM 165

Stand up to stand out: Self-advocacy for the reluctant

Susan Morris*, susan@susanmorriscoaching.com. Coaching, Susan Morris Coaching, Doylestown, Pennsylvania, United States*

Many talented scientists and technical professionals abide by the myth that it's unbecoming to talk about their accomplishment. Often heard is this career limiting belief: my good work should speak for itself. This disinclination among STEM women to self-promote has far-reaching consequences. Reluctance to self-advocate can affect getting promotions, negotiations on work schedules, salary and being considered for high visibility assignments. The purpose of this workshop is to uncover the benefits of advocating for oneself and explore alternative behaviors to bragging and boasting. Participants learn to teach and educate others about their accomplishments, tell their story of triumph and most

importantly, practice asking for a deserved promotion or getting recognition of a job well done.

RMRM 166

How to convince others (that safety is important and that you're serious about it)

***James A. Kaufman**, jim@labsafety.org. The Laboratory Safety Institute (LSI), Natick, Massachusetts, United States*

Throughout the world, this is the most frequently asked question. The answer is simple and, for the most part, inexpensive. The short answer is to create a more effective lab safety program.

This interesting and entertaining one-hour presentation provides an overview of some of 33 critical program elements. It confronts one of the more common excuses for not having or improving the lab safety program ... "it costs too much." This is simply not true. Excellent lab safety programs do not need to cost large amounts of money.

Participants learn how to convince others by creating a more effective lab safety program (without a purchase order or requisition). You don't want to miss this opportunity for a highly informative, worthwhile and enjoyable learning experience.

Here's a unique opportunity to take a look at your lab safety program to see how you're doing and how you can do it even better. The participants will receive the Laboratory Safety Institute's (LSI) lab safety program review checklist with 33 components. You will learn how to use this checklist to evaluate your program both qualitatively and quantitatively. The result is a simple, clear, low/no cost path for lab safety program development and improvement. And, with courage, you can score your program on a scale of zero to 100!

RMRM 167

Spotlight on the laboratory safety team workshops

***Jessica A. Martin**, jessica.a.martin@uconn.edu. Chemistry, University of Connecticut, Storrs, Connecticut, United States*

In the following presentation the graduate student and postdoctoral fellow initiated movement for workshops on “Safety” in academic and industrial environments is described. The laboratory safety team (LST) movement was triggered in 2012 by Dow Chemical’s exploration of ways to strengthen academic research safety culture from the bottom up. This necessitated a new form of leadership from graduate students and postdoctoral scholars. This movement has been spreading throughout chemistry and engineering academic research departments in the United States in a grassroots fashion. However, little information is available providing the details of LST structure and activities. In this presentation, the workshop is described and results from interviews with 16 currently active teams and outline a best practices guide for starting and sustaining LST programs.

RMRM 168

Chemical business networking with SCHB

***Joseph E. Sabol**, jsabol@chem-consult.com, George W. Ruger, Jim Skinner, Abhishek Kantak, David J. Deutsch, Jennifer L. Maclachlan. ACS Division of Small Chemical Businesses, Modena, New York, United States*

SCHB organizes informative and collaborative entrepreneurial themed symposia, programs, and other events at ACS national, regional, and local section meetings. Entrepreneurs Tool Kit is SCHB's flagship program that showcases best practices and resources from the perspective of business-minded chemists. SCHB partners with other ACS technical divisions and committees on thematic and other critical and contemporary topics that are of high interest to the chemistry enterprise. SCHB provides valuable member-only content, including deeply discounted expo booth space at national meetings, and, most of all, a strong network of members from whom you can draw on for inspiration and to conduct business.

RMRM 169

South Dakota mines ACS student chapter: Promoting green chemistry concepts through outreach demonstrations and hands-on activities

***Karen Ly**, Karen.Ly@mines.sdsmt.edu, **Lily C. Cutler**, lily.cutler@mines.sdsmt.edu, Kevin D. Barz. Chemistry, South Dakota School of Mines and Technology, Rapid City, South Dakota, United States*

The South Dakota Mines ACS student chapter is the leading ACS group in western South Dakota and is part of the Sioux Valley Local Section. Our major successes include increasing student membership, providing professional development activities, hosting social events, and continuing our tradition of chemistry outreach to elementary and middle schools in the Black Hills and Pine Ridge Reservation area. Our small, but dedicated group of students independently work and commit many hours to ensure that such events are possible. To maintain student membership, we hosted several social events to encourage social interaction between new and old members. The South Dakota Mines ACS student chapter strives to increase awareness of and promote the teachings of Green Chemistry. To do this, we organized workshops where students participated in hands-on experiments and saw our chemistry demonstrations. These hands-on activities and chemistry demonstrations showcased many of the principles of Green Chemistry such as, using

renewable feedstocks, using natural/non-toxic catalysts, and using non-hazardous reagents in our experiments. These workshops prepare elementary and middle school students to be responsible future citizens who will, hopefully, affect their local communities and society as a whole in a sustainable manner.

RMRM 170

Exploring environmentally sensitive benzothiadiazoles and their uses

Caroline Warner, cchow@iastate.edu. Sean Norris[a], Dr. Bryan Lampkin[a], Paige Bouc[a], Andrea Thooft[a], Dr. John Lukesh[b], S. Israel Suarez[b], Heather Brown-Harding[b] Brett VanVeller[a] *Chemistry, Iowa State University[a], Ames, Iowa and Wakeforest University[b], Winston-Salem, North Carolina, United States*

The benzoxadiazole scaffold has been of increasing interest due to its solvent specific emissive properties and variability of its photophysical properties. The effect of substitution of electron donating groups and withdrawing groups at the 4,7-positions have been extensively studied, but the effects of the diazole ring have not. This talk will discuss the synthesis of a series of derivatives that allow the exploration of each component of the benzoxa(thia)diazole moiety and how it affects the photophysical properties. Finally, an application of a benzothiadiazole derivative used as a lipid dye will be introduced.