Mark Your Calendars and Save the Date!!

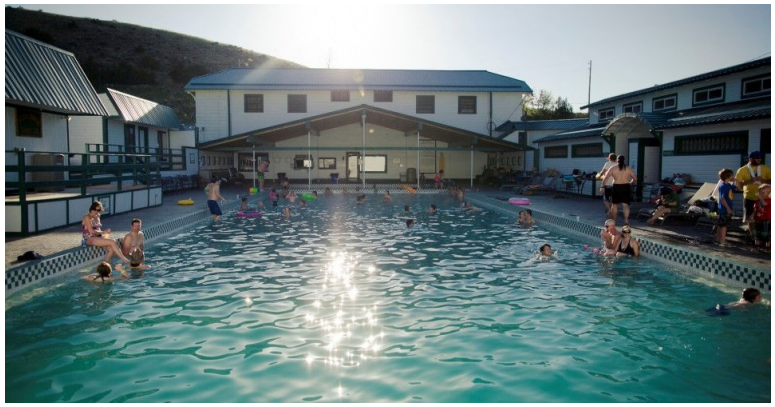
Montana Section ACS…

Spring Meeting 2018— April 6-7, 2018

Location: tba

Fall Meeting & Social 2018

October 12-14, 2018 at Chico Hot Springs



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ACS Chemistry for Life™

2017 Montana ACS Fall Meeting & Social

October 7-8, 2017

Fairmont Hot Springs Resort

Anaconda, MT

MONTANA SECTION

Meeting Schedule of Events

Friday, October 6th

Afternoon/Evening Arrival/Registration & Check-In

Saturday, October 7th

8:00 – 9:00 am Breakfast in Main meeting room

8:00 – 9:30 am Registration and Check-In

Undergraduate and Graduate Research Presentations (oral)

10:00 am Casey J. Massena, University of Montana

10:20 am Heather Cox, Flathead Valley Community College

10:40 am Haotian Lei, University of Montana

11:00 am Harrison W. VanKoten, Montana State University

11:20 am Evan McManigal, University of Montana

11:40 am Garrett Moraski, MSU Research Scientist

"Medicinal chemistry at MSU: Discovery and development of Anti-Tuberculosis Agents"

12:00 – 1:00 pm Lunch (on your own)

2:30-5:30 Beer/Wine Social

4:00-5:00 Undergraduate Poster Session

5:30 Dinner

Following dinner:

State of the Section Address & **Travel Awards Presentation** – Dr. John W. Hartman, 2017 Chair

Keynote Speaker – Dr. Nicholas R. Natale, 2017 ACS Fellow and Professor of Medicinal Chemistry - U.M.

Please join us all poolside after the conclusion of the evening and keynote presentation for more socializing and networking!!

Sunday, October 8th

8:00-9:30 Breakfast Buffet in Main Dining Room

9:00-11:30 Local Montana ACS section board and business meeting
Nominations for 2018 Section Secretary and Chair-Elect

Upcoming National and Regional Meetings…

255th ACS National Meeting & Exposition

"Nexus of Food, Energy & Water"

March 18-22, 2018 New Orleans, LA

Northwest Regional Meeting (NORM) 2018

June 24 – 27, 2016 Richland, WA

Montana Section email address:

MontanaSectionACS@gmail.com

Montana Section Website:

http://montana.sites.acs.org/

Montana Section Facebook page:

https://www.facebook.com/Montana-ACS-275145155836505/

Excerpts from Montana Section ACS Bylaws…

BYLAW V. Officers, Executive Committee, and Councilors

Section 1. The officers of the Section shall be members of the SOCIETY and the Section and shall consist of the Chair, Chair-Elect, Secretary, and Treasurer. The Secretary and Treasurer positions may be held by the same person.

Section 4. The duties of the officers shall be such as usually pertain to their offices, together with those required by these bylaws and by the Constitution and Bylaws of the SOCIETY, and such other duties as may be assigned to them from time to time by the Executive Committee.

a. The duties of the Chair shall be to preside at meetings of the Executive Committee, to carry into effect the decisions and recommendations of that Committee, to preside at meetings of the Section to conduct governance business, to appoint, with the approval of the Executive Committee, all committee chairs and committee members except as stated elsewhere in these bylaws, and to carry out the duties required by the Constitution and Bylaws of the SOCIETY.

b. The duties of the Chair-Elect shall be to assist the Chair with the direction and management of the Section. In the absence of the Chair, the duties of the office shall devolve upon the Chair-Elect.

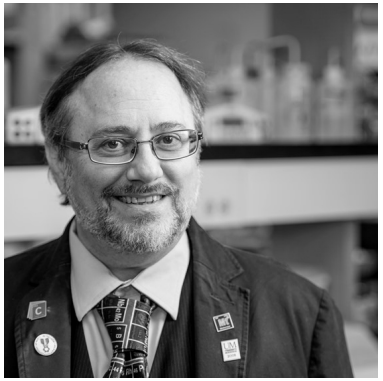
c. The duties of the Secretary shall be to keep a record of the minutes of the meetings of the Section and of the Executive Committee, to maintain a list of members and affiliates, to send to members and affiliates such notices as the business of the Section may require, to submit a report to the Section at its annual meeting, and to carry out the duties required by the Constitution and Bylaws of the SOCIETY and elsewhere in these bylaws. The Secretary shall preside over meetings in the absence of both the Chair and Chair-Elect.

d. The Treasurer shall have charge of the funds of the Section, keep an accurate record of all receipts and disbursements, receive dues, and make those disbursements approved by the Executive Committee. The Treasurer shall render an account of all transactions and of the financial condition of the Section to the Executive Committee at times set by the Committee, and shall submit such reports as are required by the Constitution and Bylaws of the SOCIETY.

Keynote Presentation:

Dr. Nicholas R. Natale

2017 ACS Fellow &
Professor of Medicinal Chemistry
University of Montana, Missoula



Nicholas R. Natale received his B.S. in Chemistry (1976), and his Ph.D. in Organic Chemistry (1979), at Drexel University in Philadelphia, under the guidance of mentor Professor Robert O. Hutchins. His research focused on synthetic methodology, and his dissertation was entitled "Trilogy of Molecular Transfiguration". He developed the first asymmetric synthesis of 4-aryl-dihydropyridines as a Postdoctoral Fellow at Colorado State University (1979-81) in the research group of Professor Albert I. Meyers. His first independent academic position was at the University of Idaho, where he rose through the ranks to Professor. He was recipient of the Idaho Academy of Science Distinguished Science Communicator Award in 2004. Nick received the 2007 American Chemical Society E. Ann Nalley Northwest Region Award for Volunteer Service. He was named Professor of Medicinal Chemistry in the Department of Biomedical and Pharmaceutical Sciences, at The University of Montana in 2007. He received the Mershon Award of the Montana Academy of Science in 2011. He has a total of over 500 publications, published abstracts, presentations at scientific meetings, and invited lectures, and was most recently selected as a 2017 Fellow of the American Chemical Society.

Student Presentations:

10:00 am A halogen bonding triple helicate: from napkin scribbles towards a synthetic anion channel

C. J. Massena, N. B. Wageling, D. A. Decato, J. Farnsworth, K. B. Hansen, and O. B. Berryman* (University of Montana)

What began as an idea, led to the synthesis and characterization of the first halogen bonding triple anion helicate to encapsulate iodide in solution and the solid state. Later, the self-assembly of its constituent phenylene ethynylene oligomers around other anions—bromide, chloride, and triiodide—was established in the same phases. Additionally, the thermodynamics and kinetics of helicate stability and anion exchange were measured, demonstrating high cohesion and long assembly lifetimes, as well as fast anion exchange kinetics. This versatility of guest inclusion and thermodynamic and kinetic analysis are unprecedented for anion helicates. Presently, we are working towards developing this prototypical anion helicate into a functional ion channel. Towards realizing a new class of halogen bonding pores that self-assemble in phospholipid bilayers and function as selective anion channels, we are conducting log P, liposome partitioning, and perforated patch clamp experiments. This fundamental work has high relevance for the study of channelopathy-related diseases like cystic fibrosis, and the development of antibiotics and chemotherapeutics.

Evening Poster Presentations…

Imidazo[1,2-a]pyridine-3-carboxyamides: A "Dual Threat" Against Mycobacterium tuberculosis and Mycobacterium avium

Garrett C. Moraski, Yong Cheng, Jeffery S. Schorey, Sanghyun Cho, and Scott G. Franzblau (Montana State University)

Electrochemically-Induced Dimerization of 2-methylthiophene

Haley Meredith, Dr. John Rowley, and Nate Burman (Carroll College)

Method Development for the Analysis of PCB's in Fish

Marietta Stringer, Sara DeJournette, and Jesse Stine (Salish Kootenai College)

Synthesis of a family of conjugated carbazole derivatives for applications in OLED technology

Dr. Caroline Pharr and **Lauren Palys** (Carroll College)

Rate comparison Studies of Diels-Alder reactions with n6-ruthenium arene complexes versus free arene dienophiles

Pierce Fix, Inderbir Bains, and David M. Hitt (Carroll College)

Investigation of Membrane Curvature Dependency on Cytochrome c Binding to Cardiolipin

Ziqing Xie, Margaret Elmer-Dixon, and Bruce Bowler (University of Montana)

Mercury Methylating Bacteria in Flathead Lake

Felicia Blandov, Japhanna Burns, and Christina L. Rush Ph.D. (Salish Kootenai College)

11:20 am

Role of Trinuclear Carbonate in Amidoxime Uptake

Evan McManigal, Dan Decatto, and Orion Berryman*
(University of Montana)

Within seawater, the uranyl cation is complexed by carbonate — aided by its high concentration—forming very stable uranyl carbonate complexes. The main species present is the mono-metallic UO2(CO3)3, but another species is also present in the environment, a tris-uranyl carbonate complex, (UO2)3(CO3)6. This trimetallic species has been extensively characterized using various spectrophotometric techniques. While there have been several ligands that have been shown to selectively bind to the uranyl ion in aqueous solution, the amidoxime functional group has been the target for extensive solution and solid state studies involving the uranyl ion. It's ability to strongly and selectively bind to the uranyl ion has made it the main candidate in the attempt to better understand the binding properties of uranyl. While the stability and nature of the trimetallic complex is well understood, the role that the trimetallic complex plays in uranyl-amidoxime interaction has yet to be explored. By probing uranyl carbonate and amidoxime complexes in both the solid and solution, we are able to elucidate the role that this complex will play within uranyl-amidoxime coordination chemistry. Based on obtained solid state data and using heteronuclear NMR, luminescence, and fluorescence we are able to probe the interaction between the trimetallic complex and simple amidoxime molecules, we are better able to understand the role that these carbonate complexes play in uranyl coordination chemistry.

10:20 am **Optimization of 4-(Dimethylamino)chalcone Synthesis**

Heather Cox and Janice Alexander*
(Flathead Valley Community College)

By reacting the substituted benzaldehyde 4-(dimethylamino) benzaldehyde with acetophenone in aqueous base, an Aldol condensation reaction takes place to produce a chalcone. The chalcone product is analyzed through infrared (IR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, melting point determination, and gas chromatography-mass spectroscopy (GC-MS). The optimization of the 4-(dimethylamino)chalcone product will occur through the manipulation of reaction conditions and be dependant on the purity of the product, determined by the instrument analyses, and the yield.

10:40 am **Effects of humanizing mutations on the heme crevice loop of yeast iso-1-cytochrome**

Haotian Lei and Bruce Bowler*
(University of Montana)

Cytochrome c (Cytc) is a small, globular protein within the inner mitochondrial membrane that plays an important role in cellular energy production by facilitating electron transport. Upon release from the mitochondria, Cytc participates in initiation of the caspase cascade leading to apoptosis, or programmed cell death. On the inner mitochondria membrane, Cytc binds cardiolipin, leading to loss of Met80-heme ligation, enabling Cytc to function as a peroxidase capable of oxidizing cardiolipin. Cytc has decreased affinity for oxidized cardiolipin and therefore can dissociate from the membrane facilitating release from mitochondrial and propagation of apoptosis. In order for the heme coordination site to open for peroxidase activity, the highly evolutionally-conserved heme crevice loop must undergo dynamic movement similar to the alkaline conformational transition. Unlike most residues in the heme crevice loop of Cytc, position 81, 83 evolves to more sterically demanding residues in higher eukaryotes. We hypothesize that a more sterically demanding residue at position 81, 83 would decrease the dynamics of the heme crevice loop and thus decrease peroxidase activity. By placing a alanine at position 81, and valine at position 83 in yeast iso-1-cytochrome c, we are able to make the yeast Cytc heme crevice loop more human-like. We observe the surprising result that this mutation stabilizes the native conformer at alkaline pH, but destabilizes it at acidic pH. As a result, the G83V mutation causes higher than wild type peroxidase activity at acidic pH and lower than wild type peroxidase activity at alkaline pH.

11:00 am **Synthesis and Biological Activity of Highly Cationic Dendrimer Antibiotics**

Harrison W. VanKoten, Wendy M. Dlakic, Robert Engel, Mary J. Cloninger * (Montana State University)

The development of pathogenic bacteria resistant to current treatments is a major issue facing the world today. Here, the synthesis and biological activity of fourth generation poly (amidoamine) dendrimers decorated with 1-hexadecyl-azoniabicylo[2.2.2]octane (C16-DABCO), a quaternary ammonium compound known to have antibacterial activity, are described. This highly cationic dendrimer antibiotic was tested against several Gram positive and Gram negative strains of pathogenic bacteria and exhibited activity against both. Higher activity towards Gram positive strains tested was observed. After the antimicrobial activity was assessed, E. coli and B. cereus were subjected to a resistance selection study. This study demonstrated that a multivalent approach to antimicrobial design significantly reduces the likelihood of developing bacterial resistance.