



# ISOTOPICS

The Cleveland Section of the American Chemical Society

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February 2017

## On Deck:

Monday 3/13/2017

MIM

Cleveland State University

## February Meeting Notice

Wednesday, February 15, 2017

Dolan Science Center

John Carroll University

1 John Carroll Blvd, University Heights

4:30 – 5:30 pm Executive Committee Meeting

5:30 – 6:15 pm Networking/social

6:15 – 7:00 pm Dinner

7:00 – 8:00 pm Presentation

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## Isotopics

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## “Evolutionary design of polymeric chemical structure”

*Dr. David Simmons*, Department of Polymer Engineering, University of Akron

One of the major challenges facing a new century of polymer science is the need for efficient strategies to design polymers with targeted material properties. This problem is particularly acute given the development over the last decade of facile strategies for synthesis of sequence-specific polymers. These polymers have the potential to offer properties meeting and exceeding those of natural sequence-specific polymers, such as proteins and DNA, that form the foundation for life. However, these chemistries pose an enormous chemical design challenge: even a binary sequence of 20 monomers has nearly half a million possible sequences; this search space rapidly becomes astronomical as the scale of the chain and number of possible constituents is increased. Nature has spent four billion years solving this design problem; how are we to do so nearly overnight? In this talk, I describe recent work in our group combining molecular simulation, artificial evolutionary algorithms, and machine learning to solve this type of chemical design problem. In particular, I describe application of this strategy to the design of model sequence-specific compatibilizers, which have the promise of reducing interfacial energies far more efficiently than non-sequence-specific polymeric surfactants.

The authors acknowledge the W. M. Keck Foundation for generous financial support of this research.

### DINNER RESERVATIONS REQUESTED:

Please RSVP to Dr. Mark Waner ([mwaner@jcu.edu](mailto:mwaner@jcu.edu)) with the names and # of people in your party by 5:00 pm on Thursday, February 9<sup>th</sup>. Dinner will be Lemon Rosemary Chicken, Shrimp Scampi, Vermicelli Pasta, Roasted Mushrooms, Mediterranean Salad, and Garlic Breadsticks. We take credit cards, checks to “Cleveland ACS”, or cash. The cost is \$20 for members and guests, \$10 for retirees or unemployed, and \$5 for students.

## **Directions and Parking**

Plan to enter campus at the main entrance off of Fairmount Circle (at Warrensville Center Rd.). The Dolan Science Center is the large building right inside the campus gate. Stop at the guard house and request a visitor parking pass. You can park in parking lots to the left or right of the building. The main entrances to the building are into the central atrium. We will meet in A202/203, which is a large conference room on the second level of the atrium. You can take the stairs in the atrium up to the second floor, or use the elevator located on the southeast side of the atrium.

<http://sites.jcu.edu/campus-maps/>

## **GO-CHEM Multi section retreat at Kalahari Resorts Feb. 24-25, 2017**

It is not too late to register for the GO-CHEM retreat at Kalahari on February 24-26<sup>th</sup>! Registration closes on February 17<sup>th</sup>. Information can be found at:

<https://www.eventbrite.com/e/go-chem-1st-annual-family-retreat-tickets-29754443341>

If you are interested in coming in for just the day on Saturday, you may do so by simply registering on EventBrite. If you want to stay overnight and get access to the water park (4 passes per room), there may still be rooms available at the discount rate even though the block of rooms reserved for this event has now been released to the public. To reserve a room, please contact Kalahari directly and refer to GO-CHEM Family Event Block (Booking ID 28191). Front Desk Reservations: 419-433-7759 or Toll Free 877-525-2427.

- People wishing to present a poster should contact Jim Zubricky ([James.Zubricky@utoledo.edu](mailto:James.Zubricky@utoledo.edu)).
- Students wishing to participate in the outreach activities should contact Lisa Ponton ([lponton@bw.edu](mailto:lponton@bw.edu)).

- If you have any questions about the event, please contact either Lisa Ponton or Jim Zubricky.

## **Weekend Agenda:**

Friday Feb. 24

6-8 pm Welcome Gathering

Saturday Feb. 25

10-11 Resume/Interview workshop

11-1 Poster session with lunch (posters available for viewing through dinner)

2-5 Outreach activities for guests of Kalahari

6-8 Dinner with Keynote speaker and awards presentation

Sunday Feb. 26

9-11 am Farewell Gathering

This event was made possible by generous donations from the Toledo, Cleveland, Columbus, Dayton, Cincinnati, Akron, Penn-Ohio Border, Northwest Central, and Upper Ohio Valley, local sections of the American Chemical Society, as well as a generous award from the ACS Local Section Committee's IPG Award Committee.

## **Call for Abstracts: Meeting-in-Miniature 2017**

Meeting-in-Miniature (MIM) of the Cleveland Section has become a much anticipated event in the calendar of many local graduate, undergraduate, postdoctoral and industrial researchers. Researchers find MIM to be a stepping stone for the presenting their work at the ACS Spring National Meeting that follows the MIM. MIM also provides a great opportunity for to network among the scientific community.

The 2017 MIM of will be held on Monday, March 13<sup>th</sup> at the Main Campus of Cleveland State University. Stemming from a strategic planning initiative, the of ACS Cleveland Section is on a mission to expand the breadth of chemistry research showcased at MIM 2017. Local area students from a number of community colleges, and researchers from area

industries will also be invited to present at this year's conference.

The half day program of MIM 2017 starting early afternoon will accommodate oral presentations of 15min and 5min questions by audience in each of its sections. Graduate and undergraduate presentations will be recognized with certificates and may be eligible for monetary awards. MIM 2017 will also include a Plenary Lecture, followed by dinner buffet.

Submission of abstracts is now open. The registration is free for this event. Please limit your abstract to 250 words and include names and affiliations of all authors. Abstracts should be submitted through the online submission system; <http://goo.gl/forms/EQCo7TRkXC>. The deadline for submission is Feb. 28<sup>th</sup>. For further information please contact Dr. David Ball, Chair - Department of Chemistry, Cleveland State University at [d.ball@csuohio.edu](mailto:d.ball@csuohio.edu).

### **Volunteering Opportunity: be a judge at NEOSEF this year!**

Every year, your ACS local section gives special awards to outstanding students in grades 7-12 who participate in the Chemistry Category at the Northeastern Ohio Science and Engineering Fair (NEOSEF). To select the award winners amongst ~100 projects, we need volunteer judges with a minimum of a Bachelor degree in Chemistry. Judging involves talking with the students, which is very rewarding. This year, NEOSEF is at John Carrol University March 7, 2017. The time commitment is a few hours in the afternoon (2:30 pm –6 :00 pm), If you are interested in judging, please contact Genevieve Sauve at [genevieve.sauve@case.edu](mailto:genevieve.sauve@case.edu).

### **Announcement: Training on Exporting Chemicals and Hazardous materials**

There is a training program coming up on Feb. 23<sup>rd</sup> on exporting chemicals and hazardous materials being offered by [Ohio SBDC-Export Assistance Network](#). They provide export assistance to small and medium-sized enterprises

(under 500 employees) in Northeast Ohio and helps to promote business growth through exporting and international trade. If you are interested in this training program, additional details can be found at: <https://www.csuohio.edu/business/global/reach>.

### **From ACS Discoveries: What's behind the durian fruit's notorious stench**

*Journal of Agricultural and Food Chemistry*

Most people who have tried durian either love it or hate it. The fruit's yellowish flesh is sweet and custard-like, but it comes with an overpowering stench of garbage. Scientists studying the unique fruit have now analyzed a set of 20 stinky and fruity chemical ingredients and found that a mere two compounds can re-create the overall smell. Their findings appear in ACS' *Journal of Agricultural and Food Chemistry*.

Native to southeast Asia – where the fruit is considered a delicacy, but also banned from some public spaces due to its odor — its appeal has spread to Westerners who relish trying distinct foods from around the world. Scientists interested in the fruit have identified several compounds that contribute to its smell, which has been said to reek of gym socks, garbage and rotting meat. Curious to better understand the complex scent, Martin Steinhaus and colleagues parsed the odor compounds further.

The researchers calculated the "odor activity values" of 19 of the durian's smelly compounds to see which ones were the most potent. Among the strongest were compounds that smelled of fruit, rotten onion and roasted onion. These were followed by chemicals with strong notes of cabbage and sulfur. Further experimentation found that putting just two specific compounds together — fruity ethyl (2S)-2-methylbutanoate and oniony 1-(ethylsulfanyl)ethanethiol — effectively resembled the fruit's entire set of odoriferous and fragrant compounds.