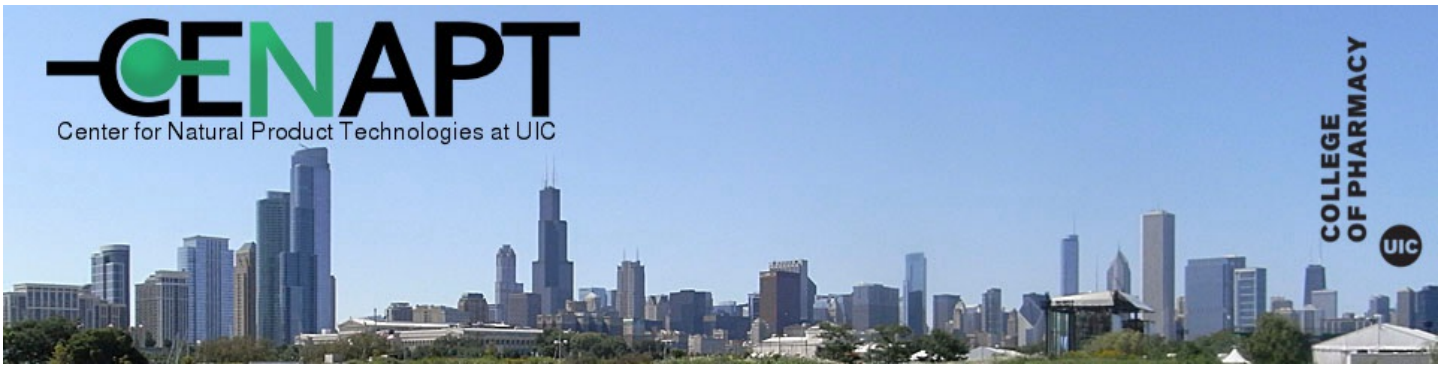

✍ The Lockdown Mass Spec Challenge Results

18 Aug, 2020
Tags: post news

What a better way to spend The Lockdown than to solve MS-MS spectra? The UIC Botanical Center and the CENAPT Center were pleased to organize The Lockdown Mass Spec Challenge. The Challenge followed the model used in the recent rounds of the CASMI contests. We provided a set of 16 MS and MS-MS spectra and asked participants to deduce the structure of compounds based on the provided data. The compounds were all derived from plants and include both known and unknown compounds. The unknown compounds were either unreported natural products or semi-synthetic analogs of known natural products. Metadata included origins of the compounds and chromatographic data were also provided. Participants could use any approach to arrive at the structures.

Follow-up wet sample challenge

We are considering organizing a ring trial in which participants will be provided a wet sample consisting of moderately complex mixture of natural products (25-35 compounds) and asked to identify compounds in the mixture. The objective of this trial would be to evaluate the current approaches for identification of natural products using mass spectrometry. If interested, please send a short email notice indicating your intent to participate as well as your willingness to contribute to the cost of shipping the sample. This notice is not binding but would help the organizers estimate the cost of running the trial, determine the workload and estimate the amount of sample necessary. Please, send the notice of interest to Dr. Dejan Nikolic at dnikol1@uic.edu.

Results

Participant	Affiliation	Correct answers (out of 16)	Correct answers (out of 20)
Team Adriano Rutz	Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Switzerland	6+1 (a)	8+1
Team Camila Crnkovic	São Carlos Institute of Chemistry, University of São Paulo, São Carlos, São Paulo, Brazil	5+1	6+1
Team Joelle Houriet	University of North Carolina at Greensboro, USA	5+1	N/A (b)
Samuel Bertrand	Groupe Mer, Molecules, Santé-EA 2160, UFR des Sciences Pharmaceutiques et Biologiques, Université de Nantes, France	4+1	N/A (b)

(a) One challenge in the contest was a publicly deposited spectrum that does not belong to the deposited structure. All participants reported the structure deposited in the database, thus that challenge was scored separately. **(b)** These participants did not submit answers to the four challenges that were added after initial announcement and per rules were not used for the final rankings.

Challenge information

All challenge data were acquired on a Waters SYNAPT quadrupole/time-of-flight mass spectrometer using electrospray ionization. Typical mass accuracy is ≤8 ppm in the MS mode and ~15 ppm or 2.0 mDa in the MS/MS mode. Some low intensity ions may have accuracies outside of these limits. Most compounds were analyzed using a generic LC method (Method A). Challenges analyzed with different methods are indicated; the corresponding methods are listed below. The flow rate was always 0.2 mL/min. Challenge 13 is a legacy spectrum for which no metadata data can be provided other than that the spectrum was acquired on a qTOF instrument. Details (including some background information, mode, collision energies, method and retention times) are given in the summary below.