

## 2016 ASMS Meeting (San Antonio)

### Metal Ions in Mass Spectrometry Interest Group Workshop (Monday, 5:45 - 7:00 pm)

Presiders: Alexandre A. Shvartsburg (Wichita State Univ.) and Cheng Lin (Boston Univ.)

Theme: Metal Cationization in MS/MS of Biomolecules

Approach: opening lecture by 2016 Biemann Medalist, Prof. Kristina Håkansson (12 min.) and five brief talks (9 min. each) focusing on different aspects of metal cationization in practical bioanalysis, followed by extensive discussion.

Estimated attendance: peak ~70, total ~80.

After a brief welcome from Alex, Cheng has kicked off the program:

- 1) Prof. Kristina Håkansson (Univ. of Michigan, Ann Arbor): “Metal ion adduction for improved utility of ExD”. She has presented several cases of ExD characterization of metal-adducted peptides and glycans and discussed how the fragmentation patterns vary depending on the peptide sequence and nature of metal charge carriers.
- 2) Prof. Robert Dunbar (Case Western Reserve Univ.): “Ni(II) peptide complexes: water changes the structure... or not”. This computational study has revealed that the propensity for charge-solvation vs. iminol binding of Ni<sup>2+</sup> to peptides depends on the chain length: an added water molecule significantly alters the complex structure for the tripeptide, but not tetrapeptide.
- 3) Prof. Igor Kaltashov (Univ. of Massachusetts, Amherst): “Can metals be used as ‘zero-interference’ protein tags in pharmacokinetic studies?”. Speaker has demonstrated metal-based quantification for metalloproteins, proteins that bind them, and His-tagged proteins.
- 4) Prof. Eric Dodds (Univ. of Nebraska, Lincoln): “Accessing alternative MS/MS pathways via metal cationization of carbohydrates and glycoconjugates”. Charge-reduced metal-adducted glycan isomers were shown to exhibit dramatically different energy-dependent fragmentation patterns, even when the original non-reduced species dissociate similarly.
- 5) Prof. Joseph Beckmann (Oregon State Univ.): “Localizing copper and zinc binding to mutant SOD in ALS-afflicted tissues”. Contrary to common belief, copper-containing compounds can halt the progression of ALS disease in lab mice. Recent results on the localization of metal binding site(s) by ECD in electromagnetostatic cells were also presented.
- 6) Dr. Laure Menin (EPFL, Switzerland): “MS.cheminfo.org: a free-access tool for analyzing complex HRMS data”. Complex MS patterns for stable isotopes of many metals challenge the data analysis. New open-access software described in this talk can assist MS and MS/MS analyses of diverse metal-containing compounds.

Participants have engaged the speakers with good questions. We have solicited nominations for the next group chair and topic suggestions for the oral and poster sessions and evening workshop.

#### Feedback

The opinions on workshop format were split. Some appreciated the short presentations, while others would prefer more interaction. We ended 15 min. over time, in part because of the late start due to equipment issues. One person suggested scheduling fewer presentations to manage the time better and allow more extensive discussion. We will seek to improve the timing and audience engagement next year.

The audience generally liked the presented topics. For the 2<sup>nd</sup> year, we have focused on the analytical utility of metal cationization of biomolecules. This shift of emphasis was deliberate in an effort to modernize the program, expand the attendance, and attract younger audience. A long-time group member has suggested revisiting the fundamental aspects of metal cationization at some point. That could possibly be achieved by shifting the emphasis in alternate years.

Alexandre Shvartsburg (co-chair for 2015 - 2016) and Cheng Lin (co-chair for 2016 - 2017)