

Workshop Report, ASMS Conference, St. Louis, MO

Metal ions in Mass Spectrometry Interest Group

Benjamin J. Bythell and Alexandre Shvartsburg, presiding

Monday, 5:45–7:00 pm

Approach: 7 short presentations (< 8 minutes) highlighting new and interesting data, followed by extensive time for discussions and questions.

Peak attendance 80, estimated total attendance ~80-100

After brief welcoming remarks from Ben, Alex kicked off the workshop portion of the interest group by introducing the first of 2 ASMS board members (due to their need to attend the board meeting too that evening).

Program:

- 1) Richard O'Hair talked about new data on DNA-bases and metal ion interactions and discussed the motivation and interest in looking at these materials.
- 2) Matthew Glover (Clemmer Group) talked about "Insights into Metal Binding Sites in Biomolecules by Multidimensional Ion Mobility Spectrometry".
- 3) Chrys Wesdemiotis (Akron University) talked about the utility of mass spectrometry and ion mobility in the analysis of synthetic polymers and related architectures.
- 4) Yury I. Kostyukevich (Nikolaev Group) showed data very new data on "super-metalization" of peptides and proteins; in the presence of zinc and high source temperature (450 °C) multiple reactions occurred that eliminated 2 protons for every Zn^{2+} ion. Multiple metal ions were added without addition of net charge which opens up additional possibilities for collisional and/or electron-based structural characterization.
- 5) Mary Rodgers (Wayne State University) – discussed "Metal Ion Effects on Glycosidic Bond Stability" using a combination of ion-trap and Guided ion beam MS techniques in conjunction with theory. High correlation between the approaches was shown for simple reactions.
- 6) Philip Ferko (University of Missouri- St. Louis, Holmes Group with Bythell Group) discussed ESI-MS of Thermochromic and Photoresponsive Cyanometalate Fe/Co Self-Assembled Squares. Experiments looking at breakdown stability and ligand binding were described.
- 7) Cheng Lin (Boston University) discussed metal-cationized complex carbohydrates and various means of structural characterization (electron- and CID-based). In addition he showed calculations on the various fragmentation processes involved utilized to elucidate the chemistry and aid interpretation.

Finally, after much discussion (~25 minute over-run) we thanked everyone for their participation and solicited nominations for chair-elect for the interest group for 2016. Given the time we decided to do this via the workgroup web list and direct e-mail to Alex. We also solicited recommendations for oral and poster sessions for 2016, and for ideas for the workshop in the same manner.

Initial feedback:

Those audience members polled were very enthusiastic about the workshop contents and variety. A few commented that our initial title was a little misleading as it implied a more applied focus than fundamental. Our mixed approach was popular and several people commented that they wished this had been a full oral session in the conference too.

Sincerely yours,

Ben Bythell (2015-Chair) and Alexandre Shvartsburg (2016-Chair)