

**2012 ASMS Polymeric Materials Interest Group Workshop Summary Report**  
**Wednesday May 22, 2012 5:45pm to 7:00pm**  
**60<sup>th</sup> ASMS Conference, May 20-24, 2012, Vancouver, BC**

Chairperson: Andrew J. Hoteling, Bausch and Lomb, Inc. (Rochester, NY)  
Co-Chairperson: William Erb, Bausch and Lomb, Inc. (Rochester, NY)

**Workshop Title: *New Capabilities for Polymeric Materials***

**Introduction:**

The attendance at this year's workshop was estimated at 70-80 attendees. This is down a little from last year, which may be due to international travel. In the conference this year, there was one polymer related oral session and one polymer related poster session. The oral session chair (William Erb, Bausch + Lomb) reported that there were 8-10 submissions, however the subject matter of the orals was well aligned with the topic of the session (Polymers MS: Materials, Medical Devices and Pharmaceuticals). The attendance at the oral session was in the range of 100-150. The polymer poster session contained 20 submissions, but there were additional polymer related posters observed during the week at other topic sessions.

The agenda for the interest group meeting included the following topics:

- General announcements
- ASMS discussion items
- Discussion of new MS capabilities and their application toward polymers/materials

**General Announcements and Business Related Topics:**

The meeting opened with an announcement from Liang Li of University of Alberta. As an editor of the *Analytica Chimica Acta* journal, he would like to put together a focus issue on polymer mass spectrometry. He discussed the need for two assistant editors that would help him arrange the issue, preferably one from industry and one from academia. He polled the audience to gauge potential authors of articles for the focus issue and approximately 15 people raised hands.

The Interest group coordinator succession plan was discussed. The expectation is that an interest group coordinator holds the position for two years. The succession plan moving forward will involve an overlap of two coordinators, one in his/her 2<sup>nd</sup> year and a new one in his/her first year. Bill Erb (Bausch + Lomb) is the recommendation from the group as the interest group coordinator starting next year. Gyorgy Vas (J & J) volunteered to be the next interest group coordinator to overlap with Bill.

A discussion of next year's ASMS polymer oral session started with volunteers for a session chair. The group agreed to recommend David Stranz (Sierra Analytics) as the oral session chair for 2012. A few suggestions were made for potential oral session topics as listed below. Attendees were encouraged to submit any additional topic suggestions to Andrew Hoteling ([Andrew.hoteling@bausch.com](mailto:Andrew.hoteling@bausch.com)) or William Erb ([william.erb@bausch.com](mailto:william.erb@bausch.com)) over the next two weeks.

- Separations and MS of Polymers
- Regulatory environment relevant to Polymeric materials
- Extractables and Leachables

To help develop the program for the next polymeric materials interest group workshop, the plan is to distribute a survey through ASMS. One of the questions of the survey will provide an opportunity to vote for your top choice among the suggested session topics. All three of the topics listed above generated lively discussion and interest among the group members. The

discussion around Extractables and Leachables was particularly interesting, and there were suggestions of trying to make that the topic of a second oral session. It was pointed out that it will be difficult to get a second oral session next year. An alternative suggestion was to attempt to make this a topic for a second workshop. Susan Weintraub (vice president in charge of programs – 2012) pointed out that an alternative could be to make this the subject of a poster session to gauge the participation level.

### **Discussion of new MS capabilities:**

In last year's workshop (2011), we began a discussion of the new Mass Spectrometry related capabilities that have emerged over the past few years, which included Ambient Ionization techniques (e.g. DESI, ASAP, LESA), Ion Mobility, and Routine Accurate Mass capability (e.g. Orbitrap, MaXis, Synapt). The discussion of this topic was continued in more detail in this year's workshop. Three short presentations were given to introduce topics and begin discussions.

The first discussion item was a combination of ASAP and Ion Mobility, with a short presentation by Eleanor Riches (Waters). The application was a co-polymer of polydimethyl acrylamide and PEG with a methacrylate end that incorporates into the backbone and extends the PEG groups as side chains. As the sample was heated to high temperature in the ASAP experiment, the side PEG chain thermally break from the backbone. The ion mobility data showed the separation of the oligomeric PDMA thermal fragments from the PEG oligomers after the ASAP experiment. The additional ion mobility separation made it easier to visualize the ASAP data. A good discussion of ion mobility followed, where a few attendees who have used ion mobility fielded a range of questions from the others who have not. Based on the discussion in the workshop, as well as the presentations in the polymer oral session, it appears that ion mobility is a new tool that is finding more applications with polymeric materials.

The second discussion item was Liquid Extraction Surface Analysis (LESA), with a short presentation by Martin Paine (University of Wollongong, Wollongong, Australia). The LESA technique is an automated coupling of a micro-droplet extraction with nano-electrospray. Examples included surface analysis of a polyester material, lipid profiling on a surface of a coil coating and contact lens surface, and surfactant on surface of a polypropylene part. The discussion involved questions about what this technique provides over a traditional extraction. The potential advantages of this technique included reproducible extraction, extraction of the surface, and spatial resolution.

The third discussion item was Direct Analysis in Real Time (DART), with a short presentation by Luke Ackerman of the FDA Center for Food Safety & Applied Nutrition. It was pointed out that DART is a technique that has potential for the direct analysis of a polymer surface. The examples that were presented involved the analysis of packaging materials for components that could potentially come in contact with food. It was noted that the low MW components were observable (e.g. polymer additives), however the signal response drops off rapidly after a few hundred Da. Luke summarized his observations from his work with DART and polymers: DART-Sample positioning affects signal; DART-MS more than sensitive enough (additives); DART-MS can be semi-quant off polymer surfaces; DART-MS can not reliably identify isomers in isomeric mixtures without MS-MS; Primarily M+H+, M+NH4+, M-H-, M+O2-, which ion varies by moiety, DART-MS inlet conditions; Polymer ions typically only after thermal decomposition, Non/less-volatiles signal increases post glass transition, Versatile sample introduction.

### **Conclusion:**

This years workshop was well attended compared with the past few years. The discussion topics seemed to be of interest to many of the participants. Overall, the presentations provided a good introduction into a few new MS techniques that are starting to show potential applications with polymers. These introductions generated a good level of discussion.

Members of the interest group are encouraged to provide feedback to the chairperson, as well as suggestions for content for next year's meeting. The group is also encouraged to search for a new LinkedIn group related to polymer mass spectrometry, where discussions can be carried on through the year. Additionally, a survey will be sent out later in the year about next year's workshop. Participation in the survey is encouraged to help shape future polymer interest group workshops.

The group recommends William Erb of Bausch + Lomb, Inc. as the new Polymeric Materials Interest Group coordinator. The group recommends David Stranz of Sierra Analytics, Inc. as the 2013 oral session chair.