



ASMS 2024 Anaheim

**Evening Workshop of the Polymeric Materials Interest Group  
“Deformation – what exists and what is lacking”**

WORKSHOP REPORT

*Date:*

Monday, June 3<sup>th</sup>, 2024

*Coordinators:*

Thierry NJ Fouquet (Bausch & Lomb, thierry.fouquet@bausch.com, thierry.fouquet83@gmail.com),  
Anthony Gies (LYB, apgies@gmail.com)

*Attendance:*

~70 attendees

*Overview:*

The main topic of the 2024 Evening Workshop of the “Polymeric Materials” Interest Group was **“deformation”** (proposed by members at the end of our workshop in 2023), with two short tutorial presentations by two invited panelists followed by an open discussion, several “flash” previews of posters / talks in addition to numerous announcements. This year again, we used the application **“Mentimeter”**. By joining the presentation via their mobile phones / tablets / laptops, the attendees were able to answer instant polls about two group projects proposed by the coordinators, ask questions or fill out forms such as our emailing list.

The slides are available in the section dedicated to our group in the ASMS website:

<https://www.asms.org/member-center/interest-groups/polymeric-materials>

## Minutes:

### ▪ Opening remarks, group business, group project 1

Thierry Fouquet discussed the Interest Group business for the first 15 minutes of the workshop, including the following topics:

- promotion of the poster and oral “polymer mass spectrometry” sessions at ASMS 2024;
- pending Sanibel/Asilomar proposal submitted on behalf of the Interest Group, need for a joint proposal with other interest groups such as “exposomics” or “energy and fuel”;
- group communication with a quick poll about the preferred channel, either via the emailing list (158 active addresses listed in July 2024), or via our LinkedIn group (<https://www.linkedin.com/groups/4009861/>, from 50 members in 2021 to 226 members in July 2024);
- our virtual informal meetings (6 gatherings between June 2023 and May 2024) and the associated recorded videos available in the group’s YouTube channel (<https://www.youtube.com/@asmsinterestgrouppolymeric2555>);
- suggestion of a first “**group project**”, namely the **co-authoring of a tutorial article about “polymer mass spectrometry”** involving as many members of the group as possible (live poll using Mentimeter: 23 members calling it a “good idea”, 12 members ready to join a writing team).

### ▪ Tutorial presentations, open discussion about “deformulation”, group project 2

Two invited panelists shared their experience in deformulation via a few slides:

- Robert B. (Chip) Cody (JEOL USA) shared an example of the combination of thermal desorption / pyrolysis (TD/Py) and Direct Analysis in Real Time (DART) for the analysis of triphenylphosphine / styrene / divinylbenzene samples. He exemplified the elucidation of triphenylphosphine derivatives using advance software tools including their newest versions powered by artificial intelligence.
- Tyler Arntz (The University of Akron, The Wesdemiotis Group “WesMass”) shared an example of deformulation of a “high gloss ceramic clear” by MALDI-MS and Kendrick analysis, the latter helping him to highlight minor poly(propylene oxide) distributions in a sample mainly constituted of poly(methyl methacrylate) series.

These two short tutorial presentations and a few questions asked to the audience (which techniques do you use first? Do you rely on databases / libraries? Are they missing for polymers? Any ethical issues with reverse engineering and competitive intelligence? Chromatography-based or chromatography-free? How do you publish your results including proprietary formulations? Will AI/ML be of any help? How do we compile training data?) were used as the basis for an open discussion with the members about the techniques used for deformulation, the existing and still missing tools especially in terms of software, the best practices...

This open discussion led up to a second “**group project**” proposed by the coordinators, namely the **creation / curation of an open access database compiling the MS fingerprints of polymers** using as many ionization techniques as possible such as MALDI, ESI, pyGCMS, DART, ... and low and high

resolution analyzers, collected from MS labs around the world and from the existing literature. Such a currently missing database would be searchable by scientists and would be a trusted source for AI/ML training (live poll using Mentimeter: 20 attendees calling it a “good idea”, 5 attendees OK to join a team, 3 being ready to share datafiles).

The two group projects will start as soon as possible and the progress shared at the next ASMS 2025.

#### ▪ **Flash previews**

Six ASMS attendees were invited to present a couple of slides about their research results dealing with polymer mass spectrometry, **but submitted in other sessions than “polymers” (poster and oral)**. It was a great occasion to remind the attendees that works related to synthetic polymers is available throughout the program of the ASMS annual conference, not only in the dedicated sessions.

- Kyle E. Lira (Vanderbilt University): Compilation of a Polysorbate CCS Database from Drift Tube and Traveling Wave Structures for Lossless Ion Manipulations Ion Mobility Measurements (poster submitted in “Ion mobility: applications II”);
- David Weil (Agilent): Non-targeted analysis, interactive visualization, and online sharing of interactive LC-HRMS/MS data of polymers using a comprehensive software PolyMatch Suite (poster submitted in “Extractables & Leachables”);
- Masaaki Ubukata (JEOL): construction of an in silico EI mass spectral library for polymeric materials analysis using pyGCMS and machine learning (oral submitted in “GC/MS: Instrumentation and Applications”);
- Alyssa Winter May (Colorado State University): Advances in block copolymer materials research enabled by MALDI-TOF mass spectrometry (poster submitted in “MALDI: Applications”);
- Bryan Katzenmeyer (JEOL): direct and indirect thermal desorption and pyrolysis of polymers by DART and GC-MS: a hot topic ! (poster submitted in “Ambient Ionization: Applications II”);
- Jens Sommertune (Polymer Factory Sweden AB): Dendrimers and their application as mass and mobility calibration standards – a case study for reliability and applicability (poster submitted in “Ion Mobility: General”).

#### ▪ **Final announcements:**

- Two breakfast seminars focused on polymer mass spectrometry proposed by Bruker and JEOL
- Open positions at Croda ISCS (presented by Wendy Yee)
- New local Mass Spectrometry Discussion Group (MSDG) for New York State gathering mass spectrometrists, chromatographers, vendors, students and LC/GC/MS enthusiasts for in-person and remote meetings  
LinkedIn group: <https://www.linkedin.com/groups/12998124/>  
Website: <https://www.newyorkms.org>
- **New coordinators!** (vide infra)

## ADDITIONAL NOTES

- Thierry Fouquet completed his 2-year term as coordinator at the end of the evening workshop.
- **Anthony Gies is the new main coordinator of the Interest Group (2025 and 2026)**, in charge of the evening workshops and informal meetings.
- The members of the Interest Group appointed **Selim Gerislioglu (PPG Industries) as the new co-coordinator**. He will later serve as main coordinator in 2027 and 2028.
- The “Polymeric Materials” interest group is hosting virtual meetings on a quasi-quarter basis, very well received by the community as a way to keep in touch throughout the year without waiting for the next ASMS conference. Typical topics include recent research results or issues, articles recently published, overview of conferences, ...

**These meetings are open to all and publicized via the interest group emailing list and LinkedIn group. Some of the presentations shared during these meetings are available on YouTube if the presenter agrees being recorded.**

○ July 21, 2023

*Focus topic:* Analysis of PEG in artifact conservation of the Vasa, a 17th century Swedish warship

*Featured speakers:* Brennan Curole and Scott M Grayson (Tulane University)

Link to video → unlisted video, link available upon request

○ Oct 16, 2023

*Focus topic:* Kendrick Analysis for Polymer Mass Spectrometry - an overview of the simple concept of Kendrick analysis and its application to polymer mass spectrometry, with examples of data processing from MALDI, ESI, DART, py, LC and GC high and low resolution MS and MS/MS.

*Featured speaker:* Thierry Fouquet (Bausch and Lomb)

Link to video → <https://www.youtube.com/watch?v=mK1SGmcK35o>

○ January 31 2024

*"Skim Thru' Your PDF":* Online Bipolar Dual Spray for the Charge State Reduction and Characterization of Complex Synthetic Polymers

*Featured speaker:* John R. Stutzman (Dow)

doi of the article: 10.1021/jasms.3c00333

This informal gathering was also the occasion to share a moment remembering Prof David M. Hercules who sadly left us on January 20 2024.

Link to video → <https://www.youtube.com/watch?v=nCOaSWS6qxE>

○ April 18, 2024

*"Skim Thru' Your PDF":* "Size-Resolved Identification and Quantification of Micro/Nanoplastics in Indoor Air Using Pyrolysis Gas Chromatography–Ion Mobility Mass Spectrometry"

*Featured speaker:* Karl J. Jobst

doi of the article: 10.1021/jasms.3c00362

Link to video → <https://www.youtube.com/watch?v=BCl6dnLpW0Q>

○ May 17 2024

*"Skim Thru' Your PDF"*: Charge Detection Mass Spectrometry for Megadalton Polymer Characterization and Measurement of Electrospray-Generated Charged Droplet Dynamics with a New "Direct Visualization of the Rayleigh Limit" Approach to Aid in  $m/z$  Calibration  
*Featured speaker*: Richard B. Cole (Sorbonne Université-Faculté des Sciences et Ingénierie)  
Doi of the article: 10.1021/acs.analchem.4c00055

Link to video → under editing, to be published

○ May 24 2024

*"Skim Thru' Your PDF"*: "Utilization of bis-MPA Dendrimers for the Calibration of Ion Mobility Collision Cross Section Calculations"

*Featured speaker*: Jens Sommertune (Polymer Factory Sweden AB)

Doi of the article: 10.1021/jasms.3c00428

Link to video → [https://www.youtube.com/watch?v=GVxMUerm\\_fs](https://www.youtube.com/watch?v=GVxMUerm_fs)