

Recent Advances in Applied Mass Spectrometry

Description, programme, and abstracts of the Mass Spectrometry Day at the KBC Umeå on 15 March 2023. Edited by Thomas Th. Kieselbach, Umeå University Library, Umeå University, Sweden, 2023.

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Mass Spectrometry Day at the KBC Umeå on 15 March 2023

Acknowledgements

The Mass Spectrometry Day at the Chemical Biological Centre (KBC) of Umeå University on 15 March 2023 would not have been possible without the help of many wonderful people, and I would like to thank everybody who made this event possible. This includes:

1. The companies who funded the Mass Spectrometry Day and who contributed to this event with their presentations and with their information material.
2. The Swedish Metabolomics Centre that co-hosted the Mass Spectrometry Day together with the Swedish Mass Spectrometry Society.
3. The people of the Mass Spectrometry Network Umeå who supported the organisation of this event through valuable discussions.
4. Agnes Rinaldo Matthis from the Swedish Chemical Society and Anna Shevtsova from the KBC Information Office who assisted with invaluable help in the organization of the event.
5. The Board of the Swedish Mass Spectrometry Society who supported the event through valuable advice.
6. Umeå University that contributed to the funding of the Mass Spectrometry Day through a conference grant.
7. My boss and my colleagues at the University Library who gave me the freedom to organize this event.

Moreover, I thank everybody who attended this event on-line and on site. Your interest in applied mass spectrometry is greatly appreciated.

Thomas Theresa Kieselbach, Umeå University Library and Swedish Mass Spectrometry Society

Contact Person

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Description

Six leading companies in the field of modern mass spectrometry present their latest news about analytical applications and technologies. The spectrum of topics covers metabolomics, proteomics and gives special attention to targeted applications. Both mass spectrometry in combination with separation by liquid chromatography and by gas chromatography is included.

The event is a collaboration between industry and academia. It is organized by the Swedish Mass Spectrometry Society in collaboration with the Swedish Metabolomics Centre, the Mass Spectrometry Network Umeå and six leading companies in the field of applied mass spectrometry. It offers a unique opportunity to learn about the latest innovations from Agilent Technologies, Bruker Nordic, SCIEX, Shimadzu, Thermo Fisher Scientific and Waters. In addition, Hamilton Nordic AB participates with a presentation table and information about their products but without an oral presentation.

The event is on-site at the Chemical Biological Centre of Umeå University (KBC Umeå) and provides a unique opportunity to attend the presentations of the application experts of the companies and to meet company representatives for discussion of analytical applications and instrumental technology.

In addition, the Mass Spectrometry Day is an opportunity for the local mass spectrometry community to meet and to exchange news and experiences. There is also an opportunity to attend the presentations at the event in Zoom. However, to meet the representatives of the companies attending the event on site is required.

Funding

The Mass Spectrometry Day at the KBC Umeå on 15 March 2023 was a non-profit event that was organized on a self-cost basis. The funding came from a conference grant from Umeå University (dnr: FS 2.1.6-2211-22) and from the companies who presented their innovations at this conference. These companies are Agilent Technologies, Bruker Nordic, Hamilton Nordic, SCIEX, Shimadzu Sweden, Thermo Fisher Scientific, and Waters.

Organizers

[Swedish Mass Spectrometry Society \(SMSS\)](#), [Swedish Metabolomics Centre \(SMC\)](#), Mass Spectrometry Network Umeå.

Programme

- | | |
|---------------|--|
| 9:00 | Reception desk of the event opens in the KBC Hall |
| 10:15 – 10:20 | Thomas Th. Kieselbach, Swedish Mass Spectrometry Society, Welcome Address (Carl-Kempe Hall) |
| 10:20 – 11:00 | Tony Wiklund, <i>Thermo Fisher Scientific</i> , Setting a new horizon for PFAS -workflow applications (Carl Kempe Hall) |
| 11:00 – 11:40 | Ross Chawner, <i>Waters</i> , SELECT SERIES: Redefining Performance of Next Generation Ion Mobility and High-Resolution Mass Spectrometry (Carl Kempe Hall) |
| 11:40 – 13:10 | Lunch break and opportunity to meet company representatives (KBC Hall, Glasburen) |
| 12:30 – 13:00 | Annual assembly of the Swedish Mass Spectrometry Society (Carl-Kempe Hall) |
| 13:10 – 13:50 | Daniel McMillan <i>Sciex</i> , Direct aqueous analysis of poly- and perfluoroalkyl substances (PFAS) in drinking and bottled water (Carl Kempe Hall) |
| 13.50 – 14:30 | Anders Feldthus, <i>Agilent</i> , Ensuring robust transfer from untargeted discovery metabolomics to a reliable targeted HILIC LCMS workflow (Carl Kempe Hall) |

- 14:30 – 15:00 Coffee break and opportunity to meet company representatives
(KBC Hall, Glasburen)
- 15:00 – 15:40 Jasper Theodore Koning, *Shimadzu*, Supercritical fluid chromatography and its potential for metabolomics (Carl Kempe Hall)
- 15:40 – 16:20 Patrik Ek, Lars Kristensen and Cristian De Gobba, *Bruker Nordics*, Benefits of Trapped Ion Mobility mass spectrometry (TIMS) and Collisional Cross Section-enabled timsTOF technology for 4D-Proteomics™, 4D-Lipidomics™, 4D-Metabolomics™ and Imaging (Carl Kempe Hall)
- 16:20 – 16:30 Jonas Bergquist, Swedish Mass Spectrometry Society, Closing Address, (Carl-Kempe Hall)

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Abstracts of the Oral Presentations

Setting a New Horizon for PFAS - Workflow Applications

Tony Wiklund, *Thermo Fisher Scientific*

The analysis of PFAS has been and are still a very hot topic more often requiring Mass spectrometry. With new legislation pushing the need for specificity and the levels of detection, Thermo Fisher Scientific has launched a workflow solution that is flexible and can be implemented both as routine and research instrumentation.

Thermo Fisher are presenting a workflow solution to analyze PFAS, including sample preparation, different choices of mass analyzers and library to screen for unknown and/or create ready to use SRM/PRM methods.

Contact Person of Thermo Fisher Scientific

Tony Wiklund, Thermo Fisher Scientific. Email: tony.wiklund@thermofisher.com

Related Application Notes

Jacob, C.C., Martins, C.P.B., Atkins, A.R., & Jack, R.F. (2019). Direct analysis of selected per- and polyfluorinated alkyl substances (PFAS) in ground, surface, and waste water by LC-MS/MS. Thermo Fisher Scientific APPLICATION NOTE 65397. [Open weblink to the PDF-document of this application note.](#)

MacLennan, M.S., Ng, D., & Hope, D. (2021). Extraction and analysis of poly- and perfluoroalkyl substances (PFAS) from soil. Thermo Fisher Scientific CUSTOMER APPLICATION NOTE 73937. [Open weblink to the PDF-document of this application note.](#)

MacLennan, M.S., Ng, D., Pond, P., & Hope, D. (2021): Extraction of poly-and perfluorinatedalkyl substances (PFAS) from solid matrices. figshare. Poster. <https://doi.org/10.6084/m9.figshare.13557185.v1>

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SELECT SERIES: Redefining Performance of Next Generation Ion Mobility and High-Resolution Mass Spectrometry

Ross Chawner, *Waters*,

Mass spectrometry has seen huge innovations over the last 30 years. Significant advancements in computing, coupled with high-speed electronics, has allowed huge strides in improvements in MS performance, that have expanded the research capabilities of MS. Using hyphenated Mass Spectrometry techniques, we can determine what is in our samples and how much there is. Also, increasingly, we also want to know where analytes are, and the use of Mass Spectrometry Imaging (MSI) is growing.

Due to sample complexity, high specificity and selectivity in the analysis method is required. Depending on the question being asked, different mass spectrometer platforms can be utilised to gain the required answer.

The SELECT SERIES MRT™ shows unparalleled levels of mass resolution (>200,000 FWHM) and mass accuracy (sub-500ppb), on a Time of Flight (ToF) platform, whilst maintaining the speed characteristics of a ToF platform, and advantages of an orthogonal arrangement. The high resolving power allows the differentiation of multiple near isobaric species, whilst the mass accuracy allows confidence in identification, based on known elemental composition.

Finally, the SELECT SERIES Cyclic™ IMS, utilises enhanced Ion mobility (IM), for significantly increased peak capacity. The tuneable cyclic IMS cell allows separation of isobaric species, with pre- and post-IMS fragmentation for identification.

Contact Person of Waters

Ross Chawner, Waters. Email: ross_chawner@waters.com

Related Application Notes

King, A., Molloy, B.J., Mortishire-Smith, R.J., & Plumb, R.S. (2022). Drug Metabolite Identification Using Waters™ SELECT SERIES™ Cyclic™ Ion Mobility Mass Spectrometer and waters_connect™ Application Manager. Waters Application Note 720007579. [Open the application note on the homepage of Waters.](#) [Open a weblink to the PDF-document of this application note.](#)

Reid, L., Towers, M., Marsden-Edwards, E., & Jarvis, S. (2022). Improving Feature Detection and Putative Identification For Tissue Imaging Applications Using the SELECT SERIES™ Multi-Reflecting-ToF (MRT) Mass Spectrometer. Waters Application Note 720007810. [Open the application note on the homepage of Waters.](#) [Open a weblink to the PDF-document of this application note.](#)

Waters. (2022). MS Imaging – The SELECT SERIES™ MALDI and MRT. Waters Application Note 720007652. [Open the application note on the home page of Waters.](#) [Open a weblink to the PDF-document of this application note.](#)

Related Research Articles

Giles, K., Ujma, J., Wildgoose, J., Pringle, S., Richardson, K., Langridge, D., & Green, M. (2019). A Cyclic Ion Mobility-Mass Spectrometry System. *Analytical chemistry*, 91(13), 8564–8573. <https://doi.org/10.1021/acs.analchem.9b01838>

Cooper-Shepherd, D. A., Wildgoose, J., Kozlov, B., Johnson, W. J., Tyldesley-Worster, R., Palmer, M. E., Hoyes, J. B., McCullagh, M., Jones, E., Tonge, R., Marsden-Edwards, E., Nixon, P., Verenchikov, A., & Langridge, J. I. (2023). Novel Hybrid Quadrupole-Multireflecting Time-of-Flight Mass Spectrometry System. *Journal of the American Society for Mass Spectrometry*, 34(2), 264–272. <https://doi.org/10.1021/jasms.2c00281>

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Direct Aqueous Analysis of Poly- and Perfluoroalkyl Substances (PFAS) in Drinking and Bottled Water

Daniel McMillan, *SCIEX*

In February 2020, the European Parliament and Council of the European Union released a new directive that recasts the limit of PFAS in drinking water which was 0.5 µg/L for all PFAS compounds identified or 0.1 µg/L for a subset of PFAS compounds that are deemed particularly concerning for humans. EU member states can choose which limit to use, and they can also decide to implement both. The difference between the limits is dependent on a list of compounds stated within the directive. Directive requirements create an analytical challenge to achieving these newly set LOQs in drinking water without solid phase extraction (SPE) clean-up, but SCIEX can demonstrate method that easily achieve new limits of all required PFAS compounds. During the presentation we will also give tips on how to achieve these limits and reduce common issues associated with the analysis without the use of specialized equipment or system modifications.

Contact Person of SCIEX

Daniel McMillan, SCIEX. Email: daniel.mcmillan@sciex.com

Related Application Notes

Butt, C. (2023). Low-level quantification of PFAS in water samples with high sensitivity and precision. RUO-MKT-02-13604-A. [Open a weblink to the PDF-document of this application note.](#)

Roberts, S., Butt, C., Wright, D., Somerville, S., Hyland, K.C., & Borton, C. (2018). Analysis of PFAS in drinking water with EPA Method 537.1 and the SCIEX QTRAP® 4500 System. RUO-MKT-02-7657-B. [Open the application note on the homepage of SCIEX.](#) [Open a weblink to the PDF-document of this application note.](#)

Schreiber, A., & Noestheden, M. (2015) LC-MS/MS Analysis of Emerging Food Contaminants. RUO-MKT-02-2755-A. [Open a weblink to the PDF-document of this application note.](#)

SCIEX. (2020). Enabling new levels of quantification Using the SCIEX Triple Quad™ 7500 LC-MS/MS System – QTRAP® Ready, powered by SCIEX OS Software. RUO-MKT-02-11886-A. [Open a weblink to the PDF-document of this application note.](#)

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Standland, M., Butt, C.M., & Noestheden M. (2021). Analysis of PFAS at low ppt levels in drinking water via EPA method 533. RUO-MKT-02-13849-A. [Open the application note on the homepage of SCIEX.](#) [Open a weblink to the PDF-document of the application note.](#)

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Ensuring Robust Transfer from Untargeted Discovery Metabolomics to a Reliable Targeted HILIC LCMS Workflow

Anders Feldthus, Karen E. Yannell, Cate Simmermaker, Genevieve Van de Bittner, and Daniel Cuthbertson, *Agilent Technologies*

HILIC LCMS is seen as the gold standard for metabolomics studies. It has superseded the use of traditional reverse phase using ion-pairing reagents. Both come with challenges such as chromatographic repeatability between sample cohorts, column batches and personnel, all particular to HILIC. We have developed a comprehensive workflow for profiling polar metabolites covering all stages from sample preparation using the Bravo Sample Prep Platform, a robust HILIC chromatographic method and a highly analytically sensitive targeted analysis using our 6495C LC/TQ. We demonstrate how using the 1290 Infinity II Bio LC System gives great benefits for metal sensitive analytes. An effective workflow that's simple to implement, reliable and reproducible for over 500 commonly measured polar metabolites. This validated method allowed the direct transfer and development to our 6546 LC/QTOF for an equally robust workflow for untargeted approaches.

Contact Person of Agilent Technologies

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Related Application Notes

Sartain, M., Gomez, M., Van de Bittner, G., & Shu, H. (2020). Enabling Automated, Low-Volume Plasma Metabolite Extraction with the Agilent Bravo Platform. Agilent Application Note 5994-2156EN. [Open a weblink the to the PDF-document of this application note.](#)

Spivia, W.R., Raedschelders, K., Gomez, M., & Van Eyk, J.E. (2019). Automated Metabolite Extraction for Plasma using the Agilent Bravo Platform. Agilent Application Note 5994-0685EN. [Open a weblink to the PDF-document of this application note.](#)

Related Research Articles

Dührkop, K., Fleischauer, M., Ludwig, M., Aksenov, A. A., Melnik, A. V., Meusel, M., Dorrestein, P. C., Rousu, J., & Böcker, S. (2019). SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information. *Nature methods*, 16(4), 299–302. <https://doi.org/10.1038/s41592-019-0344-8>

Dührkop, K., Nothias, L. F., Fleischauer, M., Reher, R., Ludwig, M., Hoffmann, M. A., Petras, D., Gerwick, W. H., Rousu, J., Dorrestein, P. C., & Böcker, S. (2021). Systematic classification of unknown metabolites using high-resolution fragmentation mass spectra. *biotechnology*, 39(4), 462–471. <https://doi.org/10.1038/s41587-020-0740-8>

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Supercritical Fluid Chromatography and its Potential for Metabolomics

Jasper Theodore Koning, *Shimadzu*

The metabolome contains a complex group of chemicals with a large variety of physicochemical properties. The analytical challenge here is to try and capture as much of the metabolome as possible, which may be challenging with conventional chromatography. Supercritical fluid chromatography (SFC) has the potential to capture a wider range of the metabolome, while also increasing throughput. In SFC, CO₂ is compressed to a liquid state and can then be used as a mobile phase. This offers several advantages, such as low viscosity and high miscibility resulting in high linear velocities. An application analyzing a pesticide mixture showed that compounds ranging from a log K_{ow} of -1.4 to 6.9 could be reliably analyzed within the same chromatographic method. Moreover, SFC has also been shown to give better sensitivity than conventional LC in mass spectrometry applications. A comparison study analyzing 400 components showed that 90% of the components offered improved detection and quantitation limits with SFC, with an average increase in peak area between 2 to 5 times. Although SFC is not a new technique, it has gained a renewed interest in recent years due to advancements in instrumentation. Demonstrations are already available for highly polar molecules, pesticides, lipids, and many other chemical classes. For metabolomics, SFC promises to give both a wider coverage of the metabolome as well as an increased sensitivity.

Contact Person of Shimadzu

Jasper Theodore Koning, Shimadzu. Email: koning.j@shimadzu.dk

Related Application Notes

Fujito, Y., Tanaka, K., Ogura, T., Arakawa, K., & Hayakawa, Y. (2016). Multi-residue analysis of pesticides in agricultural products using QuEChERS and SFC/MS. ASMS 2016 TP-221. Shimadzu PO-CON1633E. [Open a weblink to the PDF-document of this application note.](#)

Shimadzu Corporation. (2018). Supercritical Fluid Extraction/Chromatography Applications Handbook. C10G-E059. [Open a weblink to the PDF-document of this handbook.](#)

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Benefits of Trapped Ion Mobility mass spectrometry (TIMS) and Collisional Cross Section-enabled timsTOF technology for 4D-Proteomics™, 4D-Lipidomics™, 4D-Metabolomics™ and Imaging

Patrik Ek, Lars Kristensen and Cristian De Gobba, *Bruker Nordic*

The timsTOF mass spectrometry platform, with its collisional cross section-enabled software and workflows, has revolutionized the field of life sciences research by enabling 4D-Proteomics™, 4D-Lipidomics™, 4D-Metabolomics™, and Imaging with unparalleled speed, selectivity, and sensitivity. The ability to separate and identify complex mixtures of molecules based on trapped ion mobility separation and high-resolution mass spectrometry detection, without sacrificing sensitivity or speed are major advantages of the timsTOF platform. In proteomics, it enables the identification and quantification of protein isoforms, post-translational modifications, and protein complexes. In lipidomics, metabolomics, environmental toxicology and other small molecule applications, it enables the identification and quantification of molecular species, including separating isomers. In imaging mass spectrometry, it enables the visualization of the spatial distribution of molecules in biological tissues with high resolution and ion mobility separation. The collisional cross section-enabled software and workflows of the timsTOF platform provide additional benefits, particularly in the separation and identification of isomeric molecules that are difficult to distinguish using traditional mass spectrometry techniques. This capability is particularly valuable in understanding complex biological processes and for developing new therapies for diseases and advancing our understanding of the fundamental biological processes that govern life.

Contact Persons of Bruker Nordic

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Cristian De-Gobba, Bruker Nordic. Email: c.de_gobba@bruker.com

Related Application Notes

Bruker Daltonics (2022). TIMScore with PaSER: Exploiting the CCS-dimension. Bruker Daltonics 02-2022, LCMS-192, 1894928. [Open a weblink to the PDF-document of this application note.](#)

Bruker Daltonics. (2023). Exploring the single cell proteome in a streamlined loss-reduced label-free approach on the timsTOF SCP. Bruker Daltonics 02-2023, LCMS-206, 1815135. [Open a weblink to the PDF-document of this application note.](#)

Related Research Articles

Meier, F., Brunner, A. D., Koch, S., Koch, H., Lubeck, M., Krause, M., Goedecke, N., Decker, J., Kosinski, T., Park, M. A., Bache, N., Hoerning, O., Cox, J., Räther, O., & Mann, M. (2018). Online Parallel Accumulation-Serial Fragmentation (PASEF) with a Novel Trapped Ion Mobility Mass Spectrometer. *Molecular & cellular proteomics: MCP*, 17(12), 2534–2545. <https://doi.org/10.1074/mcp.TIR118.000900>

Meier, F., Park, M. A., & Mann, M. (2021). Trapped Ion Mobility Spectrometry and Parallel Accumulation-Serial Fragmentation in Proteomics. *Molecular & cellular proteomics: MCP*, 20, 100138. <https://doi.org/10.1016/j.mcpro.2021.100138>

Schroeder, M., Meyer, S. W., Heyman, H. M., Barsch, A., & Sumner, L. W. (2019). Generation of a Collision Cross Section Library for Multi-Dimensional Plant Metabolomics Using UHPLC-Trapped Ion Mobility-MS/MS. *Metabolites*, 10(1), 13. <https://doi.org/10.3390/metabo10010013>

Skowronek, P., Thielert, M., Voytik, E., Tanzer, M. C., Hansen, F. M., Willems, S., Karayel, O., Brunner, A. D., Meier, F., & Mann, M. (2022). Rapid and In-Depth Coverage of the (Phospho-)Proteome With Deep Libraries and Optimal Window Design for dia-PASEF. *Molecular & cellular proteomics: MCP*, 21(9), 100279. <https://doi.org/10.1016/j.mcpro.2022.100279>

Spanier, B., Laurençon, A., Weiser, A., Pujol, N., Omi, S., Barsch, A., Korf, A., Meyer, S. W., Ewbank, J. J., Paladino, F., Garvis, S., Aguilaniu, H., & Witting, M. (2021). Comparison of lipidome profiles of *Caenorhabditis elegans*-results from an inter-laboratory ring trial. *Metabolomics: Official journal of the Metabolomic Society*, 17(3), 25. <https://doi.org/10.1007/s11306-021-01775-6>

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Information material from Hamilton Nordic

Hamilton Nordic participated in the Mass Spectrometry Day with a presentation table and information material about their products in, for instance, liquid handling and automation technology.

Related e-book

Hamilton Bonaduz AG. (2021). LC-MS Analysis for (Bio)pharmaceutical Research. [Open a weblink to the PDF-document of this e-book.](#)

Contact person for Hamilton Nordic

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