FTMS Fachgruppentagung 2025

Monday, August 25, 2025 - Tuesday, August 26, 2025
Universität Hamburg

Book of Abstracts

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Monday - Mo-I_1 - 8/25/25, 2:10 PM

Open Source Ion Dynamics Simulations - Challenges and Applications

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Talk outline:
- Ion Dynamics, physical effects acting on ions:
- Coulombic Forces / Space charge
- Background Gas Collisions / Background Gas Interaction
- Ion Chemistry
- Current situation of ion dynamics simulation tools
- The case for open source tools
- Brief introduction of IDSimF
- Verification versus other Simulation tools
- FT-QIT: Space charge modeling
- basic problem: Quadratic scaling
- Barnes Hut approach
- FT-QIT: Experiment / Introduction
- IDSimF Simulation results
- Cl / Xe isotopes
- Space Charge Effects / Peak coalescence
- Space Charge Capacity
- Conclusio: Space Charge kills FT-QIT
- Similarly: Simple FT-LIT killed by space charge effects
- Ion Collisions / Collision Models:
- Hard Sphere Modeling as coarse approximation
- Molecular Dynamics Collision Model
- Basic approach
- Implementation in IDSimF
- Benchmark experiment:
- High Field IMS (HiKE)
- Simulation Results
- Challenges:
- Molecule Coalescence / Cluster Formation with Nitrogen
- Ion Chemistry:
- HiKE with water clusters

Monday - Mo-I_2 - 8/25/25, 2:50 PM

Overcoming the Analytical Challenge of Non-Biological Complex Drug Analysis by Process Control Drug Discrimination via Comprehensive Chromatographic and Mass Spectrometric Approaches

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Medication errors are the leading cause of preventable patient harm. Globally, about 5% of patients are affected by medication-related harm, with 25% of these harms being life-threatening. Often, these errors are caused by orthographic or phonetic properties of medications. Look-alike, sound-alike errors are further aggravated by the availability of both foreign and local drugs sharing similarities in regulatory requirements and areas of application as well as the drug's complexity.

The relatively new drug group of non-biological complex drugs (NBCDs) covers complex synthetic medications and has gained significant medicinal, economic, and regulatory interest lately. Tentatively, also bituminosulfonates (BSs), obtained by sulfonation of shale oil distillates, are allocated toward the NBCD category. Their shale oil-based origin results in high isomeric and isobaric complexity and therefore cannot be fully described by physicochemical analytical means. These BSs are listed in the European Pharmacopeia (Ph. Eur.) by the brand name Ichthammol and are used for treating various dermatological diseases. Simultaneously, the Chinese Pharmacopeia (ChP) also lists a drug with dermatological application named Ichthammol. However, the ChP describes Ichthammol as a product of vegetable oil-based origin. Despite the origin differences, the Ph. Eur. and ChP share comparable bulk parameters defined in the corresponding monographs for Ichthammol.

To tackle the high error potential by unintended substitutions, we investigated Ichthammol matrices compliant with the Ph. Eur. as well as with the ChP in a comprehensive approach utilizing FT-ICR MS to resolve the isobaric complexity and comprehensive two-dimensional GC coupled to high-resolution ToF MS for isomeric information. We achieved an in-depth chemical description of different Ichthammol matrices by tracing compounds throughout the manufacturing process with high confidence in our results even without suitable standard reference materials for the Ph. Eur. compliant Ichthammol. For ChP compliant Ichthammol matrices, our results allowed confident conclusions about the manufacturing process without investigating process intermediates. Finally, we were able to transfer this information from these state-of-the-art methods to LC triple quadrupole MS, an approach that qualifies for routine differentiation between shale oil-based Ichthammol matrices derived from different distillation cuts and between Ichthammol samples derived from starting materials with different origins.

With this work, we present an approach to overcome the analytical challenges of NBCD analysis. By achieving detailed molecular-level information from state-of-the-art investigations we were able to differentiate between various Ichthammol matrices. These sophisticated results were then transferred into a routinely usable analysis method, which in the next step can be implemented into a regulated pharmaceutical environment.

Monday - Mo-I_3 - 8/25/25, 3:10 M

Metabolic Characterization of Glacier Surface Autotrophs via ^{13}C Labelling

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Ice algae inhabiting glacier surfaces are key primary producers that influence surface albedo and are integral for glacial microbial community structures. Ice surface species such as *Ancylonema nordenskiöldii* are central to carbon cycling in the supraglacial environment, yet their metabolic potential and ecological roles have not been fully characterised. Experiments using metabolic labelling by supplying and tracing $^{13}CO_3^{2-}$ with fluxomics techniques offer a powerful strategy for probing microbial metabolism. In this study, we apply $^{13}CO_3^{2-}$ based labelling and fluxomic analyses to glacier surface communities to assess their metabolism and carbon utilization strategies. High-resolution mass spectrometry (HRMS) is employed to accurately detect and identify labelled intracellular metabolites, including secondary metabolites, providing detailed insight into the metabolic pathways active in the autotrophic community. By tracking ^{13}C incorporation into intracellular metabolites, we aim to resolve active carbon assimilation pathways and secondary metabolite production with potential relevance to microbial community dynamics. Our results represent the first use of fluxomics in glacier environments targeted at surface ice-associated autotrophs. Understanding metabolic strategies is essential in light of accelerating glacier melt, which alters environmental conditions and may reshape microbial activity on glacier surfaces. As glacier surface conditions are highly vulnerable to climate-driven alterations in melt dynamics, identifying the metabolic strategies of ice surface-dominating ice algae and other autotrophs is essential for anticipating shifts in ecosystem function.

Monday - Mo-II_1 - 8/25/25, 4:10 PM

CHEMICAL CHARACTERIZATION OF WILDFIRE AEROSOL EMISSIONS AND PRODUCTS OF ATMOSPHERIC AGING BY ULTRAHIGH RESOLUTION MASS SPECTROMETRY

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Particulate matter (PM) is widely recognized as a threat to public health and a key driving force of climate change. The chemical composition significantly influences the properties of the particles, especially their interactions with solar radiation and their role in inducing adverse health effects. Atmospheric aging modifies aerosol composition, forming new compounds and increasing complexity. Despite progress, both primary and processed aerosols remain poorly characterized, contributing to uncertainties in climate models and a limited understanding of their effects on humans. The frequency and intensity of wildfires have risen in recent decades, a trend expected to persist with global warming. This study investigates aerosol emissions from wildfire and peat-burning scenarios using real-world samples and laboratory-simulated conditions. [1-7] Peatlands, which store one-third of terrestrial organic carbon, were a particular focus. [3,4]

High-resolution mass spectrometry methods combined with soft ionization techniques were applied for a systematic study of combustion-derived PM covering emissions [1,3,4], atmospheric transformation [5,7] and ambient air [2,6]. Fourier-transform ion cyclotron resonance mass spectrometry systems of magnetic field strengths from 7 to 21 T as well as Orbitrap systems were utilized to examine the complex PM chemistry, together with the development of sample preparation protocols and an improved understanding of the ionization characteristics for PM analysis.

Peat-burning emissions revealed an exceptionally complex molecular composition, with an average of more than 30,000 assigned compounds, including oxygen-, nitrogen-, sulfur-, and phosphorus-containing species. High levels of nitrogen-containing compounds (up to six nitrogen atoms) and characteristic biomass-burning markers, such as levoglucosan and terpenoids, were identified. Regional vegetation influenced the chemical profiles of peat-burning aerosols, yet over 10,000 common CHO and CHNO compounds were consistent across samples, forming a foundational set of peat-derived organic carbon. Notably, sulfur-rich compounds originating from Sphagnum moss-derived peat highlight peat combustion as a significant source of organic sulfur to the atmosphere. These findings underscore the need to consider Arctic and boreal peat smoldering as significant contributors to atmospheric sulfur cycling. [3,4]

[1] Schneider, E., et al. Environmental science. Processes & impacts 2024, 26, 1295–1309.
[2] Schneider, E., et al. Atmos. Chem. Phys. 2024, 24 (1), 553–576.
[3] Schneider, E., et al. J. Am. Soc. Mass Spectrom. 2024, 35 (8), 1713–1725.
[4] Schneider, E., et al. Commun Earth Environ 2024, 5 (1), 137.
[5] Czech, H., et al. Environmental science. Processes & impacts 2023, 26, 35–55.
[6] Schneider, E., et al. ACS Earth Space Chem. 2022, 6 (4), 1095–1107.
[7] Czech, H., et al. Environ. Sci.: Atmos. 2024, 4, 718–731.

Monday - Mo-II_2 - 8/25/25, 4:50 PM

Combining High Resolution and Speed with the Waters Xevo MRT

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The Waters Xevo MRT Mass Spectrometer marks a breakthrough in high-resolution mass spectrometry, integrating multi-reflecting time-of-flight (MRT) technology into a benchtop QTof system. It achieves up to 100,000 FWHM resolution at 100 Hz acquisition rates, while maintaining sub-ppm mass accuracy—independent of scan speed or acquisition mode. Unlike FTMS systems, where resolution typically decreases with faster scans, the Xevo MRT MS delivers consistent resolution across all acquisition conditions, enabling confident identification in complex matrices without compromising throughput.

The instrument features advanced ion optics and a novel collision cell for high sensitivity and transmission across the full m/z range. Its gridless ToF geometry and dual-gain ADC detector ensure excellent dynamic range and reproducibility, making it ideal for metabolomics, lipidomics, biopharmaceutical analysis, and clinical biomarker discovery.

Recent applications include single-cell lipidomics and Parkinson's disease stratification via sebum analysis, demonstrating its value in translational and precision medicine. The system supports open-source data formats (e.g., mzML) and integrates seamlessly with third-party software such as MS-DIAL, MZMine, Lipostar, and MARS, offering flexible and scalable data workflows.

Combined with the waters_connect software platform, the Xevo MRT MS streamlines acquisition, processing, and interpretation of high-resolution data, empowering researchers to accelerate discovery and enhance analytical confidence.

Monday - Mo-II_3 - 8/25/25, 5:10 PM

Using FTMS to study PFAS reactions with peptides and proteins

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PFASs are a diverse group of major emerging contaminants, with more than 7800 compounds identified to date. All of them possess at least one carbon atom, on which all the H substituents were replaced with F atoms. Due to the exceptional stability of the C-F bond, they are widely used as surfactants and stain repellents, in firefighting foams, cosmetics and surface coatings. The stability of the perfluorinated moiety makes it resistant to biodegradation and leads to accumulation of these substances in nature. PFASs are found in human blood, drinking water and biota in remote regions. Adverse effects such as hepatotoxicity, disturbances in lipid and protein metabolism and even carcinogenesis were attributed to these compounds. Yet the precise mechanisms by which these compounds interact with biological systems are unknown. It is known that lipid-protein interactions can affect the functioning of the proteins. Due to structural similarity between the lipid chain and the perfluorinated chain it is reasonable to expect the interactions between PFASs and proteins to have a certain effect on the latter.

In this project, reactions between PFASs and peptides or proteins were studied. Each pair of compounds (a PFAS and a biomolecule) were incubated in aqueous medium for several hours, then the resulting solution measured by HRMS. The samples were analyzed by a 7-T LTQ FT-ICR with a resolving power of R = 400 000 at m/z 400 and by LTQ-Orbitrap Elite mass spectrometer with mass resolving power of R = 480 000 (Thermo Fisher Scientific, Bremen, Germany) using ESI ionization.

Reactions between several PFASs and biomolecules were assessed. The results show that interactions are possible between the compounds, and they depend both on the PFAS and the biomolecule present. Most of the tested proteins and peptides interact with the PFSA compounds, as well as with perfluorophosphinic acids, but only a few exhibit interaction with PFCAs. Only GHK protein was found to interact with PFCAs. Each molecule of a protein or a peptide can interact with several PFAS molecules.

Tuesday - Tu-I_1 - 8/26/25, 9:00 AM

Top-Down Proteomics with FTMS: 1993-2025

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Since the early 1990s, FTMS has transformed biomolecular mass spectrometry, but its role in proteomics has been dominated by bottom-up (peptide-based) strategies. Top-down proteomics instead analyzes intact proteins, directly revealing proteoforms (the molecular variants arising from genetic variation, splicing, and post-translational modifications). By capturing the complete biochemical state of proteins, proteoforms provide a more direct link between genotype and phenotype.

FTMS is uniquely suited to this challenge, with unmatched resolution, mass accuracy, and fragmentation capabilities. Advances in ion statistics and single-ion detection now enable routine measurement and sequencing of low-abundance proteoforms and complex mixtures of proteoforms. Building on this, we developed Proteoform Imaging Mass Spectrometry (PiMS), and more recently single-cell PiMS (scPiMS), achieving >20-fold increases in throughput and direct proteoform detection at single-cell resolution.

This talk will trace the evolution of top-down proteomics with FTMS from its beginnings in 1993 to its current state.

Tuesday - Tu-I_2 - 8/26/25, 9:40 AM

Advances in Laser- and Lamp-based Photoionization High Resolution Mass Spectrometry

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Photoionization schemes have been extensively explored in both vacuum and ambient ionization mass spectrometry. In ambient ionization, atmospheric pressure photoionization (APPI) development has largely stalled, and atmospheric pressure laser ionization (APLI) remains niche. However, photoionization provides unique control over ionization characteristics and structural selectivity based on light-source wavelength. Uncommon vacuum and ambient laser/lamp-based ionization techniques are presented, offering diagnostic insights at high-resolution mass spectrometry with confident elemental composition attribution.

To expand the photoionization toolbox, atmospheric pressure single photon ionization (APSPLI) using a fluorine excimer laser and Xenon lamp APPI have been explored. [1,2] Compared to standard APLI (266 nm), APSPLI showed increased ionization for aromatic compounds with heteroatoms, while Xenon-APPI demonstrated minimal background signal.

In seeking a robust portable platform, vacuum photoionization Orbitrap mass spectrometry has been realized by deploying aromatic-selective multiphoton ionization (REMPI). [3] Online field studies have shown reliable operation under harsh conditions, recording complex emission patterns with sub-ppm mass accuracy [4]. Facing the diversity in energy transition matrices featuring various oxygen functionalities, derivatization with gas chromatographic pre-separation was evaluated. We find that the silylated species can be well ionized with REMPI. More interestingly, introducing the unique isotopic pattern of Silicon resulted in narrow mass splits. Even in complex mixtures, this characteristic isotopic fine structure could be resolved and used for increased confidence in molecular attribution. [5]

For further structural insights, a custom setup with adjustable-wavelength APLI has been built. Therefore, an optic-parametric oscillator (OPO) was used to investigate wavelength-dependent ionization characteristics in the range of 213-300 nm. Insights into the ionization behaviour of standard compounds allowed us to find structurally diagnostic patterns, with significant redshifts for alkylation or broader absorption bands for larger aromatic moieties. The first correlation of this standard library with the results from petroleum matrices indicated isomeric information. [6]

Literature:
[1] Rüger et al., *Analytical Chemistry*, **2021**, 93, 3691–3697; [2] Neumann et al., *JASMS*, **2023**, 34, 1632–1646; [3] Kösling et al., *Analytical Chemistry*, **2021**, 93, 9418–9427; [4] Kösling et al., *Analytical Chemistry*, **2022**, 94, 16855–16863; [5] Vesga-Martínez et al., *JASMS*, **2024**, 35, 3242–3255; [6] Etscheidt et al., *Analytical Chemistry*, **2025**, 97, 676–685

Tuesday - Tu-I_3 - 8/26/25, 10:00 AM

Innovations in MRMS - from feasibility to ease-of-use

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Since the invention of FT-ICRMS 1973 by Comisarow and Marshall, many innovations have been implemented in home built and commercial FT-ICR instrumentation and made available to researchers. With the change of user profile, moving from fundamental expert research to routine applications, more focus is on ease of use, often enabled by technology advances like Maxwell magnet technology and XR and 2xR detection and optimization methods. While these are now routinely available in commercial products like scimaX MRMS, innovation continues with e. g. merging trapped ion mobility spectrometry (TIMS) with Magnetic Resonance Mass Spectrometry (MRMS) or increased magnetic field strength of 18T.

Tuesday - Tu-II_1 - 8/26/25, 11:00 AM

How we can gain structural information about individual compounds in complex energy mixtures: Theoretical calculations support high resolution data and lead to surprising results

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High-resolution mass spectrometry is the method of choice for analyzing complex mixtures, as this is the only method that allows gaining detailed analytical information with high accuracy. The only problem is that mass spectrometry inherently can not provide structural information about unknown compounds per se. Liquid fuel systems are some of the most complex natural mixtures available and contain hundreds of thousands of different hydrocarbon-type compounds. Raw materials for fossil fuels are formed under geological conditions over large time frames, while biofuels are being made from a precursor source in different ways. To better understand the formation pathways it is imminent to understand how complex these mixtures are and what type of compounds are being formed under which conditions. Here, we have combined sophisticated analytical methods with different types of theoretical calculations on both the DFT- and coupled cluster level of theory to understand the structures of individual compounds in complex systems. High-resolution mass spectrometry allows the parallel detection of a vast range of different compounds, which can result in some 100,000 exactly measured signals that correspond to individual elemental compositions. Theoretical calculations allow finding the thermodynamically most stable structures of those compounds. Here, fascinating and unforeseen results from heavy fossil fuels are reported that show a surprising detection of carbon-type species. In crude oil we found naturally formed fullerenes and their building blocks, compounds that are interesting for a vast variety of applications. Fullerene synthesis happens under high-energy conditions, mostly laser ablation or high-voltage discharge is being used, while nature forms these compounds under geological conditions (ca. 150 °C and pressure). The results show, that nature forms a large variety of fullerenes and fullertubes, which can be detected up to C_{148}, while, additionally, electron microscopy allows a view into large multi-walled carbon nano tubes, which can also be detected. In all these findings, theoretical calculations support the results. These findings could open up a new interest in making different types of Fullerenes and functional carbon species in very different synthetic ways than before.

Tuesday - Tu-II_2 - 8/26/25, 11:40 AM

Compositional and Structural Analysis of Scrubber Discharge Water from a Ship Engine Using Liquid Chromatography and Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry

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Despite its crucial role in global trade, shipping significantly contributes to environmental pollution by emitting greenhouse gases and pollutants like nitrogen oxides, sulfur oxides, and particulate matter. To mitigate the harmful effects of ship emissions, the International Maritime Organization (IMO) has implemented a global limit on the sulfur content in marine fuels and introduced sulfur emission control areas (SECA). To comply with SOx emission regulations, ships can either operate on low-sulfur fuel oils or utilize alternative methods such as exhaust gas cleaning systems, commonly known as 'scrubbers'. Recent studies have shown that scrubber discharge water negatively impacts the aquatic environment and exhibits toxic effects on marine organisms. [1] While particle numbers are reduced by 40% [2], research on the molecular composition of scrubber water and its environmental fate remains limited.

This study investigates the chemical composition of scrubber discharge water from a research ship engine, as well as its photochemical transformation products. Therefore, a laboratory photo-aging setup was used to simulate natural aging processes and evaluate both primary and aged scrubber water discharges. For desalting and enrichment, aqueous samples were subjected to a preconditioned solid-phase extraction (SPE) cartridge and subsequently eluted with methanol. Extracts were analyzed by direct infusion high-resolution mass spectrometry using an electrospray ionization source (ESI FT-ICR MS, 7 T, University of Rostock) to characterize the polar fraction of scrubber discharge water. Additionally, liquid chromatography hyphenated with 21 T FT-ICR MS was employed to reduce ionization suppression and introduce an additional separation dimension. The 21 T FT-ICR MS platform at the National High Magnetic Field Laboratory (NHMFL) provides ultra-high-resolution broadband acquisition at high scan frequencies, maintaining the full chromatographic resolution of advanced HPLC systems.

Ultra-high-resolution mass spectrometric measurements revealed a high molecular complexity of scrubber discharge water, with numerous resolved signals detected in a single liquid chromatography scan. A diverse range of oxygenated compound classes was identified, including species containing up to two sulfur atoms and over ten oxygen atoms. These compounds exhibited a broad aromaticity spectrum, with double bond equivalents (DBE) ranging from naphthenic to polycyclic aromatic moieties. The findings indicate that variations in engine operating conditions significantly impact the elemental composition of scrubber water. Laboratory photo-aging of scrubber water revealed compound class-specific transformations dependent on irradiation time, along with a general increase in highly oxygenated species. These transformations alter the chemical nature of scrubber water, highlighting potential risks related to environmental persistence and ecotoxicity in marine systems.

Tuesday - Tu-II_3 - 8/26/25, 12:00 PM

Protein glycosylation probed by native MS

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High-resolution Fourier transform mass spectrometry (FTMS) combined with native electrospray ionization provides direct access to the proteoform and glycoform heterogeneity of intact glycoproteins. As a defined model system, the therapeutic antibodies adalimumab and trastuzumab were analyzed to test the ability of native MS to resolve Fc glycosylation variants with high mass accuracy. In parallel, human serum transferrin was investigated as a representative plasma glycoprotein with multiple N-glycosylation sites. The native mass spectra reveal a broad distribution of glycoforms and allow relative quantification of the dominant species, complementing NMR and UHPLC-based glycan profiling. These results highlight the utility of native FTMS for assessing microheterogeneity in glycoproteins, both in purified therapeutic antibodies and in proteins directly isolated from human serum.