

# Infrared Spectroscopy in a Mass Spectrometer – Molecular Fingerprints for Omics Research

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Tandem mass spectrometry is currently the gold standard in biomolecular analysis. The combination of robust and sensitive ionization techniques such as electrospray ionization with efficient fragmentation techniques and subsequent detection with high mass resolution enables the rapid identification of hundreds of proteins within hours. Likewise, highly complex maps of lipids and small molecule metabolites can be identified reliably from complex biological samples. However, differentiating isomeric species remains challenging through conventional mass spectrometry. In metabolomics, multiple structural candidates often exist for a given  $m/z$ , complicating precise identification. Similarly, in glycomics, isomeric glycan structures differing only in regio- or stereochemistry of a single glycosidic bond often coexist, presenting a significant analytical challenge. Recently, advances in commercially available ion mobility–mass spectrometers, gas-phase ion spectroscopy, and computational chemistry have opened new avenues to solve the isomer problem in mass spectrometry. Here we illustrate examples how small isomeric molecules such as metabolites and glycans can be unambiguously identified using ion mobility mass spectrometry and cryogenic gas-phase spectroscopy.

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## Biosketch

Kevin Pagel is Full Professor for Bioorganic Chemistry at the Department of Biology, Chemistry, Pharmacy of Freie Universität Berlin and guest researcher at the Fritz Haber Institute of the Max Planck Society. He obtained a PhD in Organic Chemistry in 2007 and subsequently spend several years abroad as researcher at the Universities of Cambridge and Oxford (UK). Research in the Pagel group is focused on the structural analysis of biological macromolecules, in particular glycans and glycoconjugates, using liquid chromatography, ion mobility-mass spectrometry and gas-phase IR spectroscopy. For his work he received several recognitions, including an ERC Consolidator Grant, and is spokesperson of an International Graduate School with the University of British Columbia in Vancouver and McGill University in Montreal.