INFRARED SPECTROSCOPY IN A MASS SPECTROMETER – MOLECULAR FINGERPRINTS FOR GLYCOMICS

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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, which represents 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 [1]. Here we illustrate examples how isomeric molecules can be unambiguously identified using a novel combination of ion mobility mass spectrometry and cryogenic gas-phase spectroscopy. Particular focus will be put on challenging glycoconjugates such as mucin-type *O*-glycans and glycosaminoglycans.

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References:

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