

Multi-dimensional Mass Spectrometry for Lipid Analysis

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Multi-dimensional mass spectrometry (MD-MS) is a newly emerging technology in mass spectrometry, which is analogous to multi-dimensional nuclear magnetic resonance spectroscopy. Each series of ramped changes in one of the instrumental conditions (i. e. , one variable) facilitate the generation of a dimension. These variables include: sample introduction (e. g. , solvents, pH, reagents, and flow rates), ionization (e. g. , temperature and voltage), fragment monitoring (e. g. , neutral fragments in neutral loss scanning and fragment ions in precursor-ion scanning), and collision-induced dissociation (e. g. , collision energy, collision gas pressure, and collision gas type), among others. Each of these variables constitutes a member of the MD-MS family. We recognized the power of MD-MS for analyses of individual lipid molecular species in lipidomics and have developed a technology based on MD-MS (i. e. , shotgun lipidomics). By varying the

pH of an infused solution, we have achieved optimal separation and maximal ionization of some specific lipid classes in the ion source (i. e. , intrasource separation and selective ionization). By monitoring certain fragments (which represent building blocks of each lipid class or group) through either neutral loss or precursor-ion scanning, we have identified and quantified hundreds to thousands of individual lipid molecular species directly from a lipid extract of a biological sample. By applying various amounts of collision energy during collision-induced dissociation, we are able to study the differential fragmentation kinetics of each individual lipid molecular species in a lipid class of interest. Collectively, MD-MS greatly facilitates not only the identification and quantitation of individual lipid molecular species by shotgun lipidomics, but also the determination of lipid biophysical properties and interactions for lipidomics.