

APPLICATIONS OF STRUCTURAL MASS SPECTROMETRY TO METABOLOMICS: CLARIFYING BOND SPECIFIC SPECTRAL SIGNATURES WITH ISOTOPE EDITED SPECTROSCOPY

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Comprehensive FTIR, MS/MS and NMR of pharmaceuticals are generally readily available but characterization of their metabolites has been an obstacle. Atorvastatin is a statin drug responsible for the maintenance of cholesterol in the body. Diovan is an angiotensin receptor antagonist used to treat high blood pressure and congestive heart failure. The field of metabolomics, however, is struggling to obtain the identity of their structures. We implement mass spectrometry with cryogenic ion spectroscopy to study gaseous ions of the desired metabolites which, in combination, not only identify the mass of the metabolite but also elucidate their structures through isotope-specific infrared spectroscopy.