

Jos Oomens FELIX, Radboud University	IR ion spectroscopy: a novel method in biomarker identification
<p>Mass spectrometry is one of the cornerstones in analytical chemistry, especially in the analysis of complex mixtures: samples that contain thousands of molecular components in varying concentrations, such as patient samples that may contain compounds that can serve as valuable biomarkers. Both the sensitivity and resolving power of MS are unparalleled by other analytical methods. However, determination of molecular structures on the basis of MS data is challenging, as a single molecular weight value may correspond to many structural isomers.</p>	
<p>The FELIX free-electron laser provides new opportunities here, as it enables the integration of MS with IR spectroscopy. IR spectra can be recorded with the selectivity of mass spectrometry, hence for individual components in the complex mixture. In contrast to a mass spectrum, an IR spectrum is very diagnostic for the molecular structure, so that for instance new biomarkers for metabolic diseases may be identified. With the molecular structure information, new strategies for diagnostics and therapeutics may be developed.</p>	
<p>The method of infrared ion spectroscopy (IRIS) is also applicable in fields beyond metabolomics. Molecular structure identification of unknown compounds is for instance also relevant environmental studies (e.g. drinking water contaminants), pharmaceutical sciences (drug metabolism) and forensic investigations (molecular structure of uncontrolled “designer” drugs).</p>	