

Infrared free electron lasers in (bio)analytical chemistry

The four FELs at the HFML-FELIX user facility (FELIX-1, FELIX-2, FELICE and FLARE) each produce their own range of wavelengths and together they provide a tuning range between 3 and 1500 micrometer (0.2-110 THz). FELICE is a unique FEL beamline dedicated to intra-cavity experiments: the intensity at the point of the experiments is 50 to 100 times higher compared to the conventional user stations. The 20 end stations provide a variety of experimental setups including mass spectrometers, pump-probe setups, synchronized laser (ns, ps, fs), cryostats etc. Additionally, the FEL beamlines are coupled to the magnets of the High Field Magnet Laboratory (HFML) providing continuous magnetic fields up to 38 Tesla (soon 45 Tesla). Research projects at FELIX include systems such as (bio)molecules, clusters and complexes, as well as semiconductors, metals and magnetic materials.

The high power IR FELs are very well suited for (bio)analytical chemistry applications. Infrared ion spectroscopy (IRIS), combining the individual analytical strengths of mass spectrometry and infrared spectroscopy, is a powerful tool for small-molecule identification in a wide range of analytical applications including metabolomics, forensics, environmental science, amongst others. At FELIX, four commercial state-of-the-art analytical mass spectrometers have been connected to the FEL beamline in order to record the IR spectra of mass-to-charge selected ions. IR spectra measured for analyte compounds provide a signature that can be matched to reference spectra, either measured from standards or predicted using quantum-chemical calculations. In combination with chromatographic separation, infrared spectroscopy of mass-selected ions provides a promising new route for the identification of the molecular structures of unknown m/z peaks in complex mixture analysis. Using currently existing experimental protocols in our laboratory an IR spectrum can routinely be measured from sub-picograms samples.

At FELIX, analytical infrared ion spectroscopy is used to elucidate the three-dimensional structure of molecules, to discover new biomarkers for metabolic diseases (in collaboration with medical institutes), to identify novel psychoactive drugs (with the forensic laboratory of the Dutch police), to identify metabolic or chemical derivatives of drugs and chemicals (for pharmaceutical and chemical companies), and to identify micro-pollutants in environmental samples (for knowledge institutes and companies).

This lecture provides of an overview of the FELIX user facility, followed by a tutorial of infrared ion spectroscopy with a focus on the applications and the opportunities to provide a commercial service for industry.

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