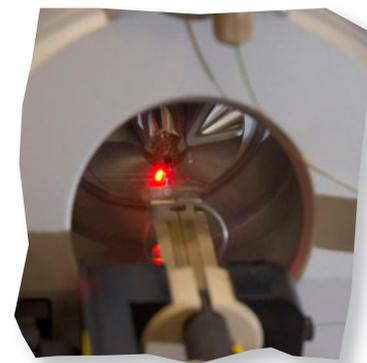


Mass Spectrometry Core Facility



The interdisciplinary nature of Mass Spectrometry (MS), which crosses the borders of physics, chemistry and biology, and the tremendous technological improvements that it has undergone have led to its increased use in biotechnology and biomedical research.

Classically, MS is considered a tool for the identification and characterisation of molecules. It has been defined as 'the art of measuring atoms and molecules to determine their molecular weight'.

Furthermore, MS has also been used to address questions about conformation and structural biology as mass analysis techniques have the capacity to detect changes in protein conformation under a wide range of conditions. Moreover, the development that MS has experienced in recent years allows intact protein complexes to be directly detected. Therefore, these analytical techniques now permit the study of non-covalent protein-protein and ligand-protein interactions, thereby improving our understanding of the mechanisms of action of these proteins in several biological processes. The capacity of MS to identify and, increasingly, to study protein-ligand interactions is expected to have a significant impact on biological and medical research. The Mass Spectrometry Core Facility provides scientific and technical support to the scientific community at IRB Barcelona, thereby combining the powerful capacity of the new MS techniques in life sciences with ongoing structural and biological research at the Institute.

The Mass Spectrometry Core Facility at IRB Barcelona is equipped with high accuracy and high resolution mass spectrometers, which are used for the identification and characterisation of a broad range of biological species, from small molecules to large biomolecules (eg intact proteins), as well as conformation, structural biology and non-covalent interactions of these biomolecules and complexes. The Facility also plans to include the study of protein biomarkers, which can indicate the presence and progression of a variety of diseases or response to drugs.

Services for IRB Barcelona researchers

The services offered include MS, MS/MS and MSⁿ analysis using atmospheric pressure ionization techniques (electrospray and APCl) coupled with LC or infusion inlets. The Facility also provides consultancy services and analytical method development for specific applications, as well as mass spectra data processing. Samples are analysed either directly by the service or by researchers trained by facility members to use mass spectrometers through an open-access system.

The Facility includes three new generation mass spectrometers, equipped with high accuracy and high resolution analysers.



LTQ FT Ultra (Thermo Scientific)

The LTQ-FT Ultra system is a fully integrated hybrid mass spectrometer consisting of a linear Ion Trap Mass Spectrometer, LTQ XL™, combined with a Fourier Transform Ion

Cyclotron Resonance Mass Spectrometer. The instrument is provided with ESI, mESI, nanoESI and ApCl ionisation sources and CID, ECD, IRMPD fragmentation technologies.

The whole configuration system has a quaternary micro LC pump attached (Mod Surveyor MS), and a micro-autosampler (Micro AS). For its installation, this mass spectrometer required the handling of 500 l of liquid N₂ and 500 l of liquid He to cool down the magnet from room temperature.

With an accuracy of 0.5-1 ppm at m/z 400, the LTQ-FT has exceptional applications in chemistry for the identification and structural characterisation of compounds. For applications in biology, it permits both bottom-up (proteomics) and top-down approaches for the analysis of intact proteins, including post-translational modifications (Instrument Mass Range: 50-4000 Da).



Core Facility Members | Mass Spectrometry Research Specialist:
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Synapt High Definition MS System (Waters-Micromass)

The Synapt is a hybrid QTOF instrument which has a Tri-wave Cell between the two analysers. This configuration allows high performance tandem MS to be combined with

high efficiency ion mobility, thus permitting the analysis of samples differentiated not only by their mass to charge ratio (like standard analysers) but also by their size and shape.

The instrument has ESI, nanoESI and ESCI™ (ESI, Apcl) capacity. Samples can be introduced by syringe pump or LC inlets. The instrument can also be attached to an Advion Triversa Nanomate, a robot which combines the strengths of LC, fraction collection and chip-based infusion into a single integrated system.

The instrument is used to analyse and study the macromolecular structure and conformation of intact proteins. It also has applications for the study of non-covalent complexes which can survive the transfer from solution to the gas phase thanks to the incorporation of 'ion cooling'. In addition, the Synapt has potential for top-down protein sequencing by increasing the sequence coverage obtained from



LCT-Premier XE (Waters-Micromass)

The LCT-Premier XE system is an orthogonal acceleration time-of-flight mass spectrometer. The system is provided with ESI, nanoESI (modified to perform H/D experiments) and

ESCI™ (ESI, Apcl) capacity. Samples can be introduced by syringe pump or LC inlets. The instrument has a UPLC Acquity Chromatography system attached.

The instrument allows the detection of large single- or multiply-charge species with accurate mass measurements. Its extended mass range up to m/z 30000 allows the detection of large biomolecule complexes. Like the Synapt, it is provided with ion cooling, or intermediate vacuums, which allow the transmission of non-covalent complexes when ejected from solution to the gas phase. This system has also been modified to achieve inert conditions inside the ionization source, in order to allow amide hydrogen H/D exchange experiments and prevent the exchange during ionization and desolvation. These kinds of experiments will permit the study of the dynamic and structural properties of proteins and their complexes.