



## Ultra-performance Liquid Chromatography – High Resolution Mass Spectrometry, U-HPLC-HRMSn (LC–MS)



### TECHNICAL DETAILS

**Manufacturer:** Thermo Scientific

**Model:** Nicolet iN10MX

**Extras:** equipped with DTGS, MCT-B and MCT Array

### HOW IT WORKS?

The system comprises a Thermo Scientific UHPLC, model Ultimate 3000, coupled to a HRMSn, model Orbitrap Elite. The mass spectrometer is a hybrid system capable of high resolution (Orbitrap) and MSn, n up to 10 (linear trap), and is equipped with Electrospray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) ion sources.

The UHPLC and the MS can work combined or separately.

The MS can detect the m/z ratio of charged molecules or molecular systems. The high resolution and high accuracy usually give the molecular form of detected ions. The system is also capable of performing sequential (multistage) Mass Spectrometry, MSn. The combination of the exact masses, isotope distributions and fragmentations patterns allows for identification of many compounds. ElectroSpray Ionization (ESI), for polar compounds, Atmospheric Pressure Chemical ionization (APCI), for less polar compounds, are available.

The system can also be used to quantify molecules by following the intensity of m/z signals or of any fragments(s) produced by MSn with very high selectivity and sensitivity. Samples can be introduced directly into the MS (infusion) or via U-HPLC. The UHPLC separates the compounds before they arrive at the MS. The high-pressure capability of the U-HPLC allows the use of thin columns and high surface stationary phases, which can separate many compounds in a short time.

The U-HPLC is equipped with a quaternary pump, a solvent degasser, an autosampler, a column compartment with temperature control and a Diode Array Detector (DAD).

This detector can be used to obtain the UV-Vis absorption spectra of separated compounds and to quantify molecules showing absorbance in the UV-Vis spectral region.

CCMAR expertise includes:

- Routine liquid chromatography separation and mass spectrometry analysis with identification and quantification of compounds.
- Analysis of complex samples.
- Development and implementation of UHPLC and UHPLC-HR-MSn methods.
- Analysis of LC-MS profiles with Compound Discoverer™.
- Analysis of regulated marine biotoxins (all) and other non-regulated biotoxins.
- Metabolomics."

### ESI/APCI-HRMSn (infusion)



Hybrid high resolution (> 200 000) mass spectrometer equipped with an Orbitrap analyzer (high field) and a linear trap capable of MS<sub>n</sub>, n up to 10, by collision-induced dissociation, CID, and high energy C-trap dissociation, HCD. The system is equipped with Electrospray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) ion sources.

CCMAR expertise includes:

- Determination of the molecular weight and molecular formula of organic and inorganic compounds.
- Structural analysis and main chemical groups of unknown molecules.
- Gas-phase structure, including weight and stoichiometry, of supramolecular structures.

### APPLICATIONS

The system can be used in any research area requiring identification and/or quantification of organic or inorganic compounds. Commonly, over 10 thousand compounds are detected in a single natural sample profile. Excalibur software, version 4.0, and all applications therein, can be used for data processing and is free. Compound Discoverer software, version 3.1, is also available for processing the LC-MS profiles.

This software analyses the gathered mass spectral information and identifies many compounds by comparing the experimental data with the available in local mass spectral libraries and online databases such as KEGG or Human Metabolome. Several workflows are available for data processing, including metabolomics and associated statistical tools, the search of metabolic pathways and the discovery of metabolites of a given compound.

### ANALYSIS REQUIREMENTS

The equipment can detect a wide range of compounds or molecular systems, ranging from high polar to non-polar. Low polarity compounds are however more difficult to ionize under ESI or APCI and usually give lower intensity signals. As the system detects the m/z ratios and large molecules usually acquire many charges upon ionization the m/z range of detection is usually not a problem.

GFP, for example, can be readily seen below m/z 1500. Samples are delivered at laboratory 1.47 as a clear solution (no particles) in transparent vials and should not contain nonvolatile salts or solvents (NaCl, phosphates, DMSO, etc). Analysis can be performed from low volumes (> 25 µL) in glass inserts placed inside transparent vials.

### ACCESS CONDITIONS

Remote