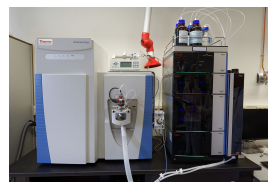


Q Exactive Focus Orbitrap LC-MS/MS

<https://labfacilities.wur.nl/SearchDetail.aspx?deviceid=d82bfd7c-bab0-44d7-a194-347c1e9bb2c7>

Brand

Thermo Scientific



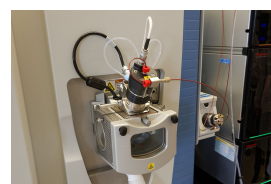
Type

Contact

Mark Sanders (mark.sanders@wur.nl)

Organisation

Agrotechnology & Food Sciences Group



Department

Food Chemistry

Description

This analytical platform is designed for use in a wide range of both metabolomics (small molecules) and proteomics analyses. With its high sensitivity, fast scan speed and fast polarity switching at high mass resolution, the Q Exactive Orbitrap FTMS mass spectrometer is an outstanding detector for fast and high-throughput chromatographic separation, for mass peak annotation and quantitation required for metabolomics and proteomics analyses. Attached to a Thermo Vanquish UHPLC system for high resolution chromatographic separation, photodiode array detector and the online (+/-) switching capability at high mass resolution the system allows the most comprehensive identification and metabolomics profiling of compounds present in complex samples and saves considerable time during experiments in which screening in both ionization modes is necessary or desired. In addition, the high resolution MS/MS data, generated by using the quadrupole (Q) option with high collision dissociation (HCD), enables identification and quantitation of many different compounds with great confidence. The precursor ion trapping option (C-trap) and fast switching Orbitrap MS/MS guarantees very high sensitivity in detection and identification providing accurate mass MS/MS spectra.

Technical Details

•Supplier: Thermo Scientific Instruments Specifications: Q Exactive Focus MS attached to a Thermo Vanquish Liquid Chromatography system. The Thermo Scientific Q Exactive Focus benchtop LC-MS/MS combines high-performance quadrupole precursor selection with very high resolution, accurate-mass Orbitrap FTMS detection to deliver high performance and tremendous versatility. All features are essential for the envisaged applications and specifications are greatly advanced compared to the existing old instruments. The key features are:

- Resolving power up to 70,000 (FWHM) at 200 m/z
- General mass range 100 – 1,200 Da up to 500 – 6,000 Da
- Mass accuracy < 1 ppm
- Maximum scan speed 12Hz
- Intra-scan dynamic range > 5000:1
- Quadrupole mass filter
- C-trap precursor ion trapping
- High-energy collisional dissociation (HCD)
- Spectral multiplexing for enhanced duty cycle
- S-Lens ion source for increased sensitivity
- HESI ion Source
- Vanquish UPLC separation
- Diode Array detection is possible

Software

Using dedicated software (Compound Discoverer 2.0) for untargeted data analyses, large series of samples can be compared for differences and similarities in the relative abundance of all small molecules detected, both known and yet unknown compounds.

This software package can identify compounds using the accurate mass MS, MS/MS and the isotope pattern in the search in several databases like mzCloud™, Chemspider, KEGG. Compound Discoverer 2.0 can predict possible metabolites from these identified compounds and uses this information to identify more unknown compounds in the samples. For quantification of targeted compounds a special software package, TraceFinder 4.0, is available.

Applications

- Targeted analyses natural and chemical compounds, like plant (secondary) metabolites, oligosaccharides and peptides
- Untargeted metabolomics: global profiling and comparison of hundreds of known and yet unknown metabolites Using dedicated software (compound discoverer 2.0) for untargeted data analyses, large series of samples can be compared for differences and similarities in the relative abundance of all small molecules detected, both known and yet unknown compounds.
- Compound identification using MS and MS/MS at ultra-high mass resolution
- Targeted quantitation of compounds in complex samples. Multiple approaches for quantitation including Selected Ion Monitoring (SIM), Parallel Reaction Monitoring (PRM) and Data-Independent Acquisition (DIA) are available. The dynamic range is >5.000:1. Linear dynamic range up to 4-6 orders of magnitude.

Publications

Mass Spectrometric Characterization of Benzoxazinoid Glycosides from Rhizopus-Elicited Wheat (*Triticum aestivum*) Seedlings. , Wouter J. C. de Bruijn, Jean-Paul Vincken, Katharina Duran, and Harry Gruppen* (2016) , J. Agric. Food Chem., 64 (32), p. 6267–6276., <https://pubmed.ncbi.nlm.nih.gov/27431363/>