GLP AGROCHEMICAL ANALYSIS

RPS' Bedford laboratory has a highly trained GLP team with many years of experience in the agrochemical industry, and we are able to manage a wide range of residues studies, following OECD Test Guidelines and EU/EC Guidance Documents.

High Resolution Accurate Mass Spectrometry (HRAMS)

At RPS, instead of using a traditional triple quadrupole (QQQ) mass spectrometer for analysis, we use a Thermo Scientific Q-Exactive Orbitrap Mass Spectrometer HRAM instrument.

What is the Q-Exactive Orbitrap HRAM instrument?

- The Q-Exactive Orbitrap HRAM mass spectrometer is an instrument that is able to deliver both high quality qualitative and quantitative analysis. Typically, qualitative analysis would need to be performed by a quadrupole-time-of-flight instrument (Q-TOF) and quantitative analysis would be performed by QQQ instrument.
- The high mass resolving power of the Q-exactive allows quantitative and qualitative analysis to occur simultaneously.
- Q-TOFs and other high resolution instruments, tend to have rapid saturation of the detector, causing serious problems with the linearity of response of the instrument. The Q-Exactive has demonstrated linearity ranges of up to 5 orders of magnitude, as it does not suffer with detector saturation.
- The Q-exactive is able to determine the accurate mass of an ion of interest. This mass accuracy can be better than 1 ppm, allowing for very selective analysis.
- Using suitable software, a suggested elemental composition of any molecular and fragment ions detected can be determined. This is a powerful tool for structural elucidation or confirmation.

How does this benefit our clients?

Retrospective Qualitative Data Analysis

- Retrospective analysis of previously acquired Full Scan data can be achieved using the Q-Exactive, not achievable using QQQ.
- This is useful to qualitatively determine unknown metabolites or contaminates at a later date.
- No re-sampling or retesting required, saving time and money.

Analysis of "tricky" compounds

- Due to the additional selectivity of the Q-exactive, compounds with poor fragementation can be confidently identified using a single fragmentation ion or the parent ion alone.
- QQQ requires at least two different fragmentation ions which is not always possible for small molecules, which therefore require additional secondary confirmation method.

More robust methods

- Different scan modes can be combined within the same run to make the analytical method more robust, providing added confidence of the analysis.

Less interference

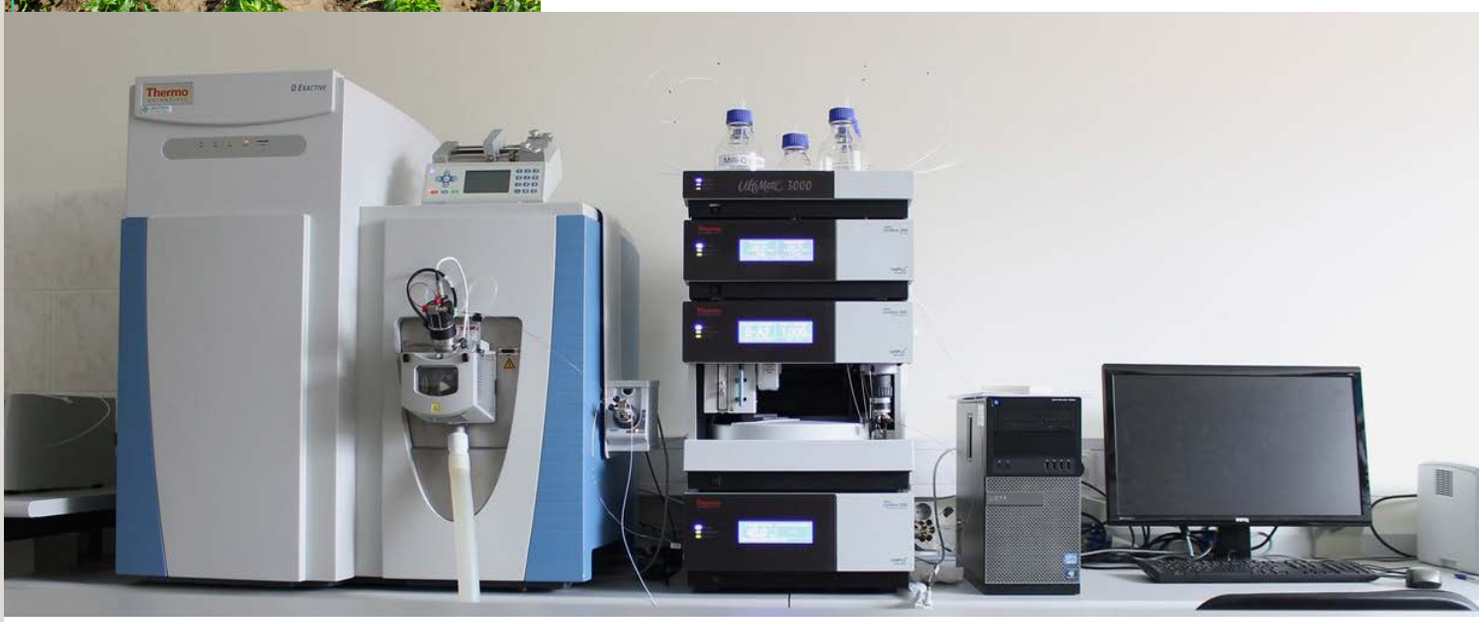
- Due to its high selectivity and resolution, there is a greater confidence that the analyte of interest can easily be resolved from any interferences.
- Less chance of any false positives or false negatives being reported.

Limits of Detection (LOD) and Limit of Quantification (LOQ)

- The Q-exactive is able to achive similarly low LOD's and LOQ's that are achievable on the QQQ.
- In some cases, due to reduced background noise and high resolving power, LOD's and LOQ's are significantly better, especially in complex matrices.

Comparison of Q-Exactive and QQQ Instruments

- Both QQQ Instruments and Q-Exactive works in a similar way, the Q-Exactive Orbitrap is a trapping device, whereas the QQQ is a scanning device.
- A QQQ uses the 1st quadrupole to scan a sample looking for specific parent ions masses. As these are not at accurate masses, the identity of the ions is highly uncertain. To gain the confidence required, the parent ions are bombarded by nitrogen gas within the 2nd quadrupole causing them to fragment and form fragmentation ions which are scanned by the 3rd quadrupole looking for specific masses. High sensitivity and selectivity can only be achieved by monitoring the fragment ions masses, known as a multiple reaction monitoring (MRM) scan.
- The Q-Exactive replaces the 3rd quadrupole with an Orbitrap, which acts as both a mass analyser and detector. The Orbitrap is comprised of a central electrode surrounded by 2 outer electrodes, which causes ions to revolve around the central electrode. Different masses will revolve at different rates, and after extensive oscillations of ions, mass separation occurs and the acurate masses can be determined.
- After initial screening using the 1st quadrupole, ions are stored in the C-Trap. The C-Trap is sends ions to the Orbitrap in waves to avoid the Orbitrap becoming saturated or any other space charging issues.
- For fragmentations, the C-Trap sends ions to the HCD cell that replaces the 2nd quadrupole. High purity nitrogen bombards the ions causing them to fragment, before sending all the fragments back to the C Trap for analysis and detection by the Orbitrap.
- Due to this extensive oscillations of ions, highly selective and sensitive data can be obtained from both the parent ion, using a Full Scan or Single Ion Monitoring (SIM) and from fragmentation ions, using Parallel Rection Monitoring (PRM) or All Ion Fragmentation (AIF) analysis.



We work with agrochemical companies of all sizes. Contact us to find out more about how we can support you to meet data requirements for the registration of your active substances or formulated products.

Brad Flegg

Business Development Manager
Analytical Services

+44 1618 743 730

brad.flegg@rpsgroup.com

Marco Lattughi

Operational Director
Analytical Services

+44 (0) 1462 480 400

marco.lattughi@rpsgroup.com

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