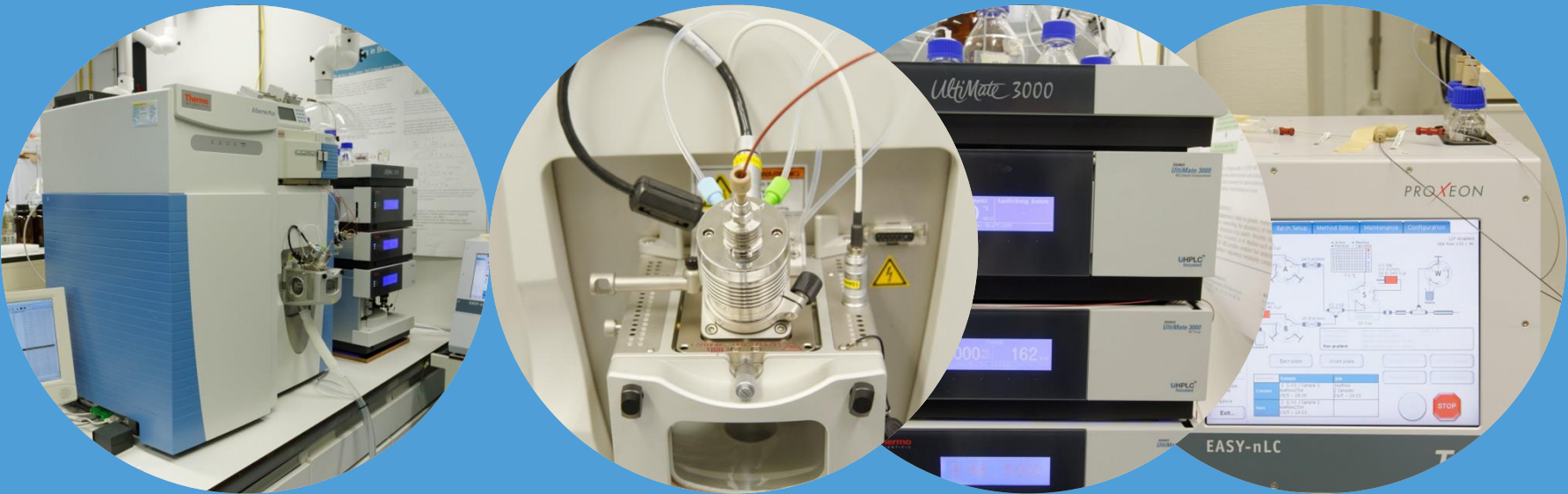


Q Exactive

Thermo Scientific Q Exactive^{Plus} Orbitrap FTMS-MS/MS

June 18th, 2014. Ric de Vos & Twan America



A benchtop model FTMS

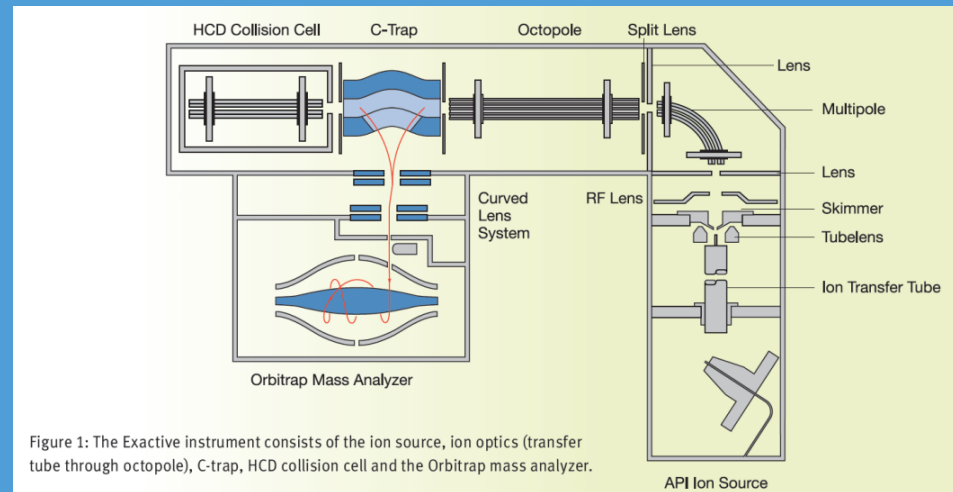


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→



Features of the Q Exactive

- Orbitrap mass analyzer
- Ultrahigh mass resolution
- Scan-to-scan polarity mode switching
- Quadrupole mass filtering ability
- Scan speed up to 12 Hz
- High-energy collision dissociation (HCD)
- Variety of MS and MS/MS methods: high flexibility



Q Exactive facility includes:

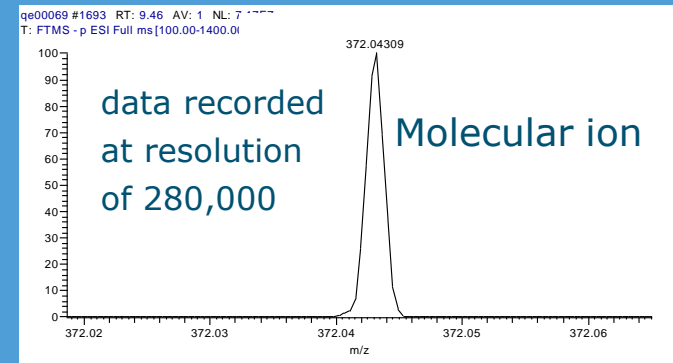
- ESI and APCI source
- U-HPLC system Ultimate 3000 (Dionex)
 - Nanomate fraction collector/injection robot (Advion) available
- PDA-detector (Thermo): 190-900nm
- Easy Nano-LC II (Proxeon)
 - 2D-LC system directly accessible

➤ For both targeted and untargeted metabolomics and proteomics !



Key feature: ultrahigh mass resolution

- Up to 280,000 FWHM
 - TOF's: max ~40,000
 - previous Orbitraps: 120,000
- Stable, high mass accuracy
 - <2 ppm deviation
- High dynamic range
 - >5 orders of magnitude
- Powerful tool for elemental formula determination

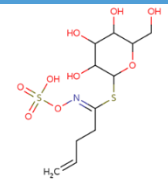
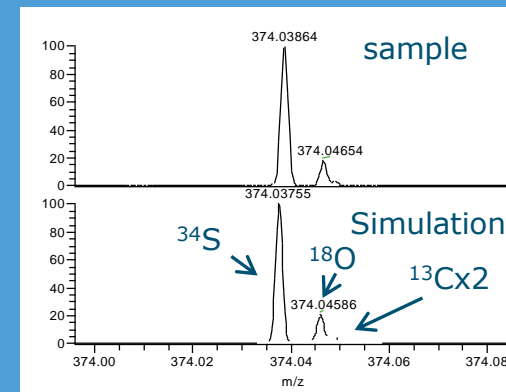
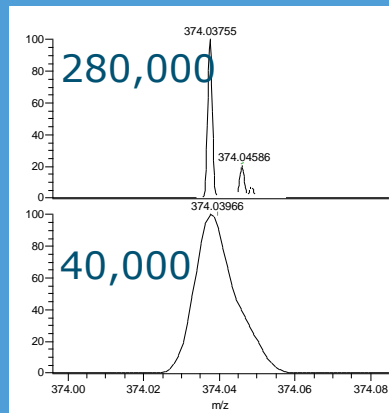


m/z	Theo. Mass	Delta (ppm)	Composition
372.04309	372.04309	0.01	C ₅ H ₂₁ O ₆ N ₅ P ₃ S
	372.04312	-0.07	C ₂₁ H ₁₁ O ₄ NP
	372.04289	0.54	C ₁₅ H ₂₂ NP ₄ S
	372.04331	-0.60	C ₁₁ H ₁₀ O ₁₀ N ₅
	372.04333	-0.66	C ₁₄ H ₁₉ ON ₃ PS ₃
	372.04285	0.66	C ₁₁ H ₁₈ O ₉ NS ₂
	372.04247	1.68	C ₁₃ H ₁₅ O ₆ N ₃ PS
	372.04374	-1.74	C ₁₃ H ₁₇ O ₄ N ₃ P ₃

☹ still 8 possibilities within 2 ppm

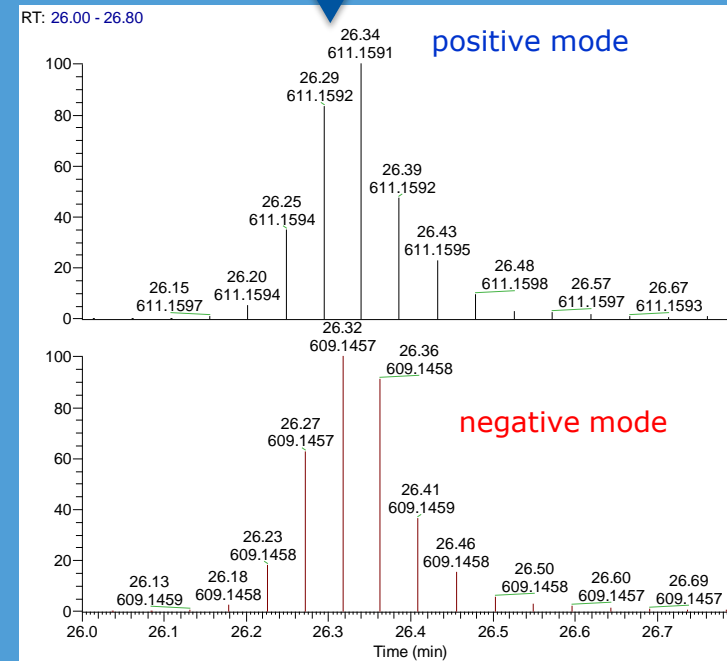
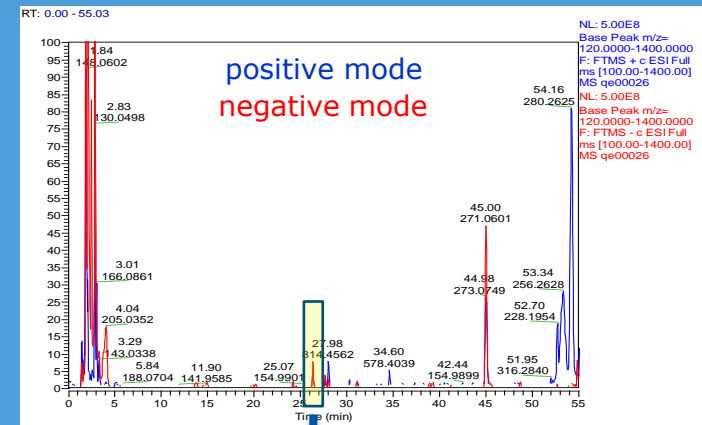
☺ solution: 2nd isotope pattern

High mass resolution is essential



Key feature 2: polarity switching at high mass resolution

- Accurate masses of positive and negative ions within same run
 - Analysis at both polarities: higher coverage of compounds present in extract
 - Similar to LCMS in each mode separately, but without any chromatographic shifts
 - Improved ability to detect and verify molecular ions

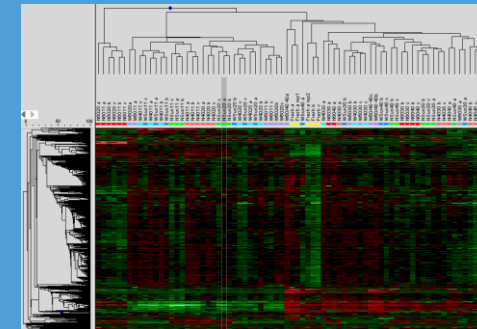
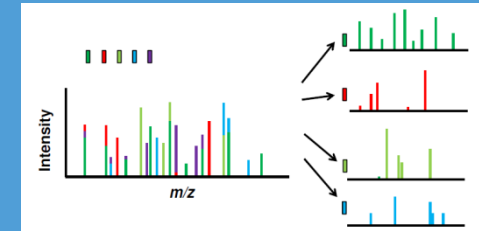


<1 ppm shift over entire
LCMS peak in both modes

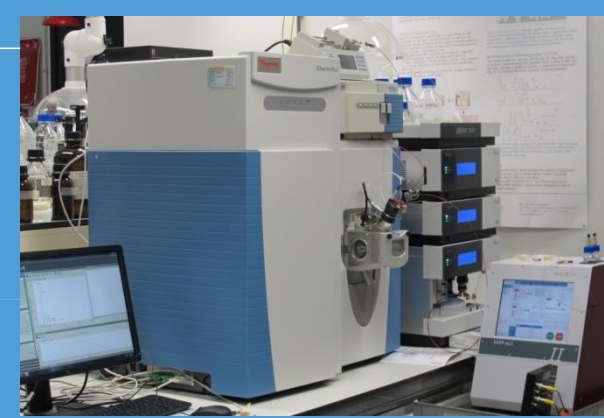
Q exactive: Metabolomics applications



- Accurate mass LC-MS and MS/MS
 - 1 or 2 polarity modes simultaneously
 - Compound identification at high mass resolution
- Targeted and untargeted analyses
 - Targeted: multiplexed MS/MS of compounds in crude extracts
 - Untargeted: relative abundance of hundreds of metabolites in extracts
 - Compare samples for differences and similarities in global metabolome



Q exactive: Proteomics applications

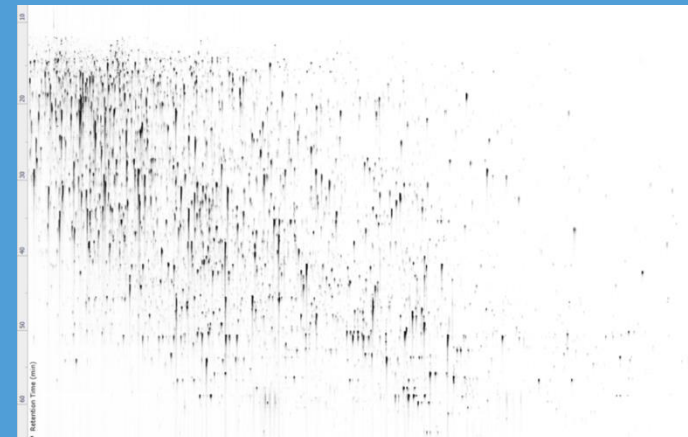


- 1D or 2D nanoLC-HD MS/MS
 - Identify ten thousands of peptides
 - Identify a few thousand proteins

- Quantification

- Untargeted: label-free
- Targeted:
 - PRM, multiplexed
 - +/- labelled standard

```
Number of filtered/unfiltered result items:  
- 970/997 protein group(s)  
- 3307/3307 merged protein(s)  
- 7465/7465 peptide(s)  
- 46500/46500 PSM(s)  
- 459766/459766 search input(s)
```



Q-Exactive: a useful tool in your research?

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Info proteomics:

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BU-Bioscience

Plant Research International

