

LTQ Orbitrap XL

Positive ionization: instrument is externally calibrated each day using Caffeine, MRFA (MET-ARG-PHE-ALA), and Ultramark 1621.

Negative ionization: instrument is externally calibrated using Caffeine, MRFA, Ultramark 1621, Sodium Dodecyl Sulfate and Sodium Taurocholate.

The LTQ Orbitrap XL also has the ability to use internal calibration with one or more ions (Lockmass).

Loop-injection method

A Thermo Scientific Surveyor MicroLC is used to provide solvent flow at 20 μ L/min., through a 2 μ L sample loop into which the sample is injected. Solvents used H₂O:MeOH (1:1). Sample preparation as per ZQ.

Advion Triversa NanoMate (nano-electrospray)

The NanoMate is used to deliver samples diluted into MeOH + 10% NH₄OAc, or suitable solvent (salts are diluted into MeOH only) at a flow of approximately 0.25 μ L/min.

<u>API source settings</u>	<u>Infusion</u>	<u>NanoMate</u>
Source Temperature	275°C	200°C
Sheath Gas flow	3 to 7 (arb. units)	2 (arb. units)
Aux Gas flow	Not used	Not used
Capillary (ionising) voltage		
positive ionisation:	+ 3.2 to 3.7kV	1.4kV
negative ionisation:	- 3.5 to - 4.0kV	-1.4kV

Mass spectra acquired at a minimum resolution of 30,000 (at m/z 400).



Specifications*

Resolution

7500, 15000, 30000, 60000 or 100,000 (FWHM) @ m/z 400 with a scan repetition rate of 1 second

Mass Range

m/z 50–2000; m/z 200–4000

Mass Accuracy

<3 ppm RMS for 2 h period with external calibration using defined conditions,
<2 ppm RMS with internal calibration

Dynamic Range

>10000 between mass spectra, >4000 between highest and lowest detectable mass in one spectrum

* Adapted from LTQ Orbitrap XL Hardware Manual, © Thermo Fisher Scientific Inc.