EI low resolution

Instrument: double focussing sectorfield mass spectrometer

Manufacturer: Thermofinnigan MAT (Bremen, Germany)

Model: MAT95XL
Resolution: 2000 (10% valley definition)

Scan: 40 – 1000 amu (1 sec/decade)
Source Temp.: 180°C
Electron energy: 70 eV

EI accurate mass:

Method: peak matching
Resolution: 10000 (10% valley definition)
Mass calibrant: PFK

ESI:

Instrument: linear iontrap coupled with orbitrap mass analyser
Manufacturer: ThermoFisher Scientific (Bremen, Germany)
Model: LTQ-Orbitrap Velos
Resolution: 100000 FWHM at (m/z = 400 amu)
Scan: 50-2000 amu (resulting in acquisition times of 1.6 sec per cycle)

Electrospraymeasurements were performed in direct infusion mode using a custom made microspray-device mounted on a Proxeon nanospray ion source. The microspray-device allows for the sample infusion through a stainless steel capillary (90 µm I. D.).

Accurate mass measurements in the orbitrap were performed using the lock mass option of the instrument control software using the cation of tetradecyltrimethylammonium bromide (256.29988 amu) as internal mass reference.

Sample concentration: approx. 50 µg/mL
Solvent: MeOH spiked with 0.1 mg/mL tetradecyltrimethylammonium bromide (unless otherwise stated)
Flow: approx. 1 µL/min
Typical sprayvoltage pos. mode: 2.3 - 2.8 kV
Typical sprayvoltage neg. mode: 1.7 - 2.5 kV