

## **ESI-TOF** (all spectra with „Agilent“ in the header (old software) or “Counts (%) vs. Mass-to-Charge (m/z)” below the graph):

Samples were measured on an Agilent 6210 ESI-TOF, Agilent Technologies, Santa Clara, CA, USA. Solvent flow rate was adjusted to 4  $\mu\text{L}/\text{min}$ , spray voltage set to 4 kV. Drying gas flow rate was set to 15 psi (1 bar). All other parameters were adjusted for a maximum abundance of the relative  $[\text{M}+\text{H}]^+$ .

(ESI-TOF = electrospray ionization - time of flight)

## **ESI-FTICRMS** (all spectra with “lonspec”, “Varian QFT” or “Varian 901-MS” in the header):

Samples were measured on an lonspec QFT-7, Varian Inc. (now Agilent Technologies), Lake Forest, CA, equipped with a 7 T superconducting magnet and a Micromass Z-Spray ESI-Source, Waters Co., Saint-Quentin, France. Solvent flow rate was adjusted to 4  $\mu\text{L}/\text{min}$ , spray voltage was set to 3.8 kV. All other parameters were adjusted for a maximum abundance of the relative  $[\text{M}+\text{H}]^+$  ( $[\text{M}+\text{Cat}]^+$  or  $[\text{M}-\text{H}]^-$ , respectively ...)

(ESI-FTICRMS = electrospray ionization - Fourier transform ion cyclotron resonance mass spectrometry)

This mass spectrometer also can be equipped with an APCI source (Z-Spray APCI Source, Waters Co., Saint-Quentin, France) or a Nanospray ion source (NSI source, MS Horizons, Almere, Netherlands).

## **EI-MS** (all spectra with “Instrument: MAT 711” in left box):

Samples were measured on a MAT 711, Varian MAT, Bremen. Electron Energy for EI was set to 80 eV. (Sometimes a temperature is given as well, may be added here ...)

## **FAB-MS** (all spectra with “Instrument: CH-5” in left box):

Samples were measured on a CH-5, Varian MAT, Bremen. Glycol (Metanitrotoluene, ...) was used as matrix.