## Templates: Instrumental Descriptions for HR-ESI-MS and -MS/MS

(Synapt G2 QTOF mass spectrometer; Laboratory for Mass Spectrometry)

## LC-HR-ESI-MS

Liquid chromatography high resolution electrospray ionization mass spectrometry (LC-HR-ESI-MS): *Acquity UPLC* (*Waters*, Milford, USA) connected to an *Acquity*  $e\lambda$  diode array detector and a *Synapt G2* HR-ESI-QTOF-MS (*Waters*, Milford, USA); injection of 1 µL sample ( $c = ca. 10-100 \mu g mL-1$  in the indicated solvent); *Acquity BEH C18* HPLC column (1.7 µm particle size, 2 × 50 mm, *Waters*) kept at 30 °C;\* elution at a flow rate of 400 µL min-1 with A: H<sub>2</sub>O + 1% HCO<sub>2</sub>H and B: CH<sub>3</sub>CN + 0.1% HCO<sub>2</sub>H, linear gradient from 5–98% B within 5 min, then isocratic for 1 min;\* UV spectra recorded from 200–600 nm at 1.2 nm resolution and 20 points s-1; ESI: positive ionization mode, capillary voltage 3.0 kV, sampling cone 40V, extraction cone 4V, N<sub>2</sub> cone gas 4 L h-1, N<sub>2</sub> desolvation gas 800 L min-1, source temperature 120°C; mass analyzer in resolution mode: mass range 100–2'000 *m/z* with a scan rate of 1 Hz; mass calibration to <2 ppm within 50–2'500 *m/z* with a 5mM aq. soln. of HCO<sub>2</sub>Na, lockmasses: *m/z* 195.0882 (caffein, 0.7 ng mL-1) and 556.2771 (Leucine-enkephalin, 2 ng mL-1).

\* check for effectively used chromatographic conditions (column and solvent system).