Templates: Instrumental Descriptions for HR-ESI-MS and -MS/MS
(*QExactive* spectrometer; Laboratory for Mass Spectrometry)

HR-ESI-MS with On-Flow Injection (routine service)

High resolution electrospray ionization mass spectrometry (HR-ESI-MS): *Dionex Ultimate 3000* UHPLC system (*ThermoFischer Scientifics*, Germering, Germany) connected to a *QExactive* MS with a heated ESI source (*ThermoFisher Scientific*, Bremen, Germany); on-flow injection of 1 μL sample (*c* = ca. 50 μg mL^{-1} in the indicated solvent) with an *XRS* auto-sampler (*CTC*, Zwingen, Switzerland); flow rate 120 μL min^{-1}; ESI: spray voltage 3.0 kV, capillary temperature 280 °C, sheath gas 30 L min^{-1}, aux gas 8 L min^{-1}, s-lens RF level 55.0, aux gas temperature 250 °C (N_2); full scan MS in the alternating (+)/(−)-ESI mode; mass ranges 80–1’200 *m/z*, 133–2’000 *m/z*, or 200–3’000 *m/z* at 70’000 resolution (full width half-maximum); automatic gain control (AGC) target of $3.00 \cdot 10^6$; maximum allowed ion transfer time (IT) 30 ms; mass calibration to <2 ppm accuracy with *Pierce*® ESI calibration solns. (*ThermoFisher Scientific*, Rockford, USA); lock masses: ubiquitous erucamide (*m/z* 338.34174, (+)-ESI) and palmitic acid (*m/z* 255.23295, (−)-ESI).

LC-HR-ESI-MS

Liquid chromatography high resolution electrospray ionization mass spectrometry (LC-HR-ESI-MS): *Dionex Ultimate 3000* UHPLC system (*ThermoFischer Scientifics*, Germering, Germany) equipped with a DAD-3000 diode array detector and connected to a *QExactive* MS with a heated ESI source (*ThermoFisher Scientific*, Bremen, Germany); injection of 1 μL sample (*c* = ca. 50 μg mL^{-1} in the indicated solvent) with an *XRS* auto-sampler (*CTC*, Zwingen, Switzerland); *Acquity BEH C18* HPLC column (1.7 μm particle size, 2 × 100 mm, *Waters*) kept at 30 °C;* elution at a flow rate of 400 μL min^{-1} with A: H_2O + 1% HCO_2H and B: CH_3CN + 0.1% HCO_2H, 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: spray voltage 3.5 kV, capillary temperature 260 °C, sheath gas 45 L min^{-1}, aux gas 15 L min^{-1}, sweep gas 2 L min^{-1}, s-lens RF level 450.0, aux gas temperature 250 °C (N_2); full scan MS in (+)-ESI (or in (−)-ESI) mode; mass ranges 80–1’200 *m/z*, 133–2’000 *m/z*, or 200–3’000 *m/z* at 70’000 resolution (full width half-maximum)**; automatic gain control (AGC) target of $3.00 \cdot 10^6$; maximum allowed ion transfer time (IT) 30 ms; mass calibration to <2 ppm accuracy with *Pierce*® ESI calibration solns. (*ThermoFisher Scientific*, Rockford, USA); lock masses: ubiquitous erucamide (*m/z* 338.34174, (+)-ESI) and palmitic acid (*m/z* 255.23295, (−)-ESI).

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

** check for effectively used resolution.