

Templates: Instrumental Descriptions for EI-, CI-, HR-EI-, HR-CI-, and GC-MS

(DFS spectrometer; Laboratory for Mass Spectrometry)

EI-MS:

Electron ionization mass spectrometry (EI-MS): double-focusing (BE geometry) magnetic sector mass spectrometer *DFS (ThermoFisher Scientific, Bremen, Germany)*; solid probe inlet; EI at 70 eV; source temperature 200 °C; acceleration voltage 5 kV; magnetic scan mode; mass range 30–900 m/z^* at 2'500 resolution (10% valley definition) and scan rate of 2 s per decade; mass calibration with perfluorokerosene (PFK, *Fluorochem, Derbyshire, UK*).

* check for effectively used mass range.

CI-MS:

Chemical ionization mass spectrometry (CI-MS): double-focusing (BE geometry) magnetic sector mass spectrometer *DFS (ThermoFisher Scientific, Bremen, Germany)*; solid probe inlet; CI with iso-butane as the reactant gas at 130–200 eV;* source temperature 200 °C; acceleration voltage 5 kV; magnetic scan mode; mass range 30–900 m/z at 2'500 resolution (10% valley definition) and scan rate of 2 s per decade; mass calibration with perfluorokerosene (PFK, *Fluorochem, Derbyshire, UK*).

* check for effectively used reactant gas, ionization voltage, and mass range.

HR-EI-MS:

High resolution electron ionization mass spectrometry (HR-EI-MS): double-focusing (BE geometry) magnetic sector mass spectrometer *DFS (ThermoFisher Scientific, Bremen, Germany)*; solid probe inlet; EI at 70 eV; source temperature 200 °C; acceleration voltage 5 kV; electric scan mode; mass range 300–350* m/z at 10'000 resolution (10% valley definition) and scan rate of 100–200 s per decade; mass accuracy ≤ 2 ppm after calibration with perfluorokerosene (PFK, *Fluorochem, Derbyshire, UK*).

* check for effectively used mass range.

HR-CI-MS:

High resolution chemical ionization mass spectrometry (HR-CI-MS): double-focusing (BE geometry) magnetic sector mass spectrometer *DFS (ThermoFisher Scientific, Bremen, Germany)*; solid probe inlet; CI with iso-butane as the reactant gas at 130–200 eV;* source temperature 200 °C; acceleration voltage 5 kV; electric scan mode; mass range 300–350* m/z at 10'000 resolution (10% valley definition) and scan rate of 100–200 s per decade; mass accuracy ≤ 2 ppm after calibration with perfluorokerosene (PFK, *Fluorochem, Derbyshire, UK*).

* check for effectively used reactant gas, ionization voltage, and mass range.

GC-EI-MS:

Gas chromatography high resolution electron ionization mass spectrometry (GC-HR-EI-MS): *Trace GC Ultra (ThermoFisher Scientific, Milano, Italy)* connected to a double-

focusing (BE geometry) magnetic sector mass spectrometer *DFS* (*ThermoFisher Scientific*, Bremen, Germany); injection of 1 μL sample ($c = 10\text{--}50\ \mu\text{g mL}^{-1}$ in the indicated solvent); split/splitless injector at 250 $^{\circ}\text{C}$; He (carrier gas) at 1 mL min^{-1} ; *OV-5MS* capillary column (*Ohio Valley Specialty*, Marietta, OH, USA), 30 m length, 0.25 mm i.d., 0.25 μm film thickness; gradient 15 $^{\circ}\text{C min}^{-1}$ from 120–300 $^{\circ}\text{C}$, then isothermal for 15 min;* transfer line at 250 $^{\circ}\text{C}$; EI at 70 eV; source temperature 200 $^{\circ}\text{C}$; acceleration voltage 5 kV; electric scan mode; mass range 30–900 m/z * at 2'500 resolution (10% valley definition) and scan rate of 0.6 s per decade; mass calibration with perfluorokerosene (PFK, *Fluorochem*, Derbyshire, UK).

* check for effectively used GC column, temperature profile, and mass range.

GC-CI-MS:

Gas chromatography high resolution electron ionization mass spectrometry (GC-HR-EI-MS): *Trace GC Ultra* (*ThermoFisher Scientific*, Milano, Italy) connected to a double-focusing (BE geometry) magnetic sector mass spectrometer *DFS* (*ThermoFisher Scientific*, Bremen, Germany); injection of 1 μL sample ($c = 10\text{--}50\ \mu\text{g mL}^{-1}$ in the indicated solvent); split/splitless injector at 250 $^{\circ}\text{C}$; He (carrier gas) at 1 mL min^{-1} ; *OV-5MS* capillary column (*Ohio Valley Specialty*, Marietta, OH, USA), 30 m length, 0.25 mm i.d., 0.25 μm film thickness; gradient 15 $^{\circ}\text{C min}^{-1}$ from 120–300 $^{\circ}\text{C}$, then isothermal for 15 min;* transfer line at 250 $^{\circ}\text{C}$; CI with iso-butane as the reactant gas at 130–200 eV;* source temperature 200 $^{\circ}\text{C}$; acceleration voltage 5 kV; magnetic scan mode; mass range 30–900 m/z at 2'500 resolution (10% valley definition) and scan rate of 0.6 s per decade; mass calibration with perfluorokerosene (PFK, *Fluorochem*, Derbyshire, UK)..

* check for effectively used GC column, temperature profile, reactant gas, ionization voltage, and mass range.