**Shimadzu 9030 Description**

Mass spectrometric measurements were performed with a Shimadzu Scientific Instruments QToF 9030 LC-MS system, equipped with a Nexera LC-40D xs UHPLC, consisting of a CBM-40 Lite system controller, a DGU-405 Degasser Unit, two LC-40D XS UHPLC pumps, a SIL-40C XS autosampler and a Column Oven CTO-40S. UV data was collected with a Shimadzu Nexera HPLC/UHPLC Photodiode Array Detector SPD M-40 in the range of 190 - 800nm. Mass spectra were subsequently recorded with the quadrupole time-of-flight (QToF) 9030 mass spectrometer.

The samples were held at 4 deg C in the autosampler compartment.

0.3uL of each spiked solution were injected into a sample loop and separated on a Shim-pack Scepter C18-120, 1.9um, 2.1x100mm Column, equilibrated at 40 deg C in a column oven.

A binary gradient was used:

Solvent A: Water, HPLC grade Chromasolv, with 0.1% Formic Acid

Solvent B: Acetonitrile, HPLC grade Chromasolv, with 0.1% Formic Acid

**Short (standard):**

Flow was held constant at 0.3000 mL/min and the composition of the eluent was changed according to the following gradient:

0 to 0.5 min, held at 95% A, 5% B

0.5 to 3 min, change to 5% A, 95% B

3 to 4 min, held at 5% A, 95% B

4 to 4.01 min, change to 95% A, 5% B

4.01 to 5min, held at 95% A, 5% B

**Medium:**

Flow was held constant at 0.3000 mL/min and the composition of the eluent was changed according to the following gradient:

0 to 2 min, held at 95% A, 5% B

2 to 8 min, change to 5% A, 95% B

8 to 10 min, held at 5% A, 95% B

10 to 10.01 min, change to 95% A, 5% B

10.01 to 12min, held at 95% A, 5% B

**Long:**

Flow was held constant at 0.4000 mL/min and the composition of the eluent was changed according to the following gradient:

0 to 2 min, held at 95% A, 5% B

2 to 10 min, change to 2% A, 98% B

10 to 18 min, held at 2% A, 98% B

18 to 18.01 min, change to 95% A, 5% B

18.01 to 20min, held at 95% A, 5% B

The ionization source was run in "ESI" mode, with the electrospray needle held at +4.5kV.

Nebulizer Gas was at 2 L/min, Heating Gas Flow at 10 L/min and the Interface at 300 deg C. Dry Gas was at 10 L/min, the Desolvation Line at 250 deg C and the heating block at 400 deg C.

Mass spectra were recorded in the range of 50 to 2000 m/z in positive ion mode.

Measurements and data post-processing were performed with LabSolutions 5.97 Realtime Analysis and PostRun.