

GC data acquisition method

GC-TOF-MS was performed as described by Lindeque et al. (2013) with slight modifications. The GC-TOF-MS system consisted of an Agilent© 7890A series gas chromatograph with Agilent© 7693 autosampler coupled to a LECO Pegasus HT time-of-flight mass analyzer. Samples (1 µL) were injected with a split ratio of 1:10. The front inlet temperature was kept at 250 °C and helium was used as carrier gas at a constant flow rate of 1.5 mL/min. Chromatography was performed on a Restek Rxi-5Sil MS (30m x 250 µm x 0.25 µm) column. The initial GC oven temperature was held at 70 °C for 1 min. Thereafter the oven temperature was increased by 7 °C/min until 120 °C, then 10 °C/min until 230 °C and finally 13 °C/min until 300 °C, where the temperature was held for 1 min before returned to 70 °C. For mass spectrometry, the separated compounds were subjected to electron impact ionization (EI) (70 eV), with the transferline and ion source temperatures were held at 225 °C and 200 °C respectively. After a solvent delay of 230 seconds, mass spectra were acquired (50-950 m/z) at a scan rate of 20 spectra/second. Peaks with 5 apexing masses were detected using an expected peak width of 3 seconds and a signal-to-noise (S/N) ratio of > 20. The LECO Corporation ChromaTOF software (v 4.5x) was used for data acquisition and extraction. This included automatic baseline removal via the “spanning” tracking method (offset of 1; just above the noise) and auto smoothing, with the software’s Statistical Compare feature used to align peaks.