GC sample preparation protocol

For GC-TOF-MS sample extracts (BR: 200 µL; OB: 150 µL) containing internal standards were evaporated under a stream of nitrogen gas at 37°C. Derivatisation was achieved via oximation and silylation. To oximate the samples, methoxyamine hydrochloride (20 mg/mL in pyridine, BR: 50 µL; OB: 25 µL) was added and the samples were vortex mixed (~ 1 min) to dissolve the dried compounds. The samples were then incubated at 60 °C for 1 hour. Thereafter, the samples were silylated by adding BSTFA (BR: 50 µL; OB: 25 µL) containing 1 % (v/v) TMCS and incubated at 60 °C for 1 hour. For the BR samples, the final volume (100 µL) was then transferred to 250 µL pulled point glass inserts. Due to the small volumes used during derivatisation, OB samples (50 µL) were derivatised in micro-vials designed to maximise recovery for small sample volumes. Finally, each vial was loaded onto an Agilent© 7693 auto sampler for GC-TOF-MS analysis.