

| <u>Variable</u> | <u>Set Parameter</u> |
|---|----------------------|
| Carrier Gas | Helium |
| Carrier gas flow rate (ml.min ⁻¹) | 1 |
| Injection Mode | Split |
| Inlet temperature (°C) | 270 |
| Sample volume injected (µl) | 1 |
| Split ratio | 1 in 3 |
| Initial GC temperature (°C) | 70 |
| Start temp hold time (min) | 2 |
| Ramp rate (°C.min ⁻¹) | 24 |
| Final temp (°C) | 280 |
| Hold final temp (min) | 5 |
| Mass spectrometer acquisition rate (Hz) | 20 |
| Transfer line temperature (°C) | 250 |
| Source temperature (°C) | 230 |
| Mass Range (Da) | 30-500 |

Table S30

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Table S30. GC-TOF-MS instrumental conditions.