

<u>Variable</u>	<u>Set Parameter</u>
Carrier Gas	Helium
Carrier gas flow rate (ml.min <sup>-1</sup> )	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 <sup>-1</sup> )	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.