

Table 3 Instrument parameters

Item	Parameter
Sample volume	1 $\mu$ L
Front inlet mode	Splitless mode
Front inlet septum purge flow	3 mL/min
Carrier gas	Helium
Column	DB-5MS (30 m $\times$ 250 $\mu$ m $\times$ 0.25 $\mu$ m)
Column flow	1 mL/min
Oven temperature ramp	50°C hold on 1 min, raised to 310°C at a rate of 10°C/min, hold on 8 min
Front injection temperature	280°C
Transfer line temperature	280°C
Ion source temperature	250°C
Electron energy	-70 eV
Mass range	50~500 m/z
Acquisition rate	12.5 spectra/s (12.5 spectra per second)
Solvent delay	6.03 min