

## GC conditions

### *Inlet*

Inlet: MultiMode inlet

Injection mode: Split 10:1

Split Flow: 12 mL/min

Injection volume :1 µL

Injection program

60°C for 0 minutes

9°C/min to 250°C hold 2.5 minutes

Column: Agilent J&W HP-5ms Ultra Inert GC Column, 30 m, 0.25 mm, 0.25 µm, 7-inch cage

Carrier gas: helium, 1.2 mL/min constant flow

### *Oven program*

55°C for 5 minutes

8°C/min to 200°C

6°C/min to 310°C, hold 5minutes

Equilibration time: 0.5 minutes

## MS conditions

Source temperature: 230°C

Quadrupoles temperature: 150°C

Ionisation mode: Electron Impact, 70eV

Gain factor: 4

Scan type: dynamic MRM (Multiple Reaction Monitoring)

Compound	Retention time (min)	Precursor Ion (Da)	Qualifier 1 (Da)	Qualifier 2 (Da)
Butyric Acid (C4)	13.20	144.9	75.0	60.0
Hexanoic acid (C6)	16.81	172.8	131.1	75.0
Heptanoic acid (C7)	18.48	186.8	95.1	75.0
Octanoic acid (C8)	20.06	201.0	131.0	75.0
Nonanoic acid (C9)	21.57	215.0	131.0	75.0
Decanoic acid (C10)	23.00	228.8	131.1	75.0
Undecanoic acid (C11)	24.40	242.7	131.1	75.0
Dodecanoic acid (C12)	25.80	256.7	130.9	75.1
Myristic acid (C14)	28.60	284.7	130.9	75.0
9-Hexadecenoic acid(C16:1)	31.12	310.7	130.8	75.0
Palmitic Acid (C16)	31.36	312.7	130.9	75.0
Linoleic acid (C18:2)	33.66	336.9	95.0	75.0
Oleic Acid (C18:1)	33.70	338.7	130.9	75.0
Linolenic acid (C18:3)	33.77	334.8	130.8	90.8
Stearic acid (C18)	34.00	340.6	130.8	75.0