

4000 Qtrap parameters:

CUR: 30
IS: -3500
TEM: 450
GS1: 50
GS2: 50
Ihe: on
CAD: LOW
DP: -110
CES: 0
CE -5

Scan Type: EMS
Scan range: 350 to 1200 m/z

dynamic fill time

Shimadzu HPLC parameters:

Phenomenex Luna Silica column 2x250 mm 5 micron

Mobile phase A: IPA:Hexane: 100 mM NH₄CO₂H 58:40:2

Mobile phase B: IPA:Hexane: 100 mM NH₄CO₂H 50:40:10

Flow rate: 300 uL/min

Initial %B 50

Gradient program:

<u>Time</u>	<u>Event</u>	
0.01	Controller	Start
5.00	Pump B	50%
30.00	Pump B	100%
40.00	Pump B	100%
41.00	Pump B	50%
50.00	Controller	Stop

Autosampler parameters:

20 uL injection (samples dissolved in 100 uL of mobile phase A)