

4000 Qtrap parameters:

CUR: 30  
IS: -3500  
TEM: 450  
GS1: 50  
GS2: 50  
Ihe: on  
CAD: LOW  
DP: -110  
CES: 0  
CE -10

Scan Type: EMS  
Scan range: 400 to 1200 m/z

dynamic fill time

Shimadzu HPLC parameters:

Mobile phase A: IPA:Hexane: 100 mM NH<sub>4</sub>OAc 58:40:2

Mobile phase B: IPA:Hexane: 100 mM NH<sub>4</sub>OAc 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