

Data File: C:\LabSolutions\Data\Chemistry\Griffin\M4-190117-003.lcd

Elmt	Val.	Min	Max	Use Adduct												
H	1	0	30	Si	4	0	0	Fe	2	0	0	Ag	1	0	0	H
2H	1	0	0	P	3	0	0	Co	2	0	0	I	3	0	0	Na
C	4	0	30	S	2	0	0	Ni	2	0	0	Re	2	0	0	K
N	3	0	5	Cl	1	0	0	Cu	2	0	0	Ir	3	0	0	NH4
O	2	0	5	V	2	0	0	Br	1	0	0	Pt	2	0	0	
F	1	0	0	Cr	2	0	0	Ru	2	0	0					

Error Margin (ppm): 25

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 1000.0

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: AND

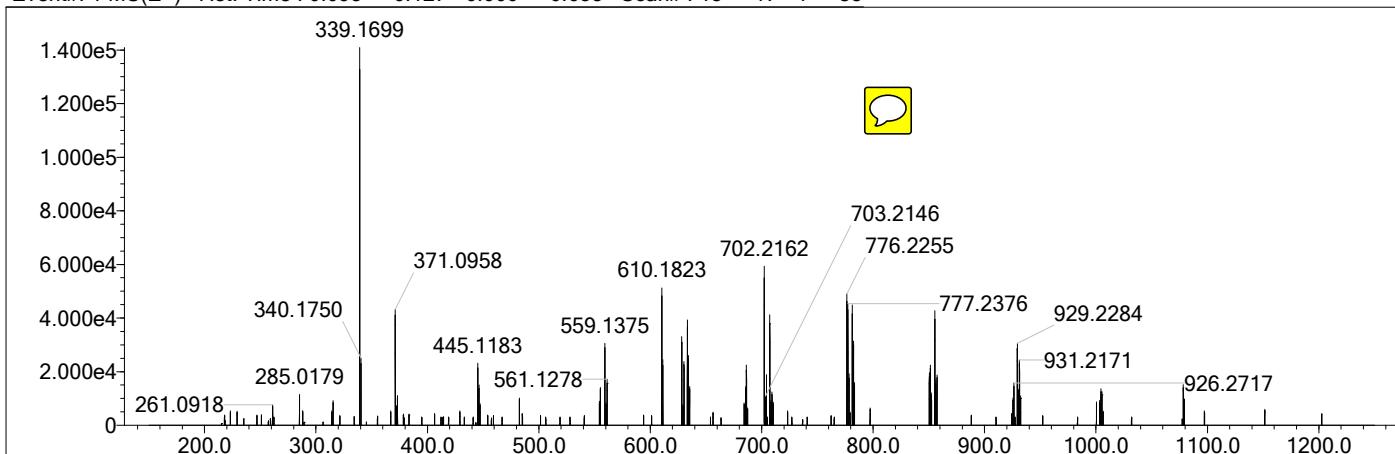
Electron Ions: both

Use MSn Info: yes

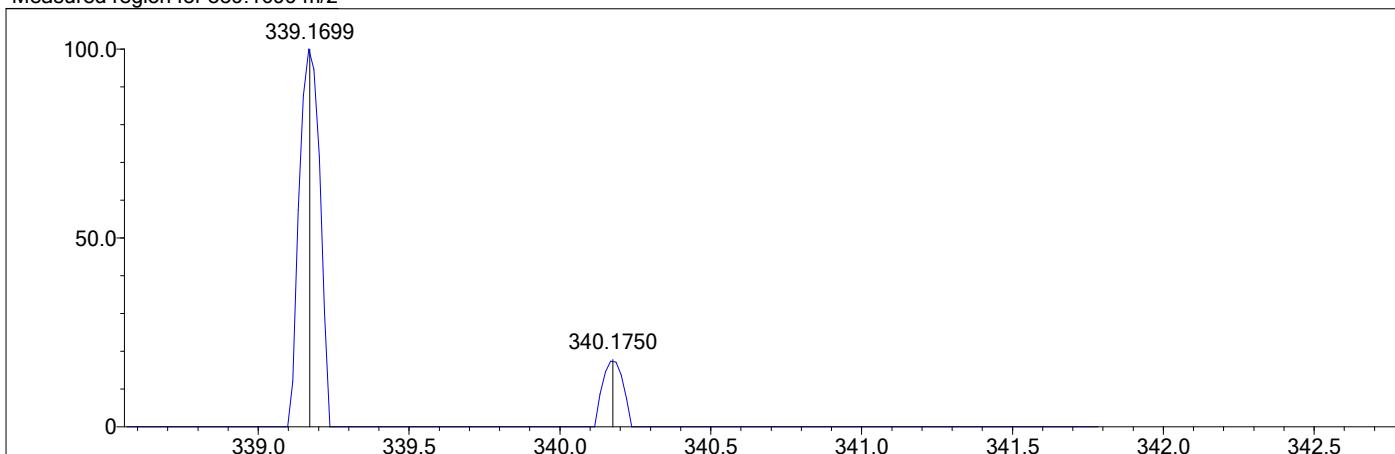
Isotope Res: 4000

Max Results: 500

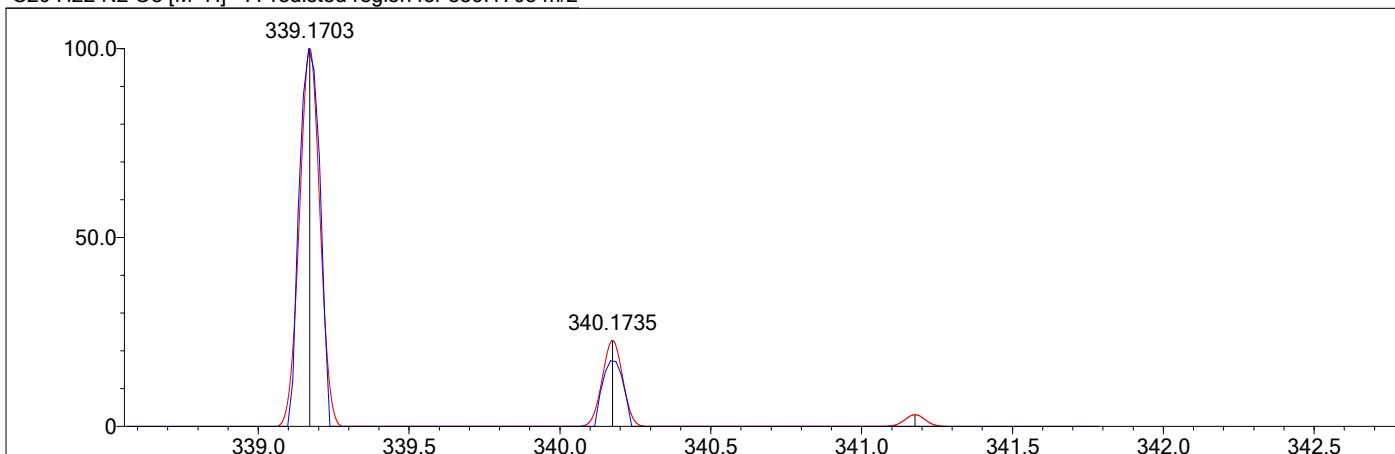
Event#: 1 MS(E+) Ret. Time : 0.095 -&gt; 0.127 - 0.000 -&gt; 0.653 Scan# : 13 -&gt; 17 - 1 -&gt; 83



Measured region for 339.1699 m/z



C20 H22 N2 O3 [M+H]+ : Predicted region for 339.1703 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	79.71	C20 H22 N2 O3	[M+H]+	339.1699	339.1703	-0.4	-1.18	80.07	11.0