

Data File: C:\LabSolutions\Data\1. Chemistry\Evans (CHEM)\Barlow, Sean\SB80-220124-003.lcd

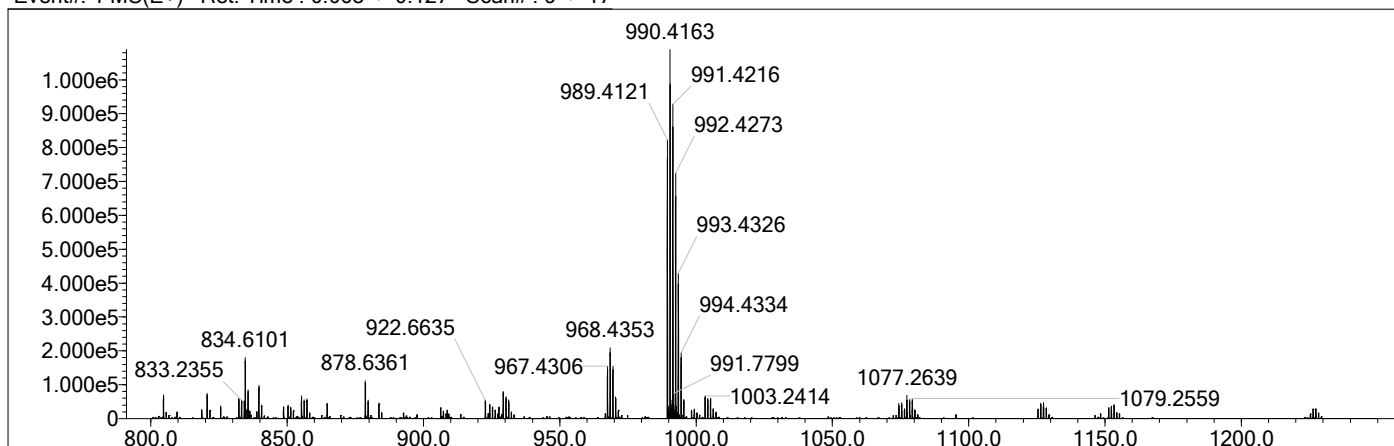
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	55	60	Na	1	0	0	Fe	2	0	0	I	3	0	0	H
2H	1	0	0	Si	4	0	0	Co	2	0	0	Re	2	0	0	Na
B	3	0	0	P	3	0	0	Ni	2	0	0	Ir	3	0	0	K
C	4	50	55	S	2	0	0	Cu	2	0	0	Pt	2	0	0	NH4
N	3	5	10	Cl	1	0	1	Br	1	0	2					
O	2	10	15	V	2	0	0	Ru	2	0	0					
F	1	0	0	Cr	2	0	0	Ag	1	0	0					

Error Margin (ppm): 200
 HC Ratio: unlimited
 Max Isotopes: all
 MSn Iso RI (%): 75.00

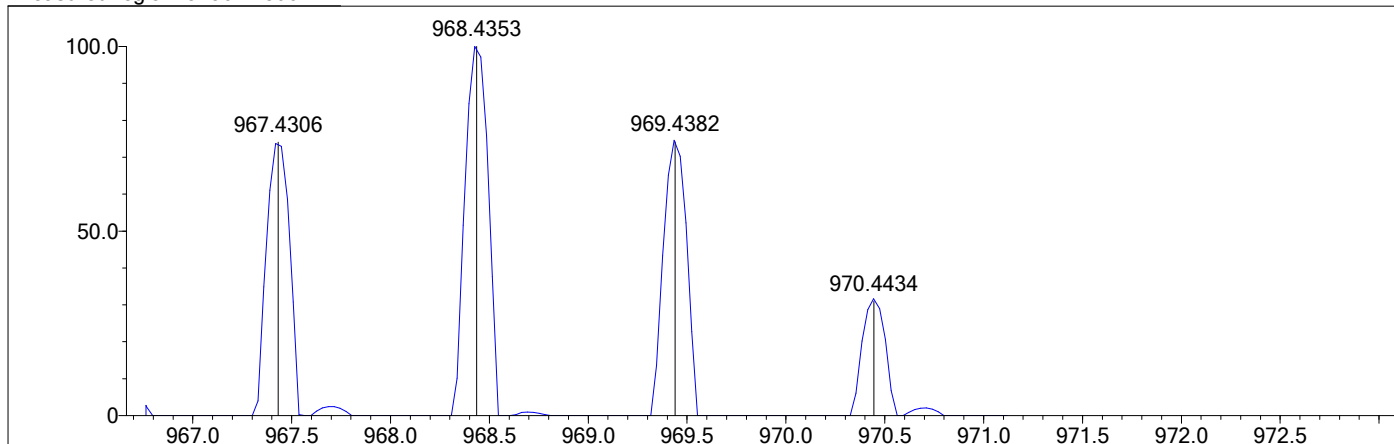
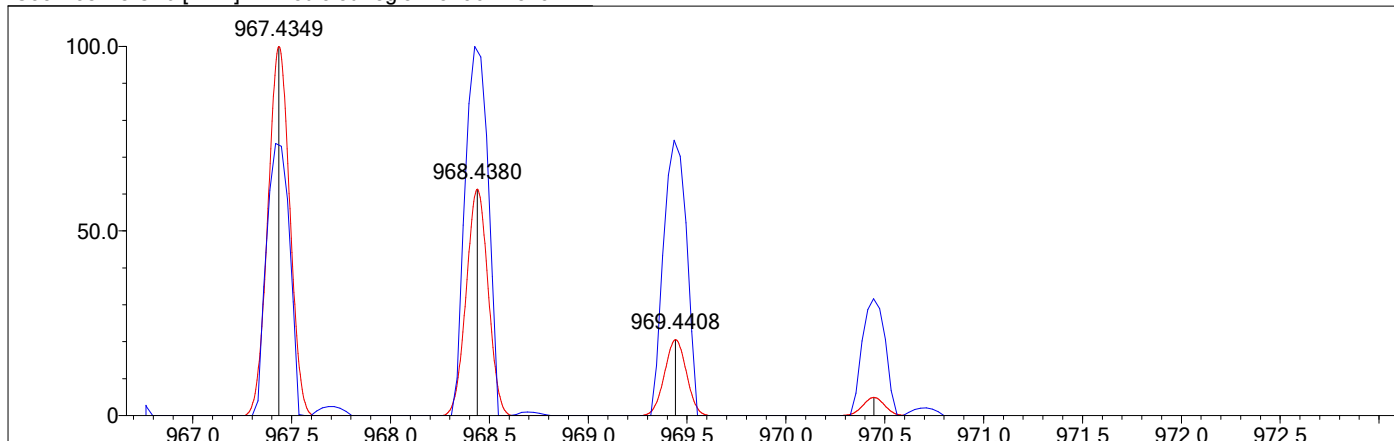
DBE Range: -2.0 - 1000.0
 Apply N Rule: no
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: yes
 Isotope Res: 7000
 Max Results: 500

Event#: 1 MS(E+) Ret. Time : 0.063 -> 0.127 Scan#: 9 -> 17



Measured region for 967.4306 m/z

C53 H58 N8 O10 [M+H]⁺ : Predicted region for 967.4349 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	45.70	C53 H58 N8 O10	[M+H] ⁺	967.4306	967.4349	-4.3	-4.44	50.00	29.0