

## Supplementary Material

### An efficient debromination technique using PMHS with a number of ligands containing different functional groups

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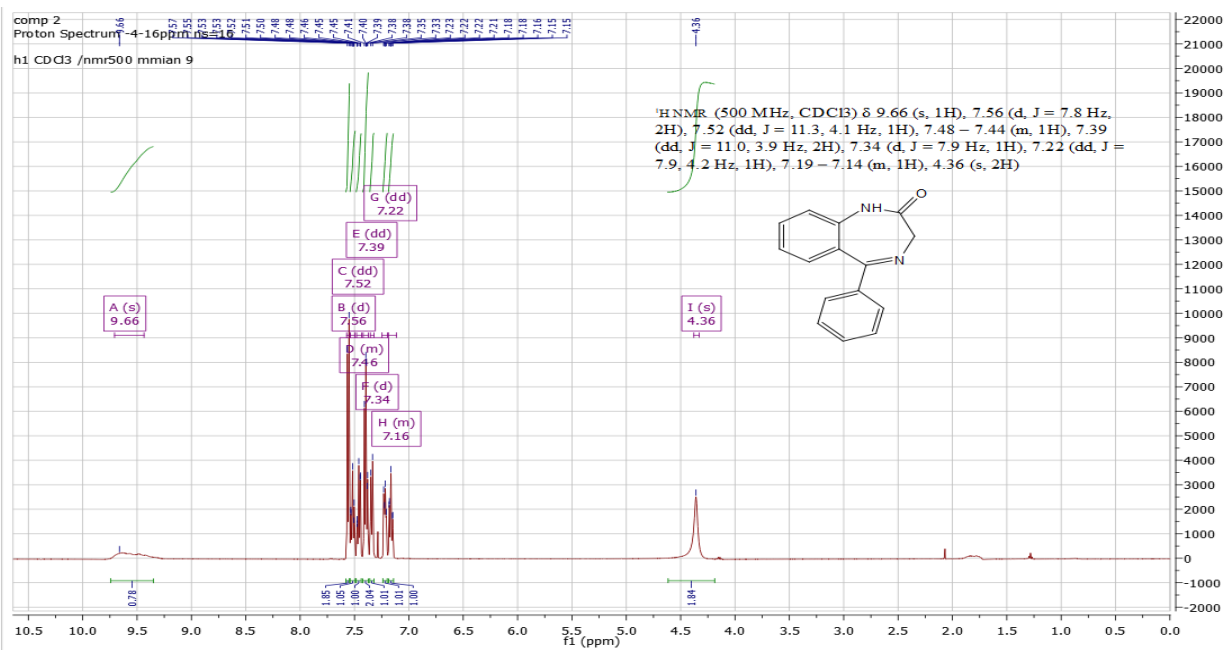
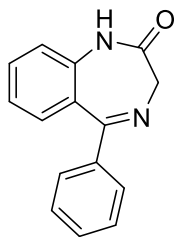
E-mail: [capncook@uwm.edu](mailto:capncook@uwm.edu)

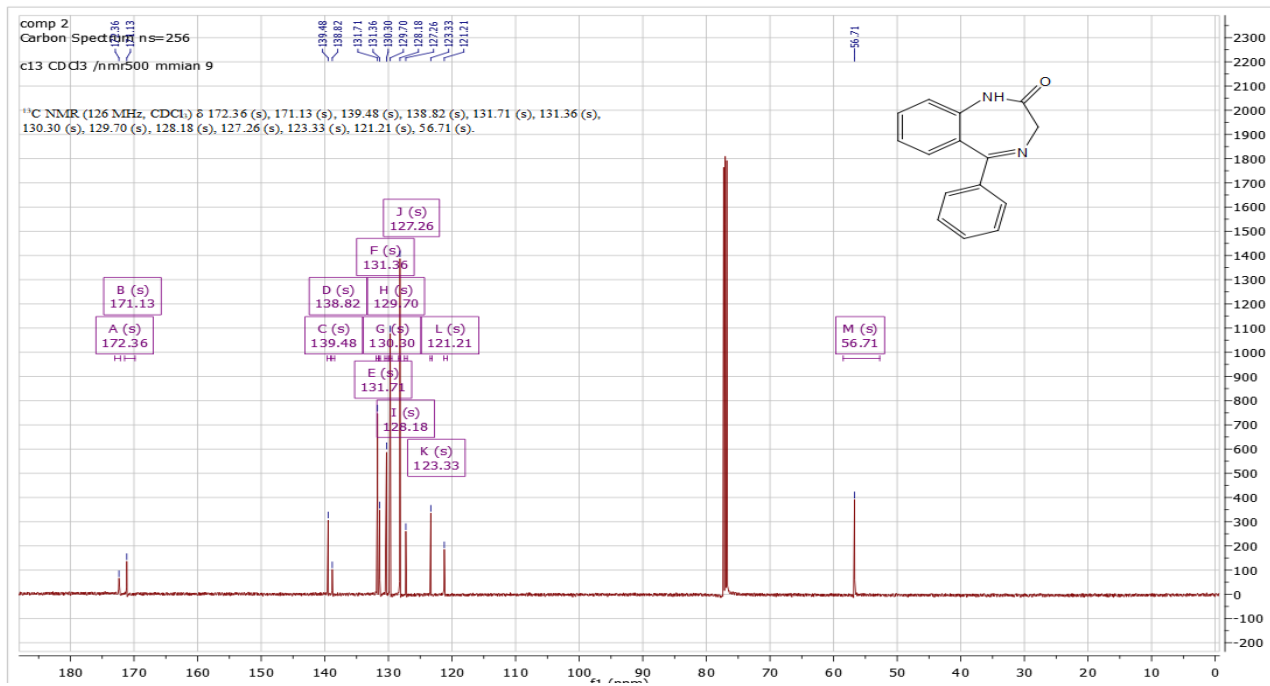
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## 5-phenyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(2)





Formula Predictor Report - COMP\_2\_12082020 Analysis\_49.lcd

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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP\_2\_12082020 Analysis\_49.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	15	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	0					

Error Margin (ppm): 300

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -100.0 - 2000.0

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: AND

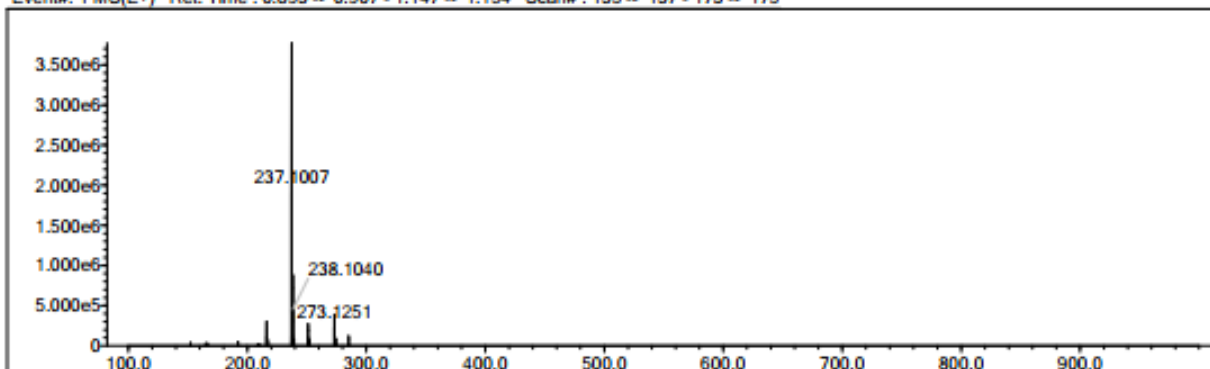
Electron Ions: both

Use MSn Info: yes

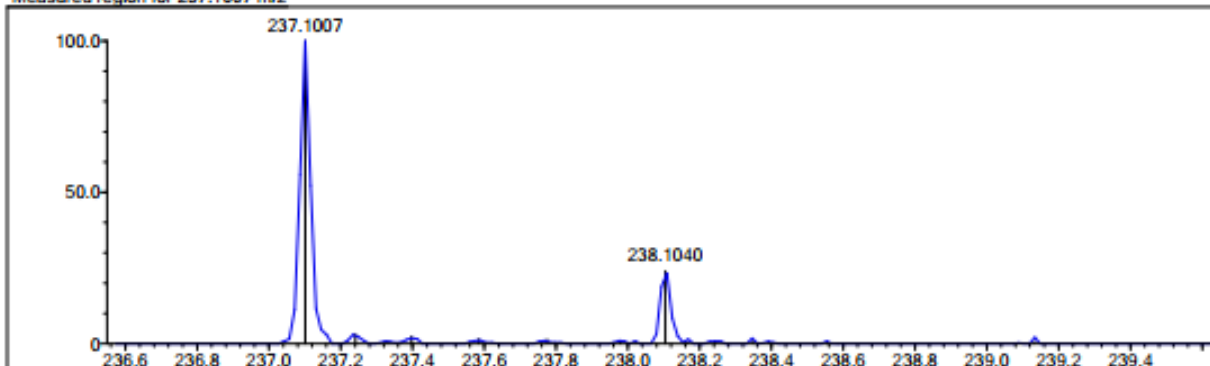
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Max Results: 10

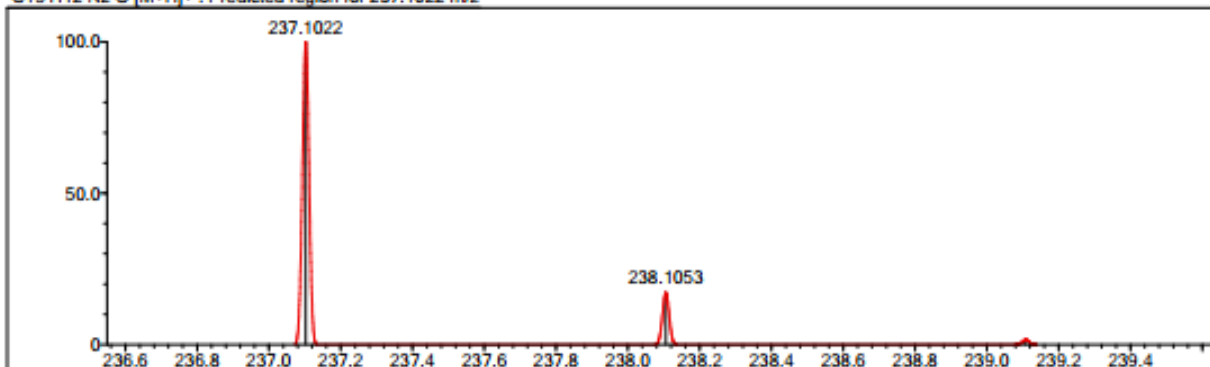
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Measured region for 237.1007 m/z

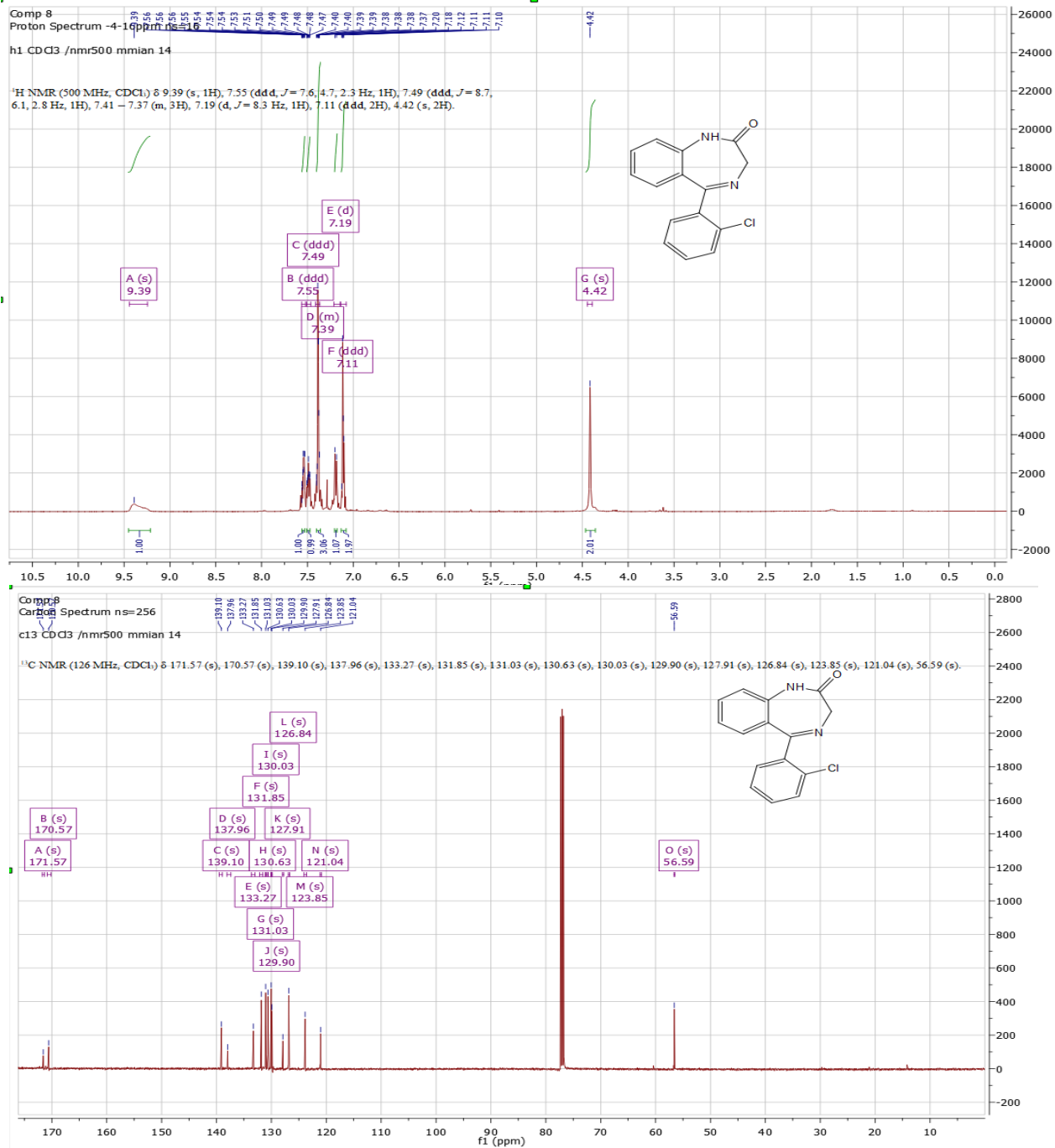
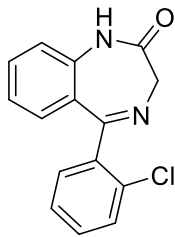


C15 H12 N2 O [M+H]<sup>+</sup> : Predicted region for 237.1022 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	27.96	C15 H12 N2 O	[M+H] <sup>+</sup>	237.1007	237.1022	-1.5	-6.33	36.45	11.0

## 5-(2-chlorophenyl)-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(3)



Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 8\_12082020 Analysis\_37.lcd

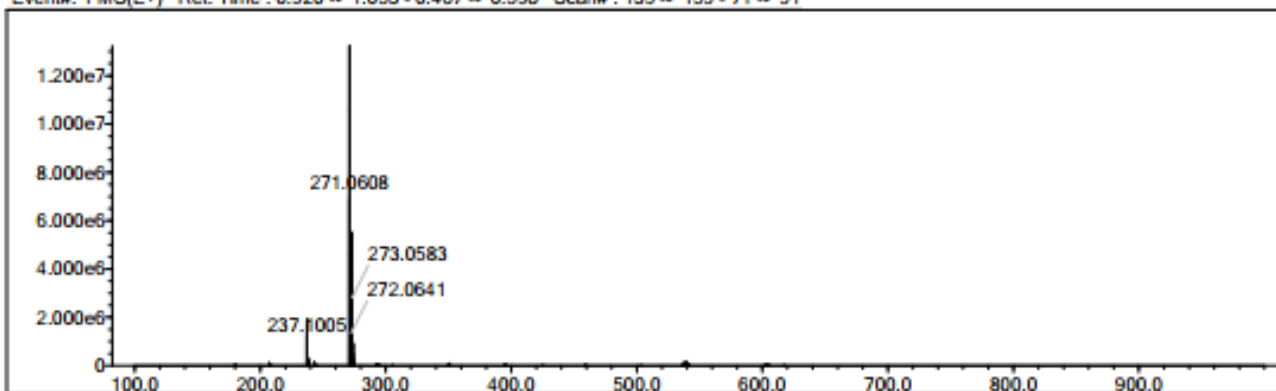
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

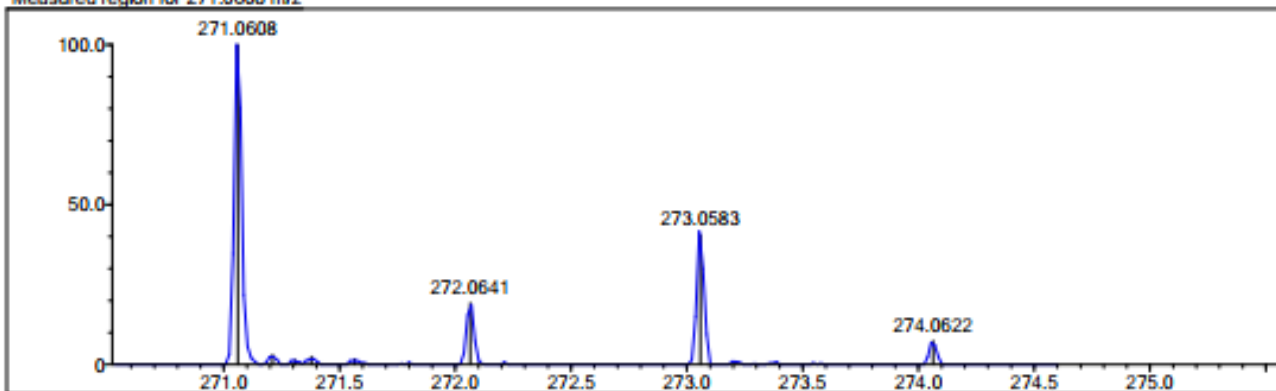
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

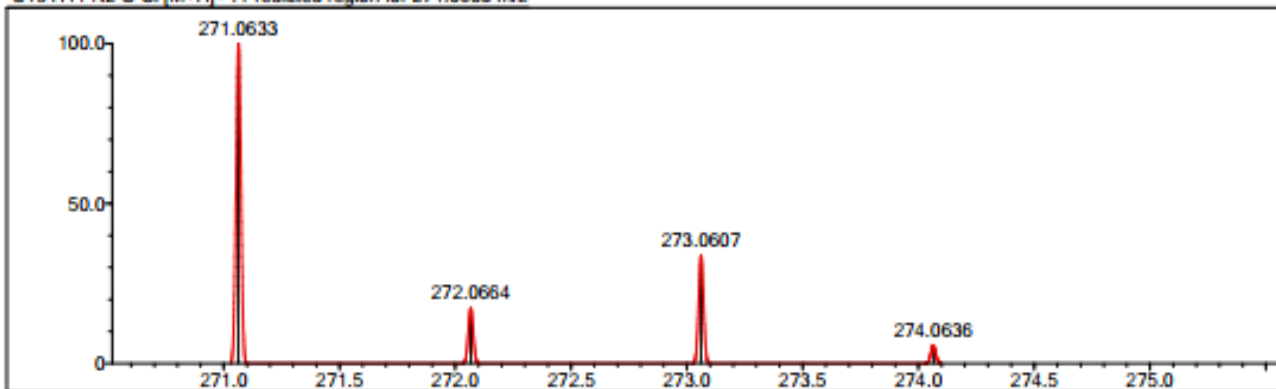
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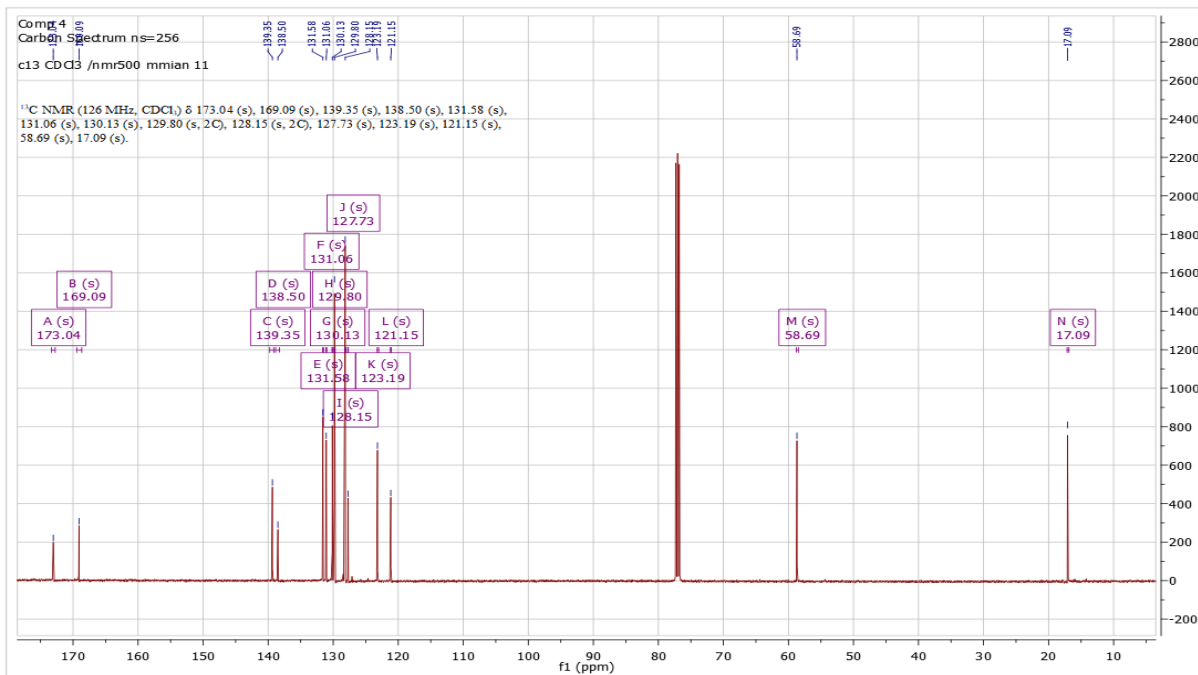
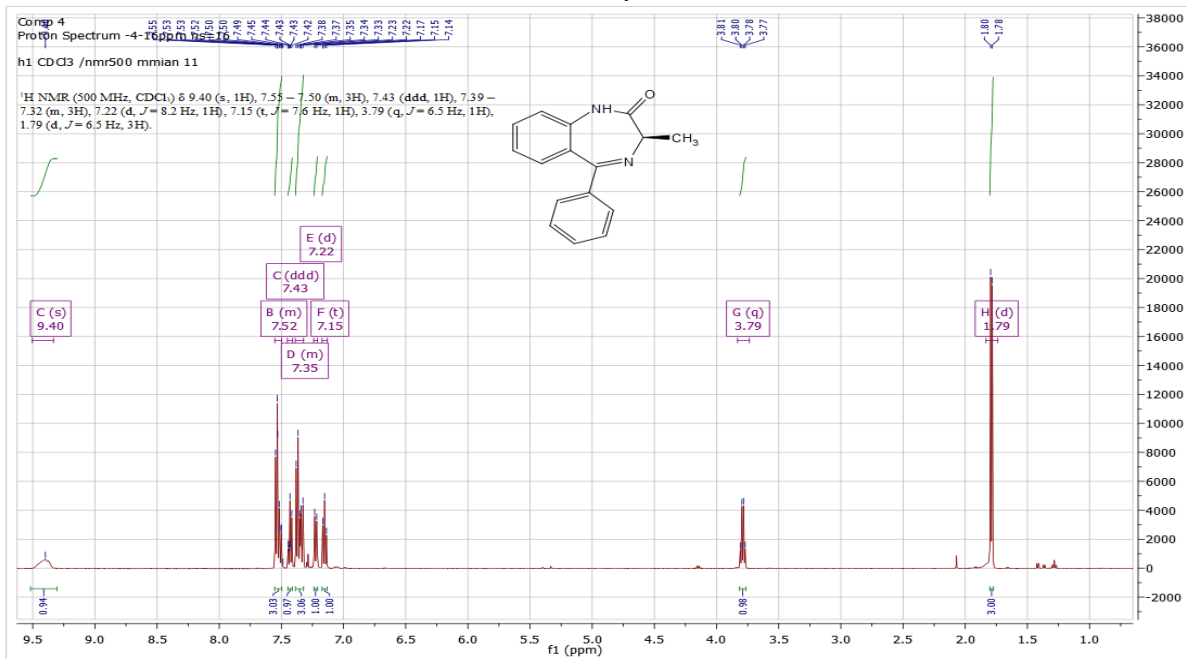
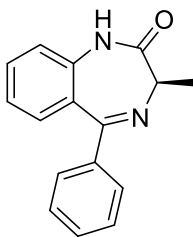
Measured region for 271.0608 m/z



C15 H11 N2 O Cl [M+H]<sup>+</sup> : Predicted region for 271.0633 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	31.61	C15 H11 N2 O Cl	[M+H] <sup>+</sup>	271.0608	271.0633	-2.5	-9.22	66.12	11.0

**(R)-7-bromo-3-methyl-5-phenyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(5b)**



Formula Predictor Report - COMP 4\_12082020 Analysis\_45.lcd

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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 4\_12082020 Analysis\_45.lcd

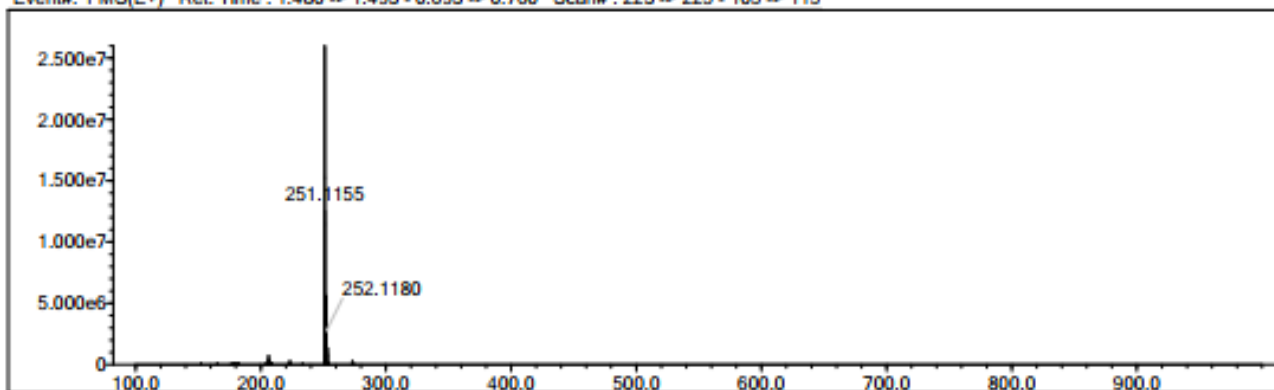
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2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	0	Cl	1	0	0					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

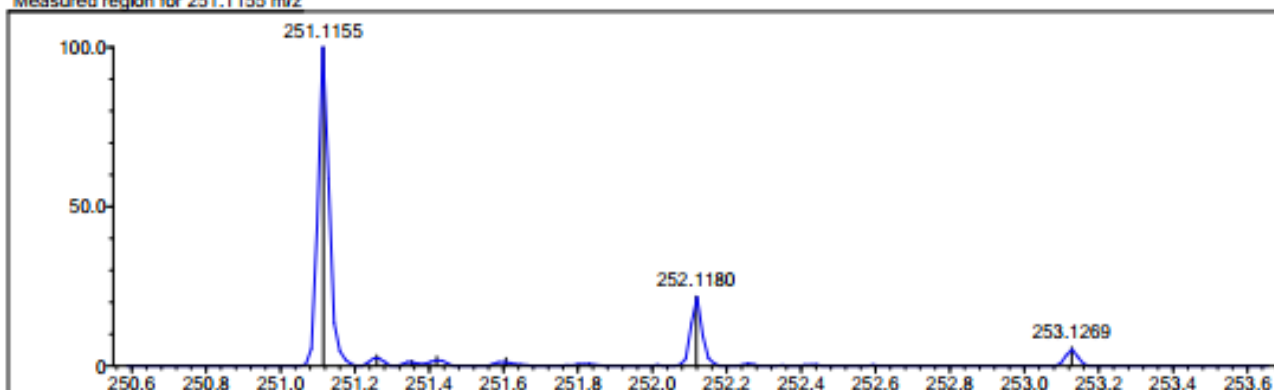
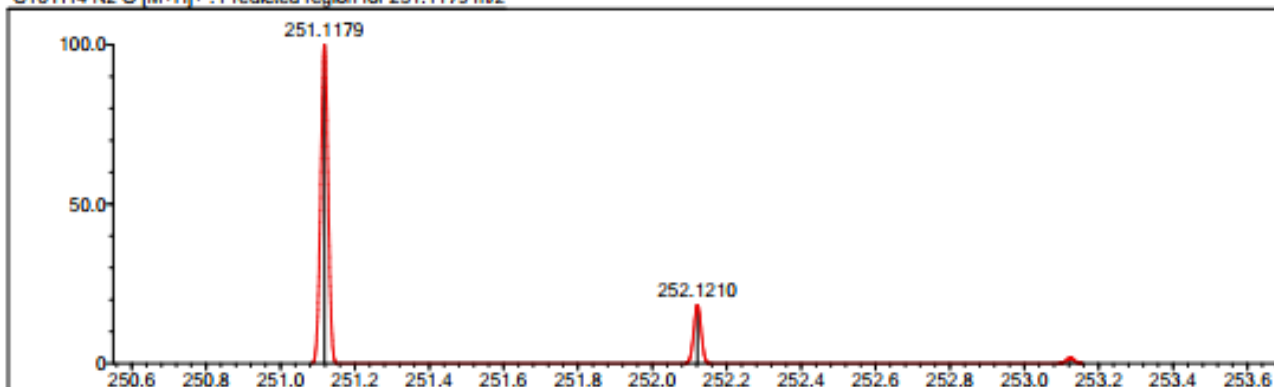
DBE Range: -100.0 - 2000.0  
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 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

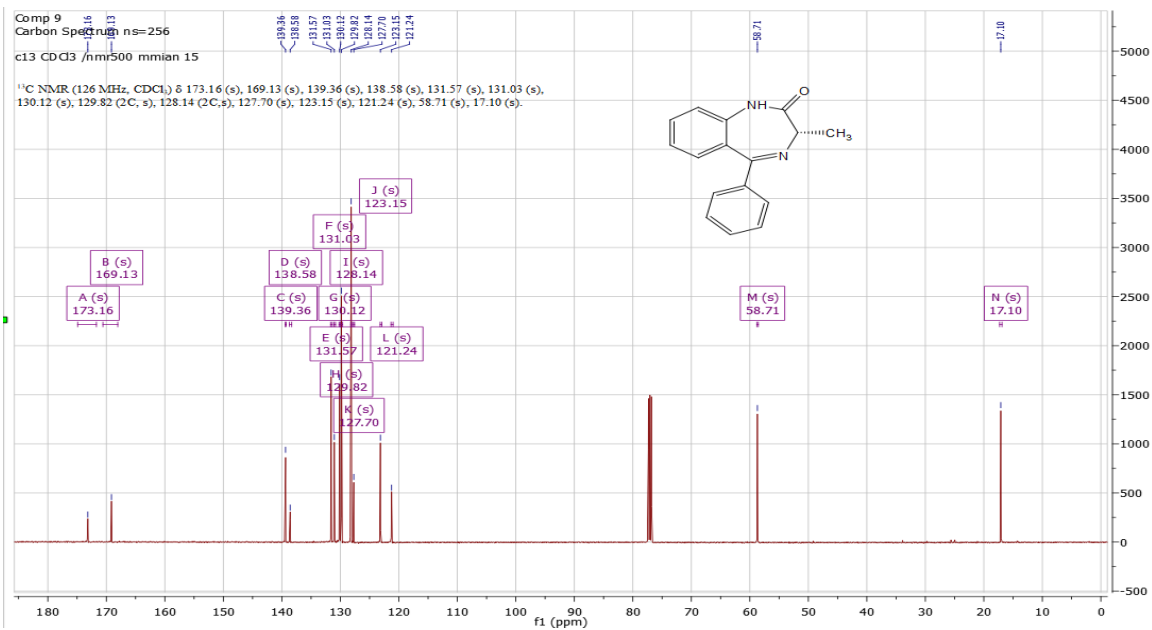
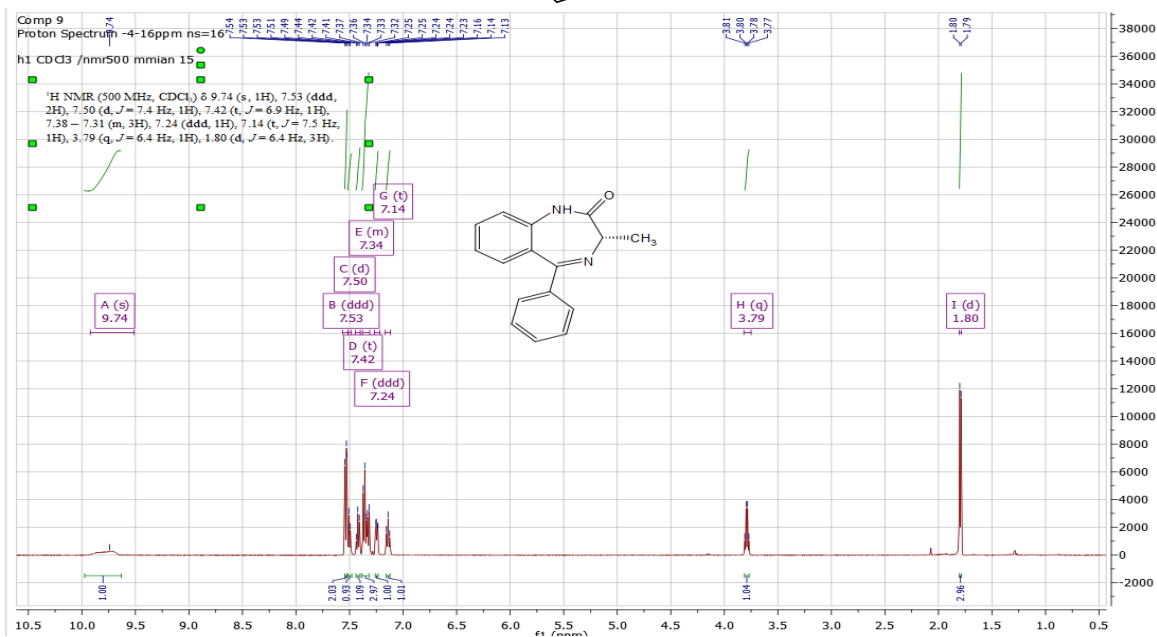
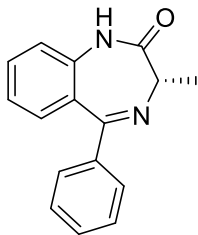
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Measured region for 251.1155 m/z

C16 H14 N2 O [M+H]<sup>+</sup> : Predicted region for 251.1179 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	25.99	C16 H14 N2 O	[M+H] <sup>+</sup>	251.1155	251.1179	-2.4	-9.56	58.54	11.0

**(S)-7-bromo-3-methyl-5-phenyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(5c)**

Data File: C:\LabSolutions\Data\Wilashini Rajaratnam\12082020 Analysis\COMP 9\_12082020 Analysis\_35.lcd

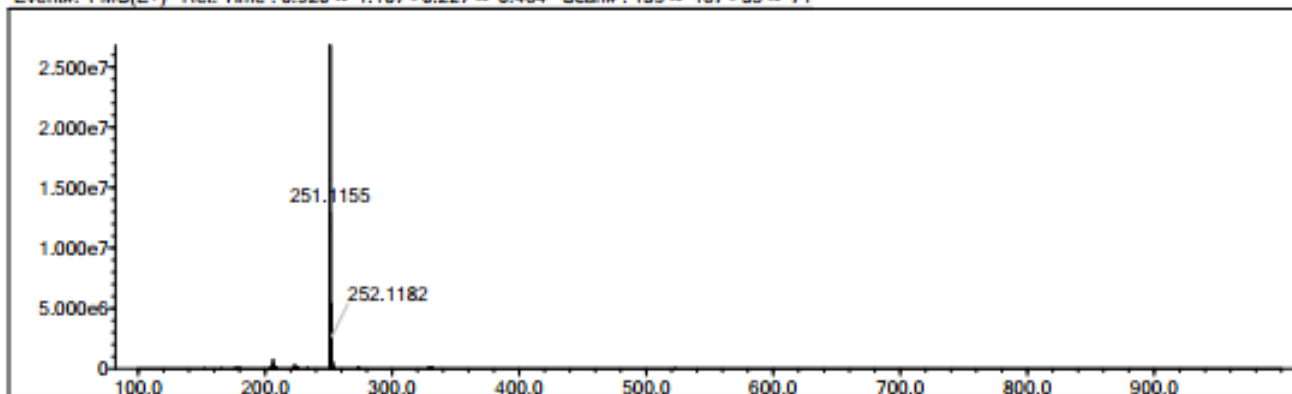
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H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

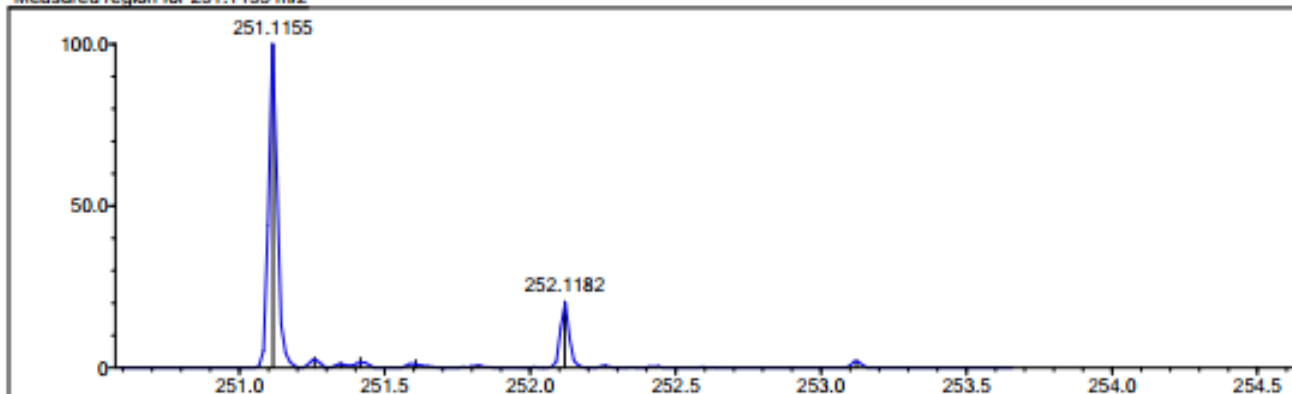
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

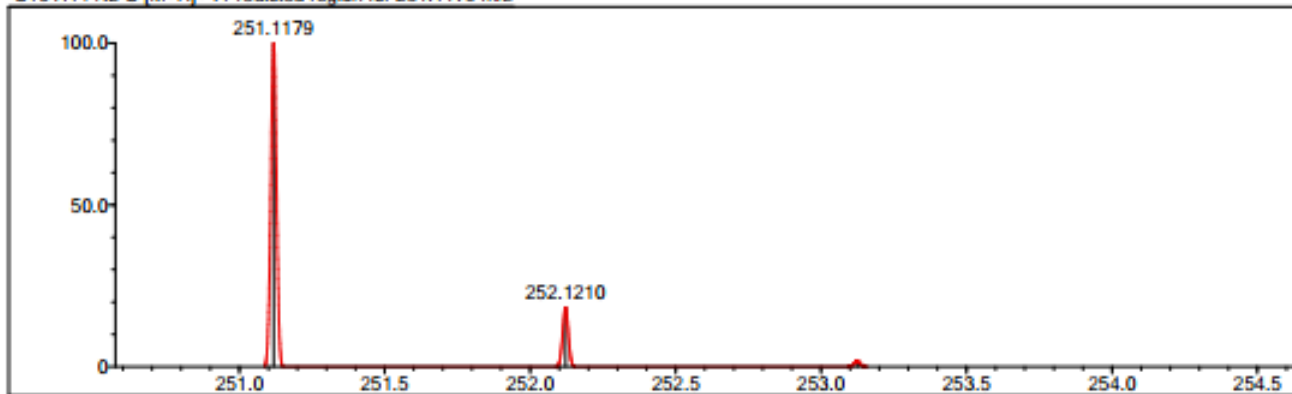
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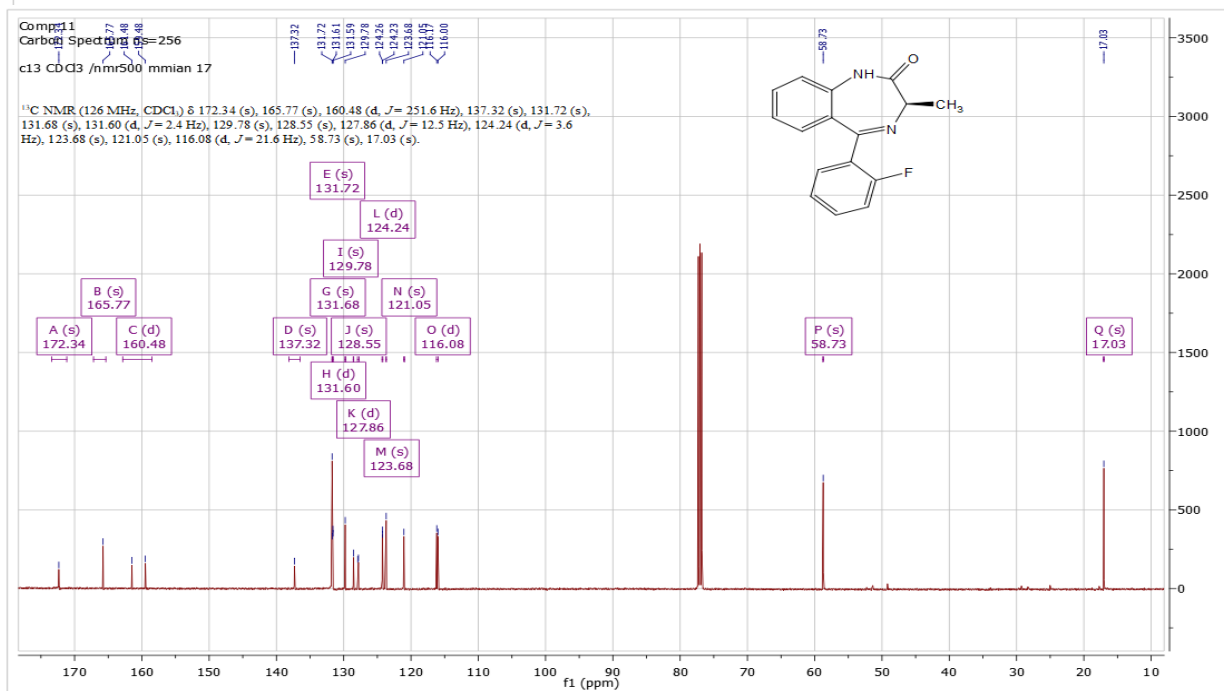
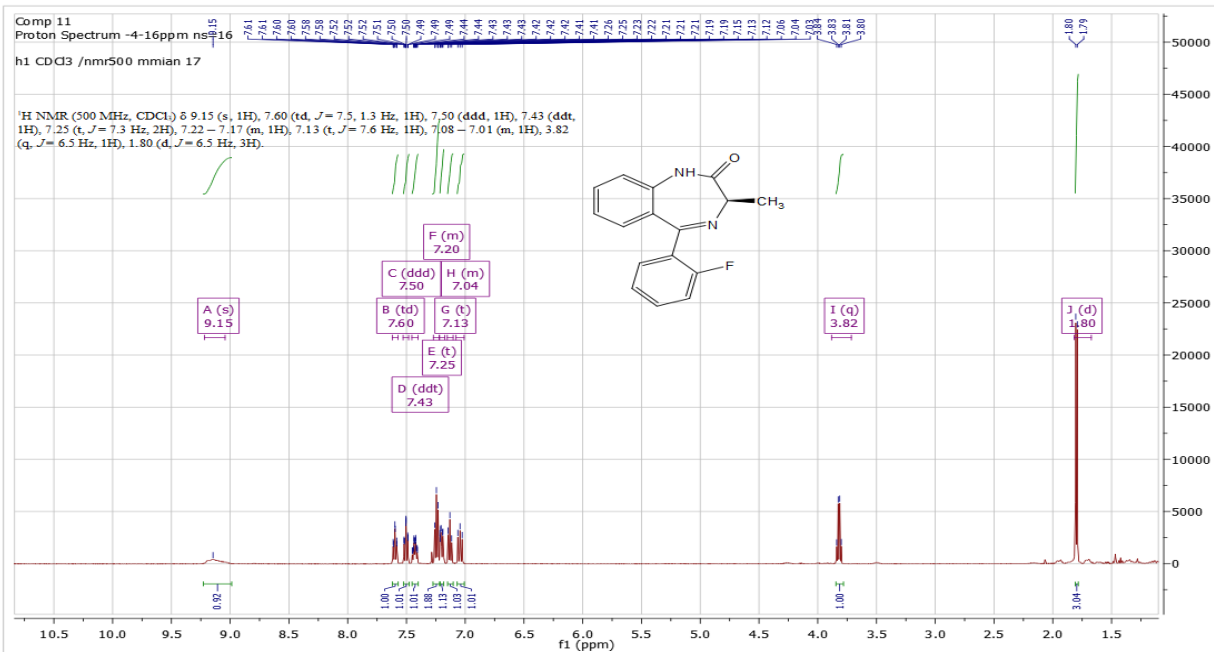
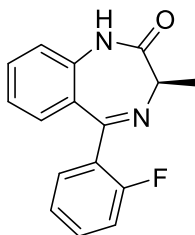
Measured region for 251.1155 m/z



C16 H14 N2 O [M+H]+ : Predicted region for 251.1179 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	25.80	C16 H14 N2 O	[M+H] <sup>+</sup>	251.1155	251.1179	-2.4	-9.56	58.11	11.0

**(R)-5-(2-fluorophenyl)-3-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(5d)**

Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 11\_12082020 Analysis\_31.lcd

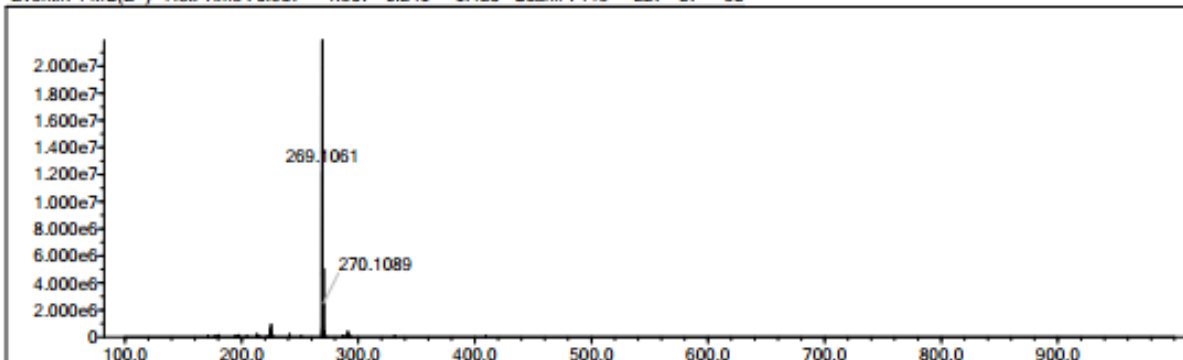
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H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

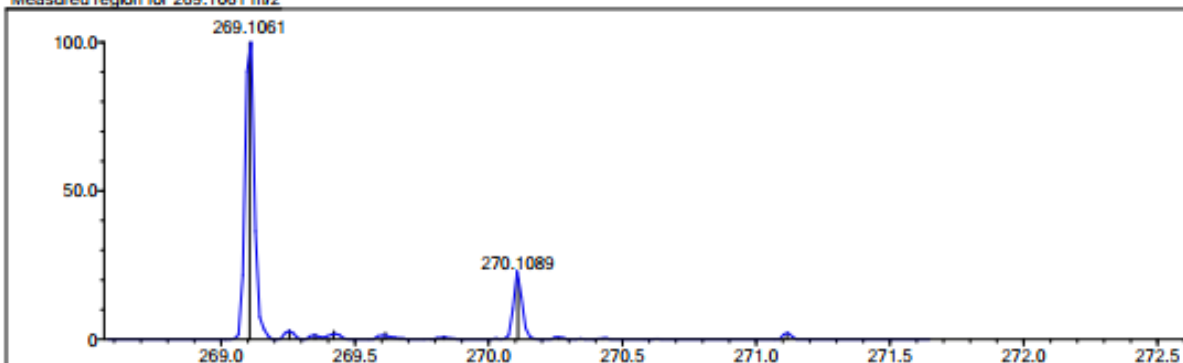
DBE Range: -100.0 - 2000.0  
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 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

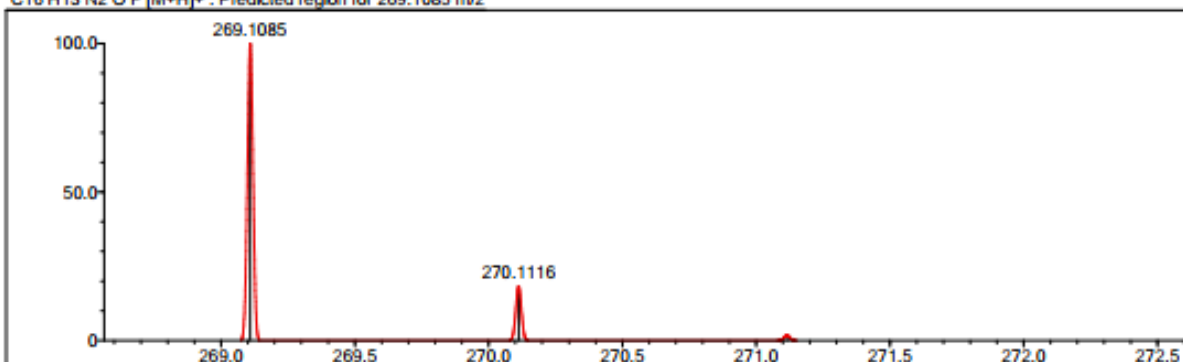
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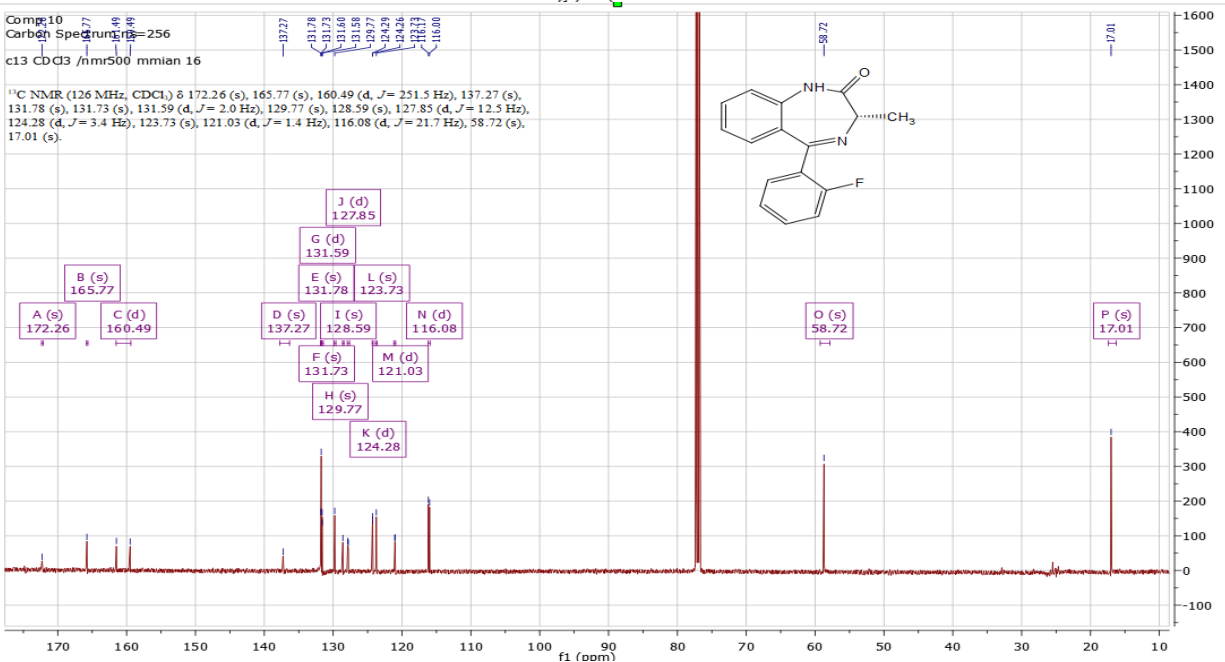
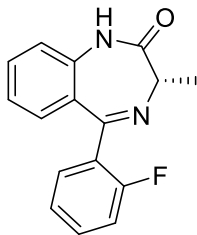
Measured region for 269.1061 m/z



C16 H13 N2 O F [M+H]+ : Predicted region for 269.1085 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	47.48	C16 H13 N2 O F	[M+H] <sup>+</sup>	269.1061	269.1085	-2.4	-8.92	93.47	11.0

**(S)-5-(2-fluorophenyl)-3-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (5e)**

Formula Predictor Report - COMP 10\_12082020 Analysis\_33.lcd

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Data File: C:\LabSolutions\Data\Wilashini Rajaratnam\12082020 Analysis\COMP 10\_12082020 Analysis\_33.lcd

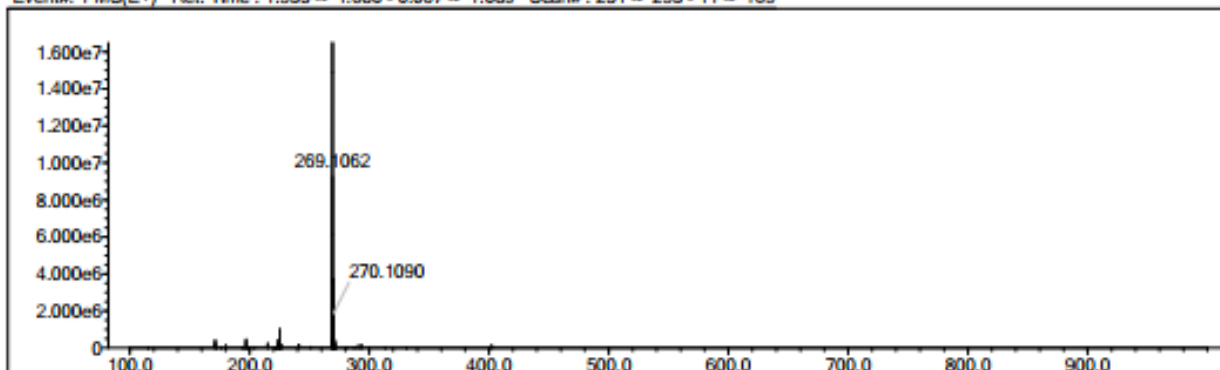
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2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

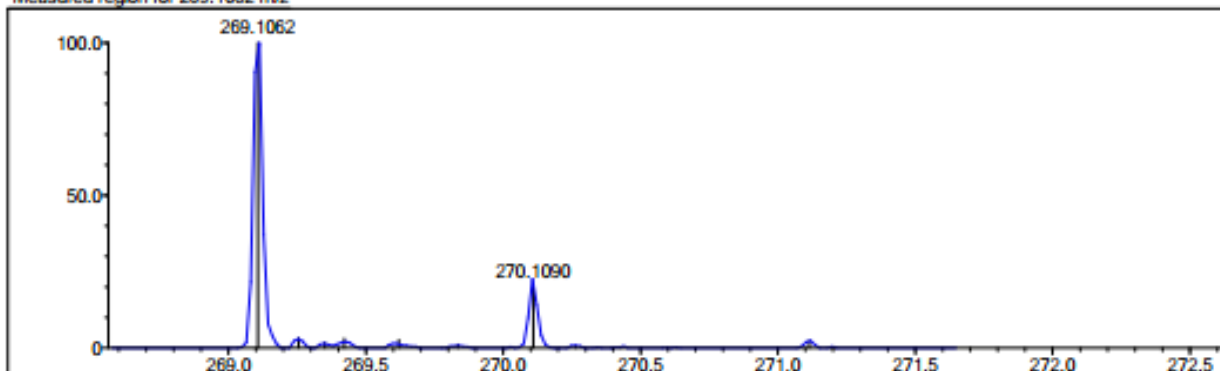
DBE Range: -100.0 - 2000.0  
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 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

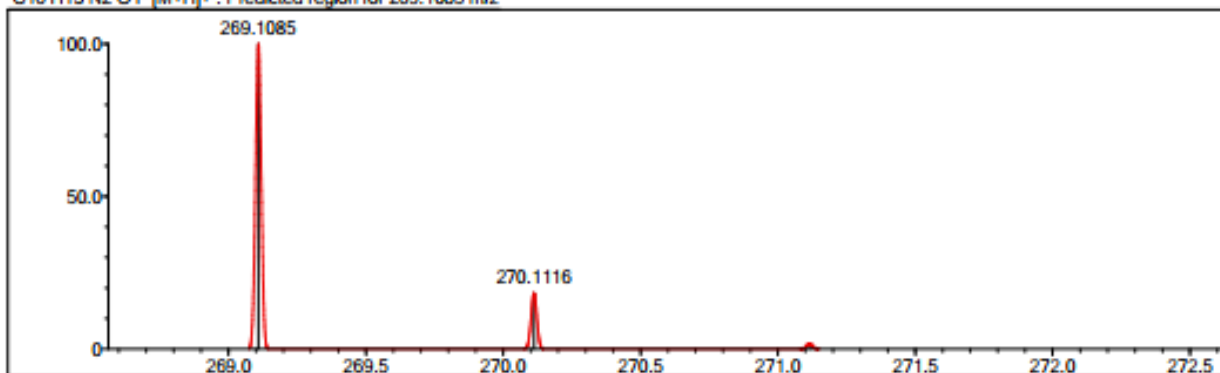
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Measured region for 269.1062 m/z

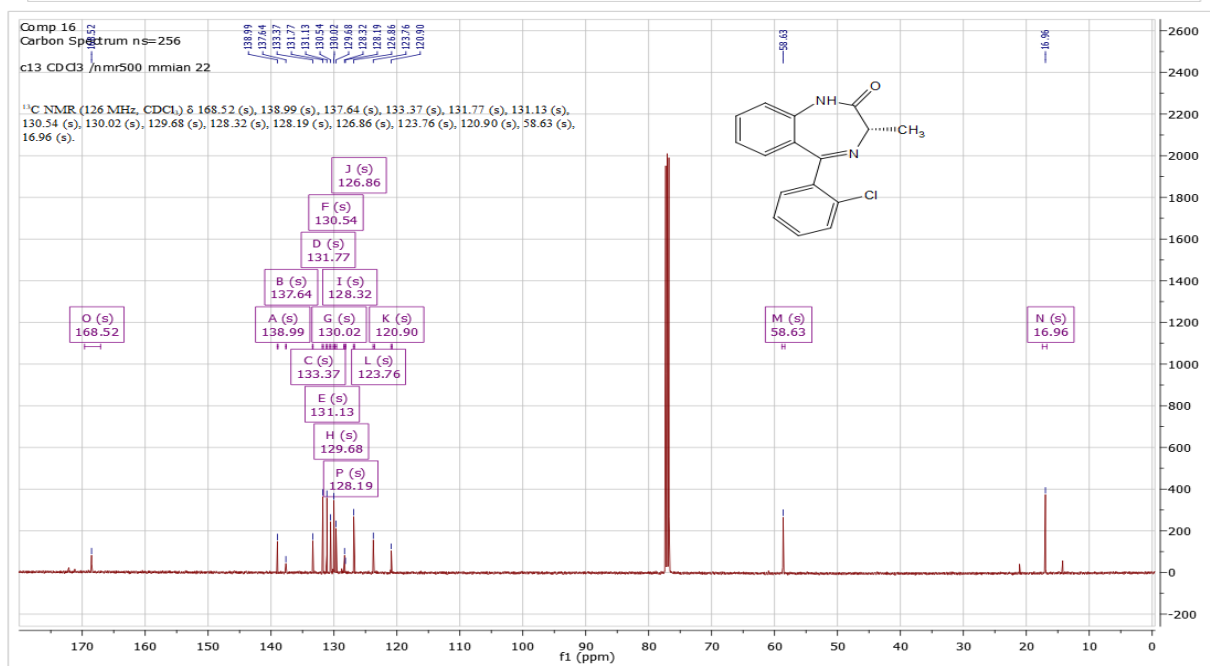
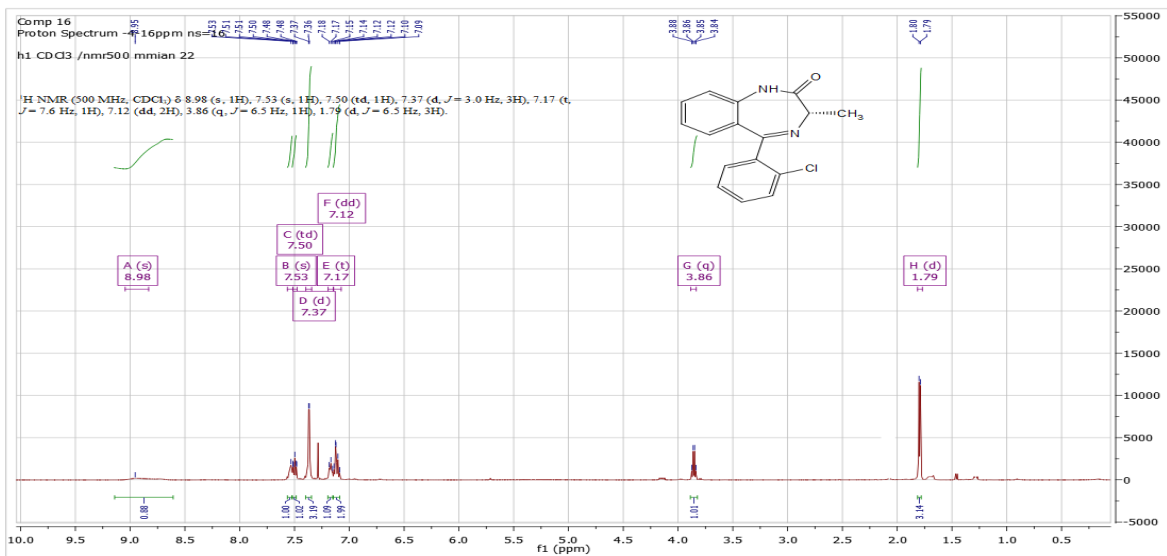
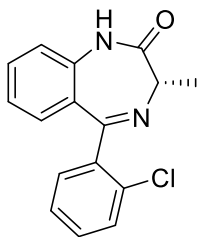


C16 H13 N2 O F [M+H]<sup>+</sup> : Predicted region for 269.1085 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	46.02	C16 H13 N2 O F	[M+H] <sup>+</sup>	269.1062	269.1085	-2.3	-8.55	84.45	11.0

(S)-5-(2-chlorophenyl)-3-methyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one (5f)





Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\MYMV6\_12082020 Analysis\_19.lcd

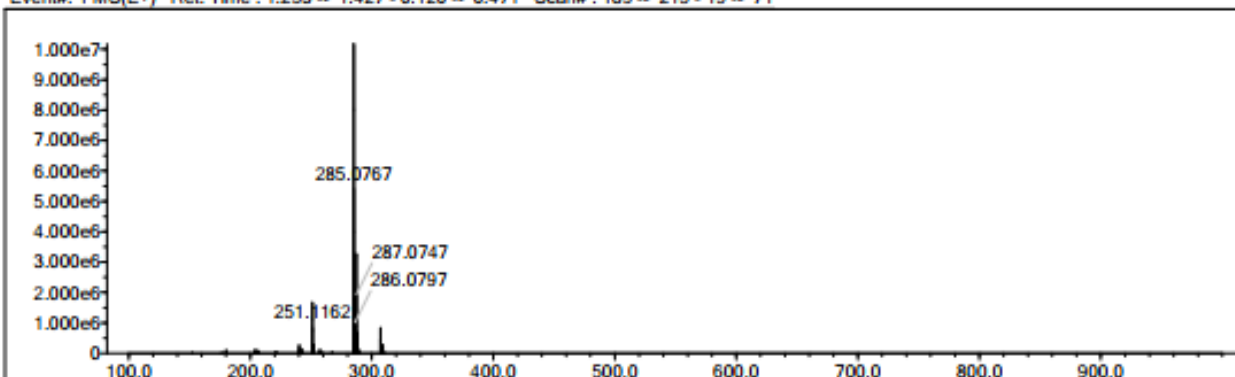
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	0	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

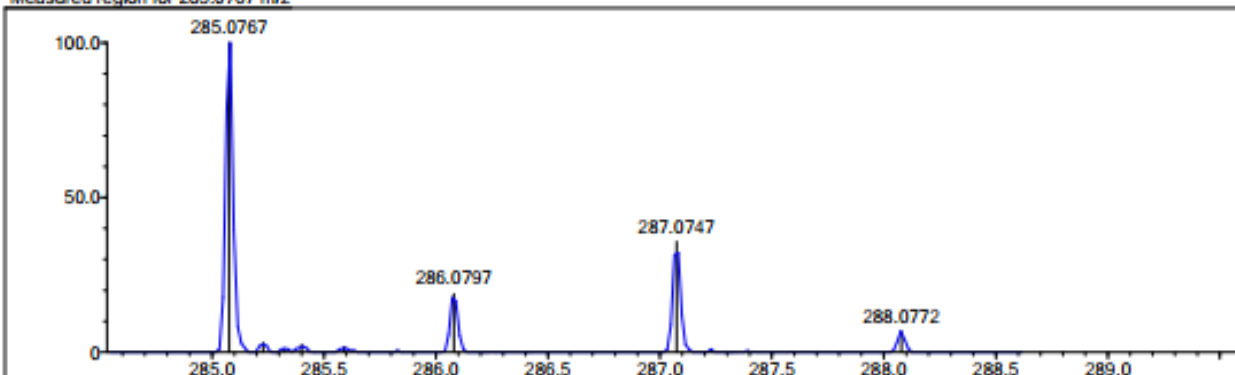
DBE Range: +100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

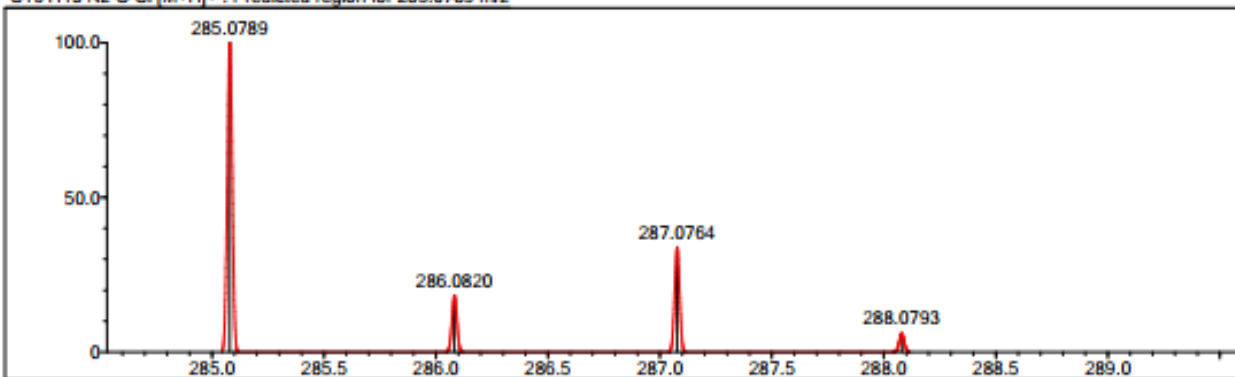
Event#: 1 MS(E+) Ret. Time : 1.253 -> 1.427 - 0.120 -> 0.471 Scan#: 189 -> 215 - 19 -> 71



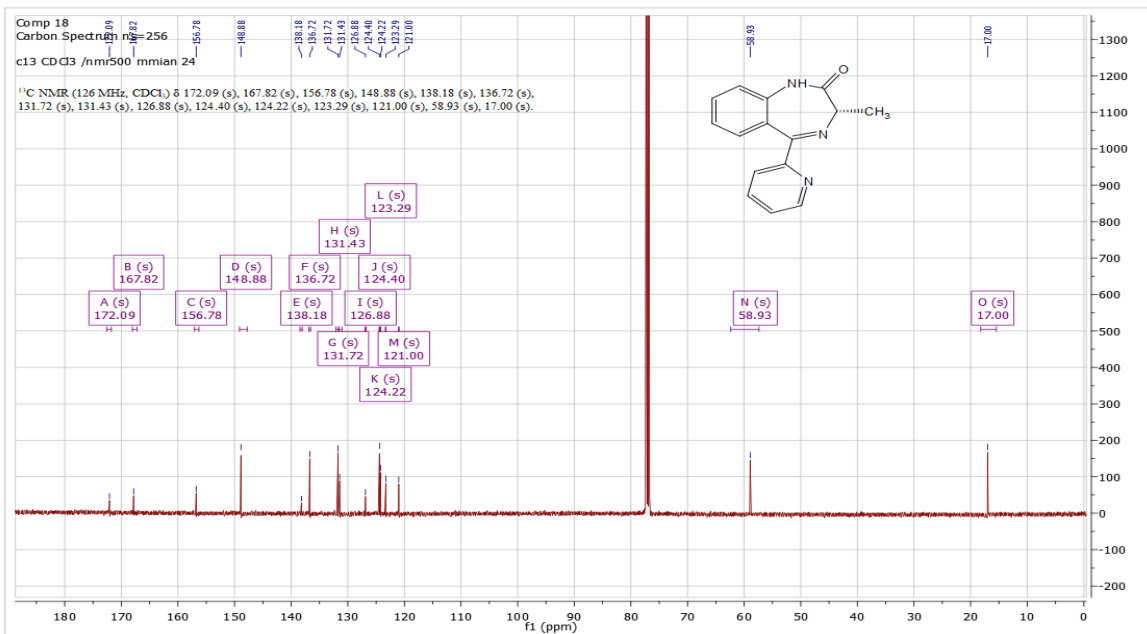
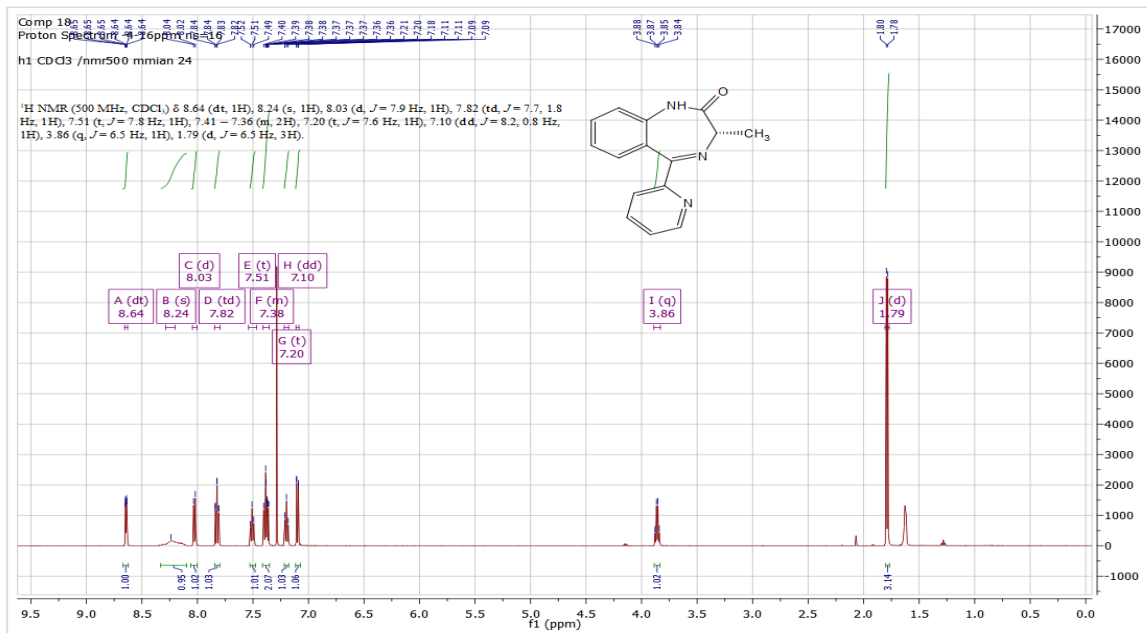
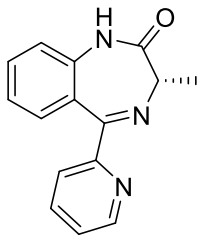
Measured region for 285.0767 m/z



C16 H13 N2 O Cl [M+H]<sup>+</sup> : Predicted region for 285.0789 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	62.41	C16 H13 N2 O Cl	[M+H] <sup>+</sup>	285.0767	285.0789	-2.2	-7.72	99.38	11.0

**(S)-3-methyl-5-(pyridin-2-yl)-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one(5g)**

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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 18\_12082020 Analysis\_21.lcd

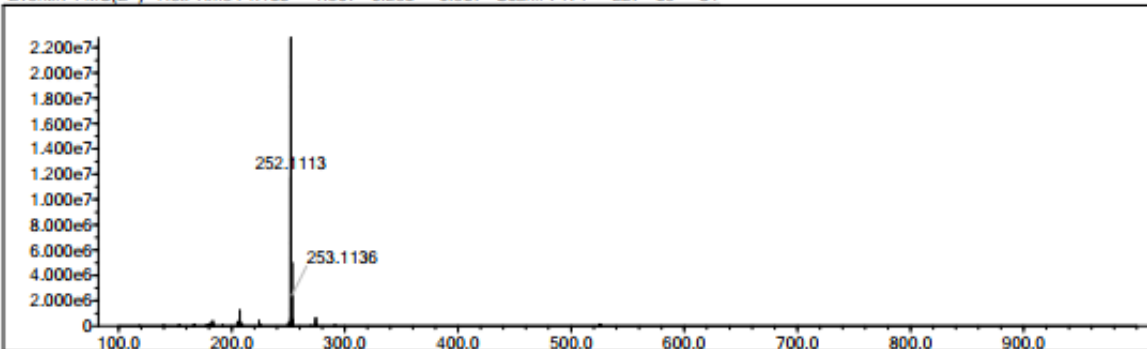
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	0	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

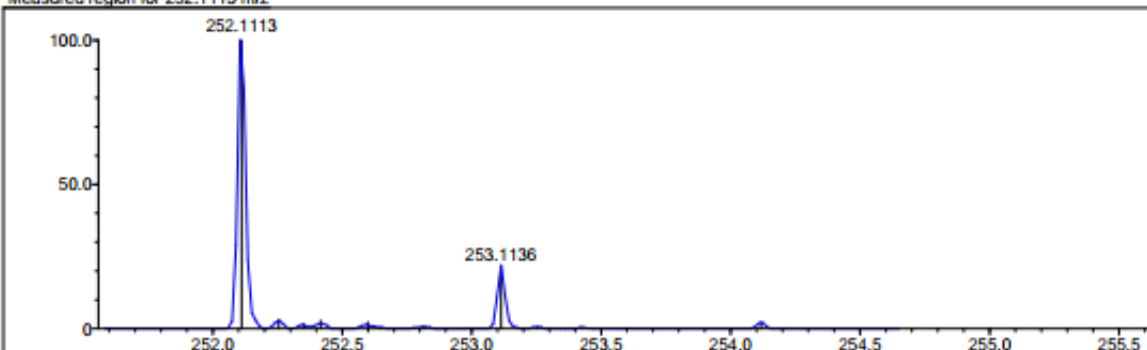
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

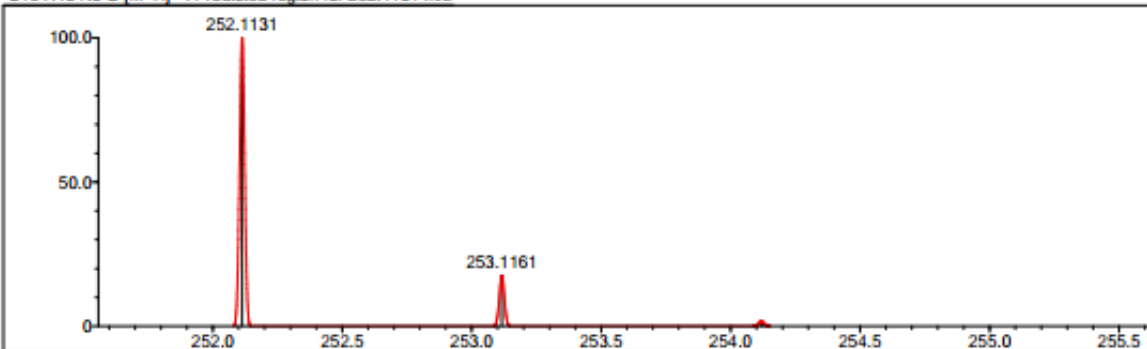
Event#: 1 MS(E+) Ret. Time : 1.133 -> 1.507 -> 0.253 -> 0.537 Scan#: 171 -> 227 - 39 -> 81



Measured region for 252.1113 m/z

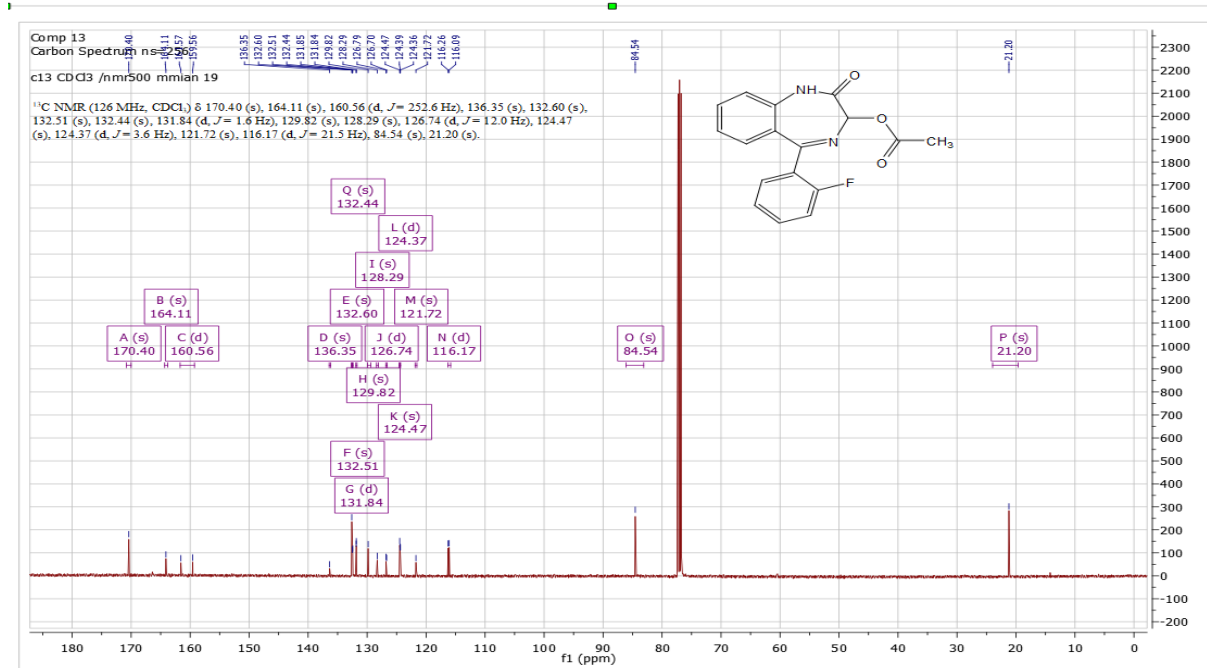
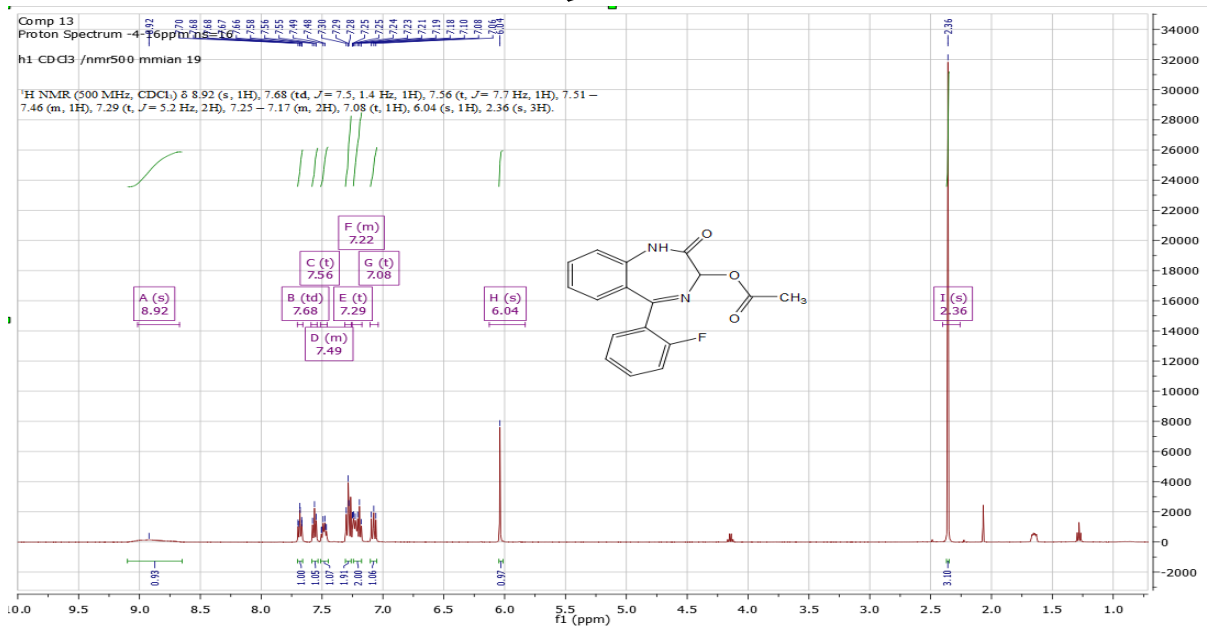
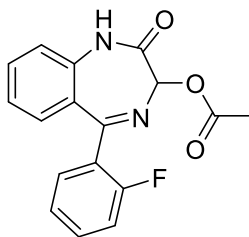


C15 H13 N3 O [M+H]<sup>+</sup> : Predicted region for 252.1131 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	43.70	C15 H13 N3 O	[M+H] <sup>+</sup>	252.1113	252.1131	-1.8	-7.14	63.70	11.0

## 5-(2-fluorophenyl)-2-oxo-2,3-dihydro-1H-benzo[e][1,4]diazepin-3-yl acetate(5h)



Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 13\_12082020 Analysis\_27.lcd

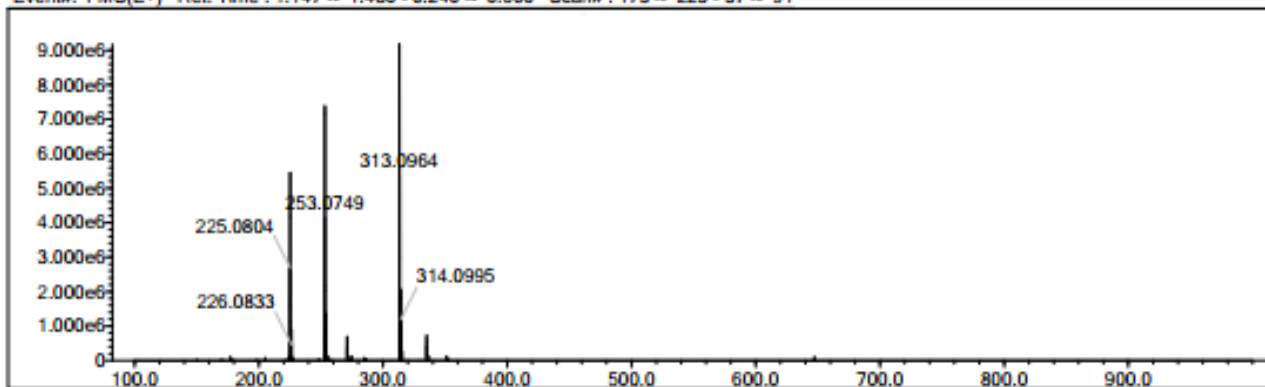
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

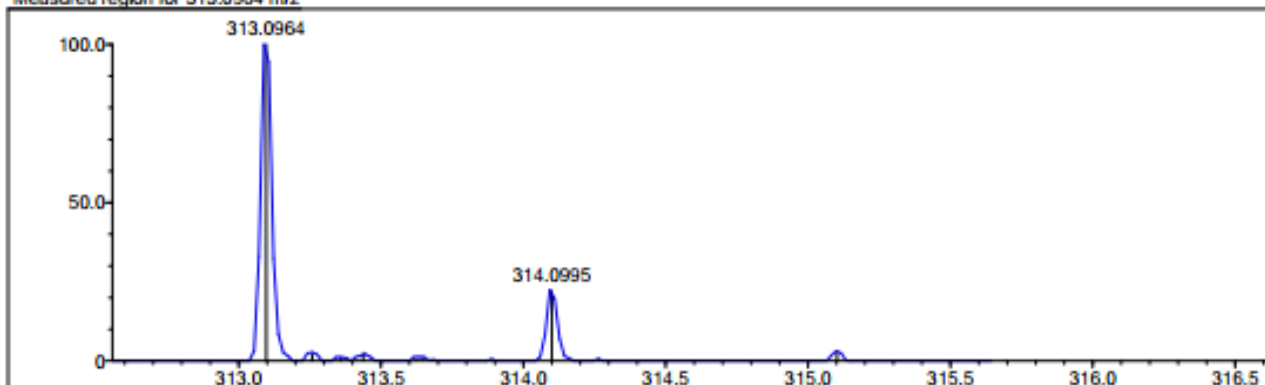
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

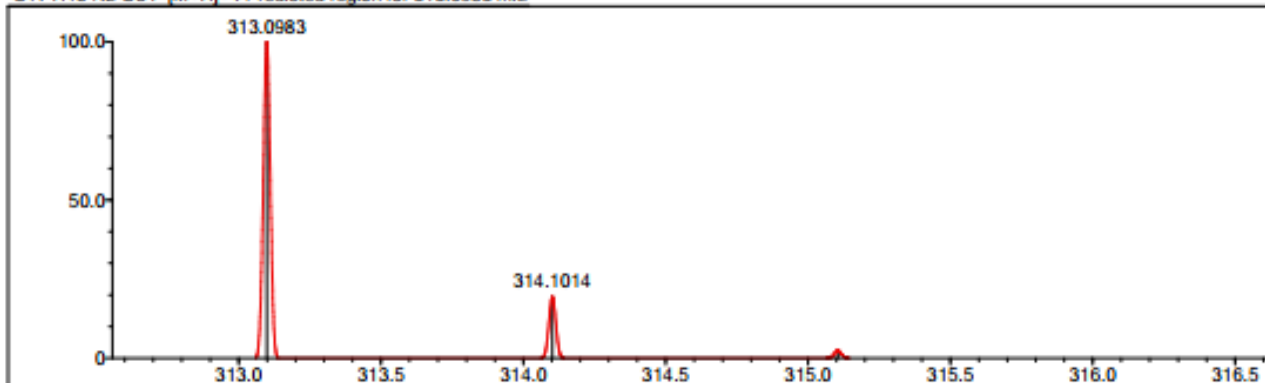
Event#: 1 MS(E+) Ret. Time : 1.147 -> 1.480 - 0.240 -> 0.600 Scan#: 173 -> 223 - 37 -> 91



Measured region for 313.0964 m/z

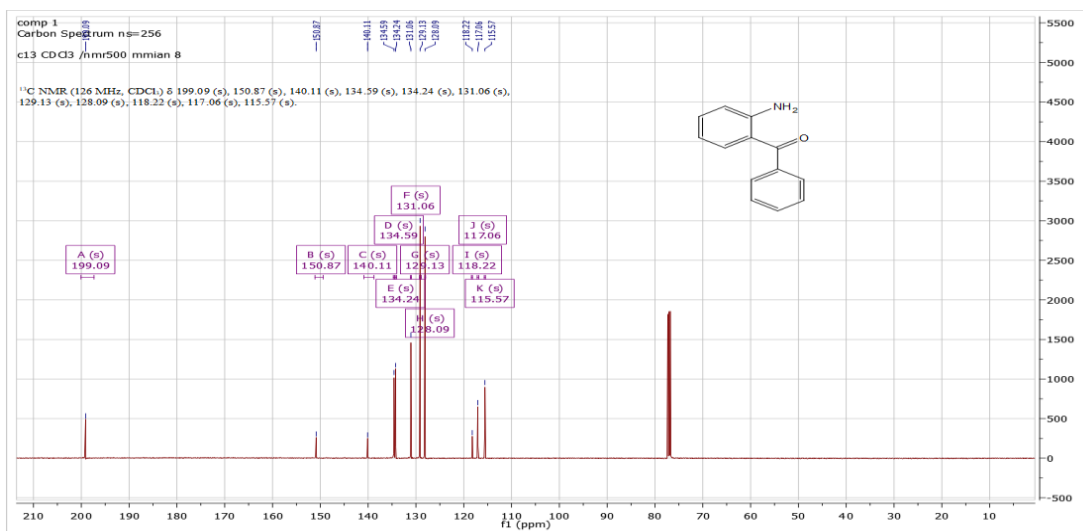
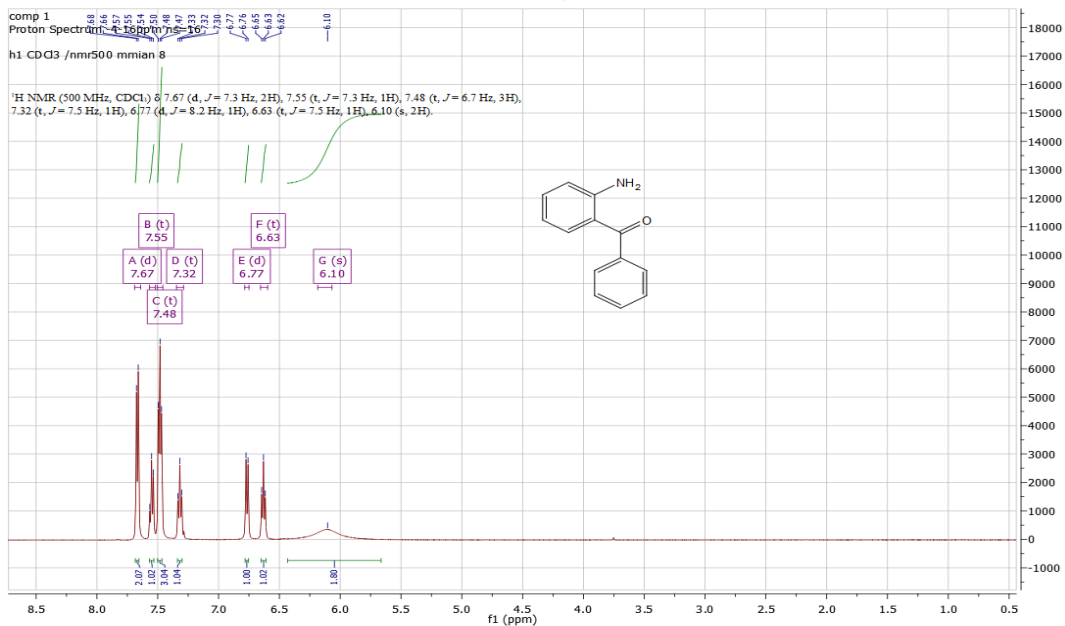
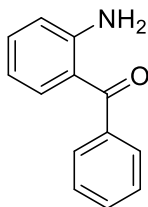


C17H13N2O3F [M+H]<sup>+</sup> : Predicted region for 313.0983 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	74.08	C17H13N2O3F	[M+H] <sup>+</sup>	313.0964	313.0983	-1.9	-6.07	93.42	12.0

## (2-aminophenyl)(phenyl)methanone (7a)



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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 1\_12082020 Analysis\_51.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	15	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	0					

Error Margin (ppm): 300

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -100.0 - 2000.0

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: AND

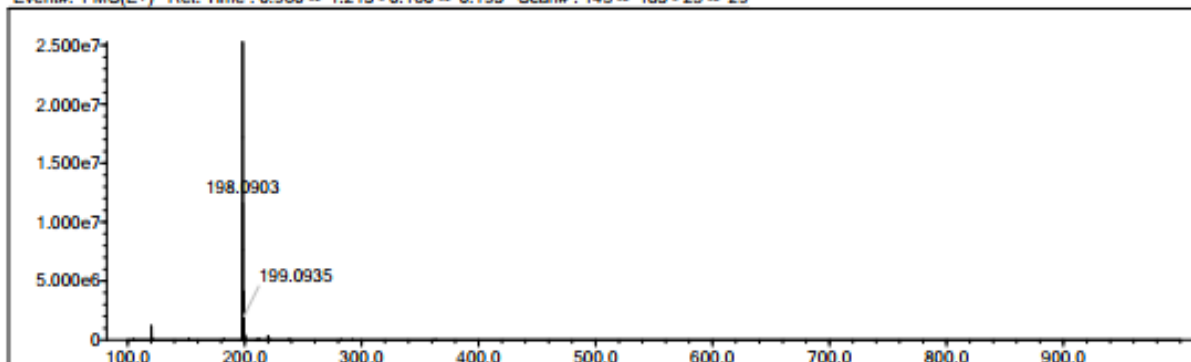
Electron Ions: both

Use MSn Info: yes

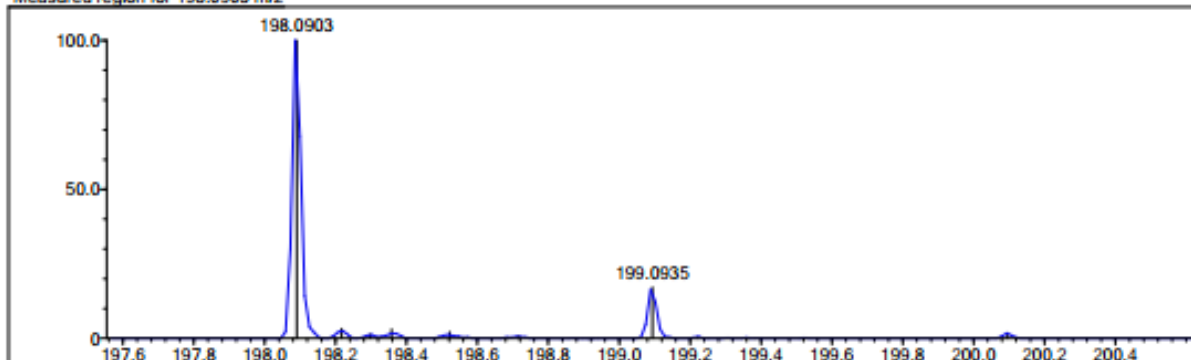
Isotope Res: 10000

Max Results: 10

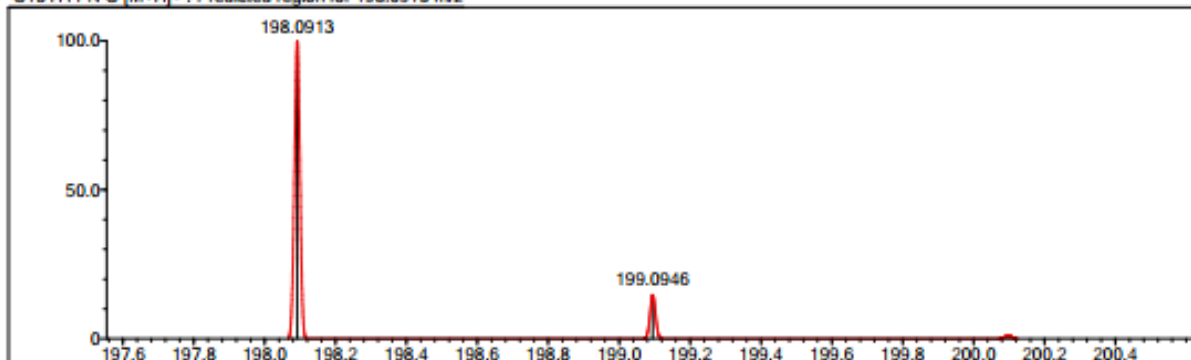
Event#: 1 MS(E+) Ret. Time : 0.960 -> 1.213 - 0.160 -> 0.193 Scan#: 145 -> 183 - 25 -> 29



Measured region for 198.0903 m/z

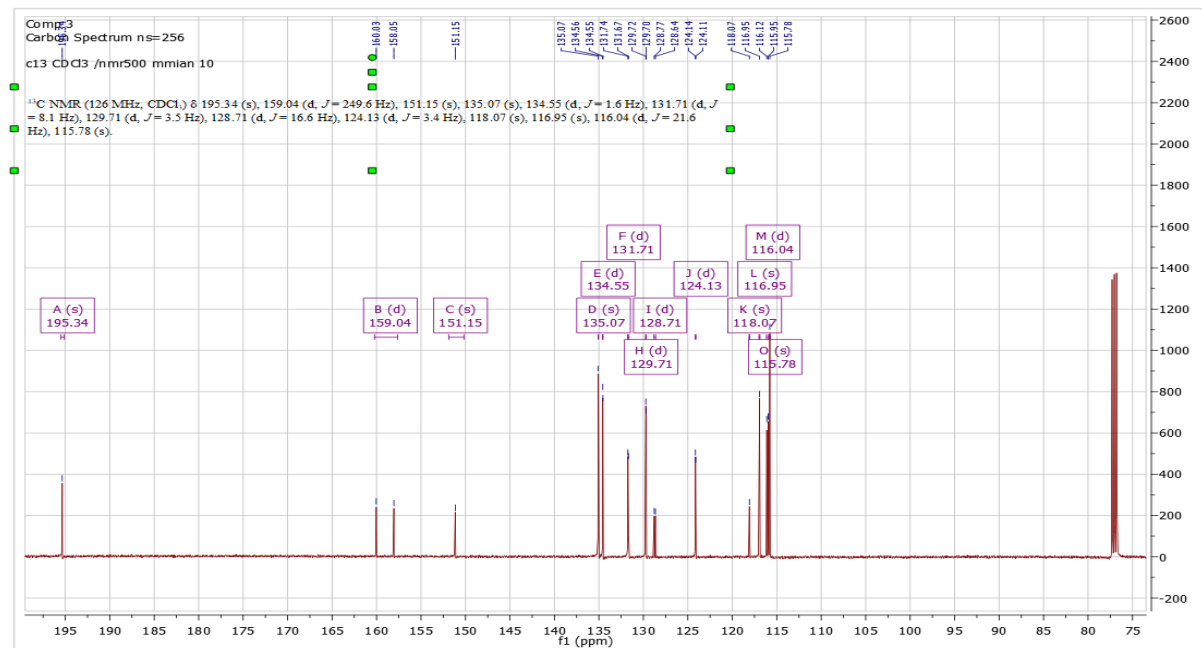
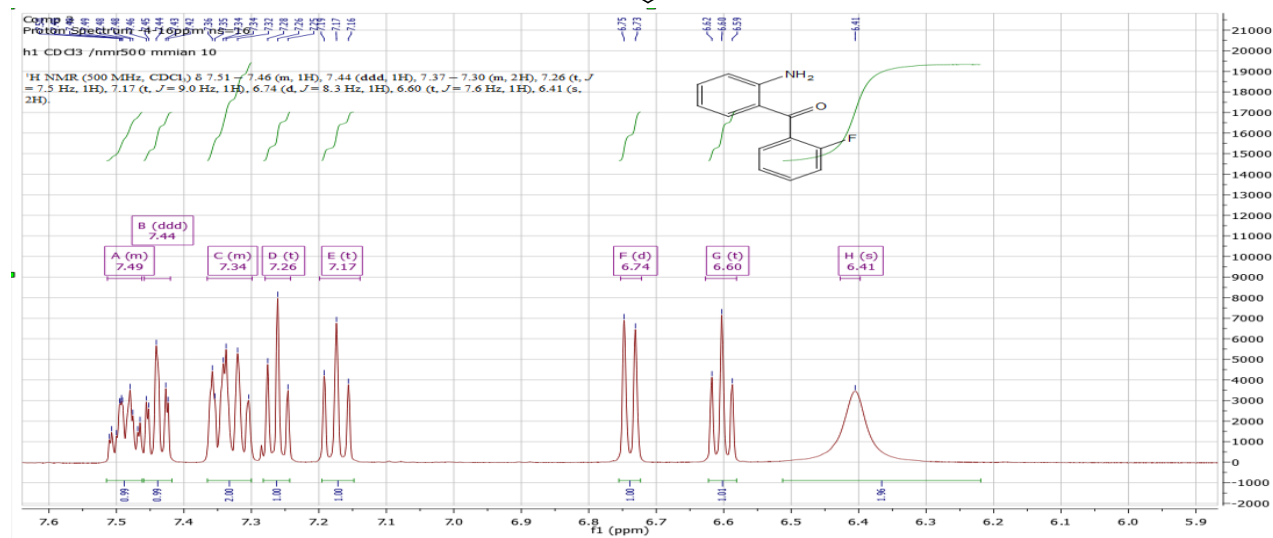
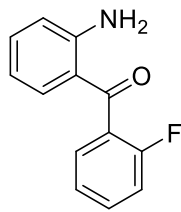


C13 H11 N O [M+H]+ : Predicted region for 198.0913 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	53.40	C13H11NO	[M+H] <sup>+</sup>	198.0903	198.0913	-1.0	-5.05	59.66	9.0

## (2-aminophenyl)(2-fluorophenyl)methanone(7b)





Formula Predictor Report - COMP\_3\_12082020 Analysis\_47.lcd

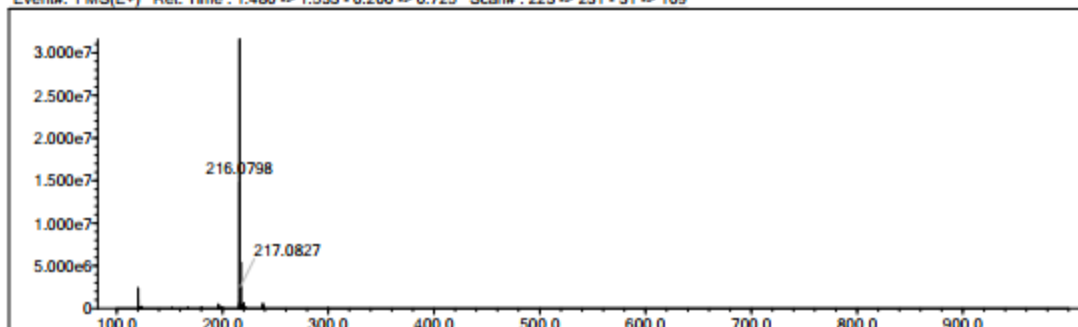
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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP\_3\_12082020 Analysis\_47.lcd

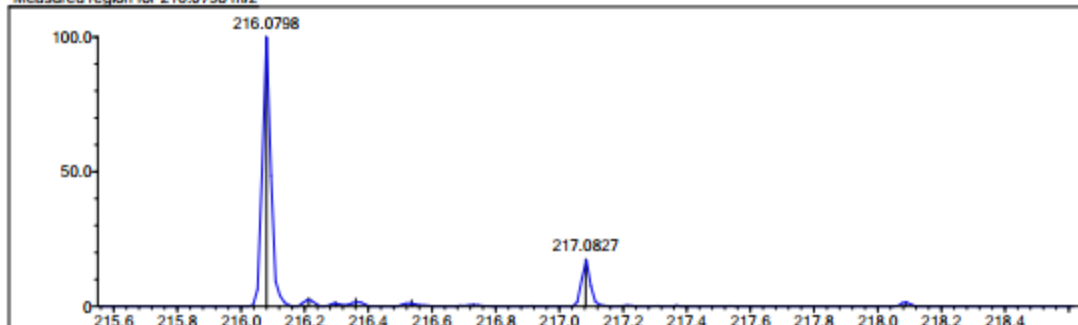
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	0					

Error Margin (ppm): 300  
 DBE Range: -100.0 - 2000.0  
 Electron Ions: both  
 HC Ratio: unlimited  
 Apply N Rule: no  
 Use MSn Info: yes  
 Max Isotopes: all  
 Isotope RI (%): 1.00  
 Isotope Res: 10000  
 MSn Iso RI (%): 75.00  
 MSn Logic Mode: AND  
 Max Results: 10

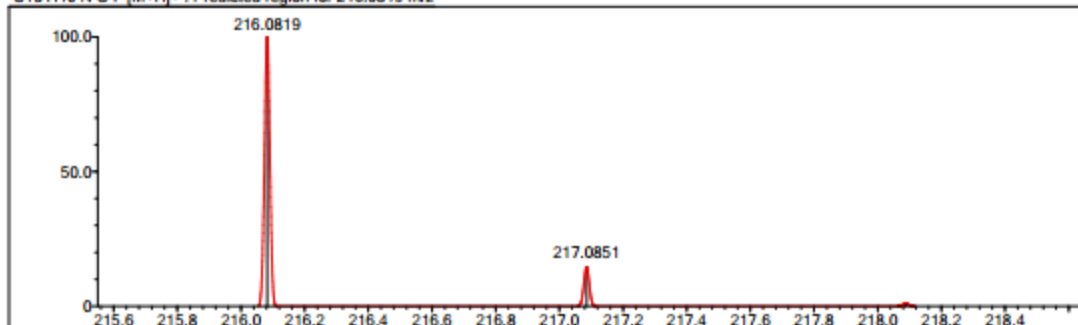
Event#: 1 MS(E+) Ret. Time : 1.480 -> 1.533 - 0.200 -> 0.725 Scan# : 223 -> 231 - 31 -> 109



Measured region for 216.0798 m/z

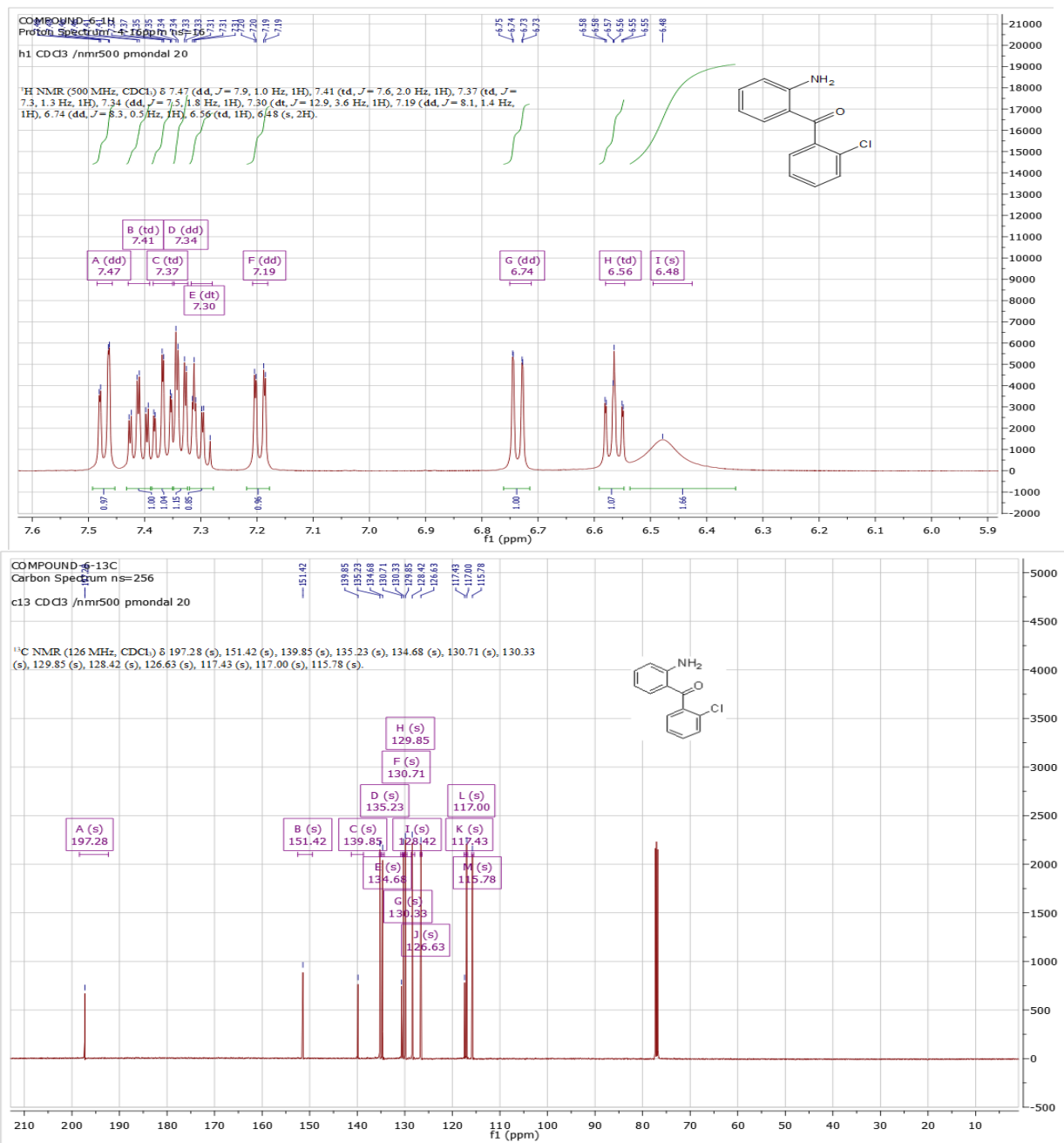
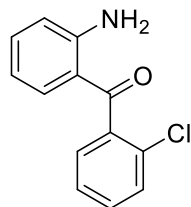


C13 H10 N O F [M+H]+ : Predicted region for 216.0819 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	33.60	C13 H10 N O F	[M+H] <sup>+</sup>	216.0798	216.0819	-2.1	-9.72	78.51	9.0

## (2-aminophenyl)(2-chlorophenyl)methanone(7c)



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Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 6\_12082020 Analysis\_41.lcd

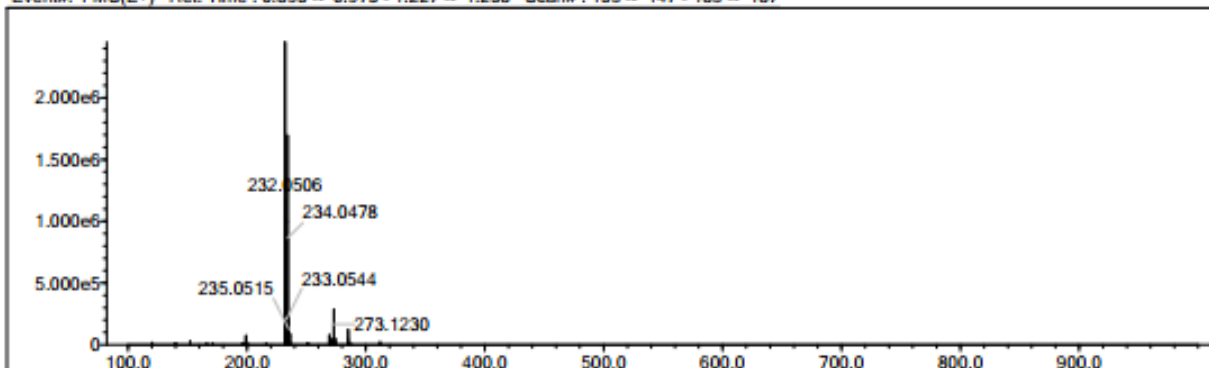
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	25	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

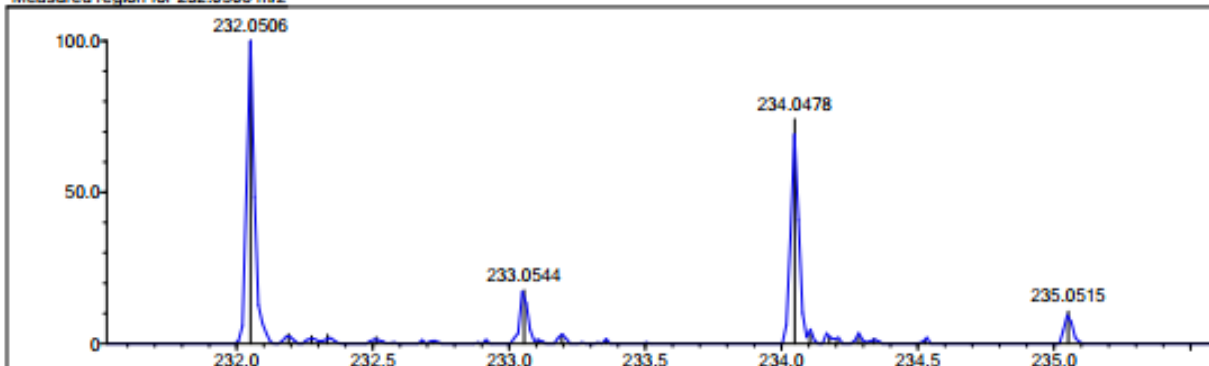
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

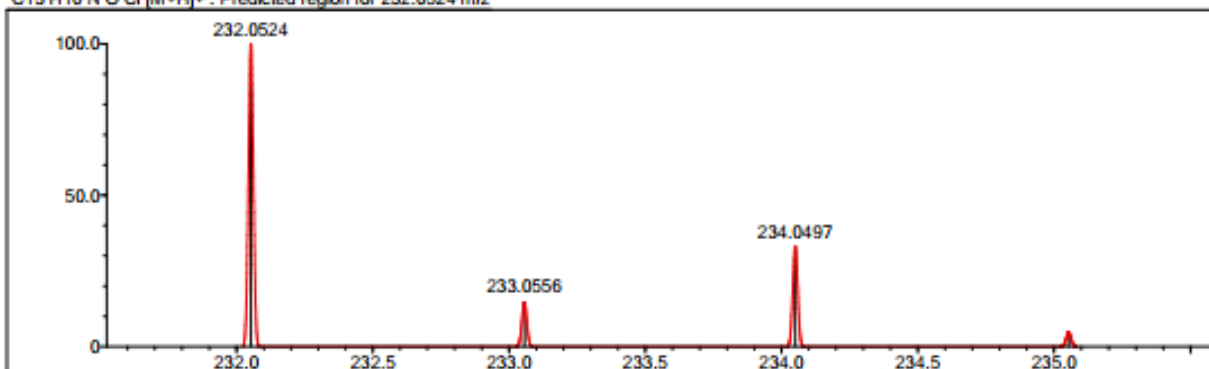
Event#: 1 MS(E+) Ret. Time : 0.893 -> 0.973 - 1.227 -> 1.238 Scan#: 135 -> 147 - 185 -> 187



Measured region for 232.0506 m/z

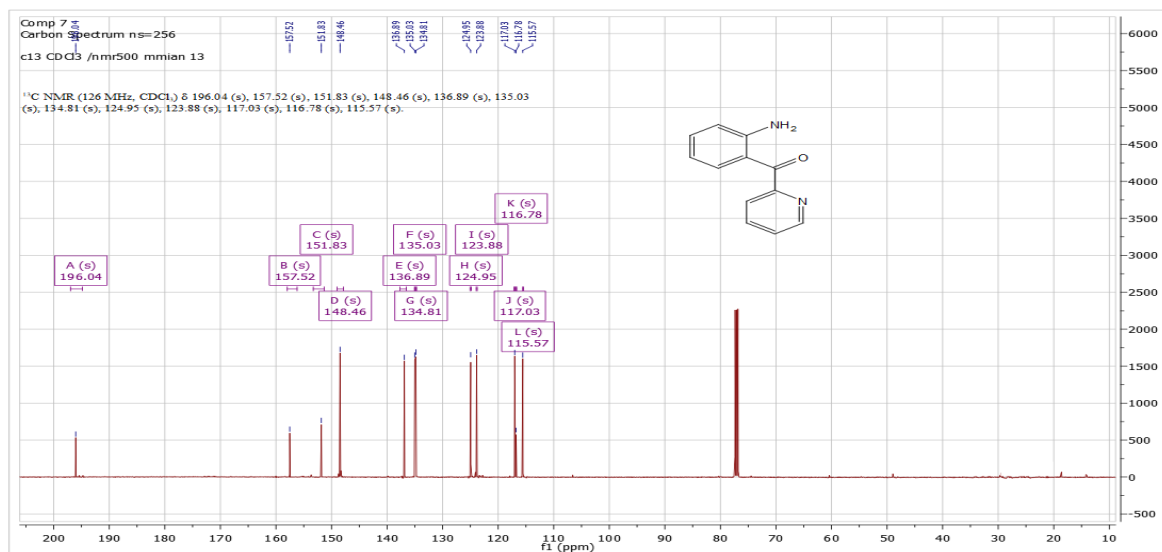
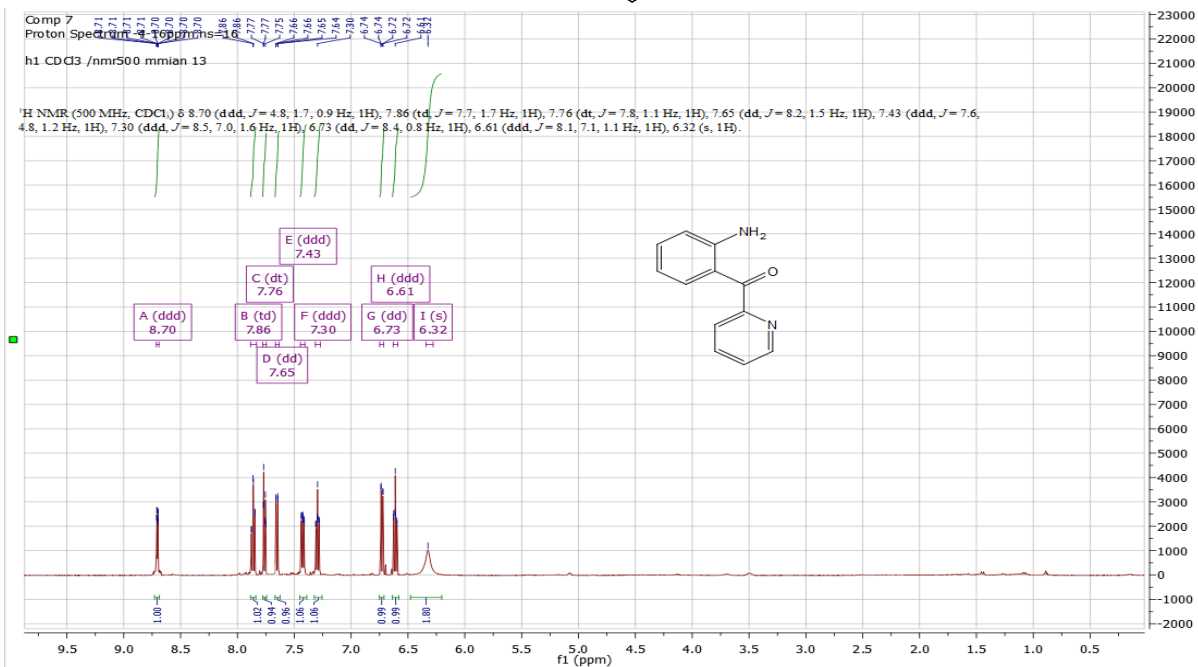
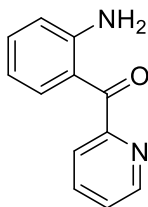


C13 H10 N O Cl [M+H]<sup>+</sup> : Predicted region for 232.0524 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	30.35	C13 H10 N O Cl	[M+H] <sup>+</sup>	232.0506	232.0524	-1.8	-7.76	48.64	9.0

## (2-aminophenyl)(pyridin-2-yl)methanone (7d)



Data File: C:\LabSolutions\Data\Vilashini Rajaratnam\12082020 Analysis\COMP 7\_12082020 Analysis\_39.lcd

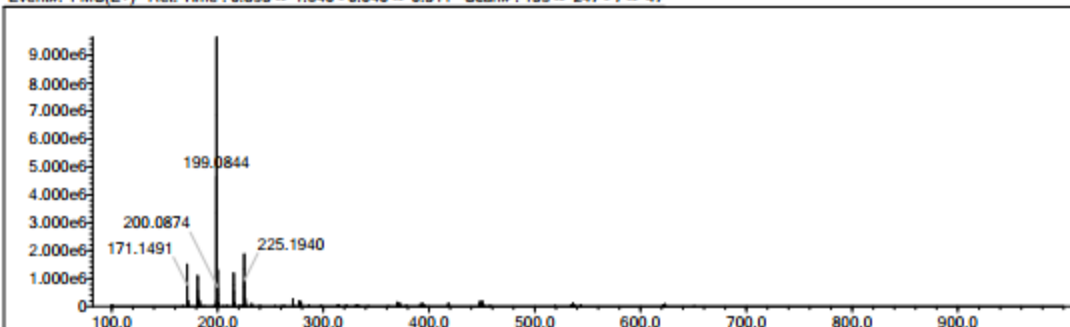
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	N	3	1	3	Si	4	0	0	Br	1	0	0	H
2H	1	0	0	O	2	1	3	S	2	0	0	I	3	0	0	K
C	4	10	25	F	1	0	1	Cl	1	0	1					

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

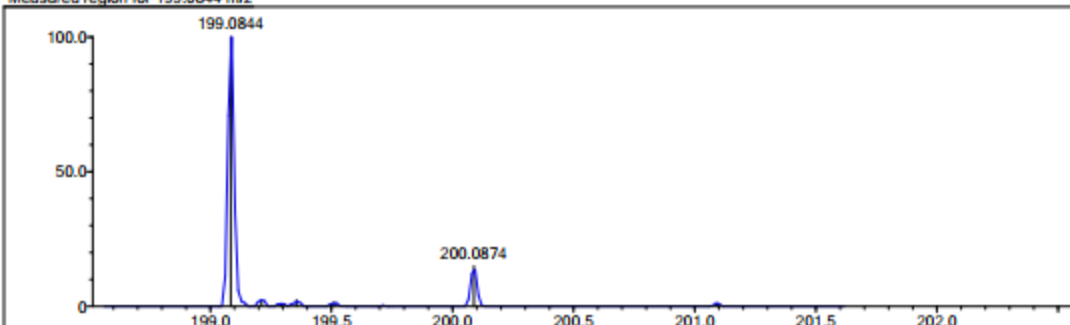
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

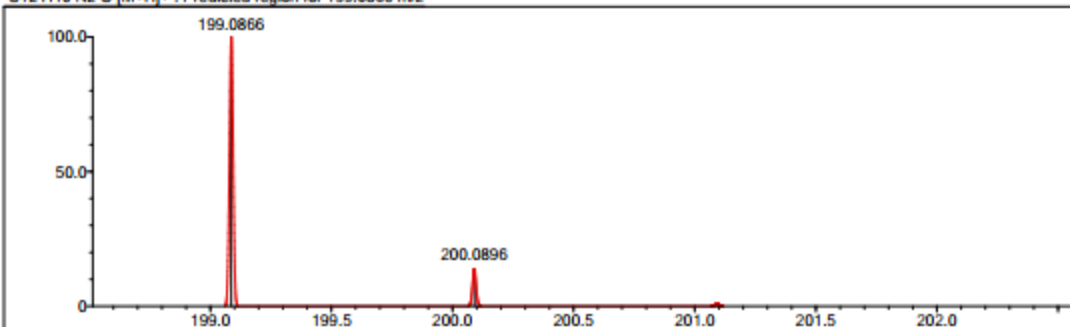
Event#: 1 MS(E+) Ret. Time : 0.893 -> 1.640 - 0.040 -> 0.311 Scan#: 135 -> 247 - 7 -> 47



Measured region for 199.0844 m/z

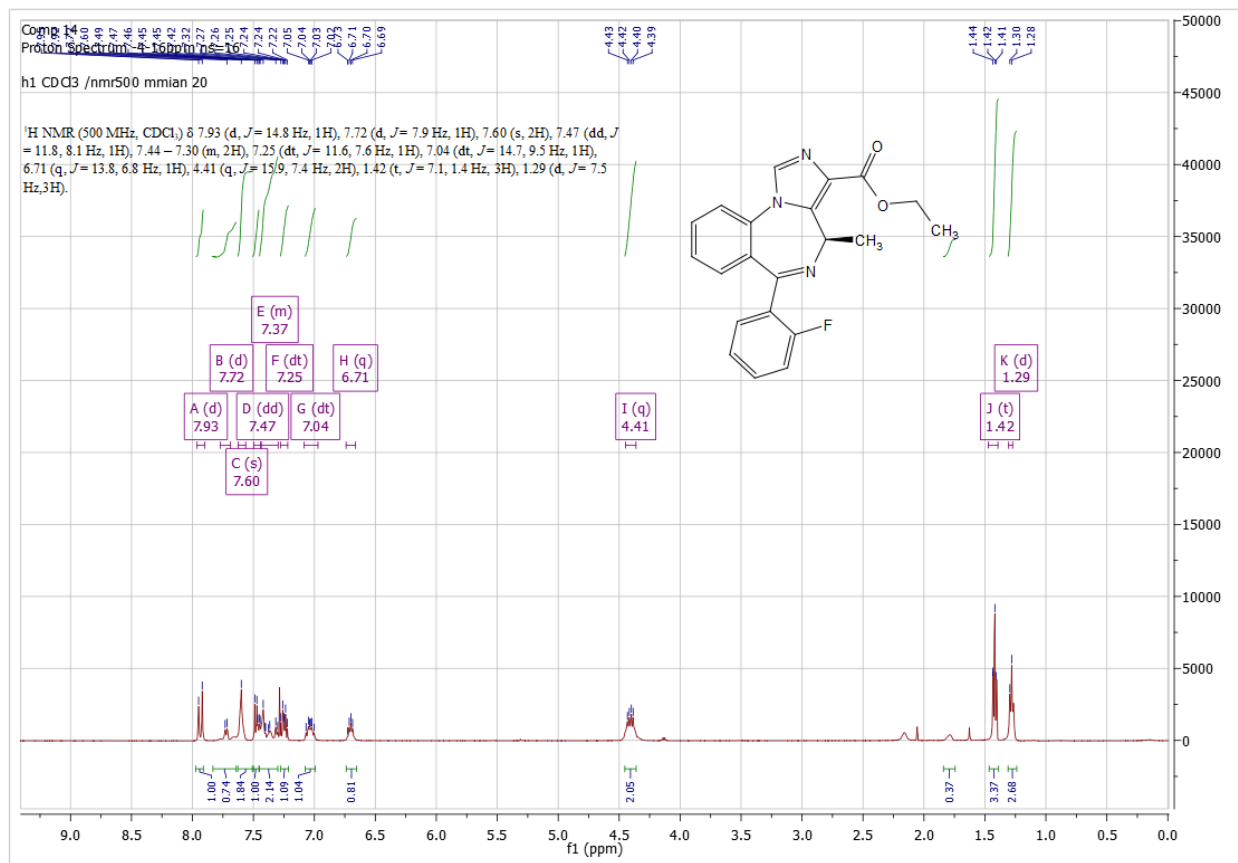
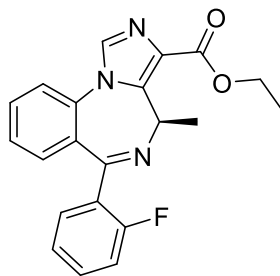


C12 H10 N2 O [M+H]<sup>+</sup> : Predicted region for 199.0866 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	35.70	C12 H10 N2 O	[M+H] <sup>+</sup>	199.0844	199.0866	-2.2	-11.05	95.97	9.0

## ethyl (R)-6-(2-fluorophenyl)-4-methyl-4H-benzo[f]imidazo[1,5-a][1,4]diazepine-3-carboxylate(9a)



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Data File: C:\LabSolutions\Data\Witashini Rajaratnam\12082020 Analysis\COMP\_14\_12082020 Analysis\_25.lcd

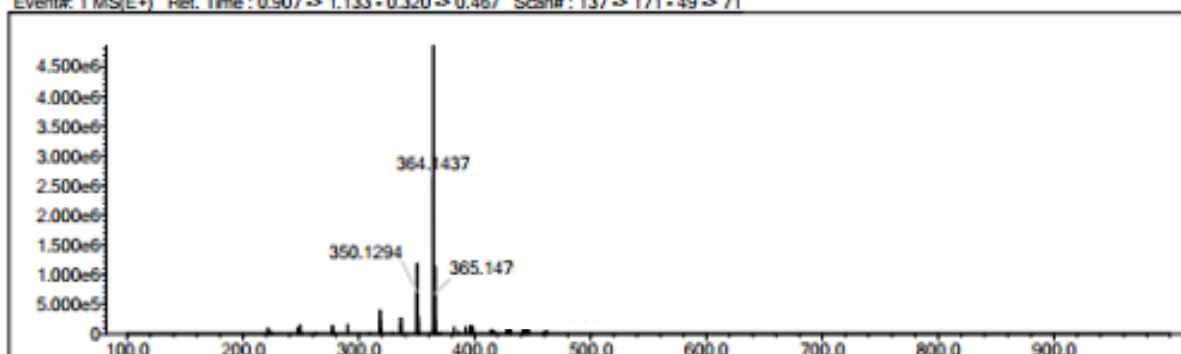
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	30	O	2	1	3	Cl	1	0	0	H
2H	1	0	0	F	1	1	4	Br	1	0	0	Na
C	4	10	25	Si	4	0	0	I	3	0	0	K
N	3	1	3	S	2	0	0					NH4

Error Margin (ppm): 300  
 HC Ratio: unlimited  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

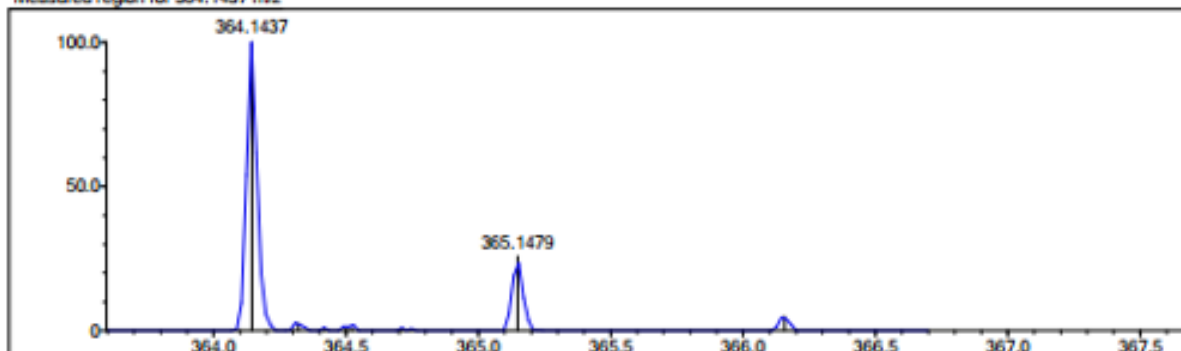
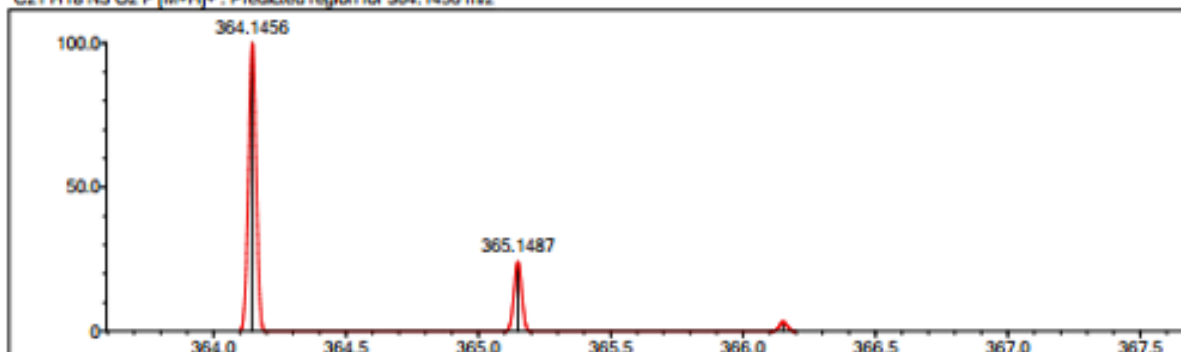
DBE Range: -100.0 - 2000.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: yes  
 Isotope Res: 10000  
 Max Results: 10

Event#: 1 MS(E+) Ret. Time : 0.907 -&gt; 1.133 - 0.320 -&gt; 0.467 Scan#: 137 -&gt; 171 - 49 -&gt; 71

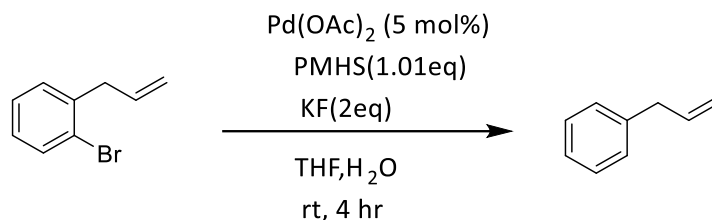


Measured region for 364.1437 m/z

C21 H18 N3 O2 F [M+H]<sup>+</sup> : Predicted region for 364.1456 m/z

Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	72.18	C21 H18 N3 O2 F	[M+H] <sup>+</sup>	364.1437	364.1456	-1.9	-5.22	82.21	14.0

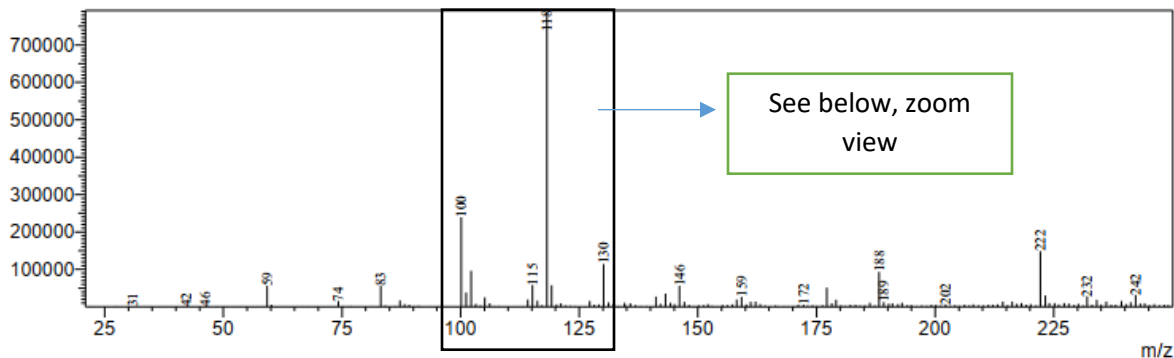
## Debromination on a double bond containing substrate



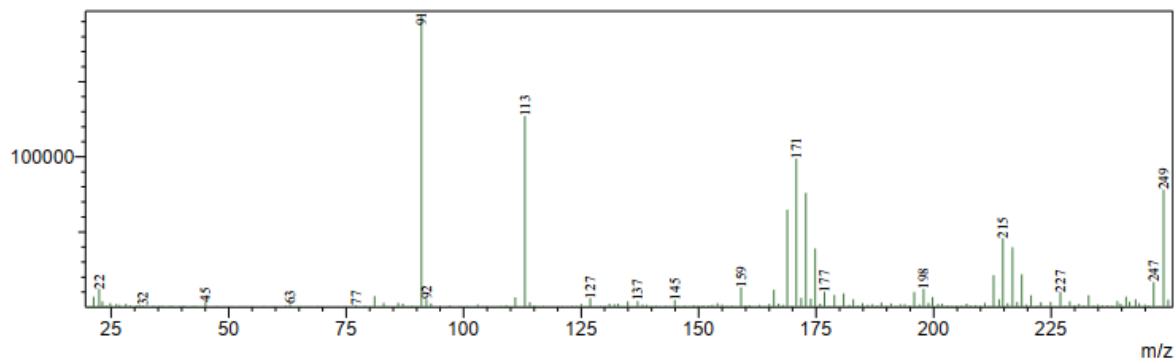
PHMS debrominated the bromine group selectively without interfering with the double bond. The debromination was confirmed by running the crude products on a single quadrupole LCMS 2020.

## &lt;Spectrum&gt;

R.Time:----(Scan#:----)  
MassPeaks:221 BasePeak:118(784464)  
Spectrum Mode:Averaged 0.093-0.313(29-95)  
BG Mode:None Polarity:Positive Segment 1 - Event 1

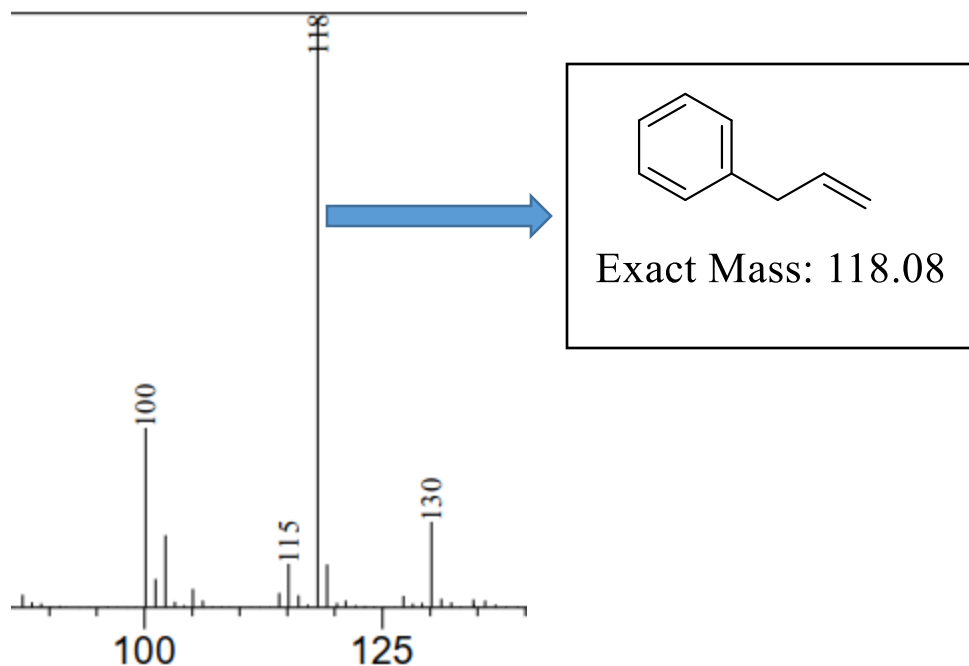


R.Time:----(Scan#:----)  
MassPeaks:231 BasePeak:91(194980)  
Spectrum Mode:Averaged 0.097-0.317(30-96)  
BG Mode:None Polarity:Negative Segment 1 - Event 2

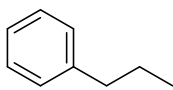


Prithu 2020 - 3-87/3-526-1 - 3.lcd



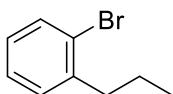


If double bond is reduced, then the mass will be 120, there is no peak here.



Exact Mass: 120.09

If double bond is reduced before debromination, then the mass will be 198 and a double peak will appear but there is no such peak in the whole spectra



Exact Mass: 198.00