Supporting Information

For

Design of new quinolin-2-one-pyrimidine hybrids as sphingosine kinases inhibitors

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[b]*Departamento de Química y Biología, Universidad del Norte, Km 5 vía Puerto Colombia, Barranquilla 081007, Colombia.*

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[e]*Research Group of Heterocyclic Compounds, Department of Chemistry, Universidad del Valle, A. A. 25360, Cali, Colombia..*

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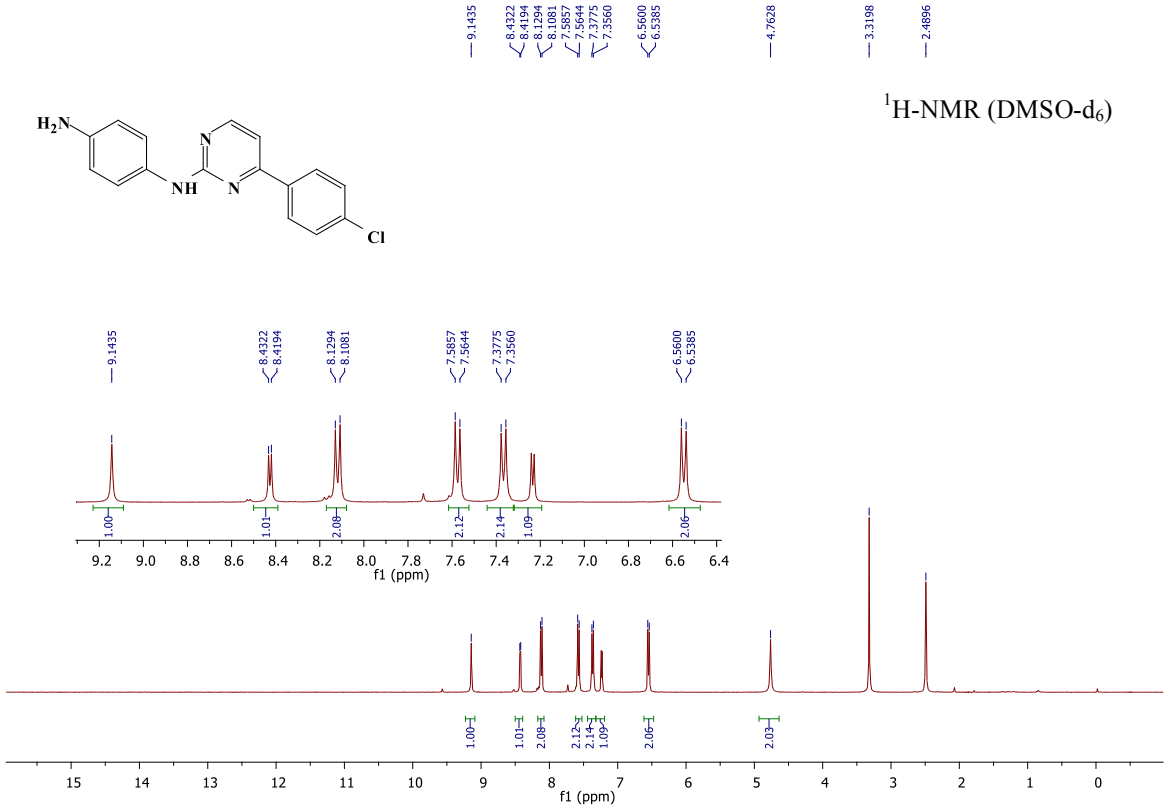
Compound-3a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8.1081
7.5857
7.5644
7.3775
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6.5385
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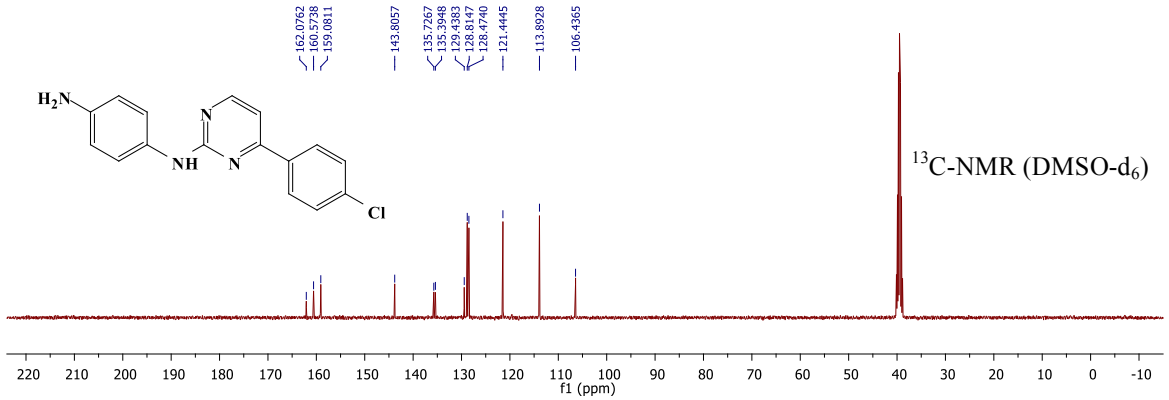
3.3198
2.4896
^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)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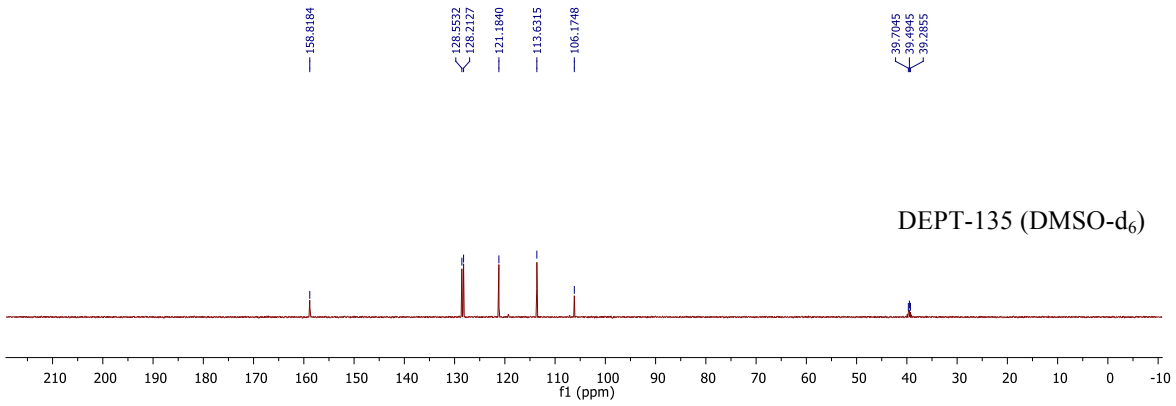
159.0811
143.8057
135.7267
135.3948
129.4383
128.8147
128.4740
121.4445
113.8928
106.4365
^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)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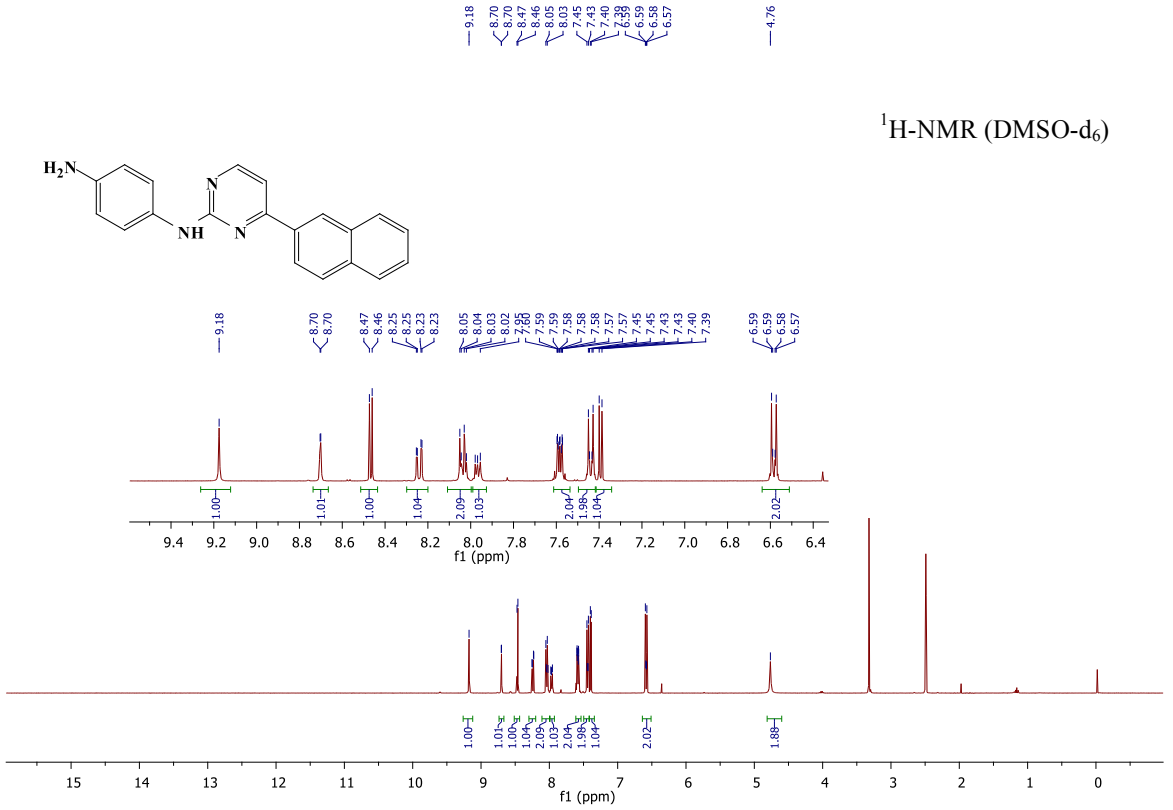
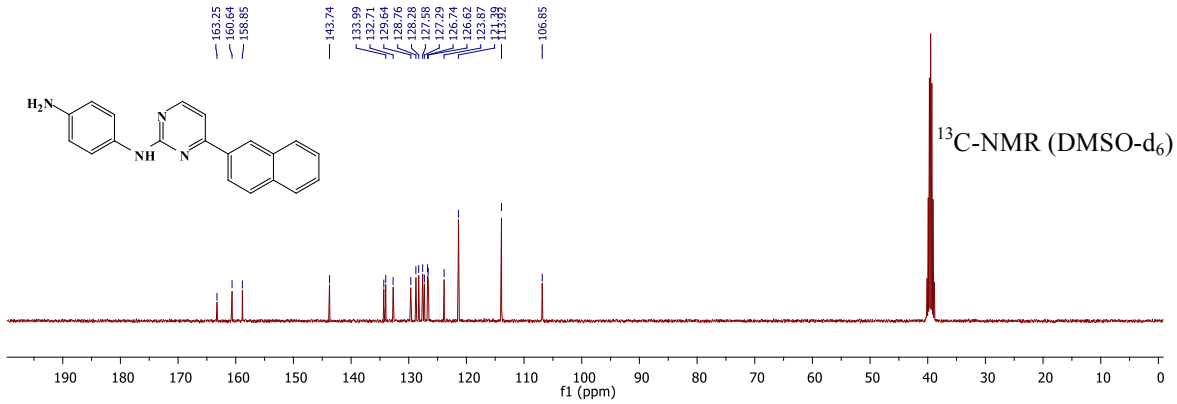
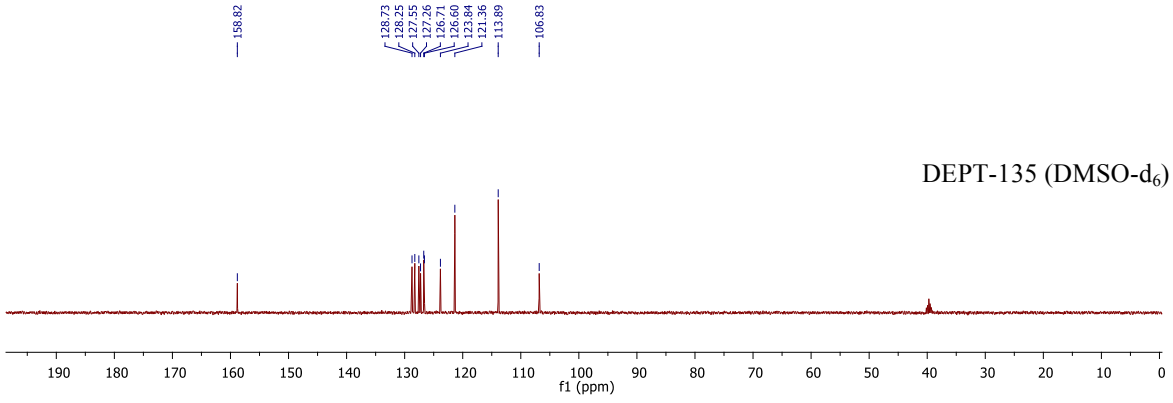
128.5532
128.2127
121.1840
113.6315
106.1748
39.7045
39.4945
39.2855
DEPT-135 (DMSO-d$_6$)
f1 (ppm)

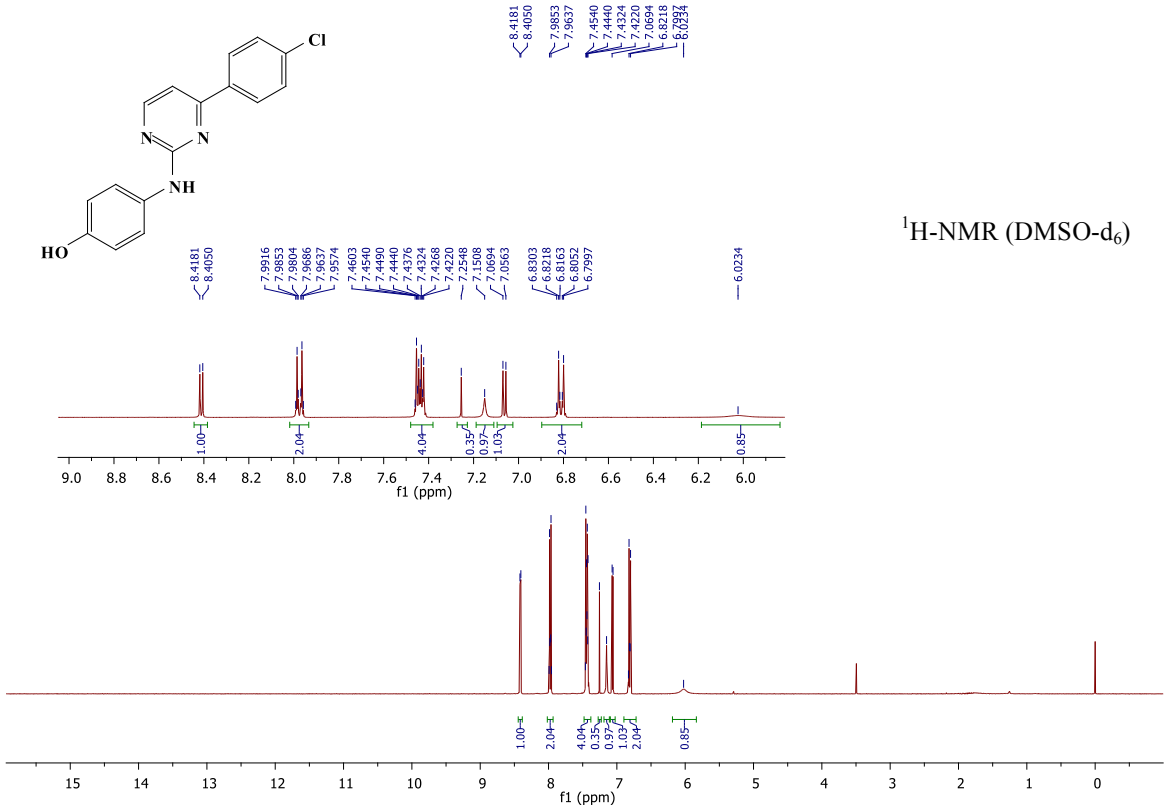
Compound-3b


^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)


^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)


DEPT-135 (DMSO-d$_6$)
f1 (ppm)

Compound-4a



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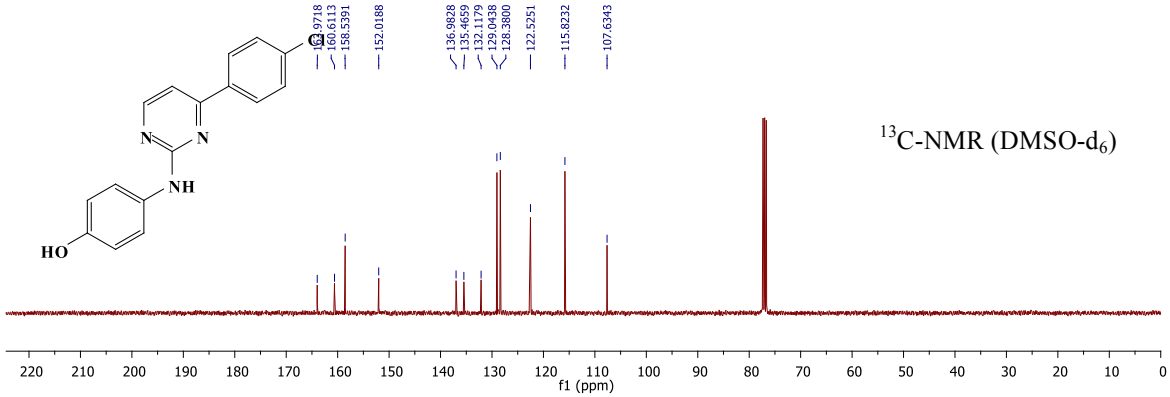

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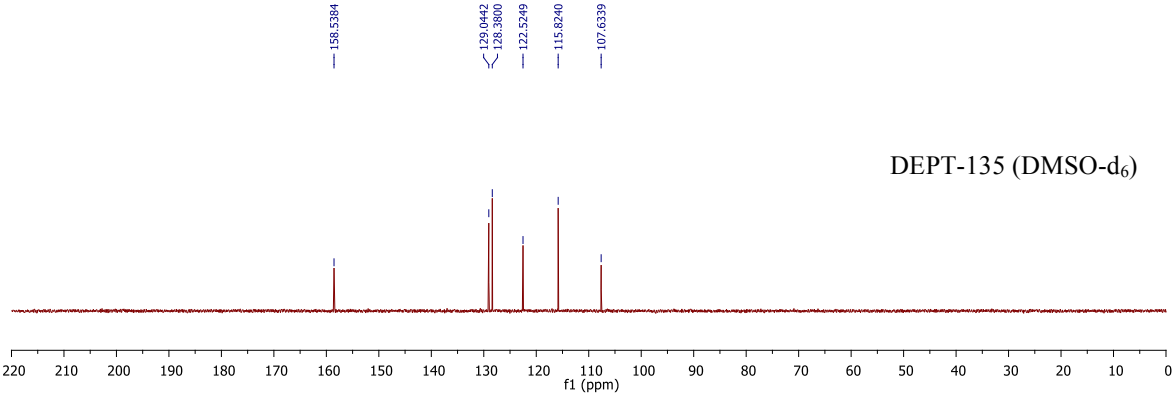
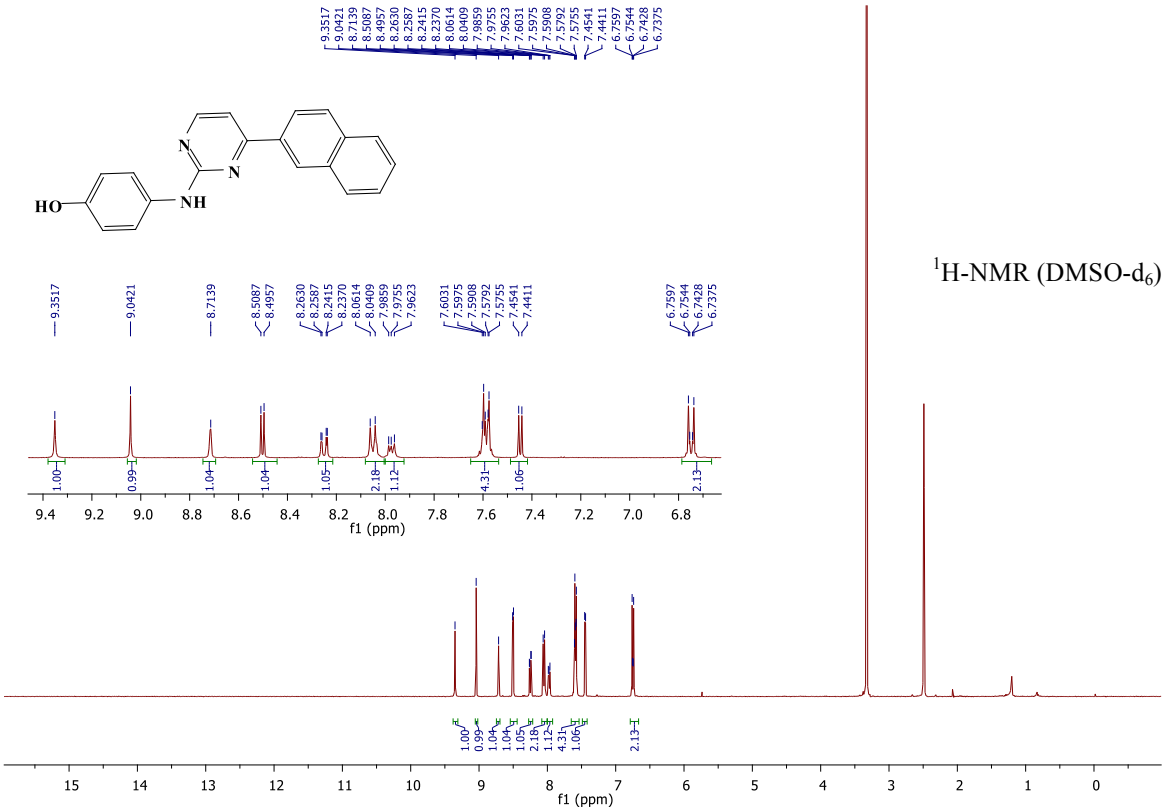


DEPT-135 (DMSO-d$_6$)

Compound-4b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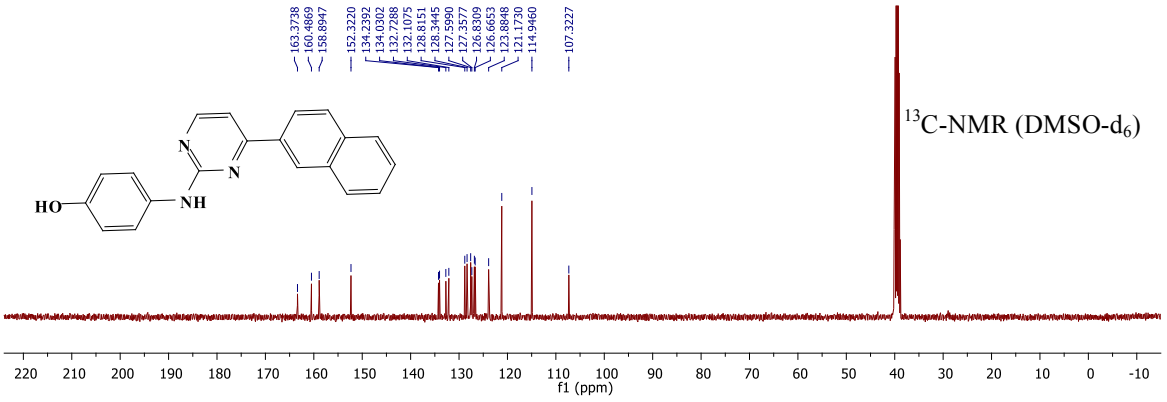
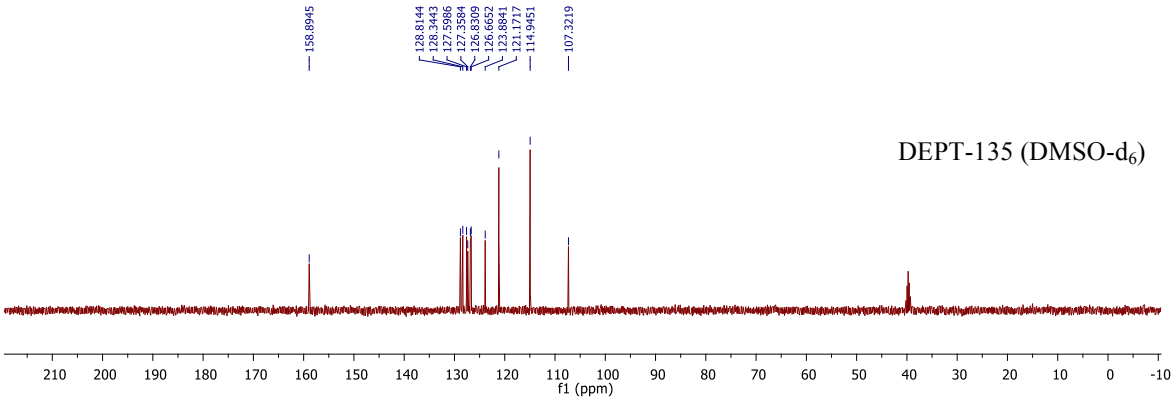
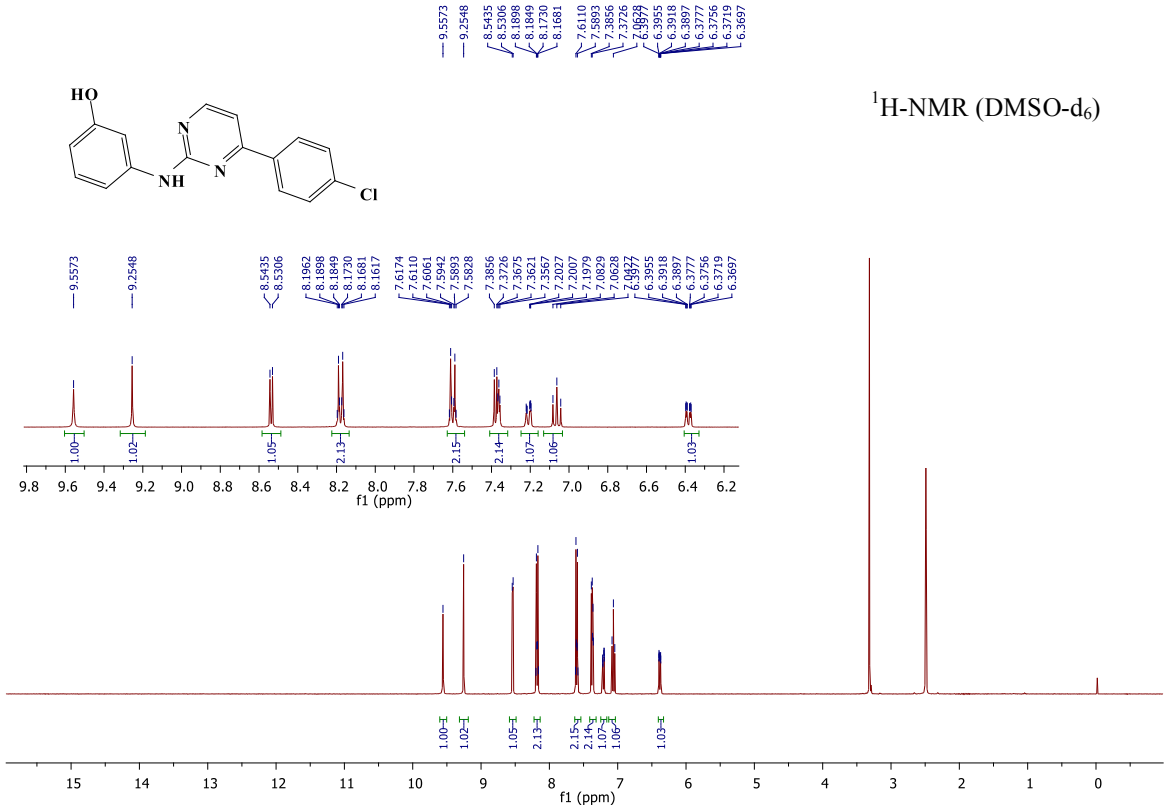
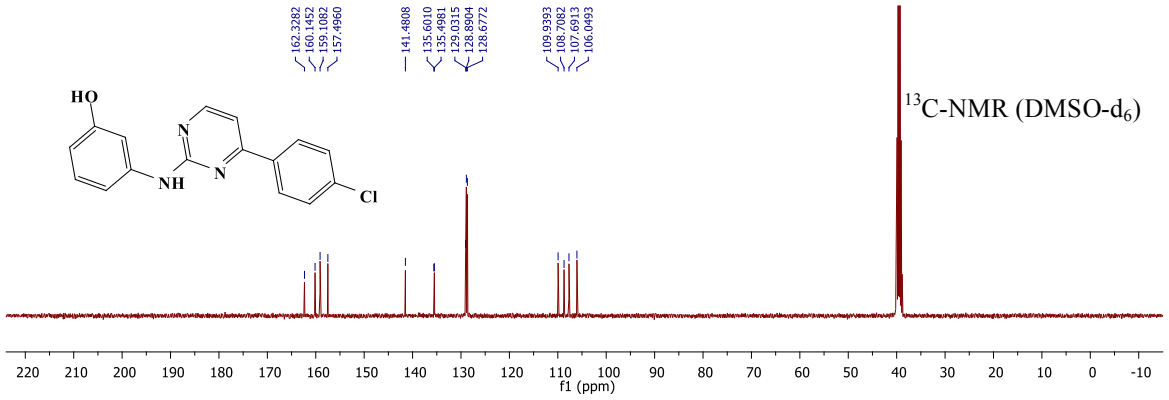
^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)

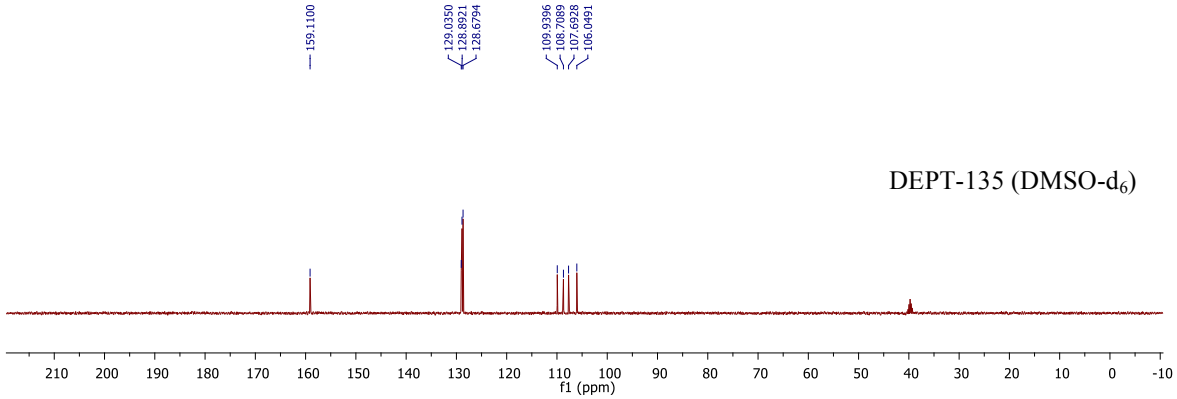

HO
NH
N
N
^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)


DEPT-135 (DMSO-d$_6$)
f1 (ppm)

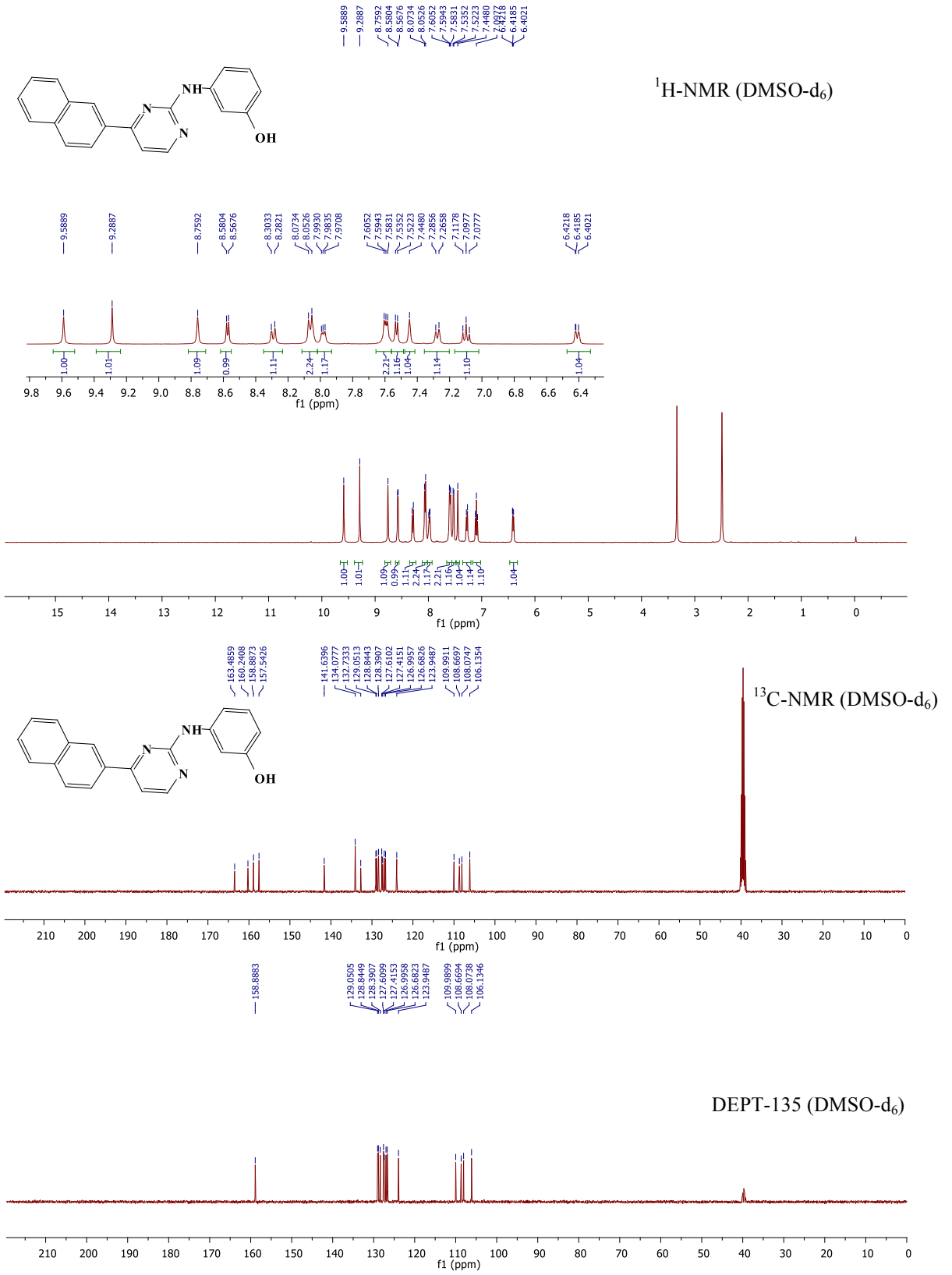
Compound-5a


HO
N
NH
N
Cl
^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)


HO
N
NH
N
Cl
^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)


DEPT-135 (DMSO-d$_6$)
f1 (ppm)

Compound-5b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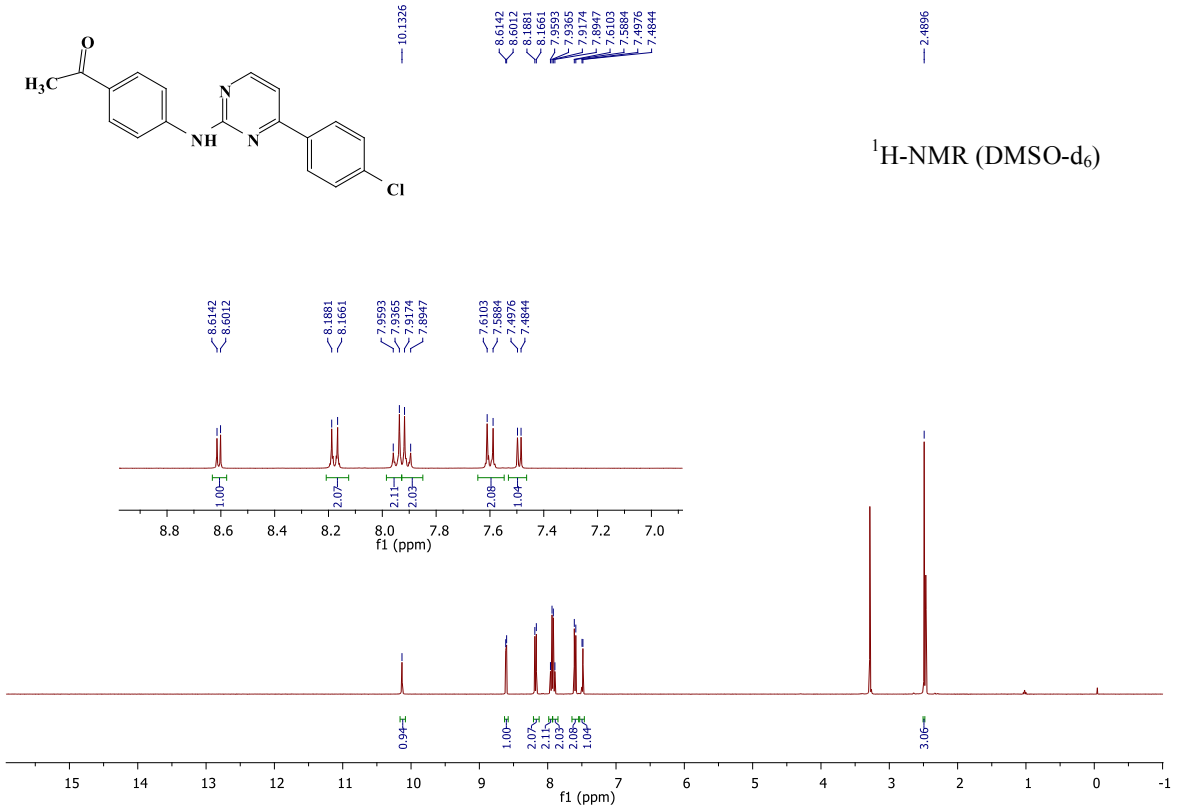
8.5804
8.5676
8.0734
8.0526
7.6052
7.5943
7.5831
7.5352
7.5223
7.4480
7.2856
7.2658
7.1178
7.0977
7.0777
6.4218
6.4185
6.4021
NH
N
N
OH
1H-NMR (DMSO-d6)
f1 (ppm)
163.4859
160.2408
158.8873
157.5426
141.6396
134.0777
132.7333
129.0513
128.8443
128.3907
127.6102
127.4151
126.9957
126.6826
123.9487
109.9911
108.6697
108.0747
106.1354
13C-NMR (DMSO-d6)
158.8883
129.0505
128.8449
128.3907
127.6099
127.4153
126.9958
126.6823
123.9487
109.9899
108.6694
108.0738
106.1346
DEPT-135 (DMSO-d6)

Compound-6a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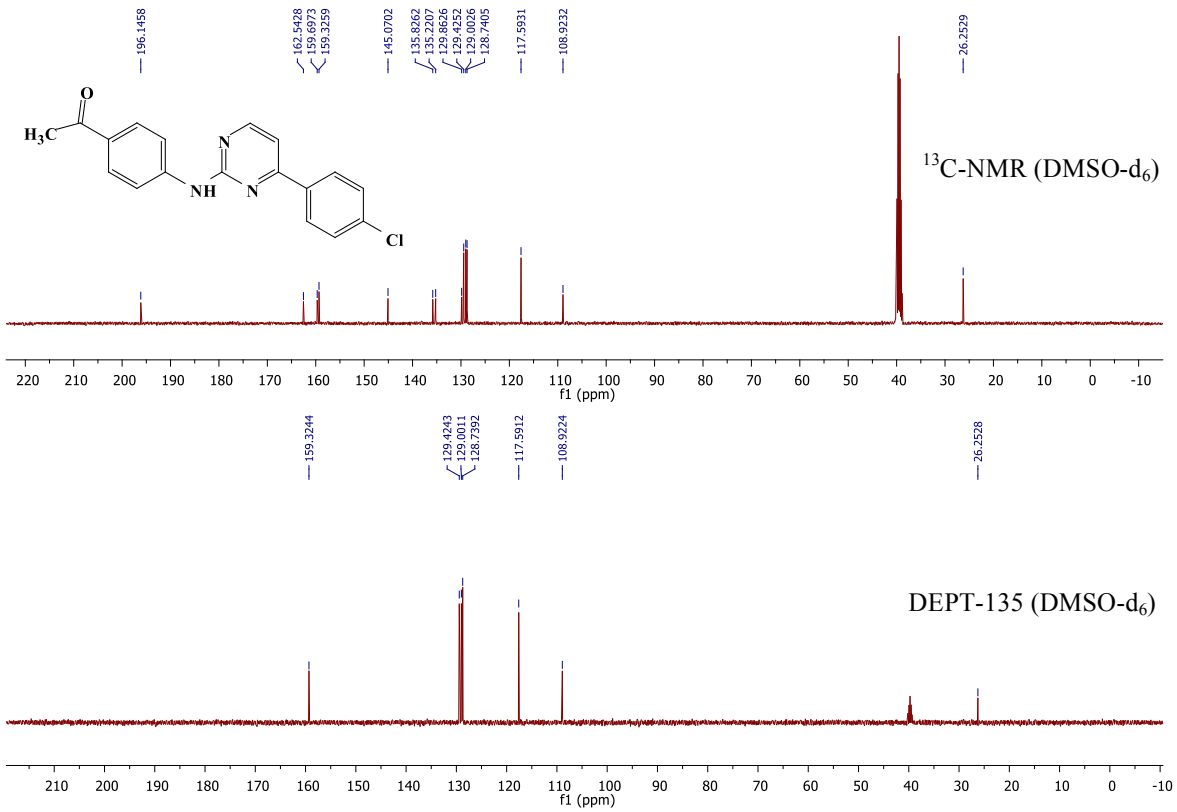
8.6012
8.1881
8.1661
7.9593
7.9365
7.9174
7.8947
7.6103
7.5884
7.4976
7.4844
2.4896
^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)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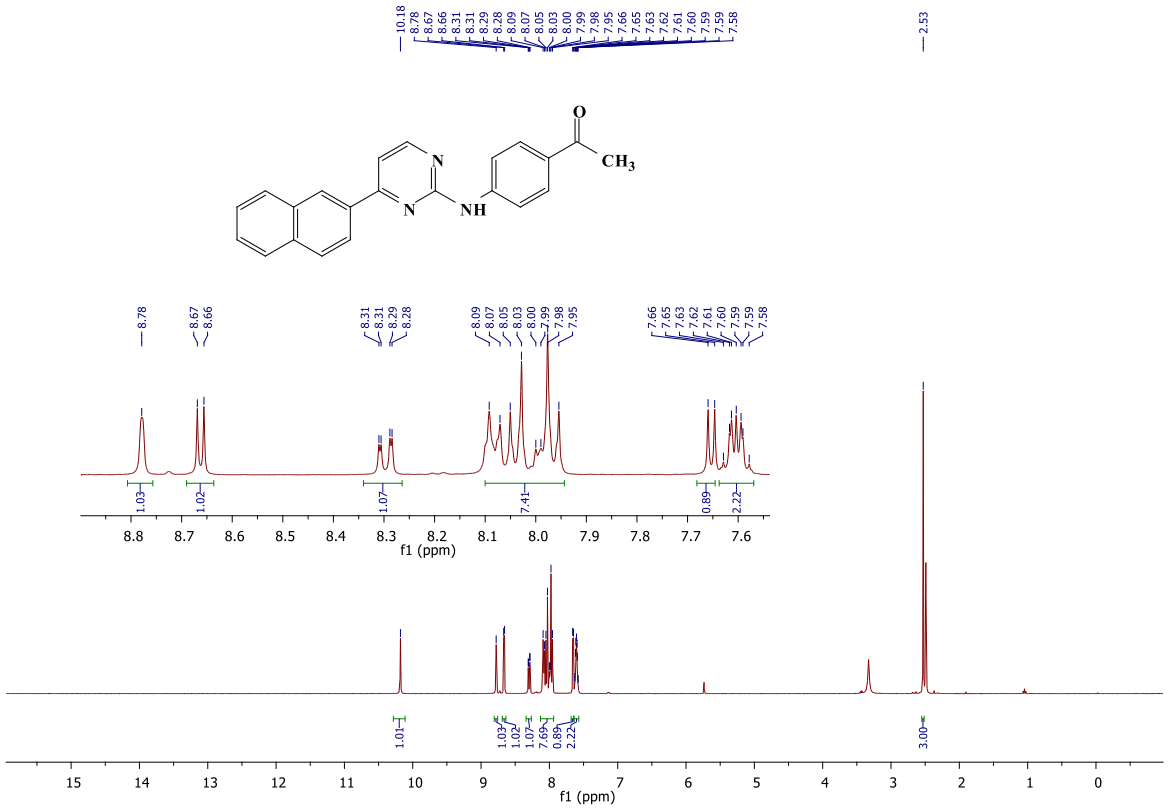
159.6973
159.3259
145.0702
135.8262
135.2207
129.8626
129.4252
129.0026
128.7405
117.5931
108.9232
26.2529
^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)

159.3244
129.4243
129.0011
128.7392
117.5912
108.9224
26.2528
DEPT-135 (DMSO-d$_6$)
f1 (ppm)

Compound-6b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8.67
8.66
8.31
8.31
8.29
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8.09
8.07
8.05
8.03
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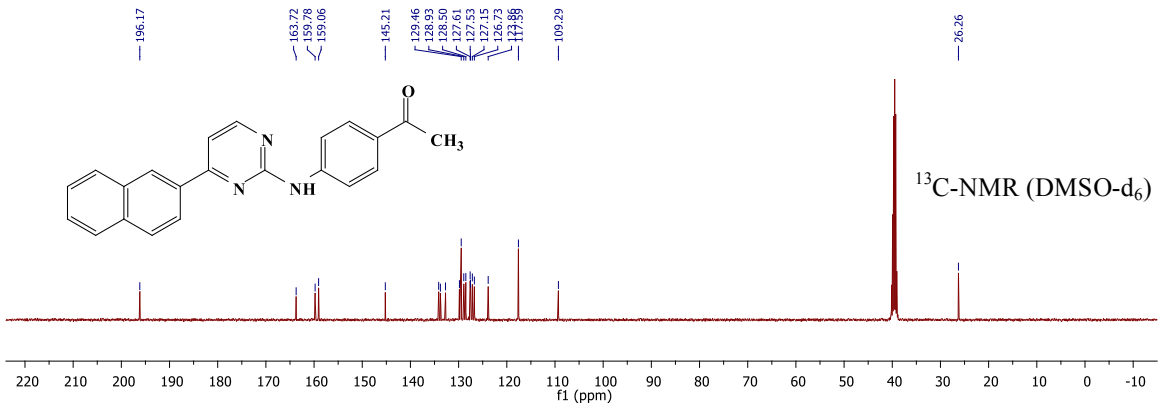
7.99
7.98
7.95
7.66
7.65
7.63
7.62
7.61
7.60
7.59
7.59
7.58
2.53
O
CH3
N
N
NH
f1 (ppm)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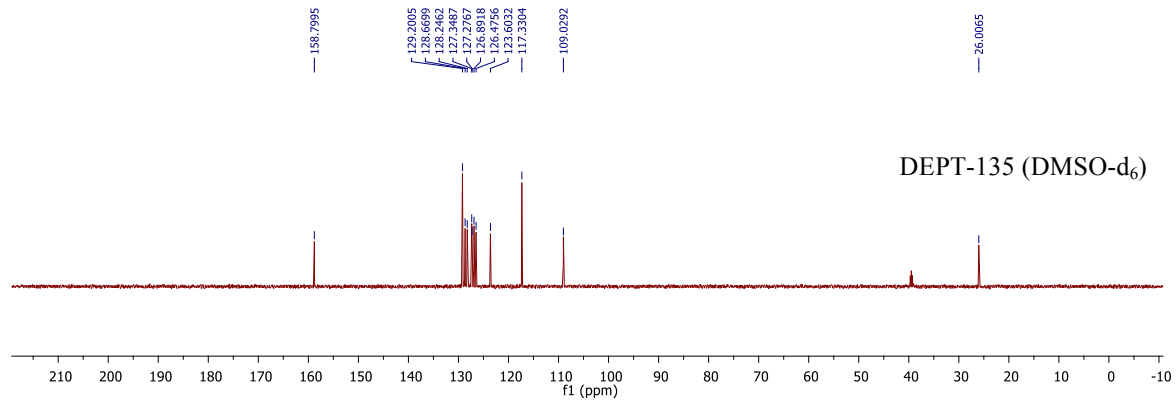
159.78
159.06
145.21
129.46
128.93
128.50
127.61
127.53
127.15
126.73
109.29
26.26
O
CH3
N
N
NH
13C-NMR (DMSO-d6)
f1 (ppm)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128.6699
128.2462
127.3487
127.2767
126.8918
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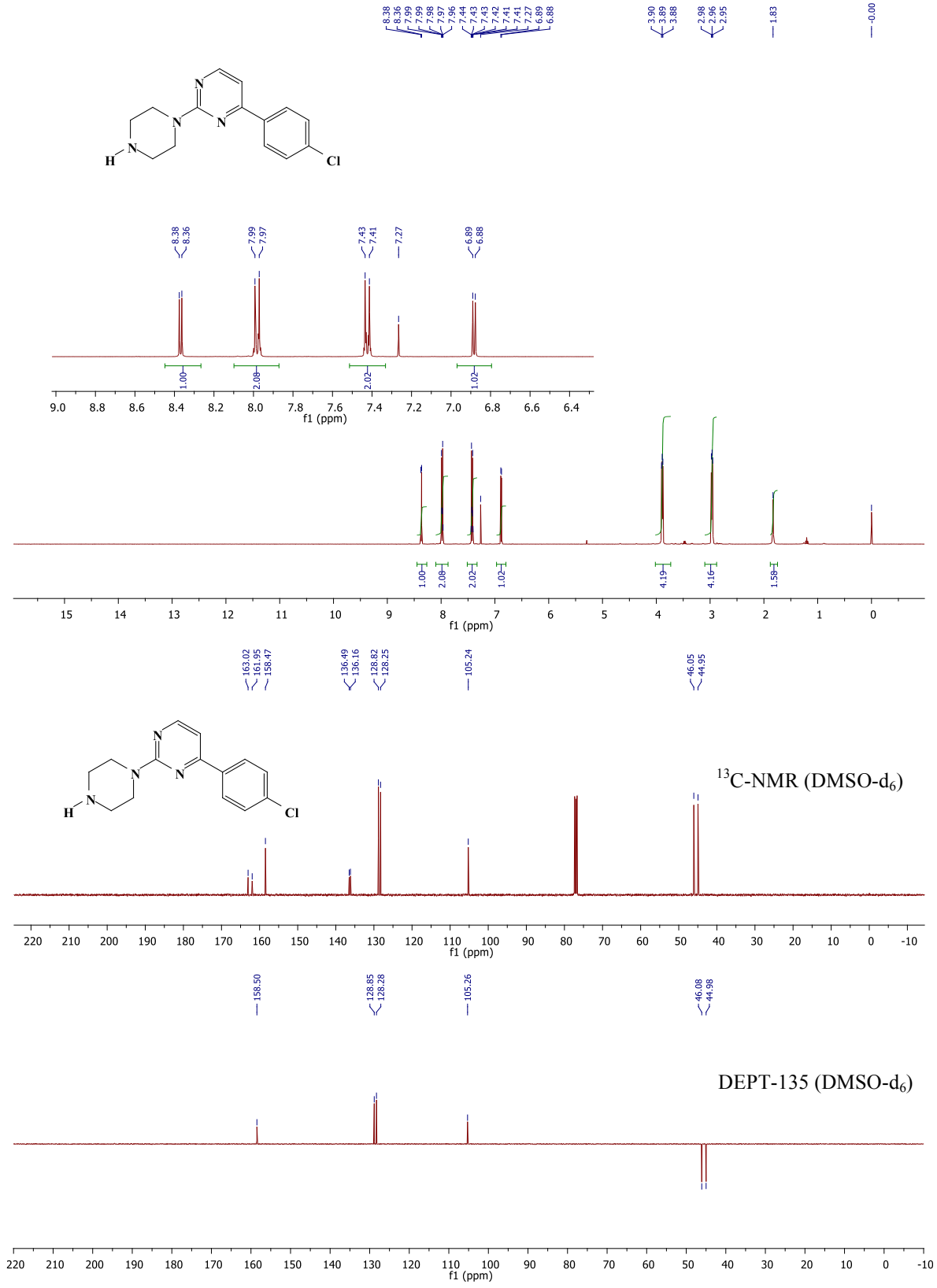
123.6032
117.3304
109.0292
26.0065
DEPT-135 (DMSO-d6)
f1 (ppm)

Compound-7a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7.99
7.99
7.98
7.97
7.96
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7.43
7.43
7.42
7.41
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7.27
6.89
6.88
3.90
3.89
3.88
2.98
2.96
2.95
1.83
-0.00
N
N
N
H
Cl
8.38
8.36
7.99
7.97
7.43
7.41
7.27
6.89
6.88
1.00
2.08
2.02
1.02
9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4
f1 (ppm)
1.00
2.08
2.02
1.02
4.19
4.16
1.58
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)
163.02
161.95
158.47
136.49
136.16
128.82
128.25
105.24
46.05
44.95
N
N
N
H
Cl
13C-NMR (DMSO-d6)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
158.50
128.85
128.28
105.26
46.08
44.98
DEPT-135 (DMSO-d6)
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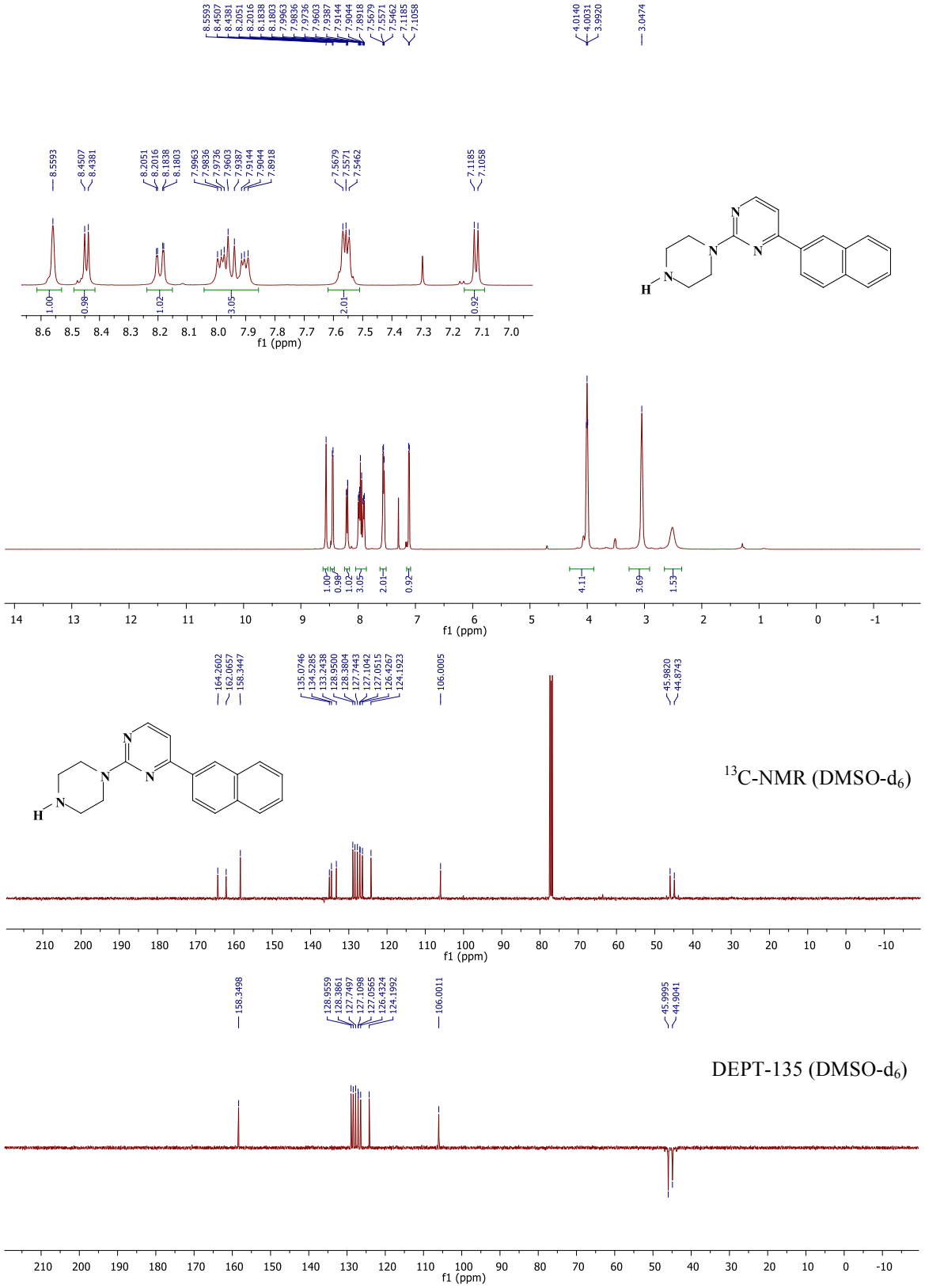
f1 (ppm)

Compound-7b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7.9144
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7.8918
7.5679
7.5571
7.5462
7.1185
7.1058
4.0140
4.0031
3.9920
3.0474
f1 (ppm)
^{13}C-NMR (DMSO-d$_6$)
164.2602
162.0657
158.3447
135.0746
134.5285
133.2438
128.9500
128.3804
127.7443
127.1042
127.0515
126.4267
124.1923
106.0005
45.9820
44.8743
DEPT-135 (DMSO-d$_6$)
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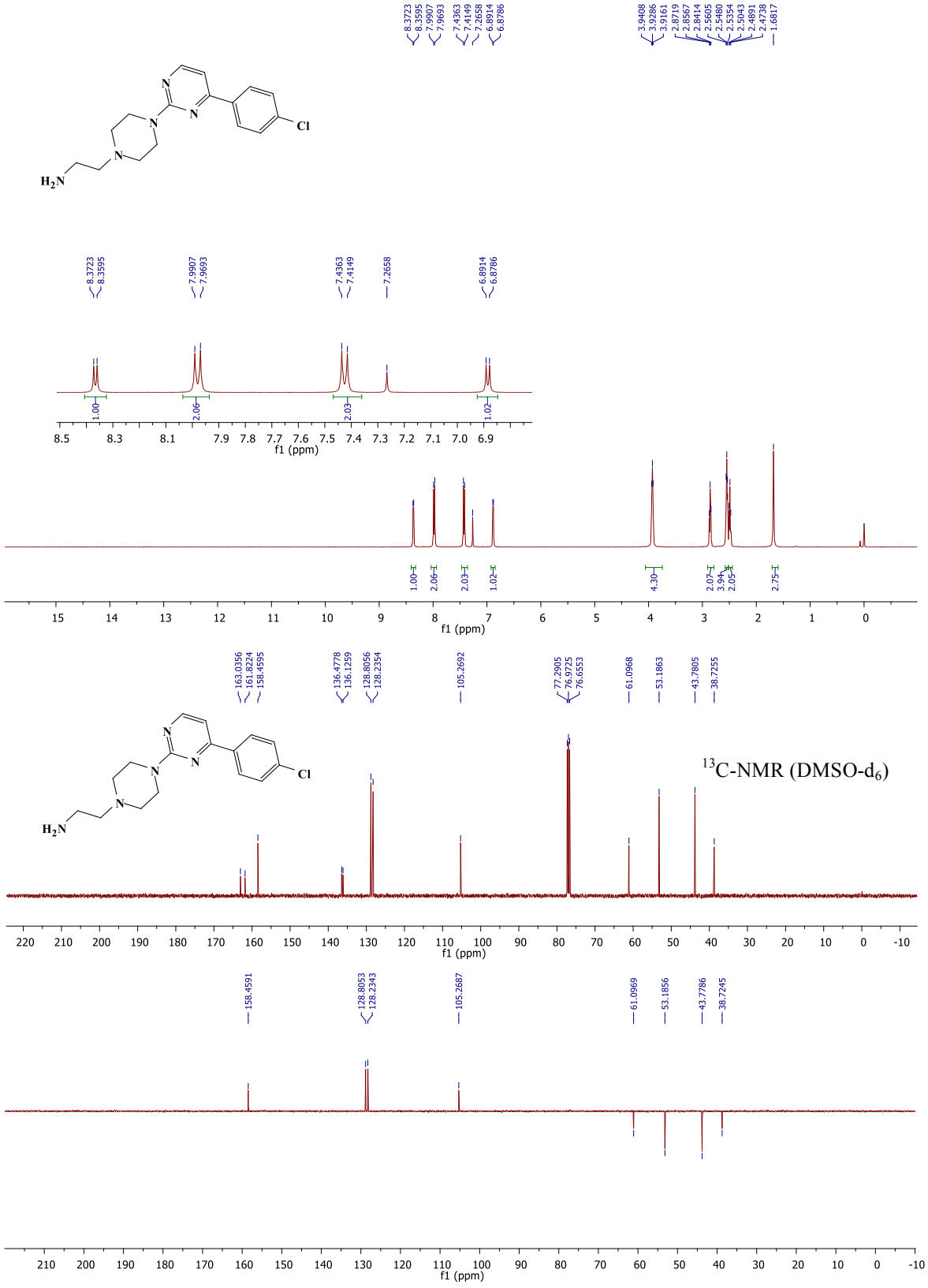
45.9995
44.9041

Compound-8a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7.9693
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3.9286
3.9161
2.8719
2.8567
2.8414
2.5605
2.5480
2.5354
2.5043
2.4891
2.4738
1.6817
Cl
H2N
f1 (ppm)
163.0356
161.8224
158.4595
136.4778
136.1259
128.8056
128.2354
105.2692
77.2905
76.9725
76.6553
61.0968
53.1863
43.7805
38.7255
13C-NMR (DMSO-d6)
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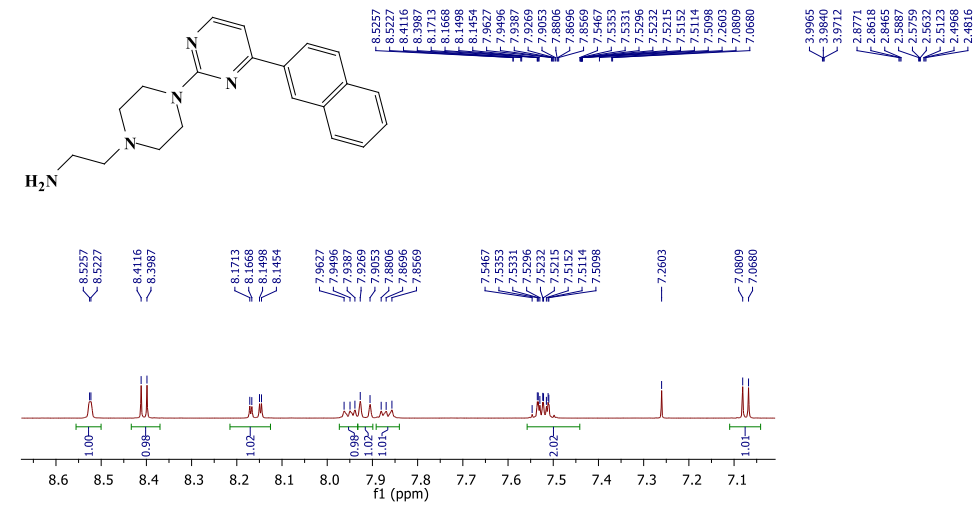
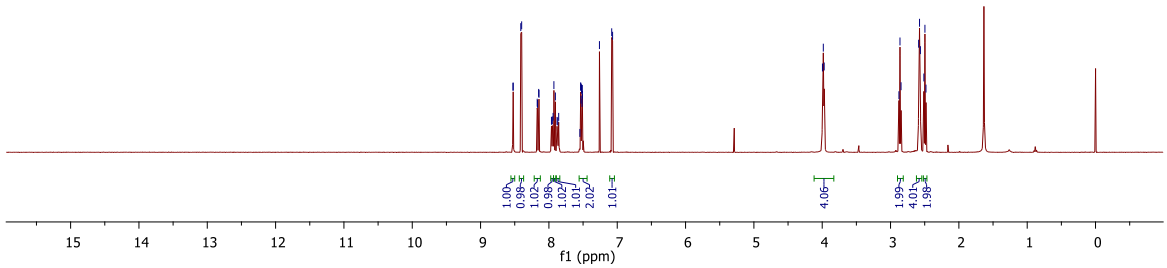
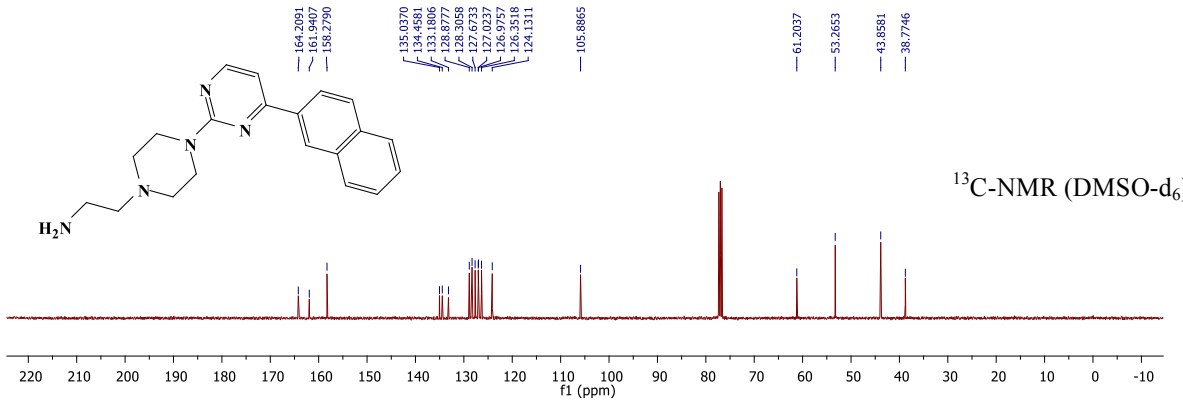
105.2687
61.0969
53.1856
43.7786
38.7245

Compound-8b

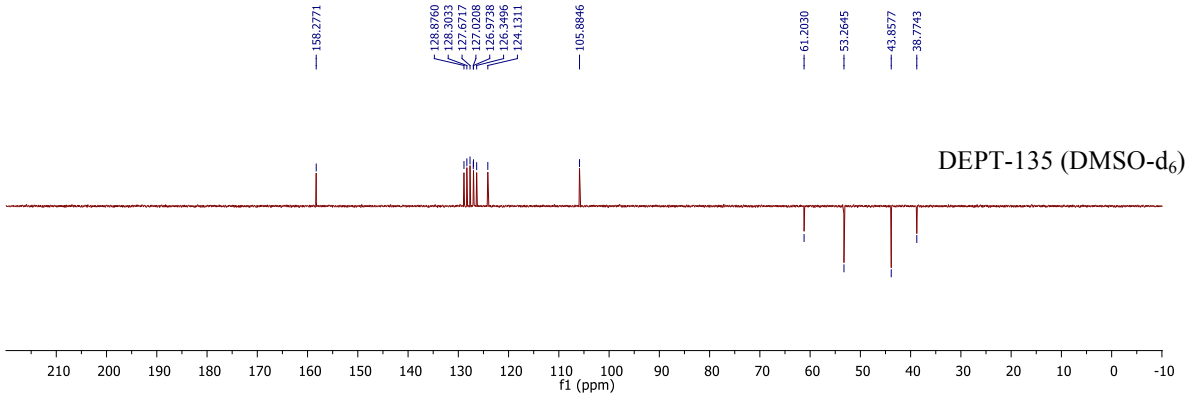




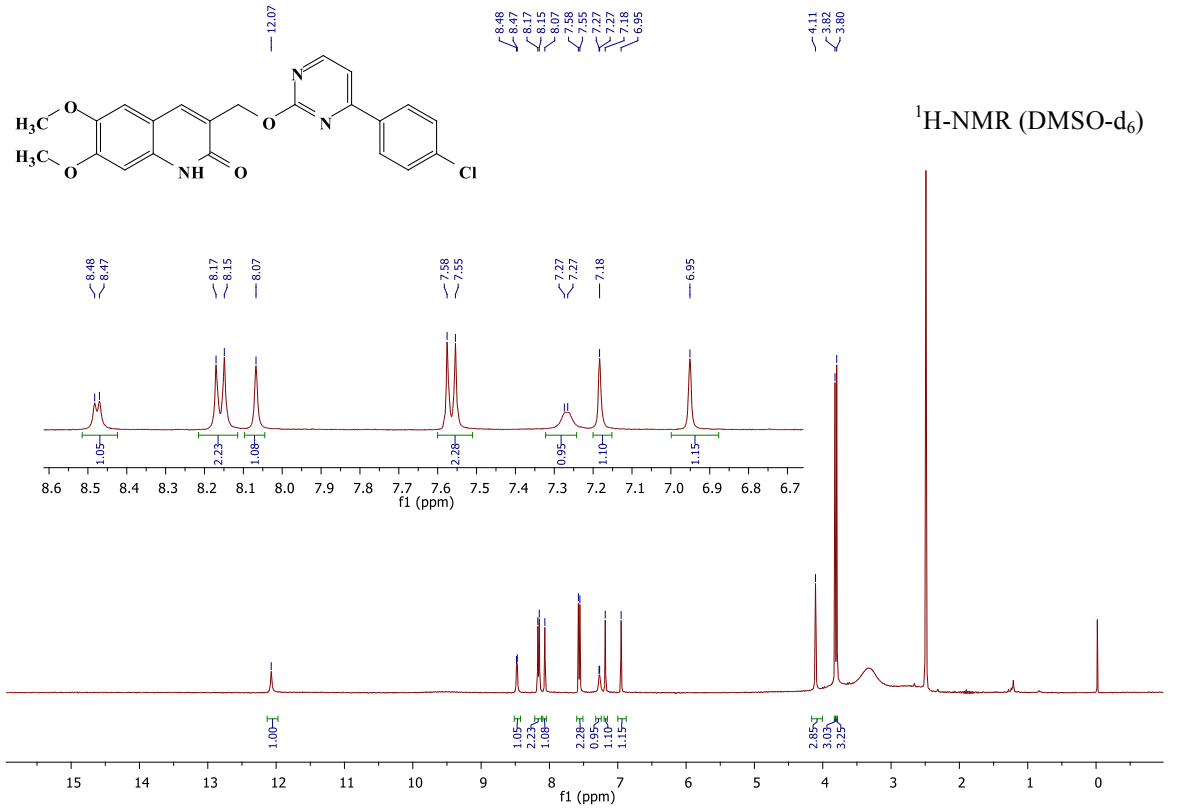
^{13}C-NMR (DMSO-d$_6$)

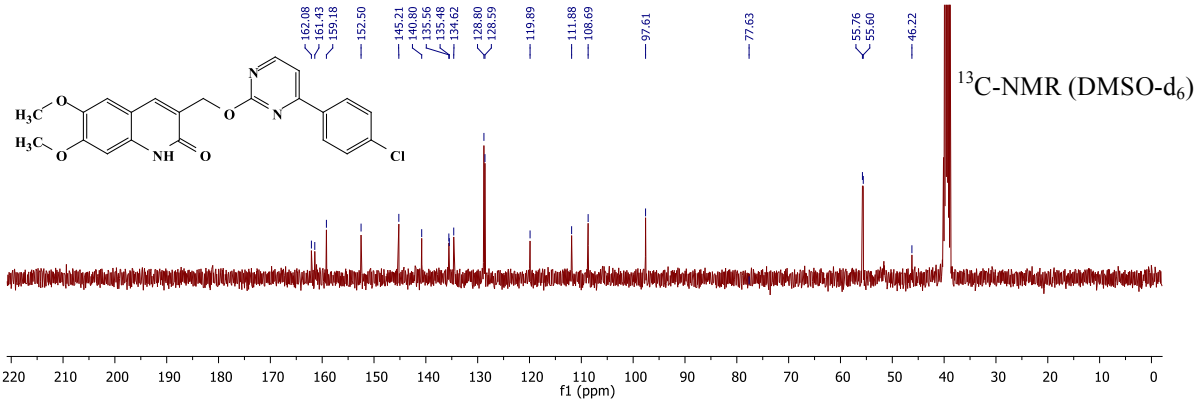


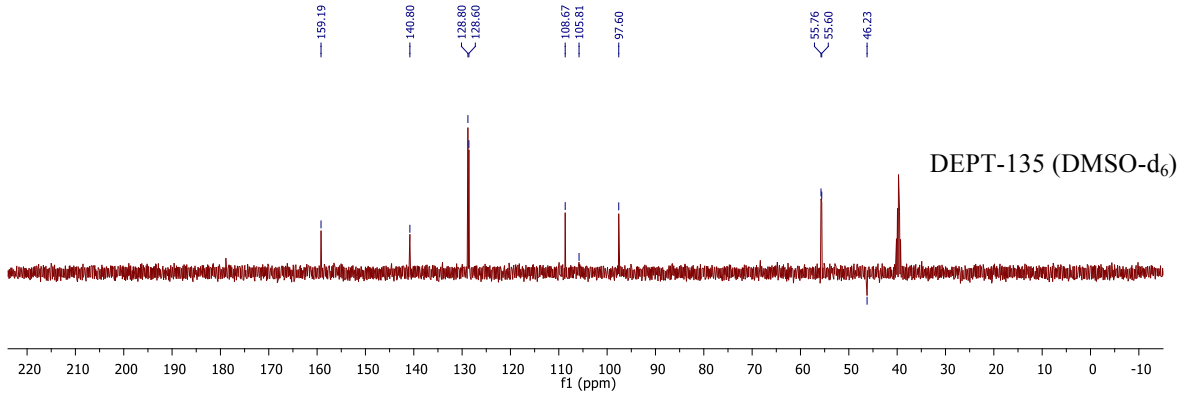
DEPT-135 (DMSO-d$_6$)



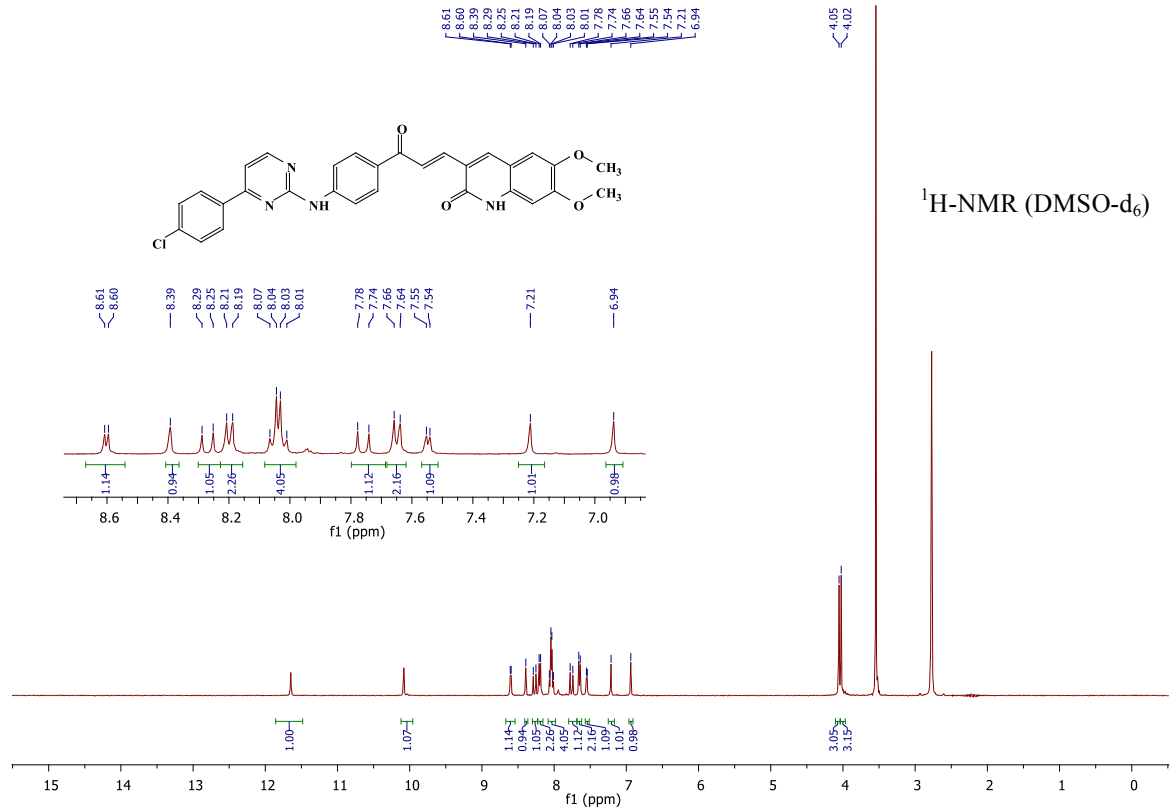
Compound-9


^{1}H-NMR (DMSO-d$_6$)
f1 (ppm)

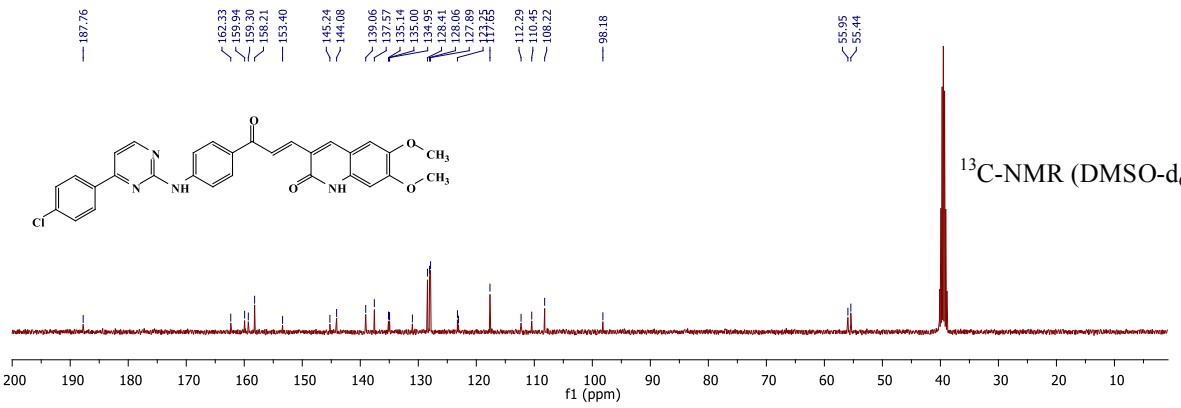

^{13}C-NMR (DMSO-d$_6$)
f1 (ppm)


DEPT-135 (DMSO-d$_6$)
f1 (ppm)

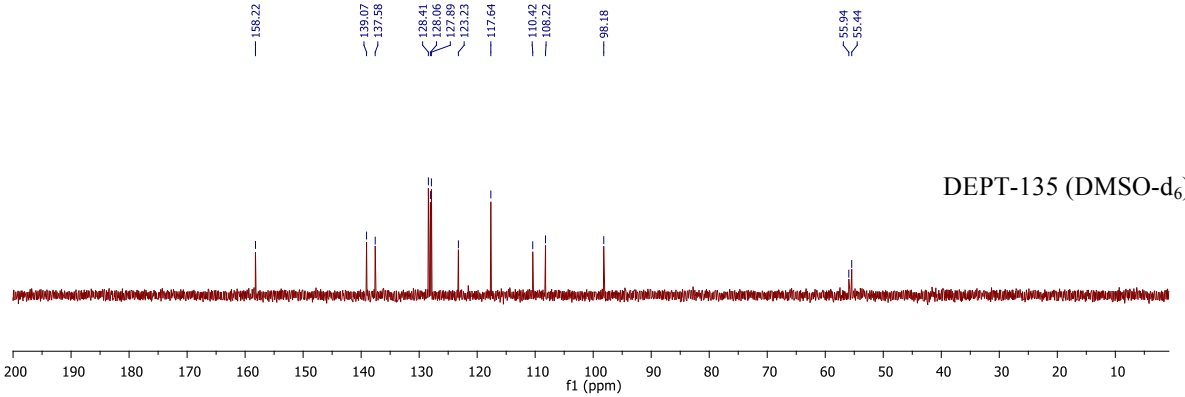
Compound-10a



^{1}H-NMR (DMSO-d$_6$)

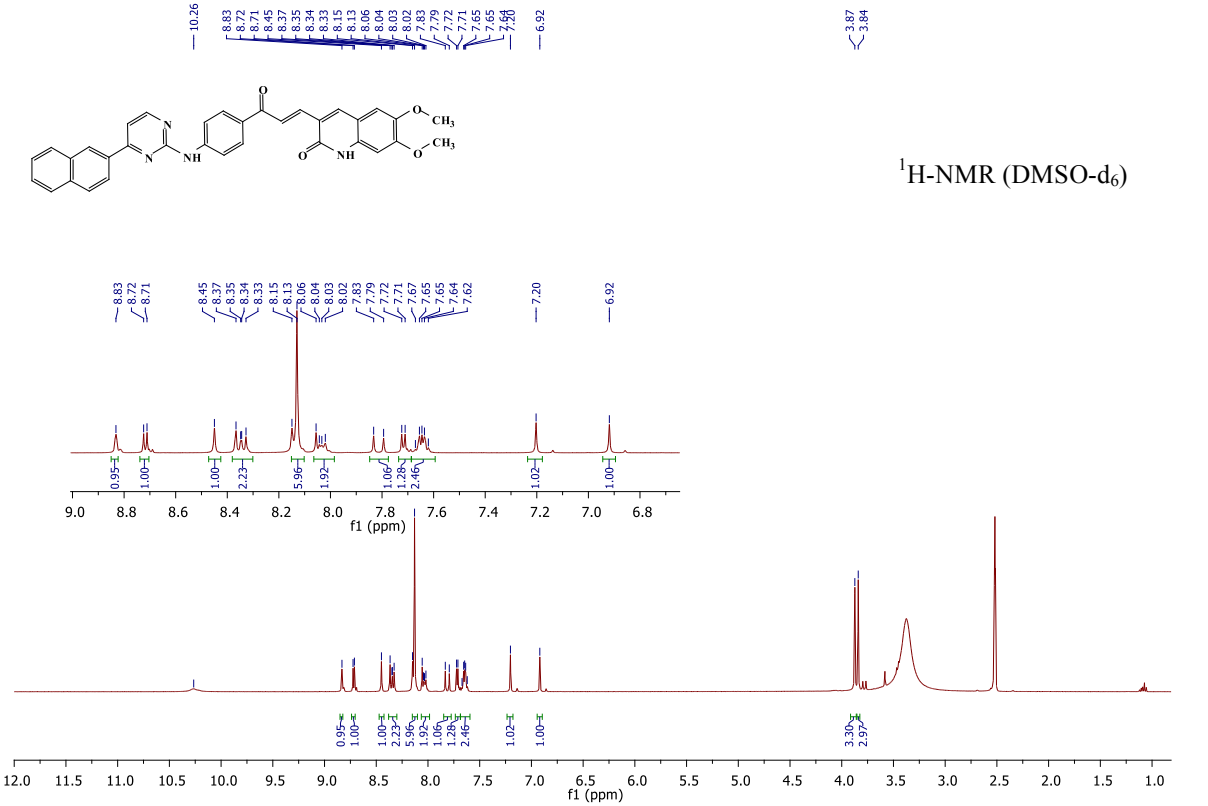


^{13}C-NMR (DMSO-d$_6$)

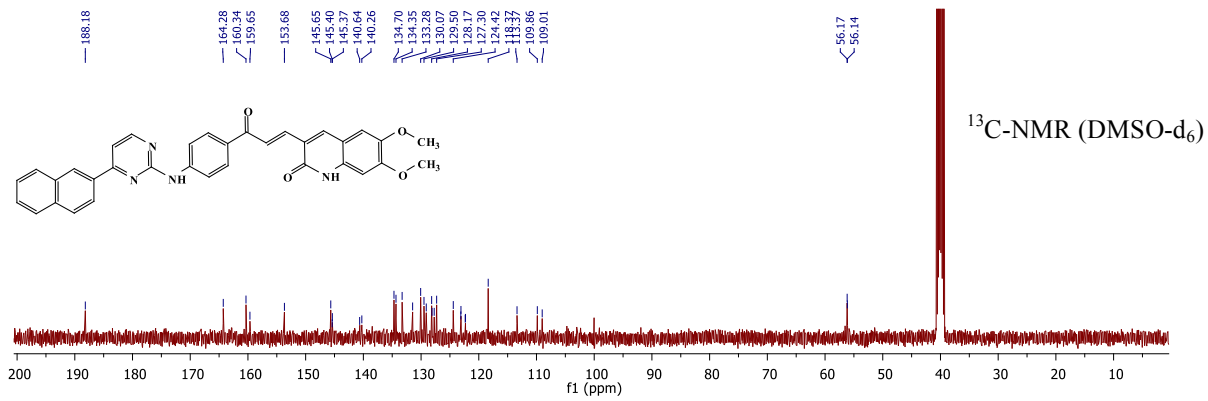


DEPT-135 (DMSO-d$_6$)

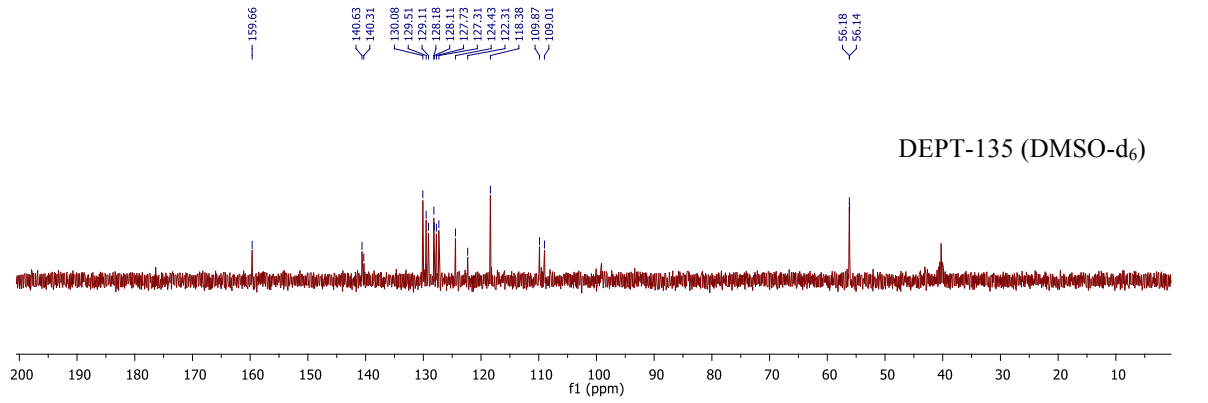
Compound-10b



^{1}H-NMR (DMSO-d$_6$)

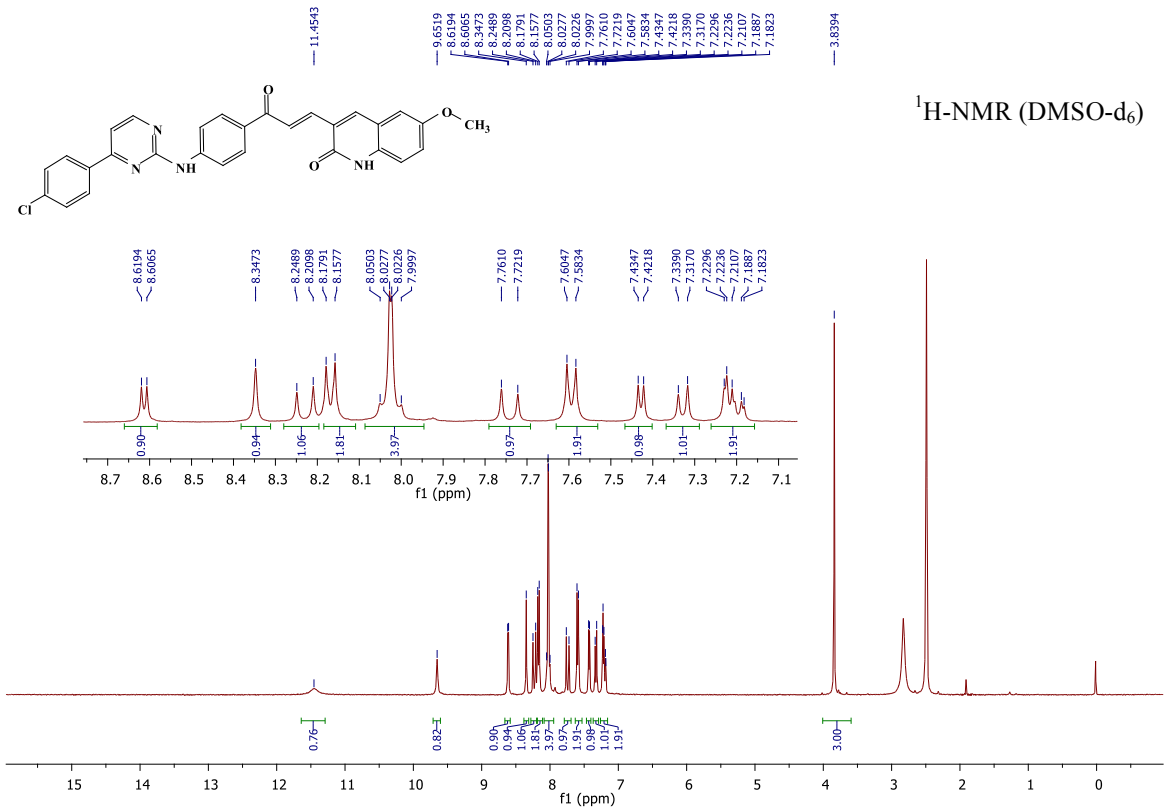


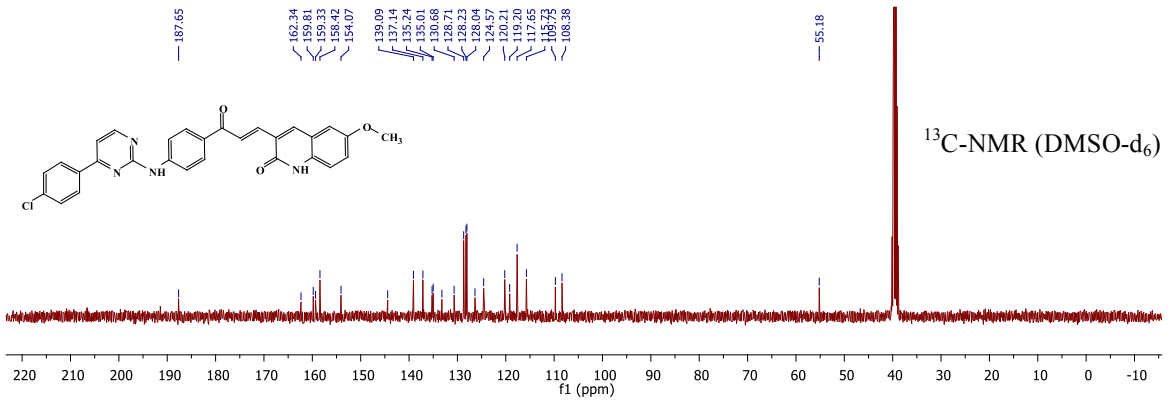
^{13}C-NMR (DMSO-d$_6$)

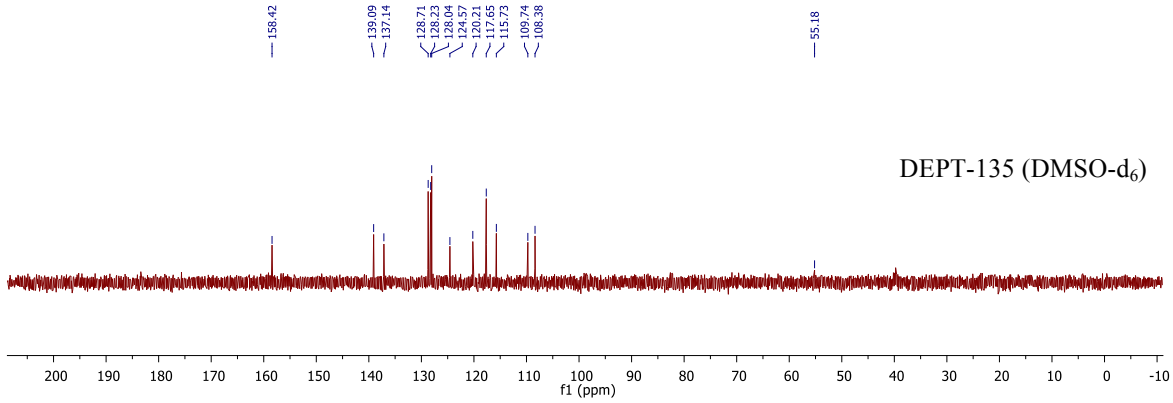


DEPT-135 (DMSO-d$_6$)

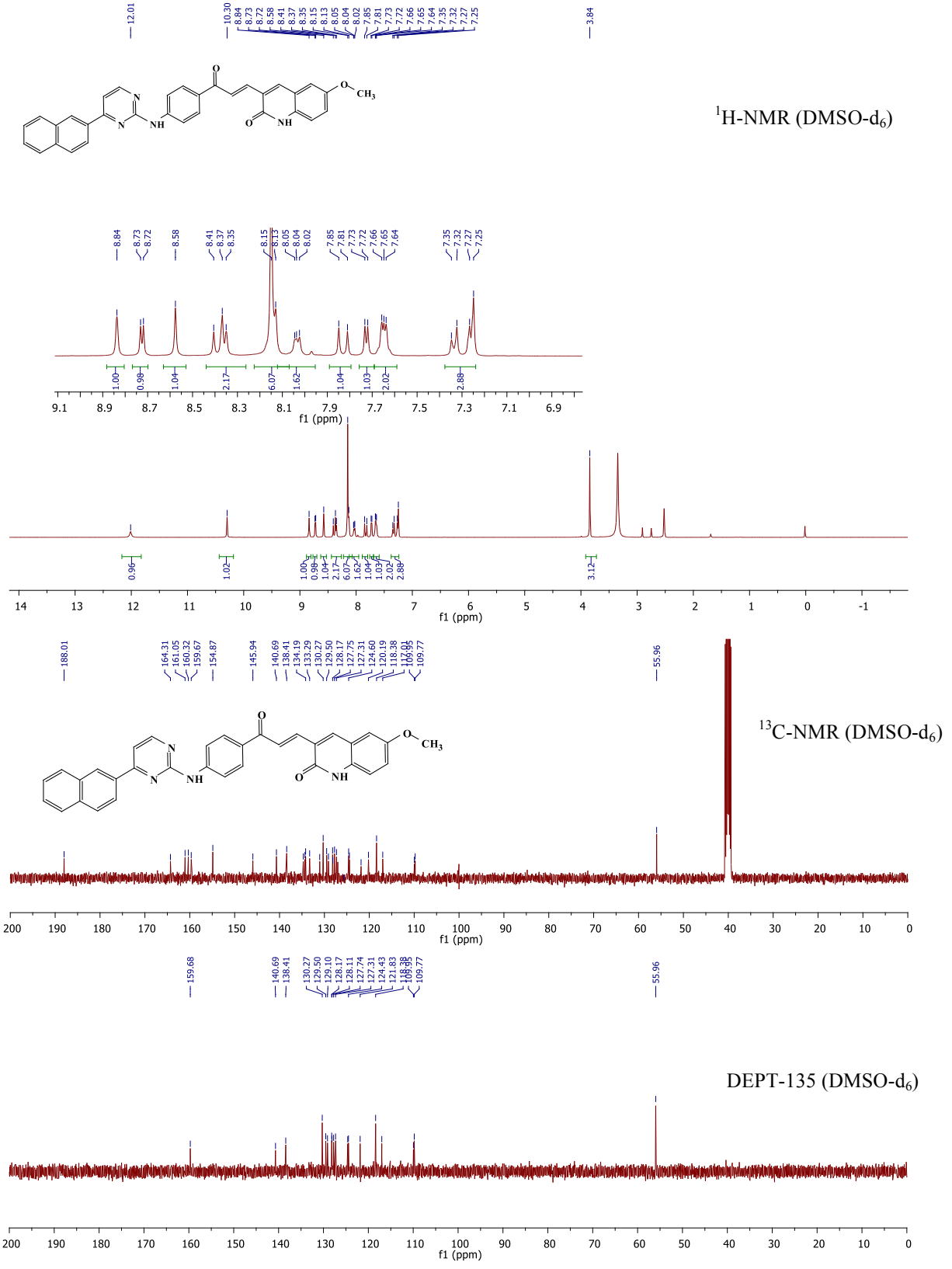
Compound-11a







Compound-11b

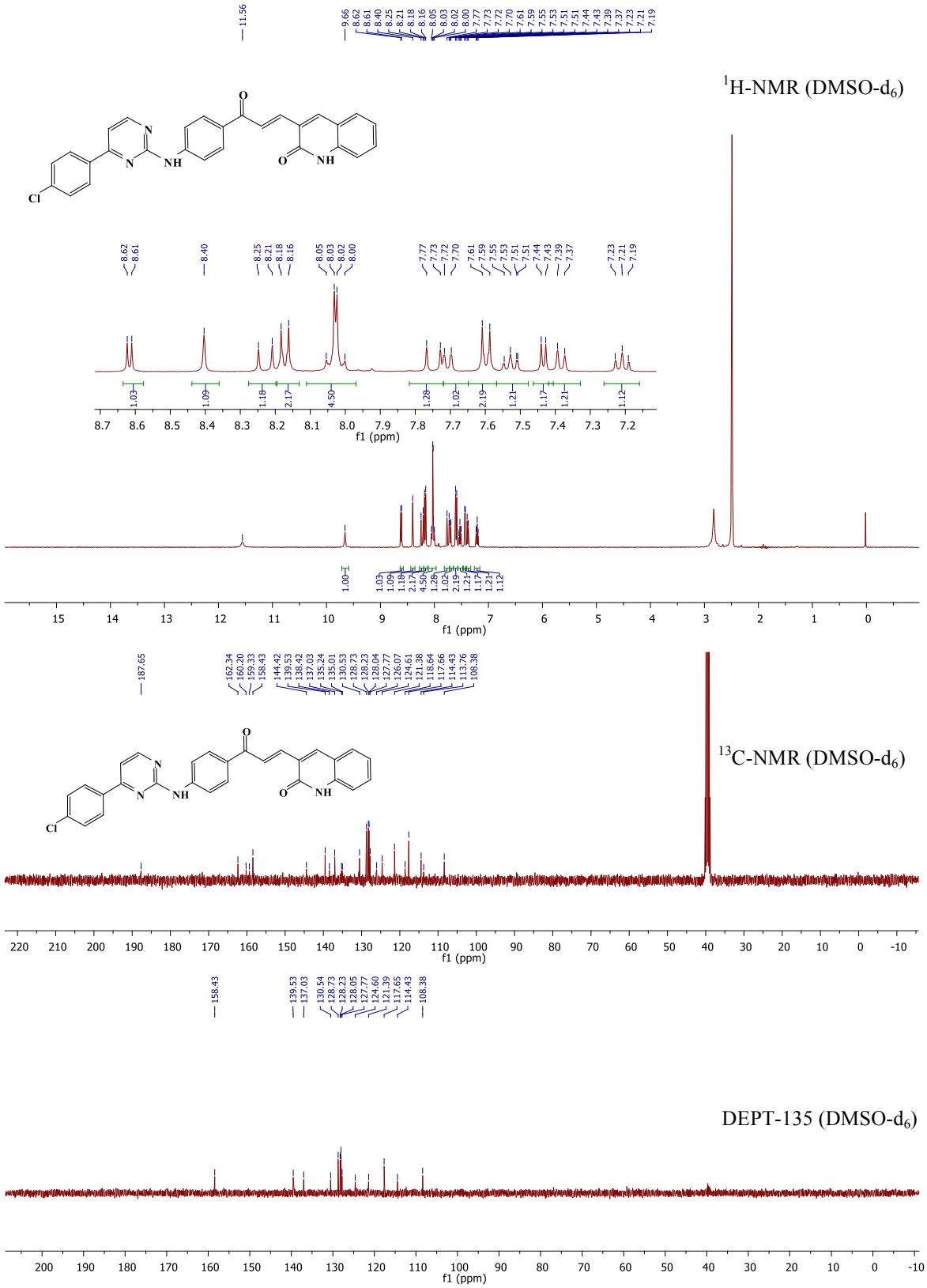


^{1}H-NMR (DMSO-d$_6$)

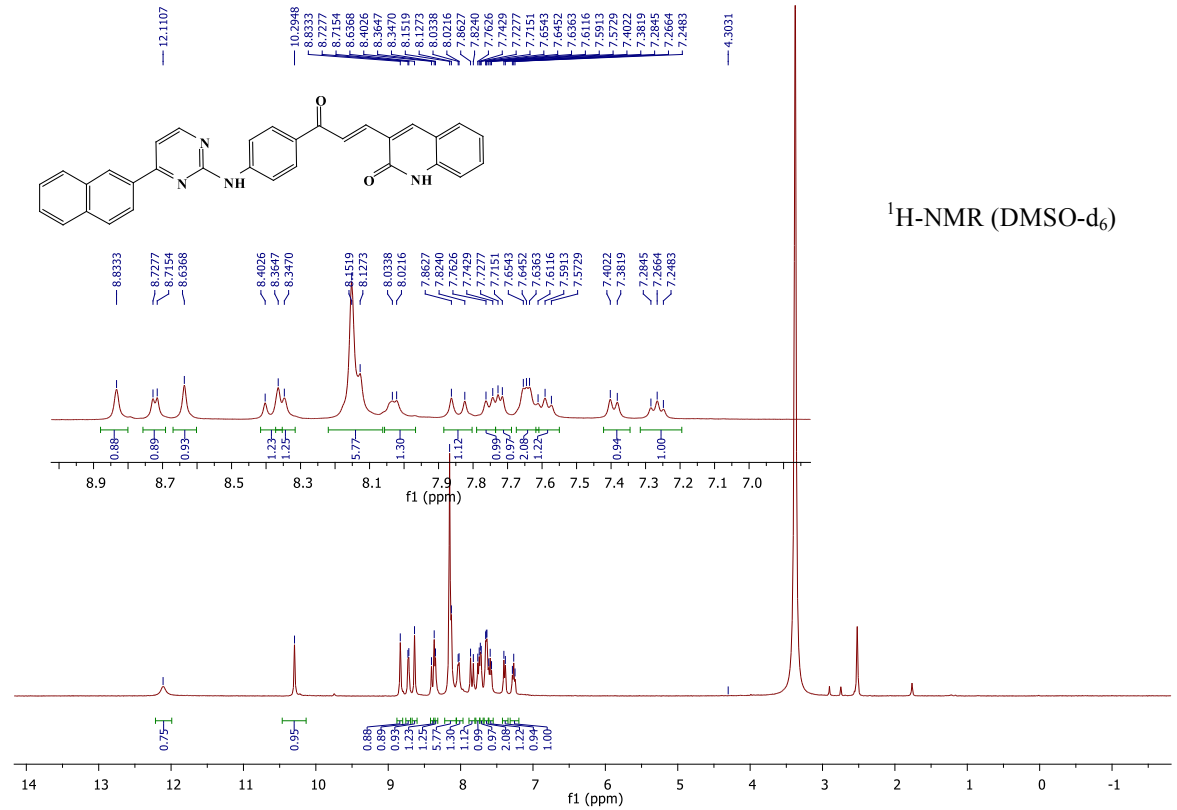
^{13}C-NMR (DMSO-d$_6$)

DEPT-135 (DMSO-d$_6$)

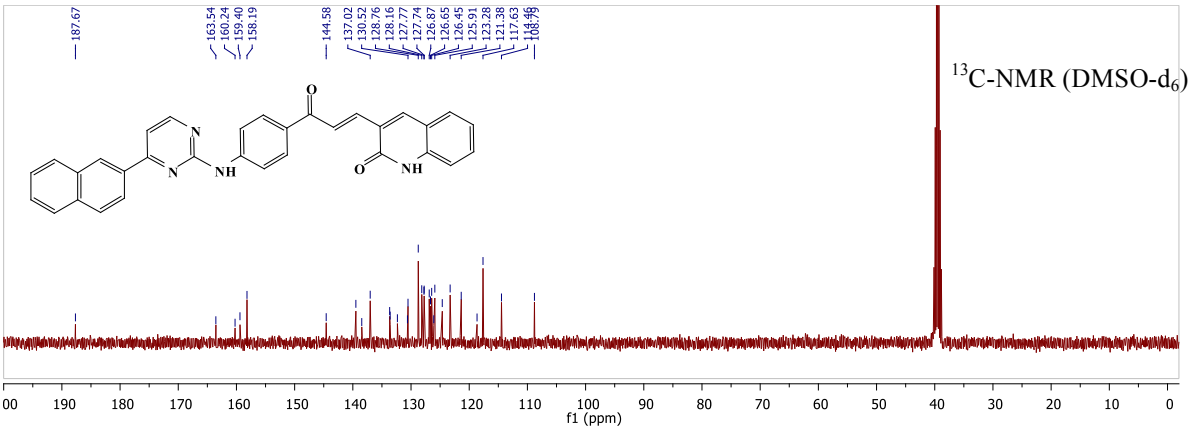
Compound-12a



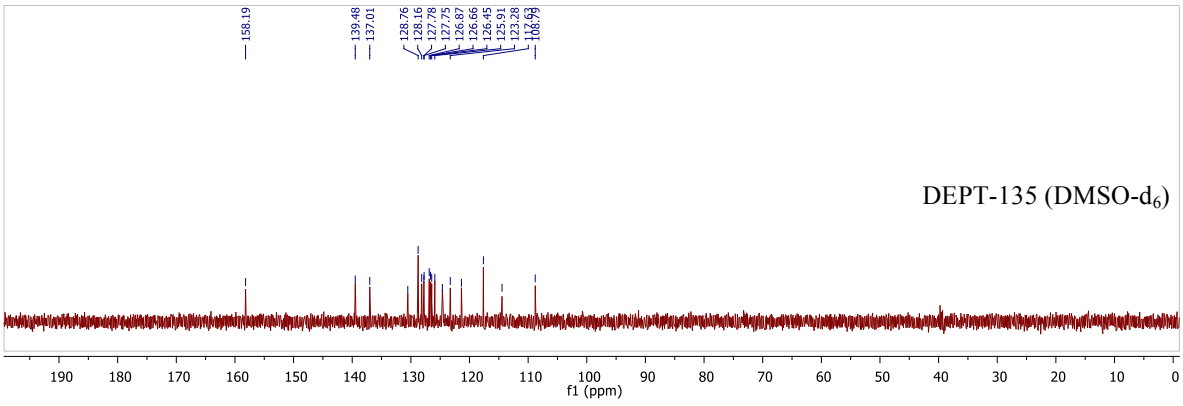
Compound-12b



^{1}H-NMR (DMSO-d$_6$)

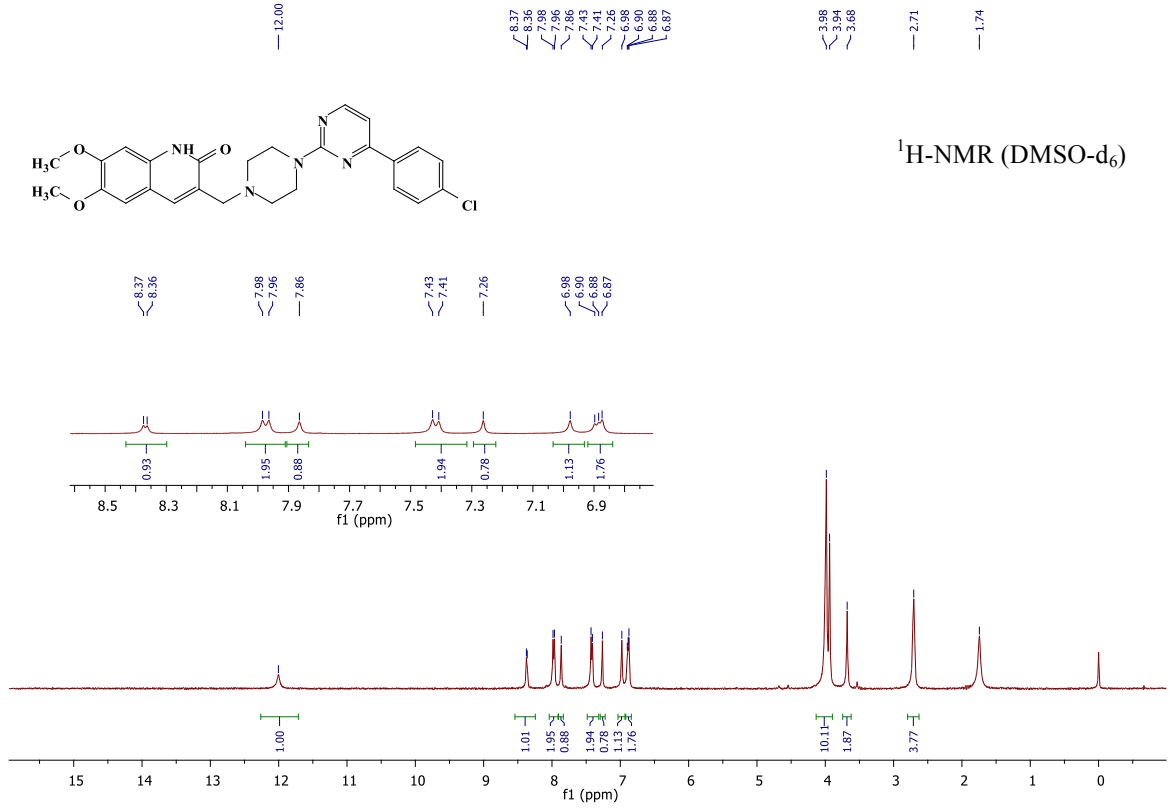


^{13}C-NMR (DMSO-d$_6$)

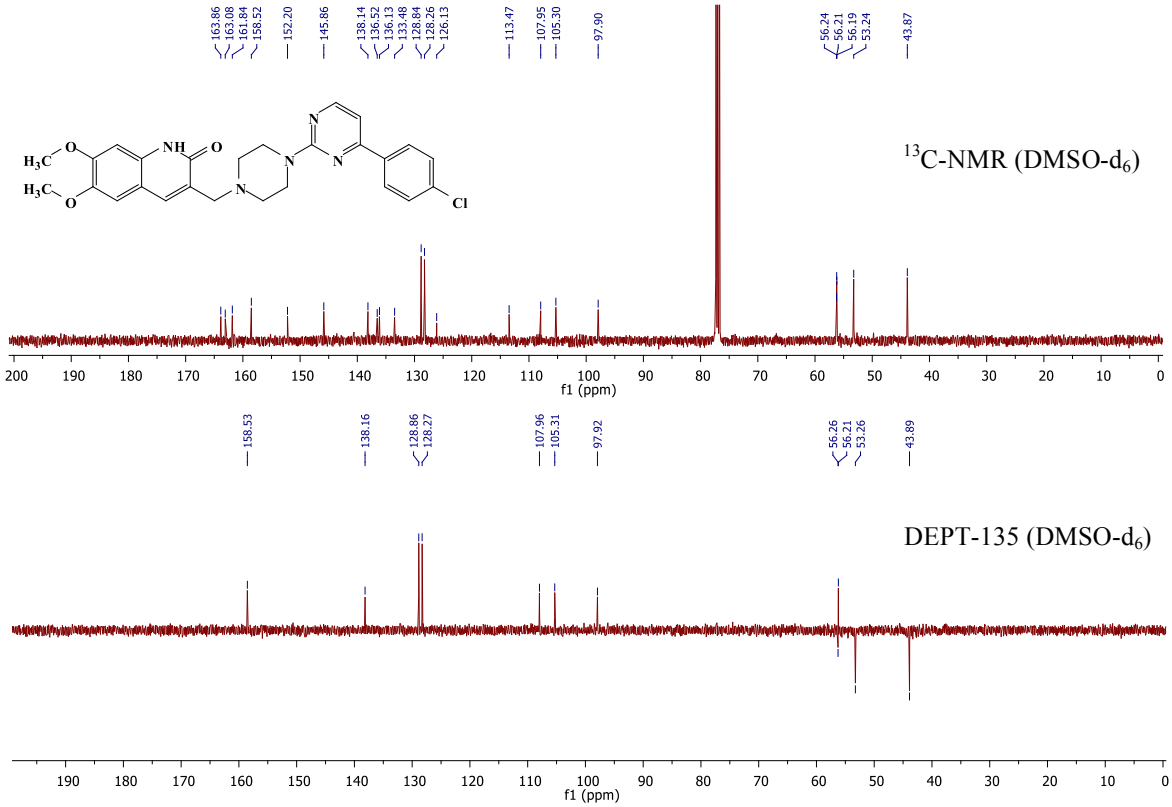


DEPT-135 (DMSO-d$_6$)

Compound-13a



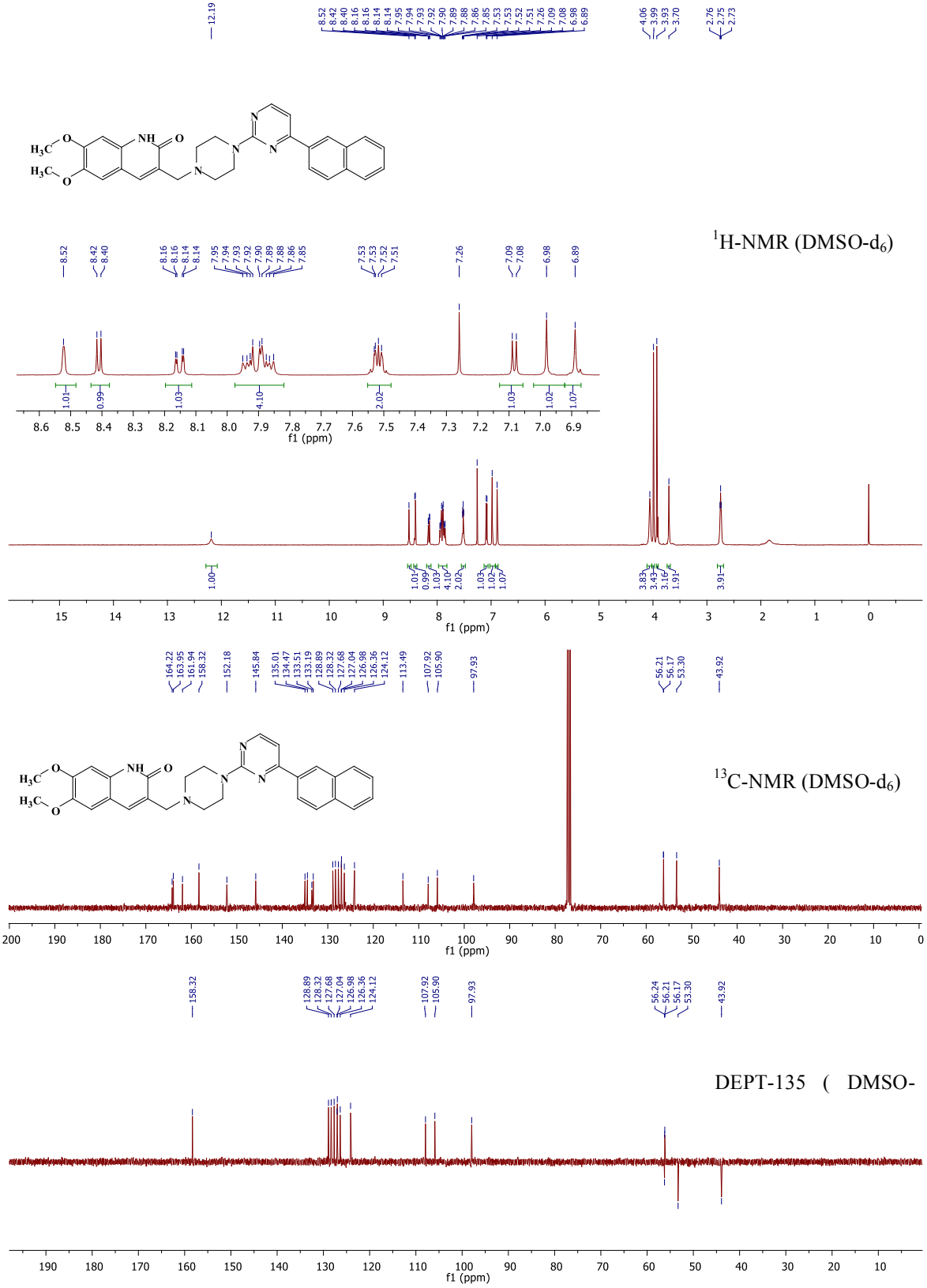
^{1}H-NMR (DMSO-d$_6$)



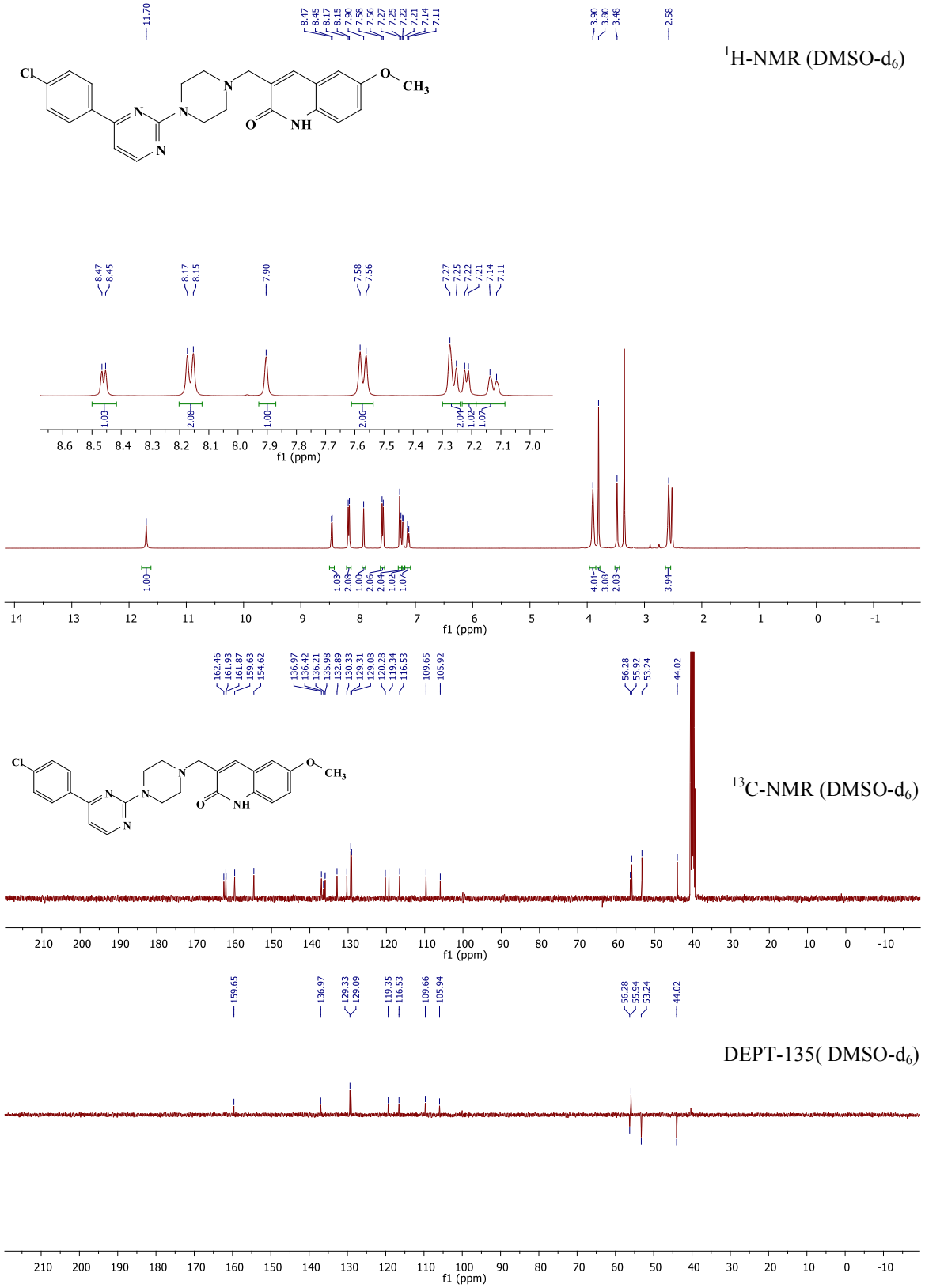
^{13}C-NMR (DMSO-d$_6$)

DEPT-135 (DMSO-d$_6$)

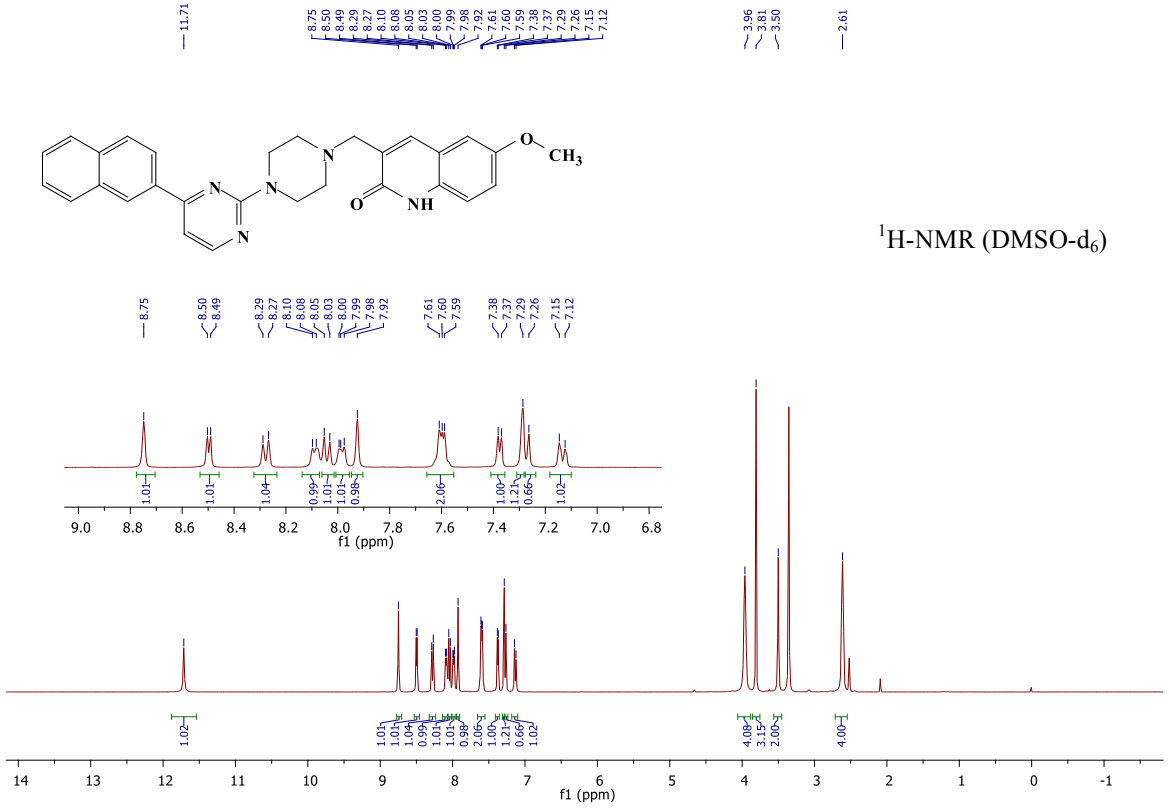
Compound-13b

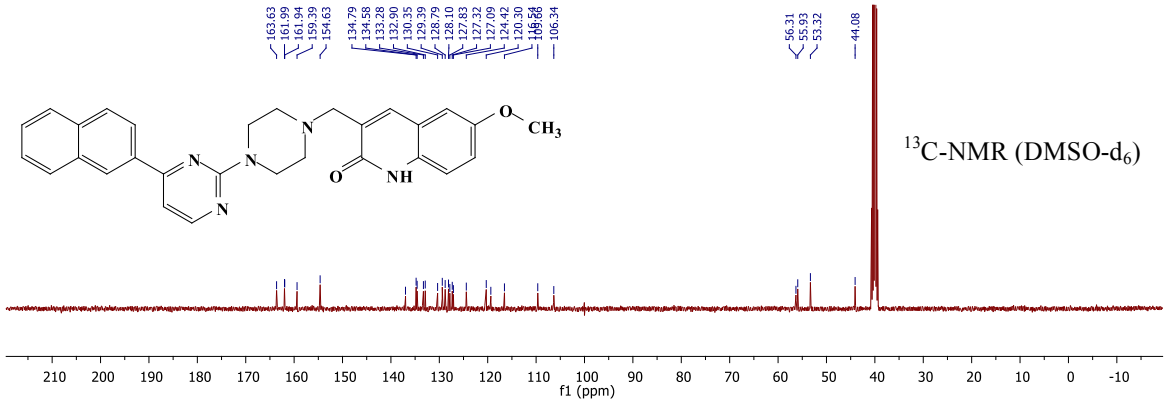


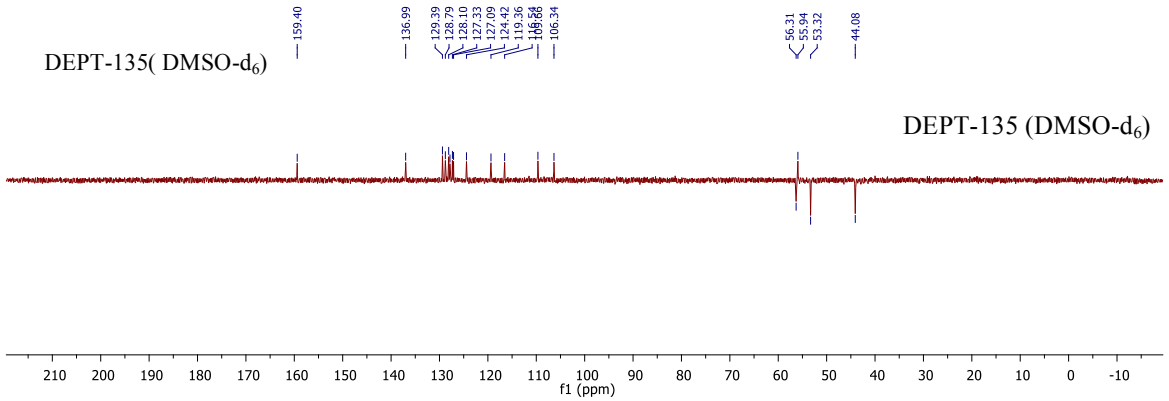
Compound-14a



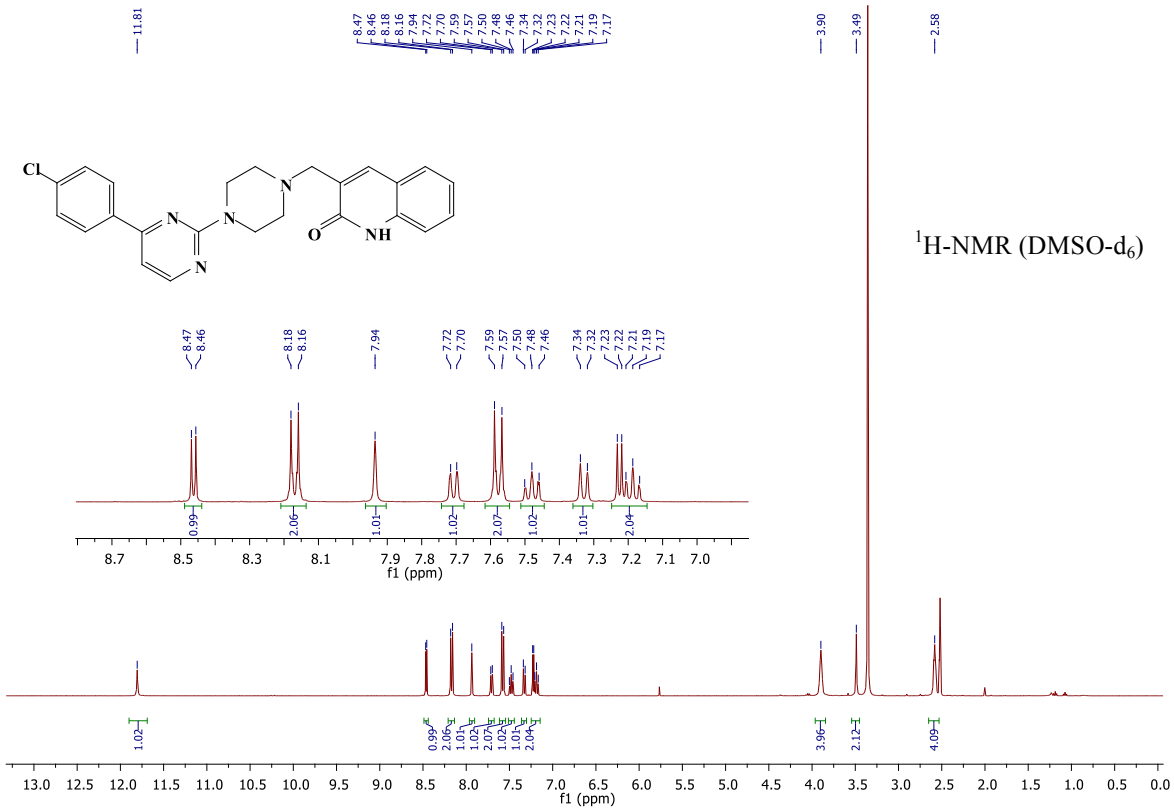
Compound-14b

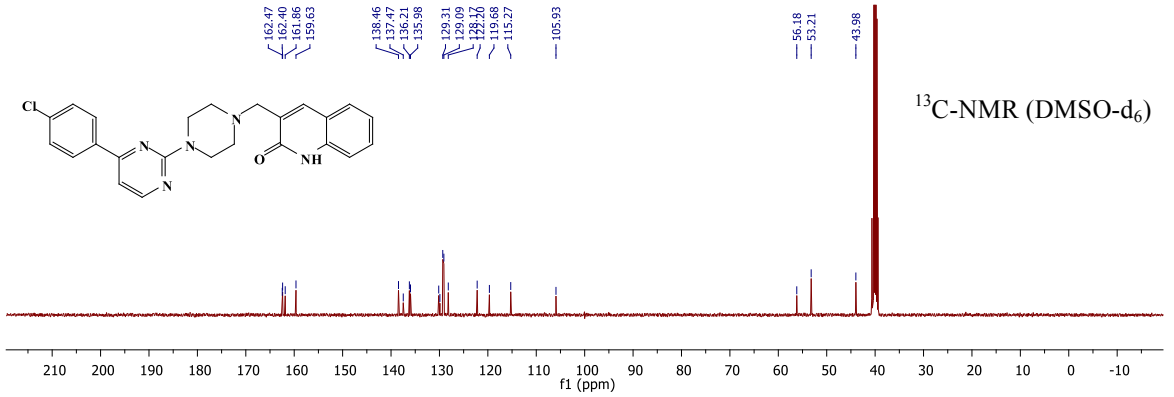


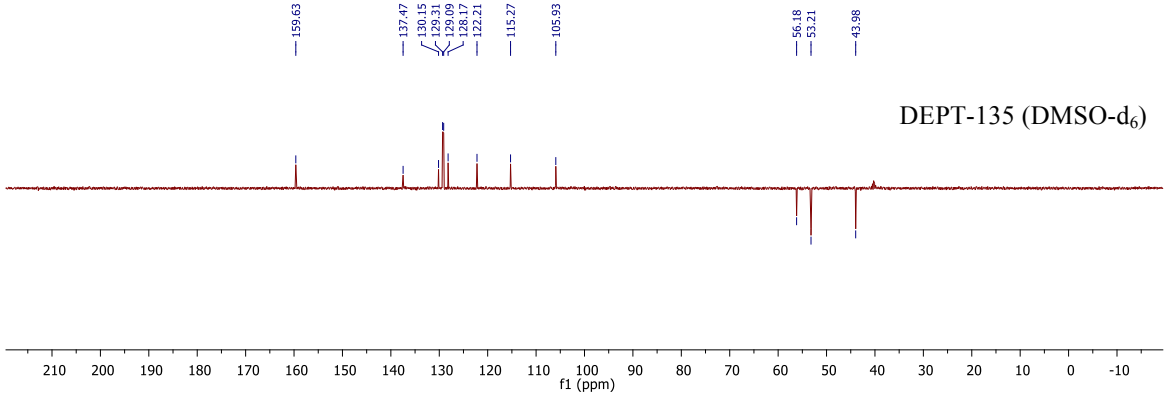




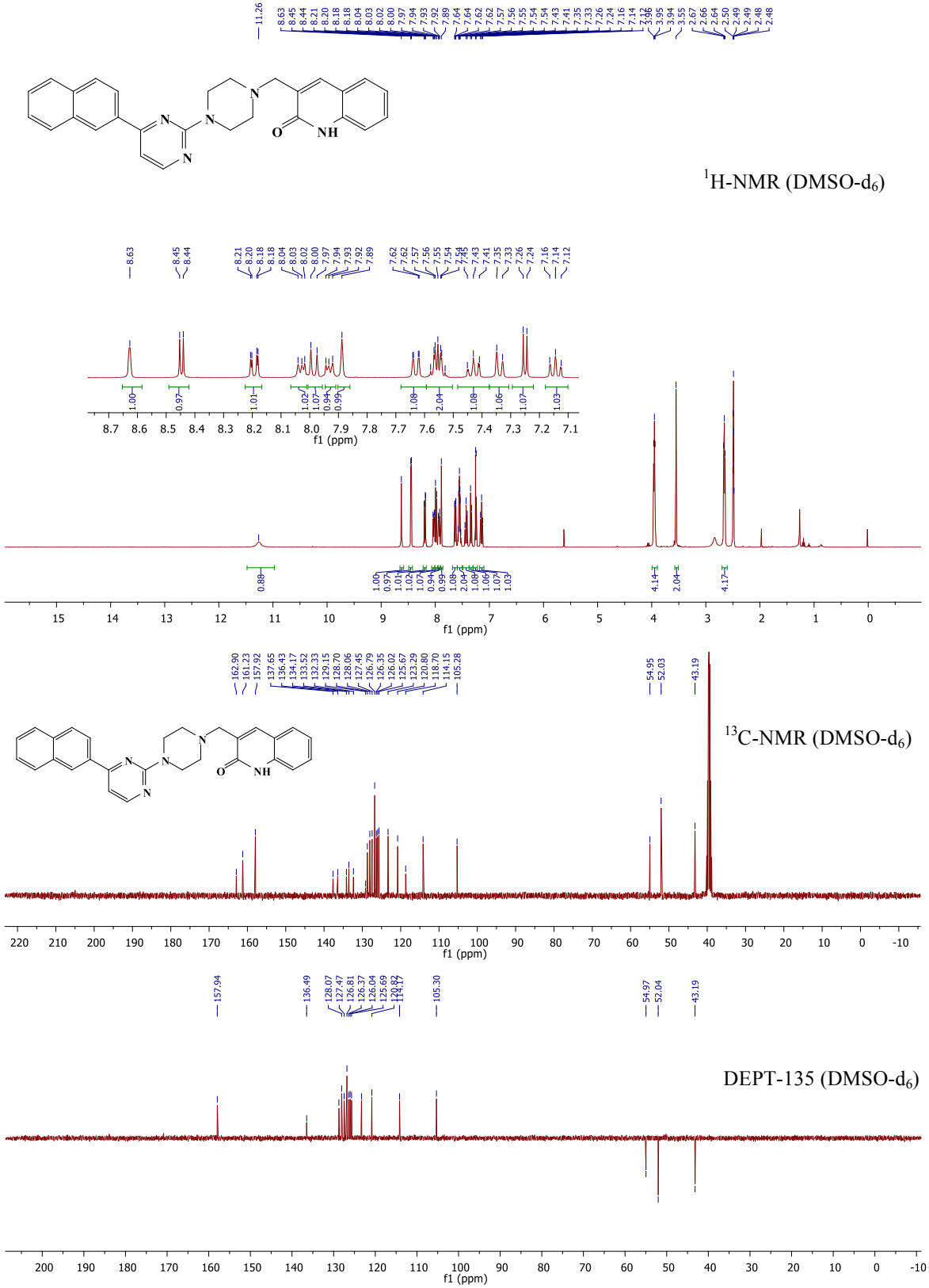
Compound-15a



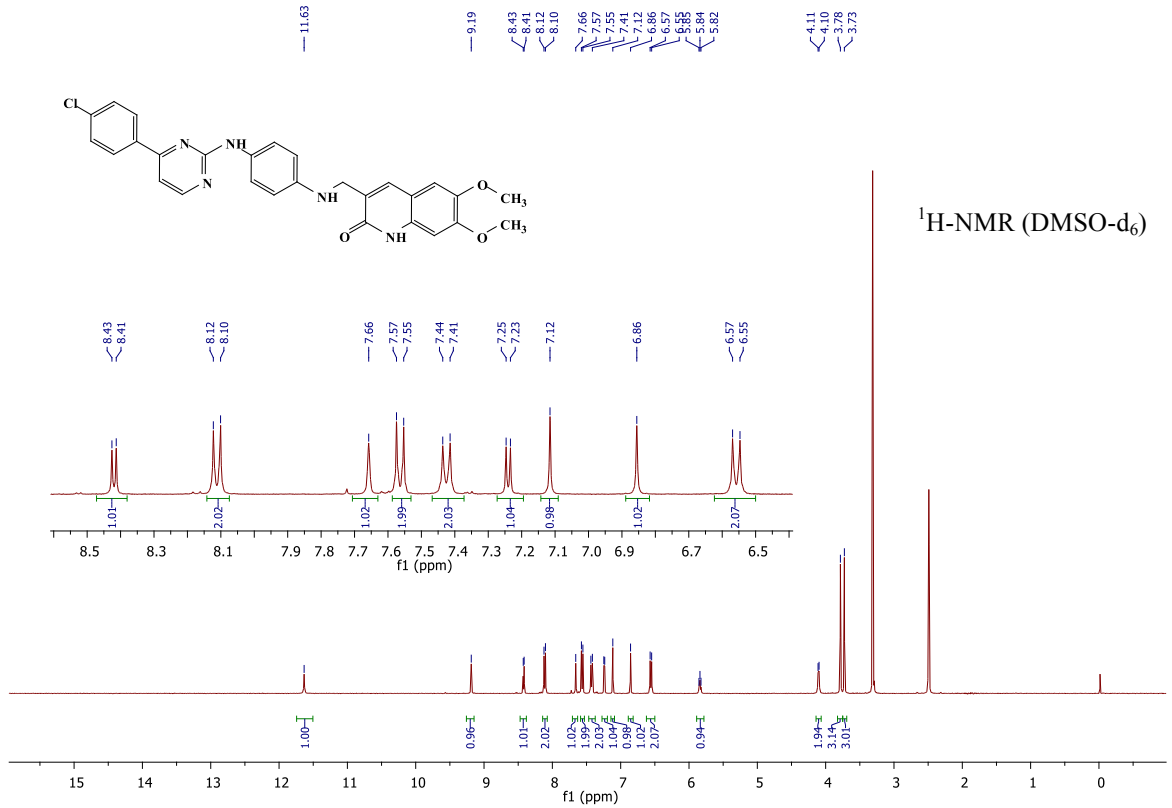


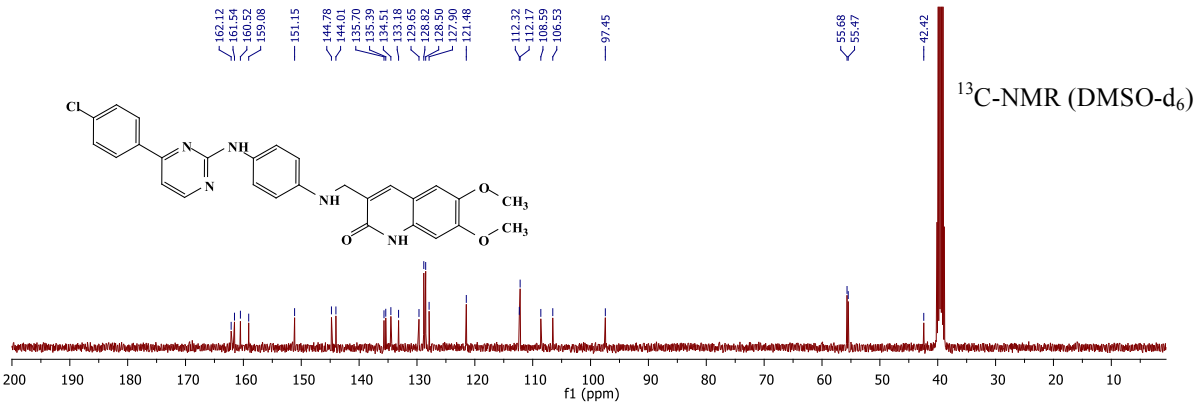


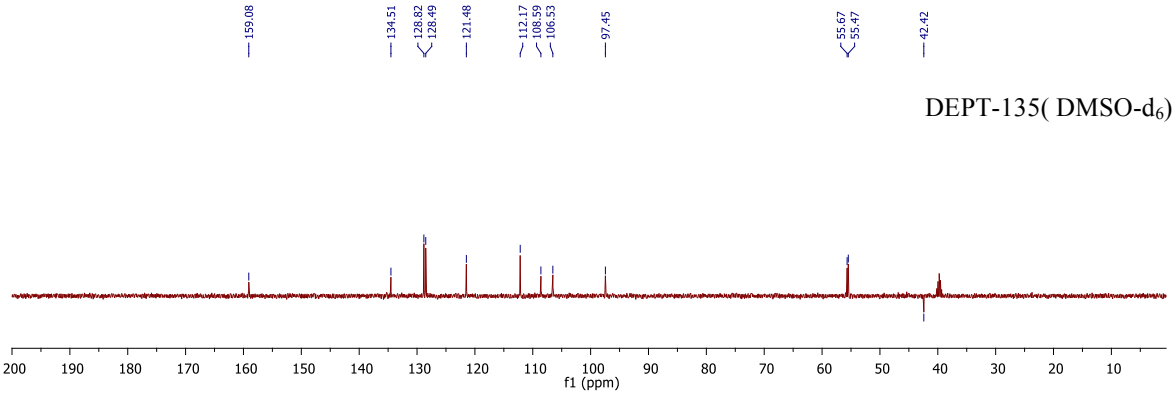
Compound-15b



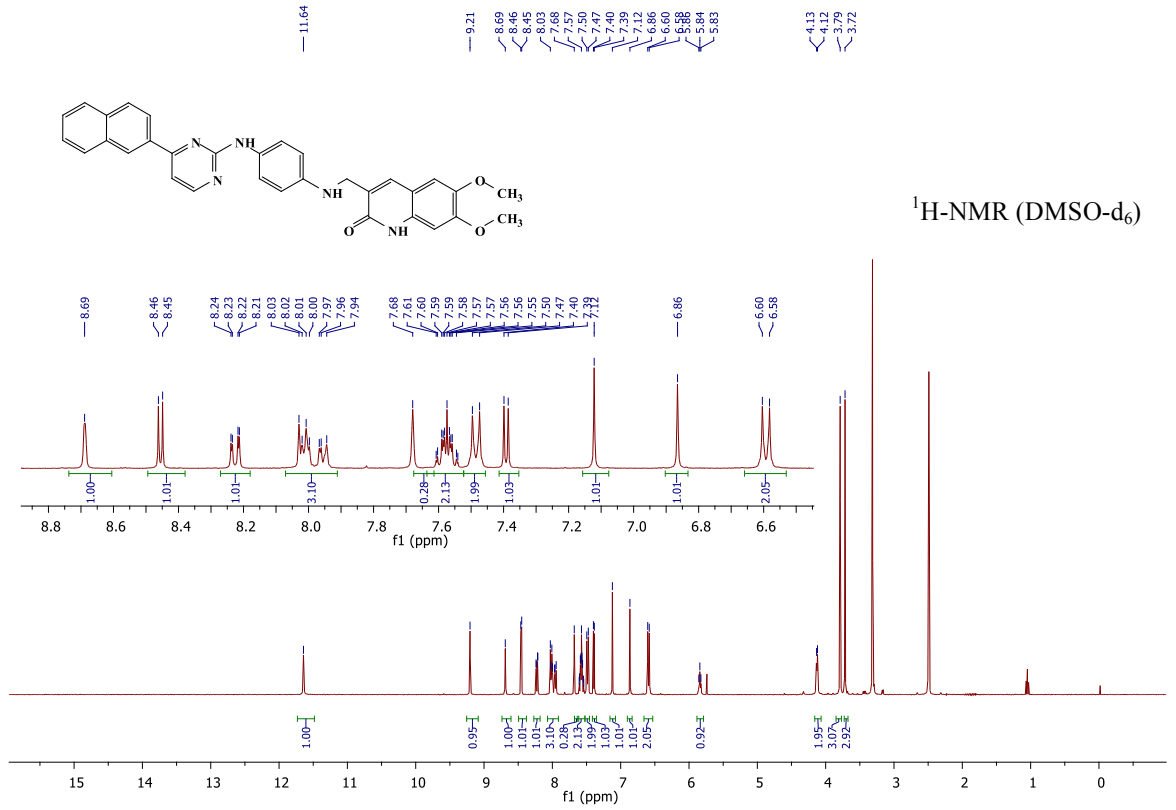
Compound-16a

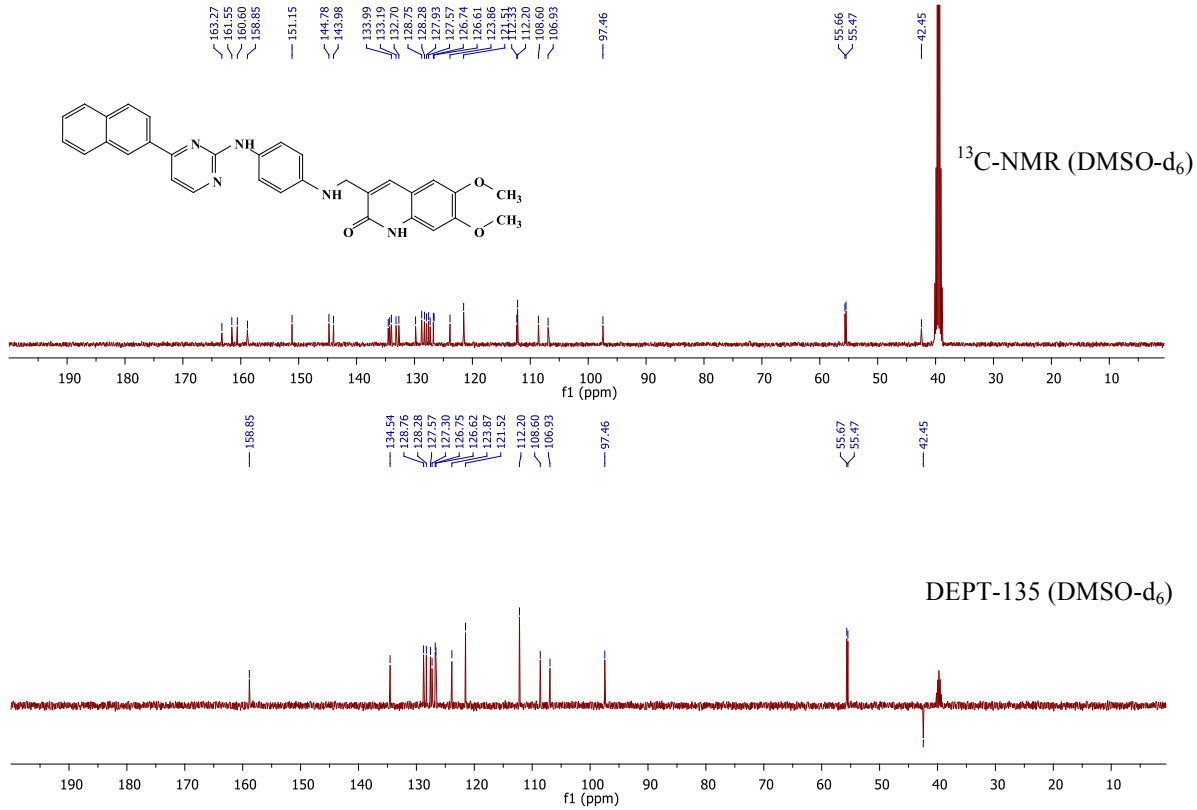




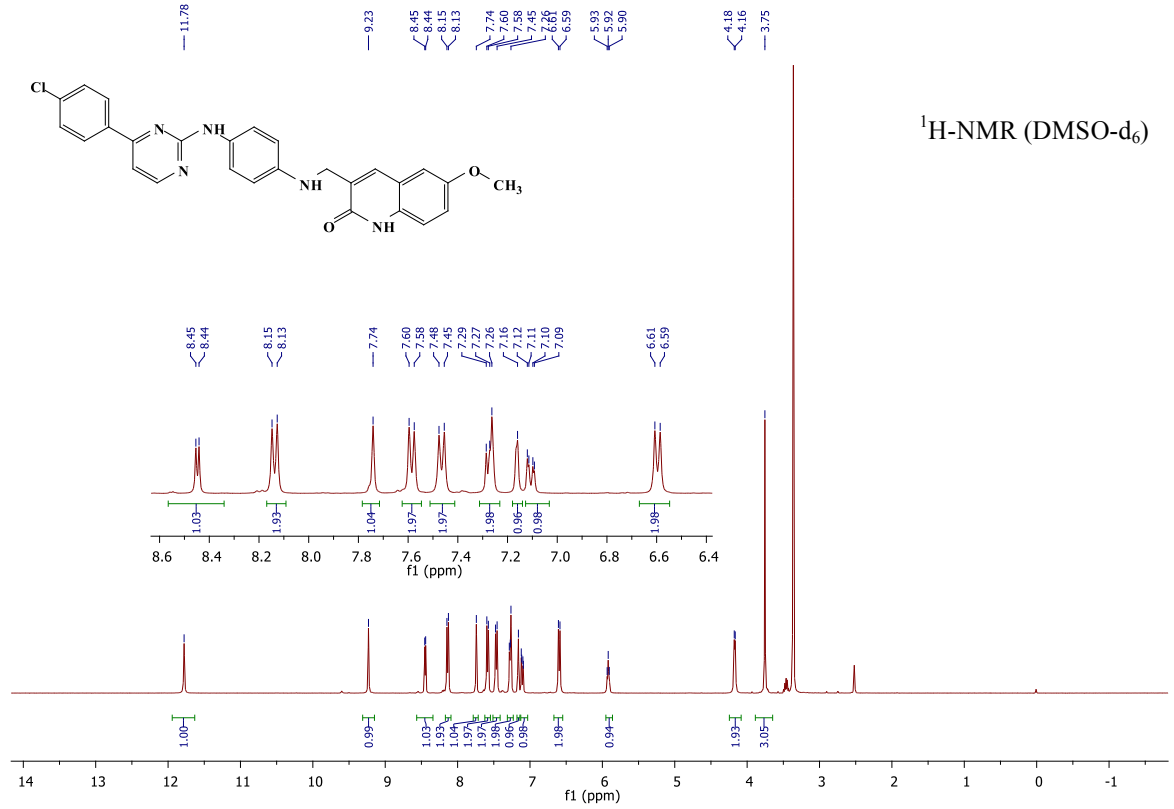


Compound-16b

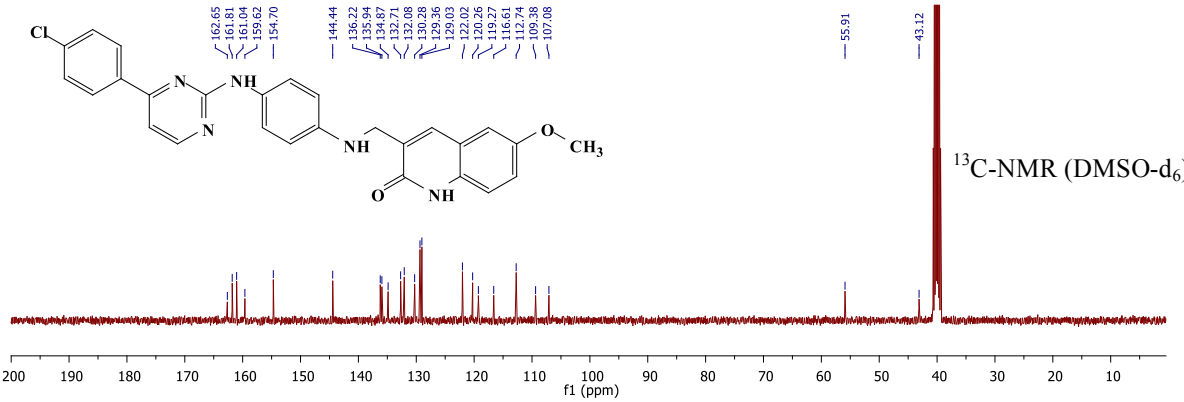




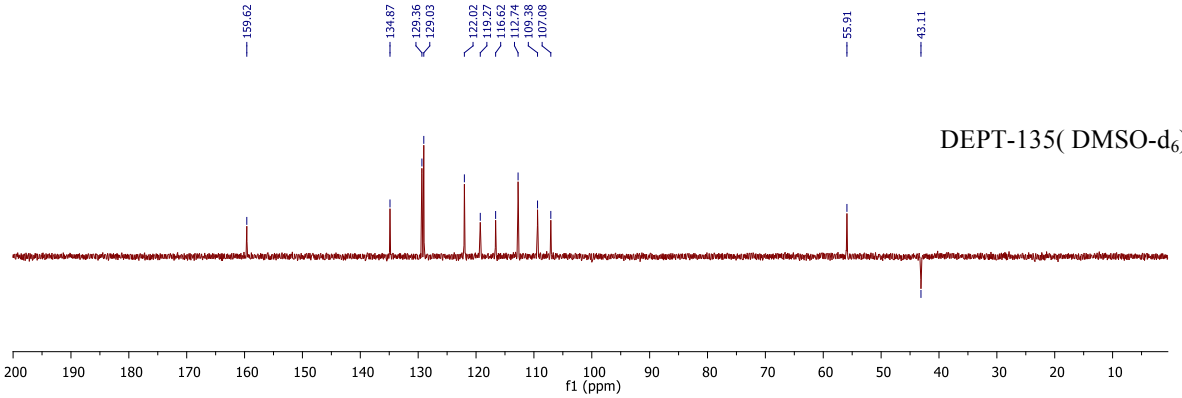
Compound-17a



^{1}H-NMR (DMSO-d$_6$)

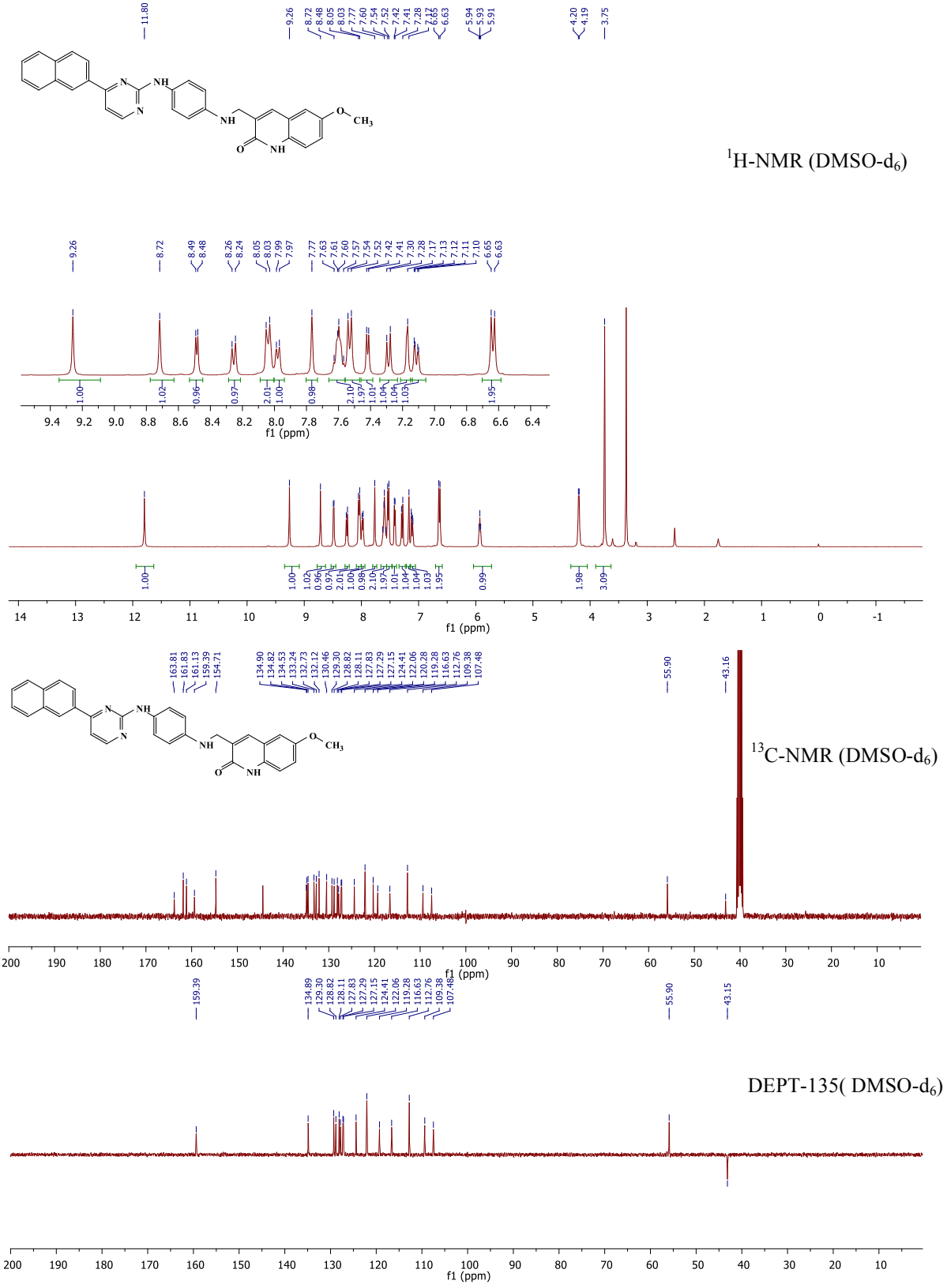


^{13}C-NMR (DMSO-d$_6$)

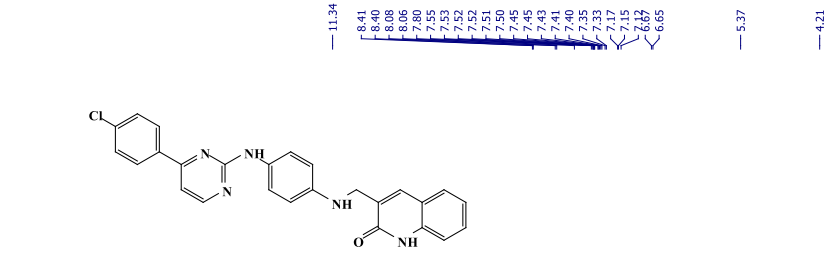


DEPT-135(DMSO-d$_6$)

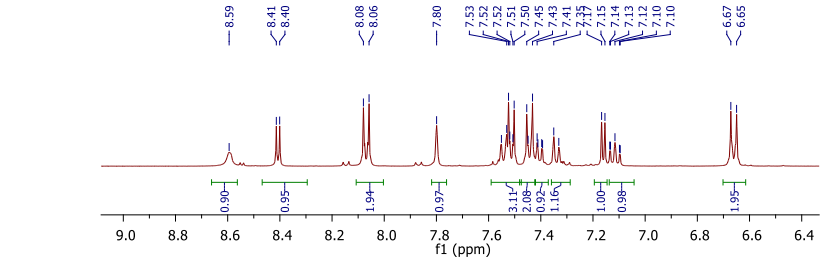
Compound-17b

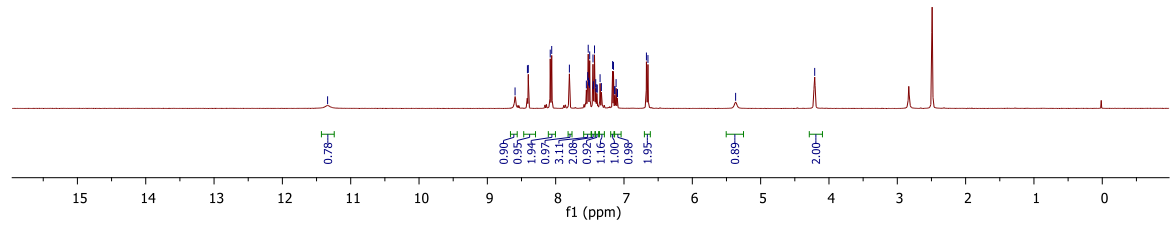


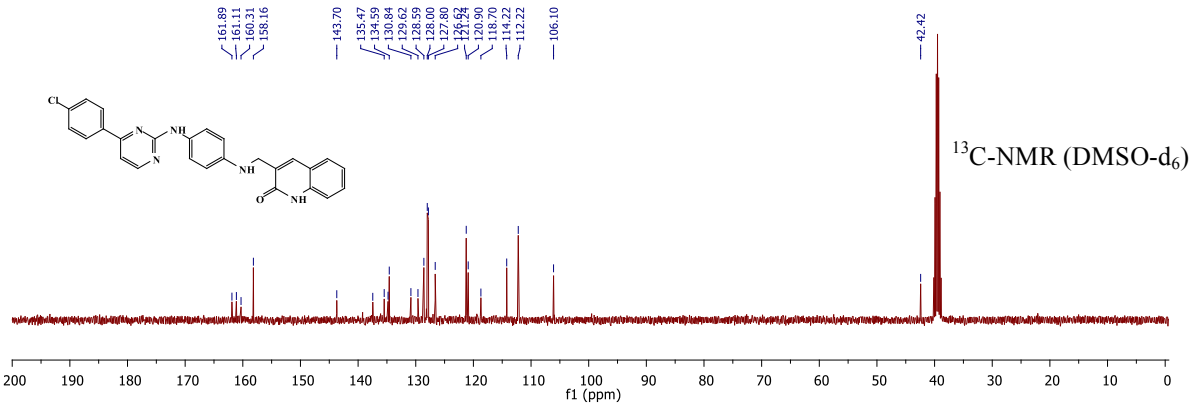
Compound-18a



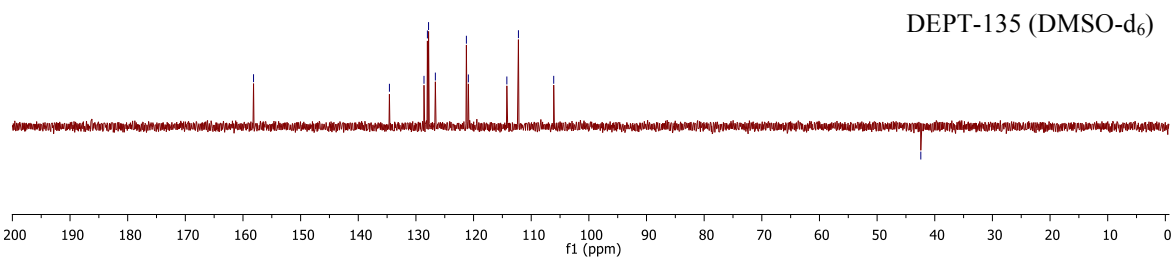
^{1}H-NMR (DMSO-d$_6$)





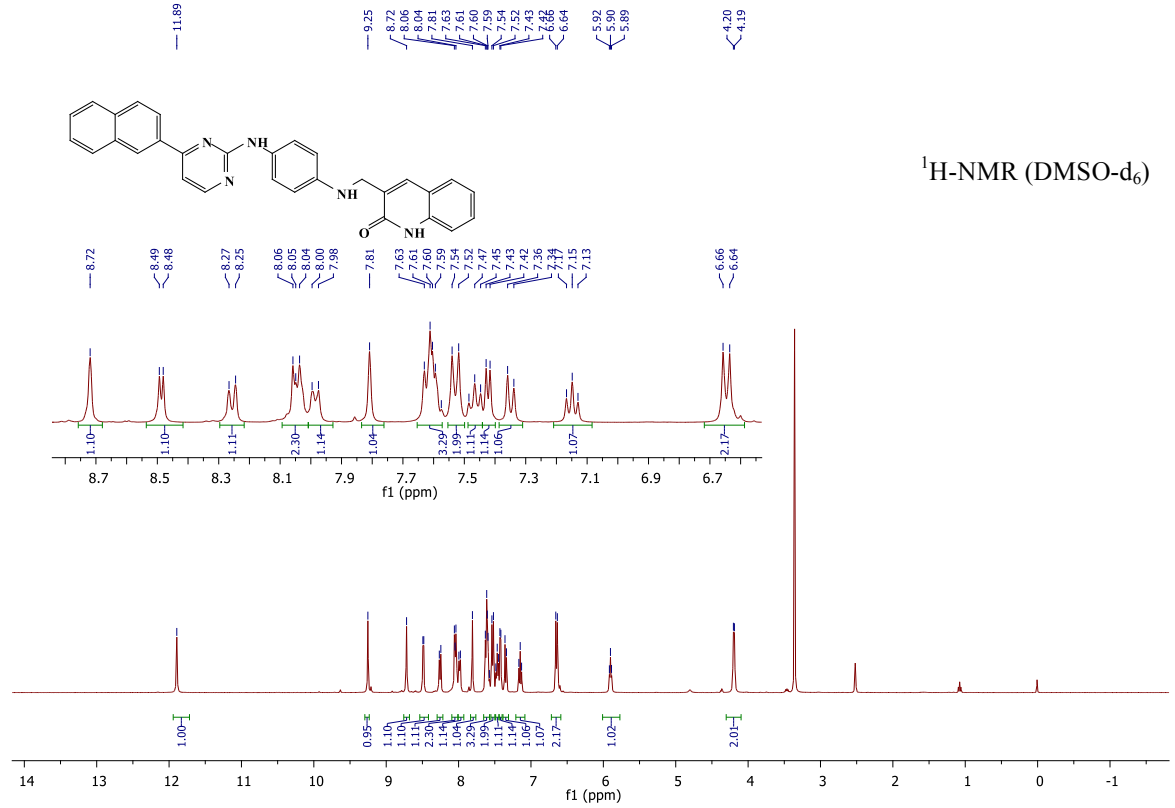


^{13}C-NMR (DMSO-d$_6$)

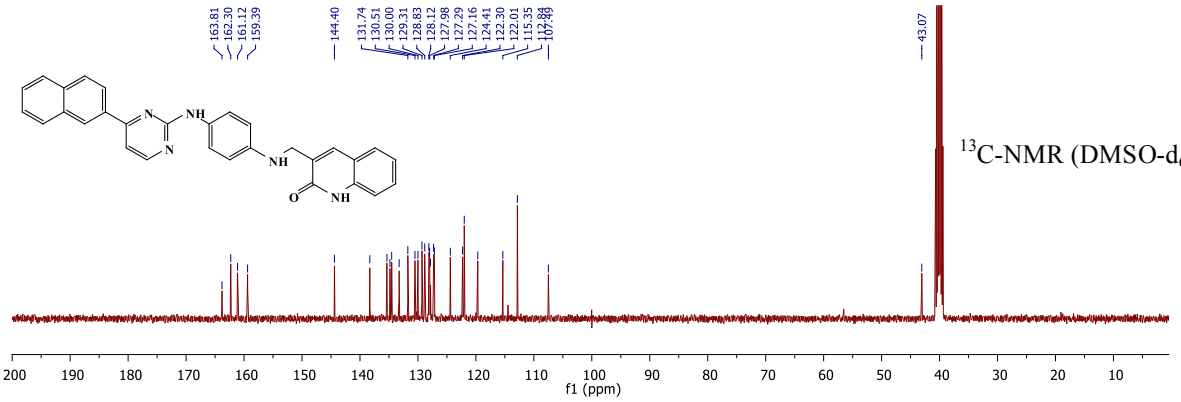


DEPT-135 (DMSO-d$_6$)

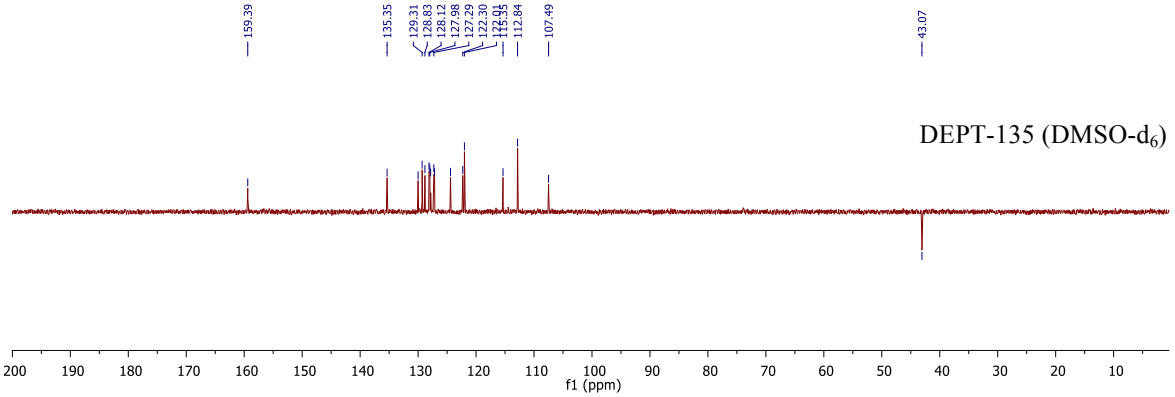
Compound-18b



^{1}H-NMR (DMSO-d$_6$)

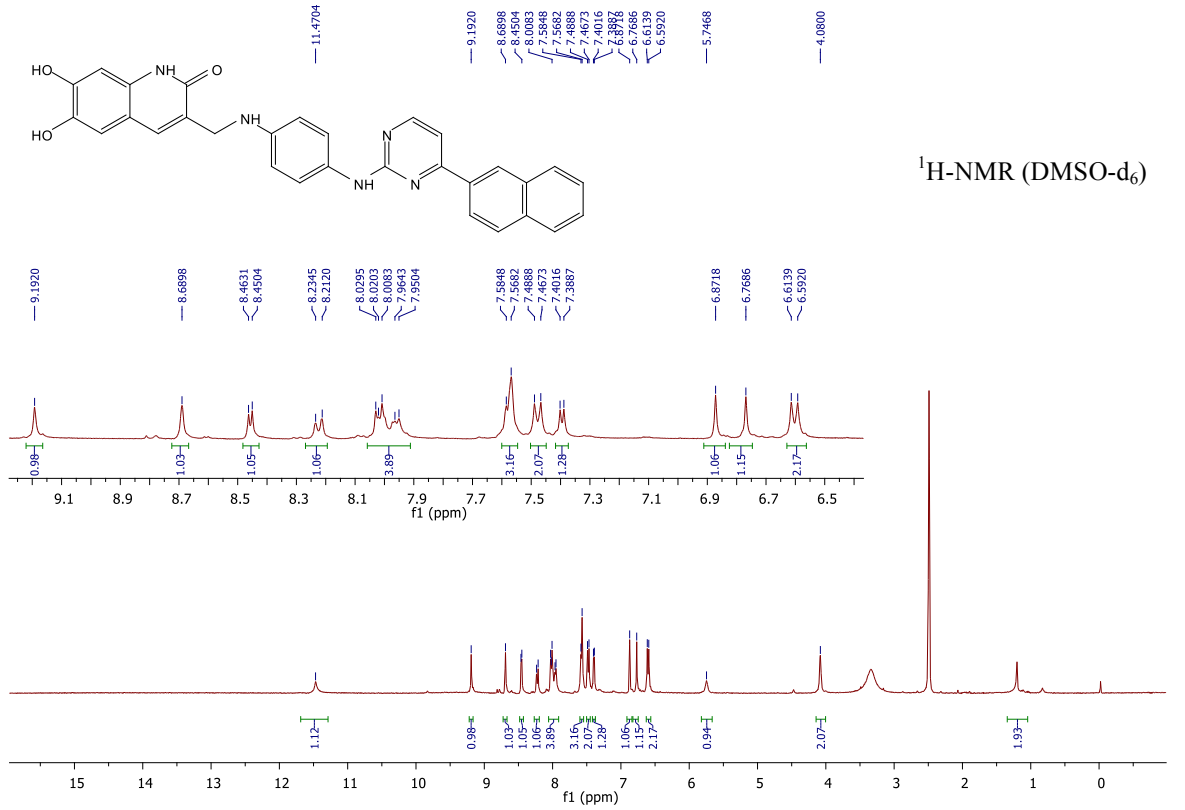


^{13}C-NMR (DMSO-d$_6$)

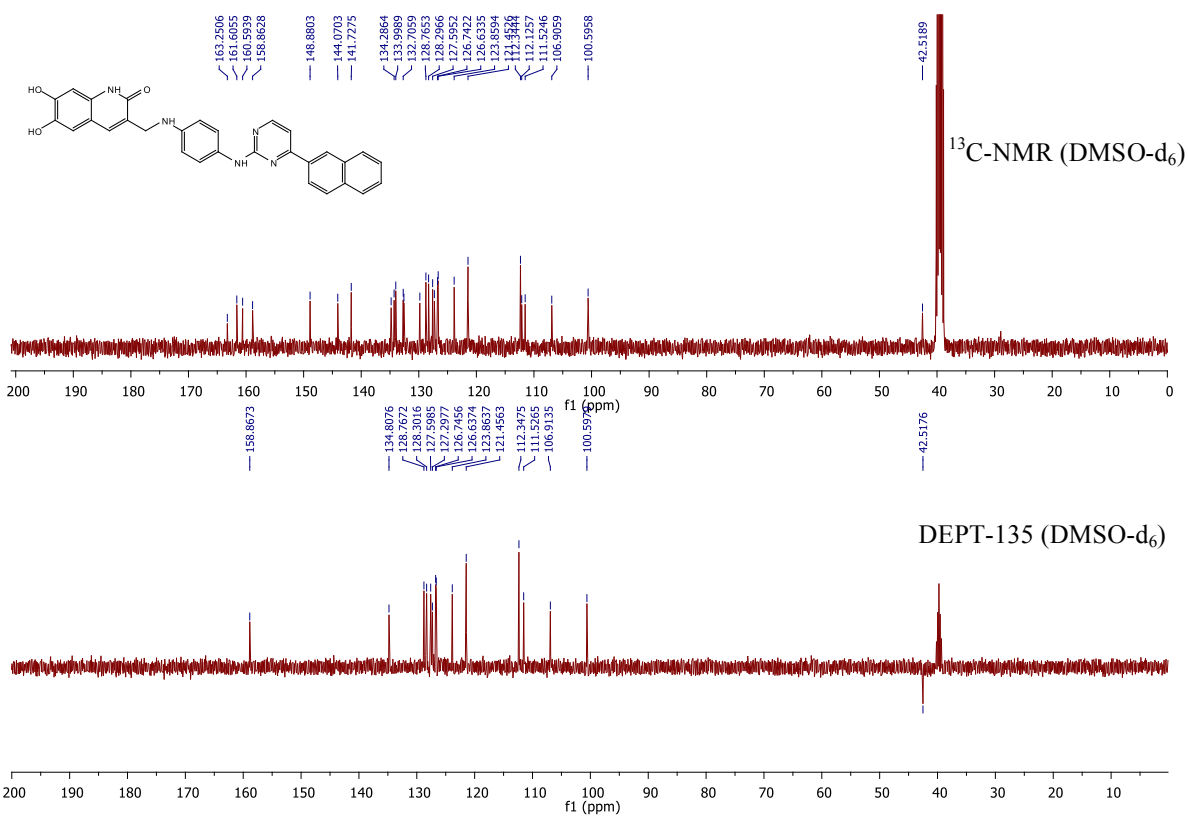


DEPT-135 (DMSO-d$_6$)

Compound-19b



^{1}H-NMR (DMSO-d$_6$)

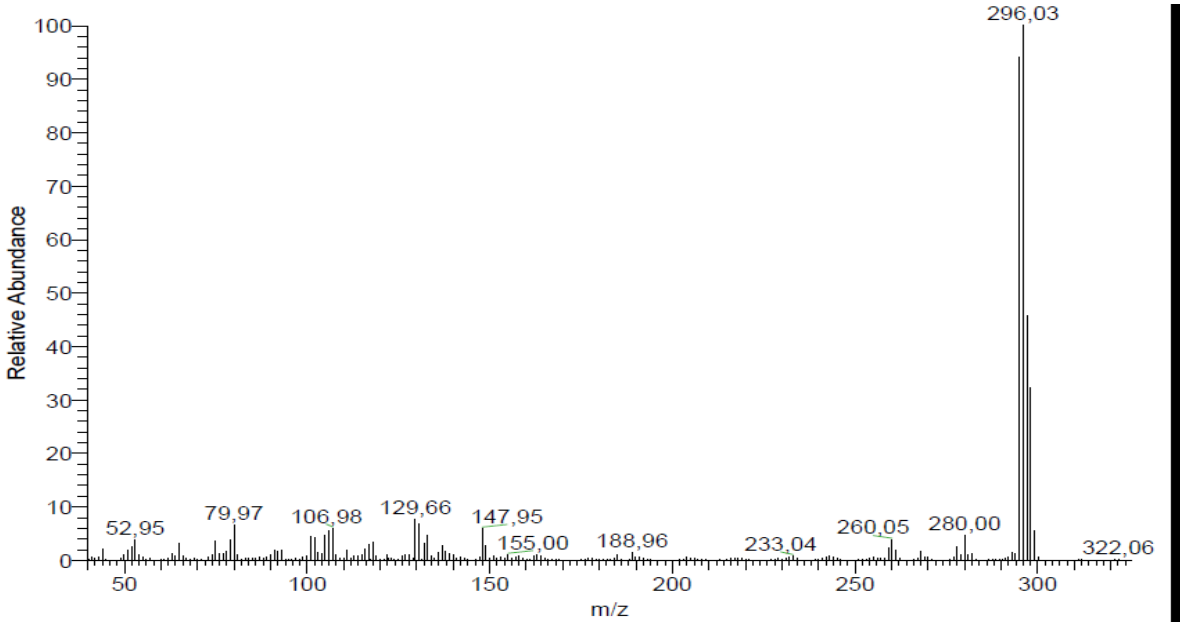


^{13}C-NMR (DMSO-d$_6$)

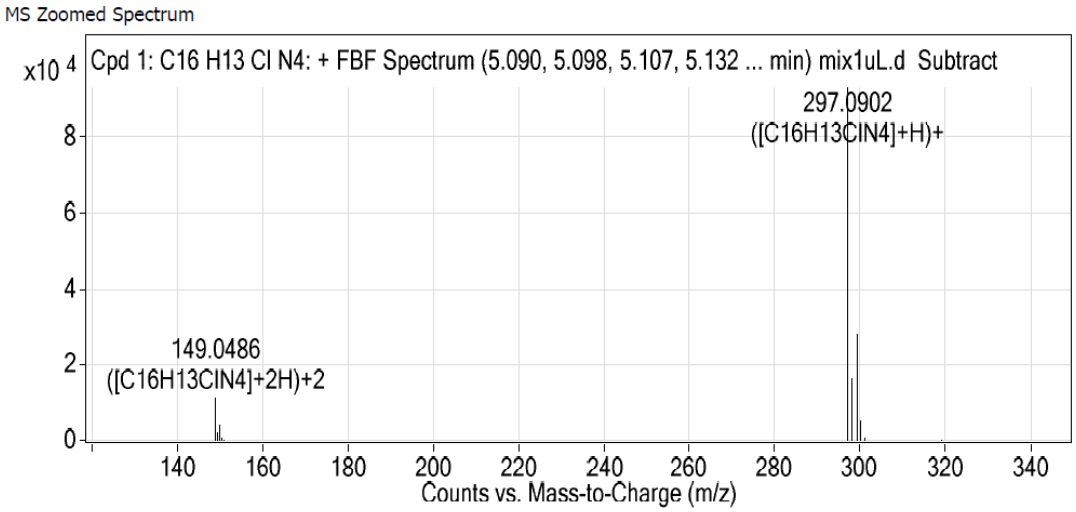
DEPT-135 (DMSO-d$_6$)

Compound-3a

EI MS (70 eV):



ESI-QTOF (positive ionization)

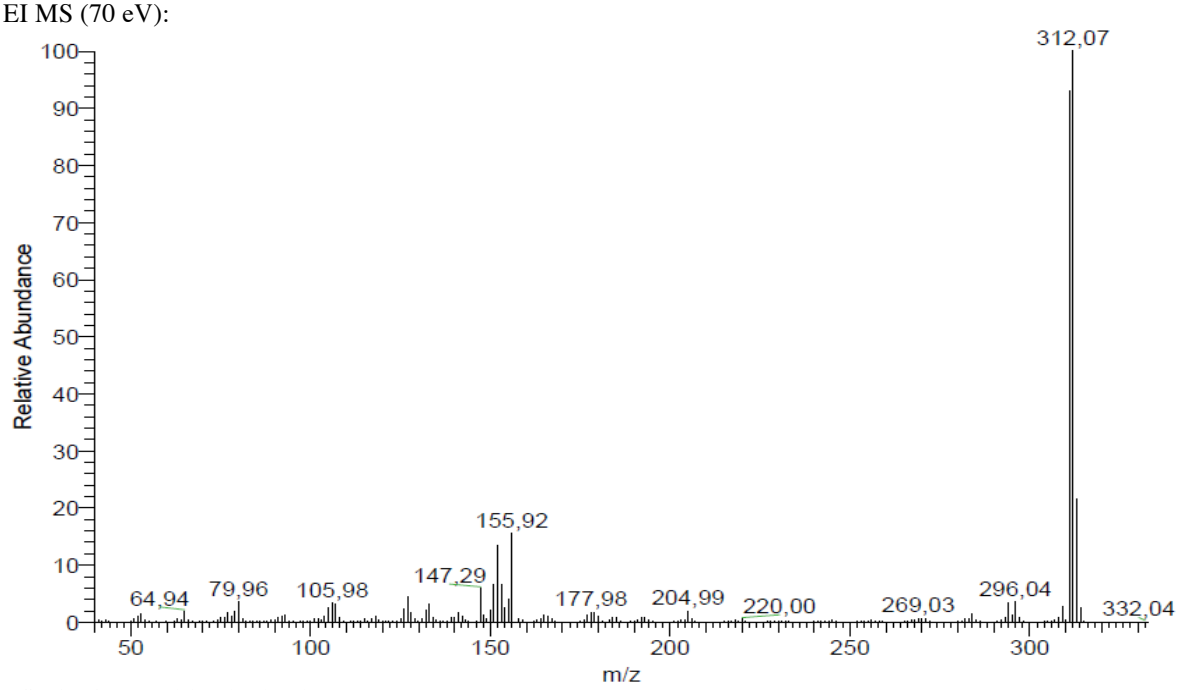


MS Spectrum Peak List

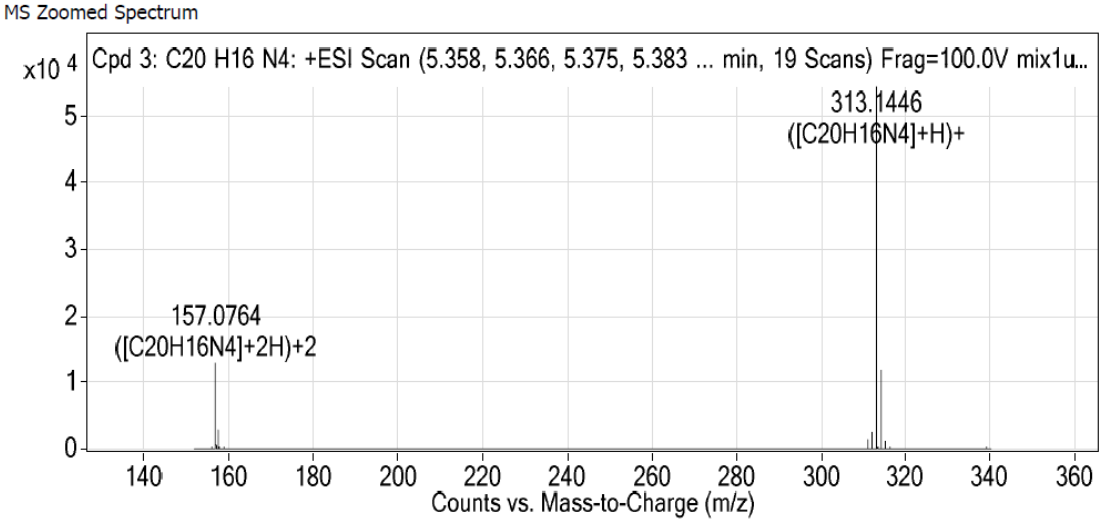
m/z	z	Abund	Formula	Ion
149.0486	2	11263.39	C16H13ClN4	(M+2H)+2
149.5497	2	2081.65	C16H13ClN4	(M+2H)+2
150.0472	2	3663.54	C16H13ClN4	(M+2H)+2
150.5486	2	692.96	C16H13ClN4	(M+2H)+2
297.0902	1	93136.22	C16H13ClN4	(M+H)+
298.0928	1	16208.65	C16H13ClN4	(M+H)+
299.0875	1	27865.41	C16H13ClN4	(M+H)+
300.0904	1	5187.81	C16H13ClN4	(M+H)+

Compound-3b

EI MS (70 eV):



ESI-QTOF (positive ionization)

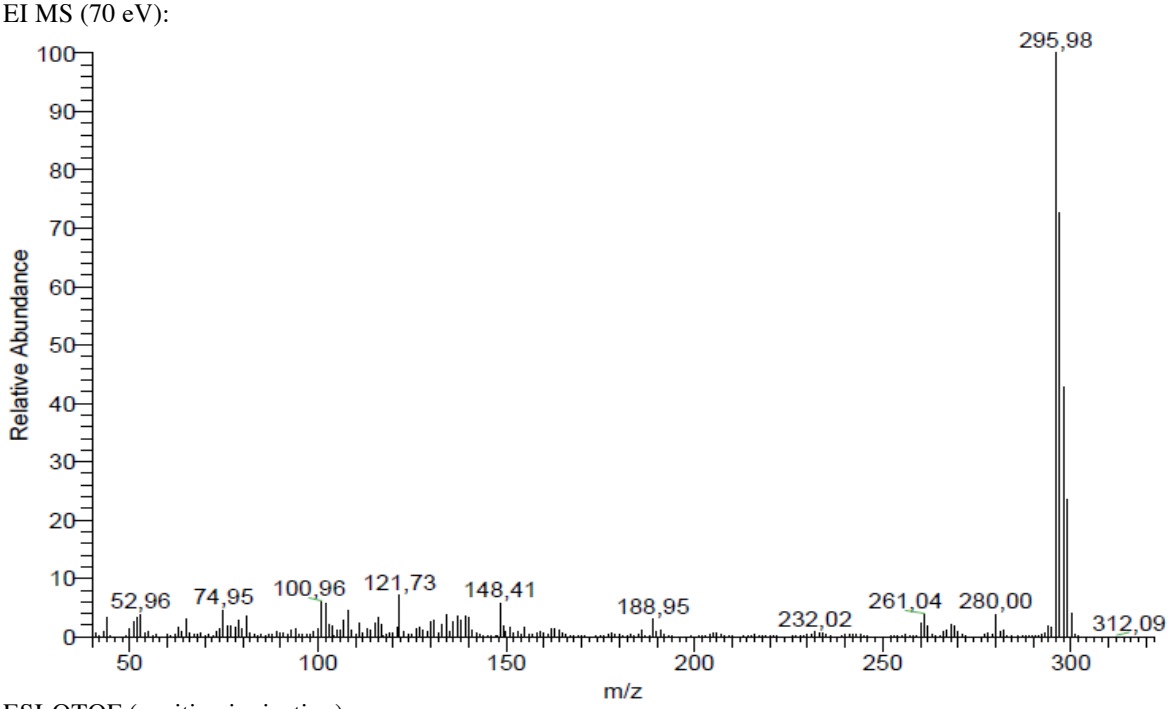


MS Spectrum Peak List

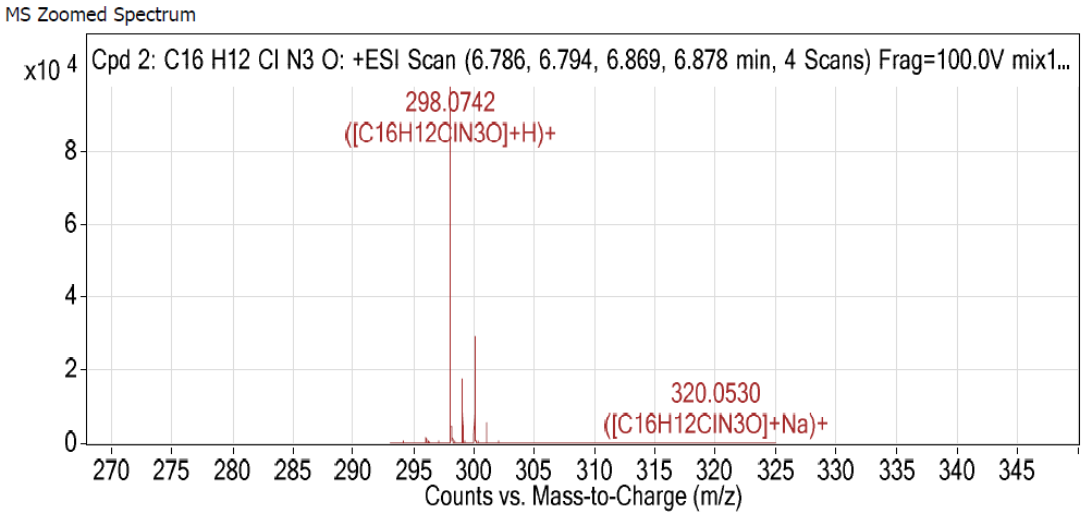
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
157.0764	157.076	-2.19	2	12568.78	C20H16N4	(M+2H)+2
157.5776	157.5775	-0.31	2	2819.89	C20H16N4	(M+2H)+2
158.0793	158.079	-2.13	2	444.36	C20H16N4	(M+2H)+2
313.1446	313.1448	0.68	1	54342.16	C20H16N4	(M+H)+
314.1476	314.1478	0.64	1	12099.22	C20H16N4	(M+H)+
315.154	315.1507	-10.28	1	1062.96	C20H16N4	(M+H)+
316.1573	316.1537	-11.58	1	174.2	C20H16N4	(M+H)+
335.1268	335.1267	-0.1	1	178.45	C20H16N4	(M+Na)+

Compound-4a

EI MS (70 eV):



ESI-QTOF (positive ionization)

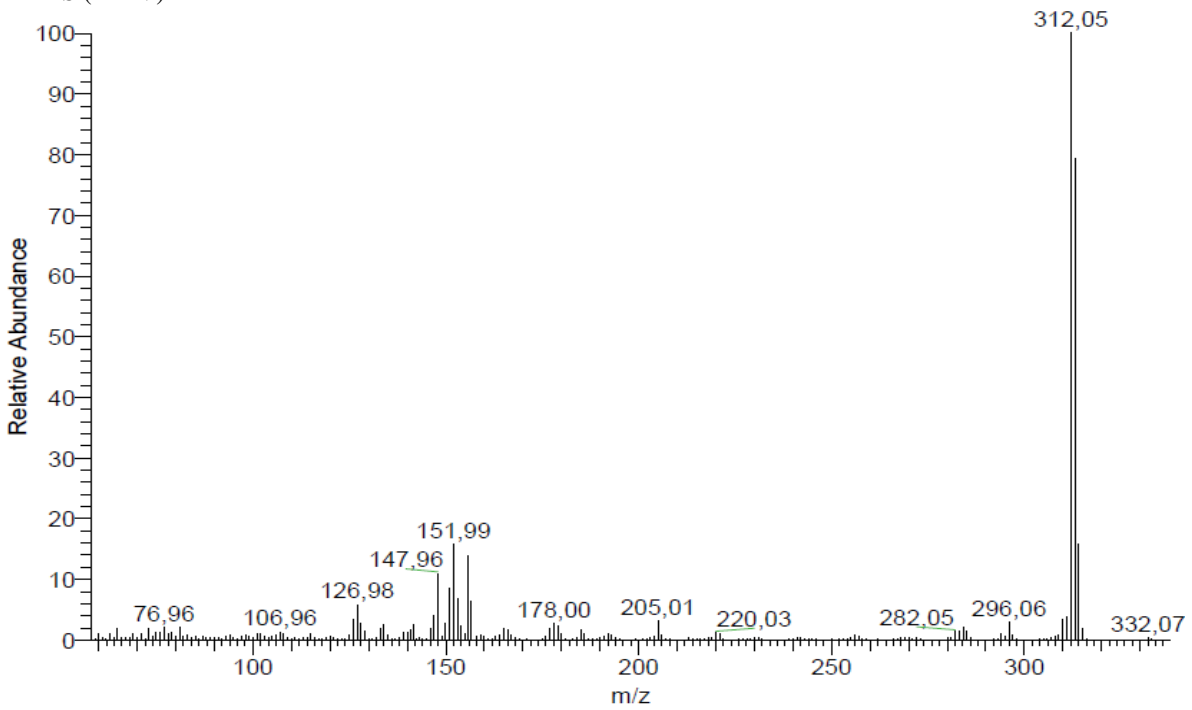


MS Spectrum Peak List

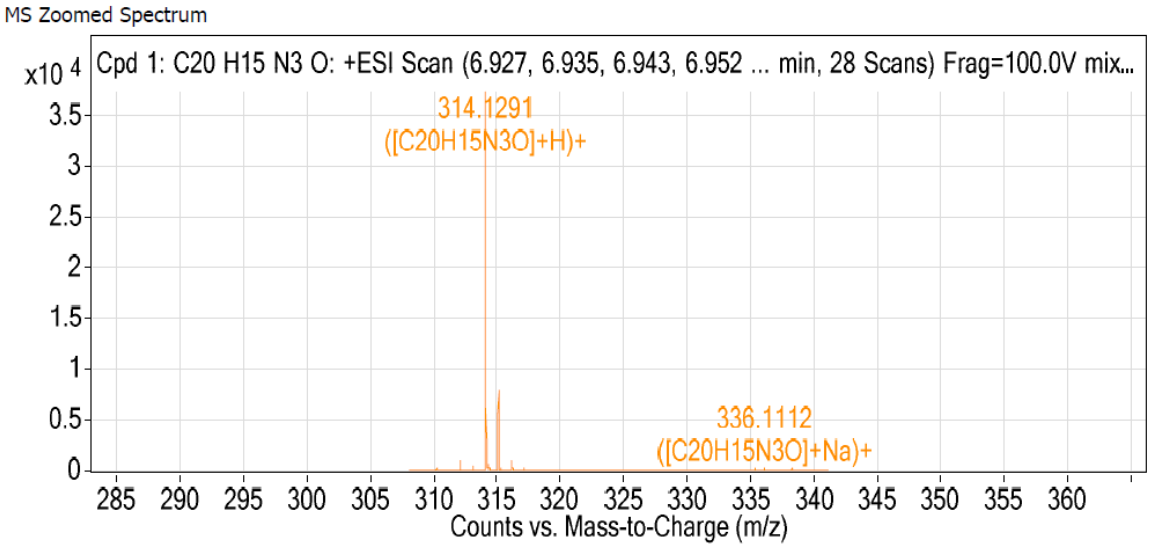
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
298.0742	298.0742	-0.11	1	101744.8	C16H12ClN3O	(M+H)+
299.0773	299.0772	-0.41	1	17875.09	C16H12ClN3O	(M+H)+
300.0718	300.0717	-0.48	1	30274.79	C16H12ClN3O	(M+H)+
301.0742	301.0744	0.8	1	5547.51	C16H12ClN3O	(M+H)+
302.0764	302.0771	2.47	1	645.22	C16H12ClN3O	(M+H)+
320.053	320.0561	9.64	1	159.12	C16H12ClN3O	(M+Na)+

Compound-4b

EI MS (70 eV):



ESI-QTOF (positive ionization)

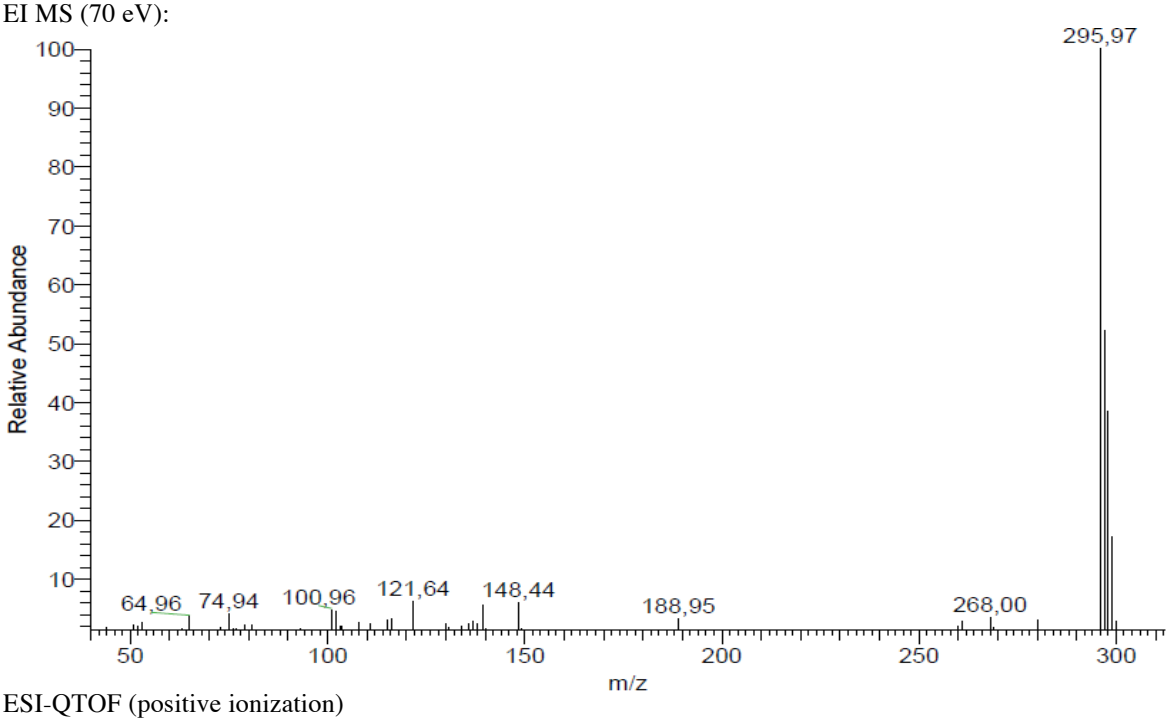


MS Spectrum Peak List

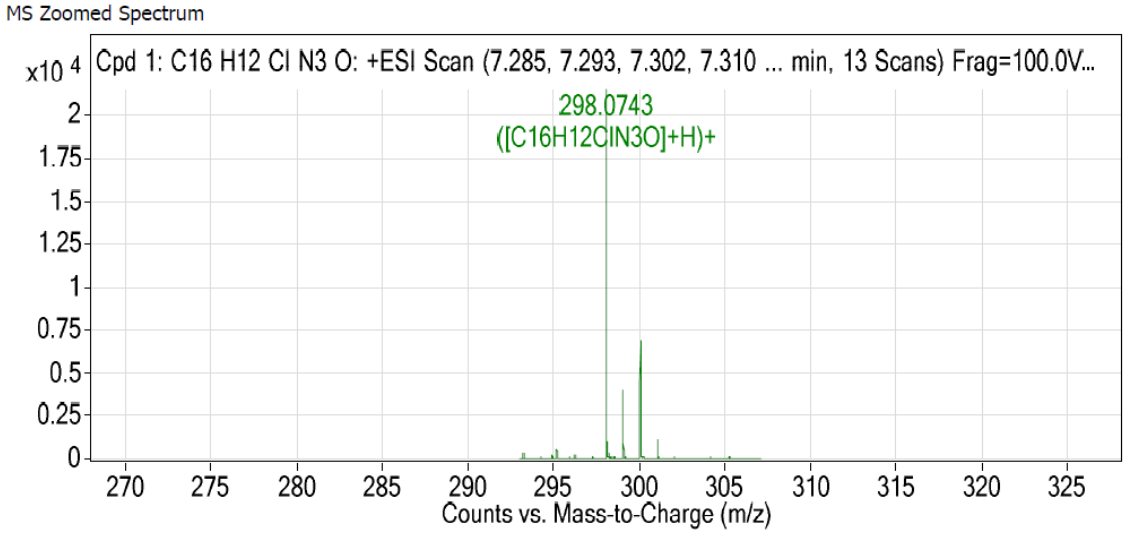
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
313.1161	313.121	15.54	1	118.96	C20H15N3O	M+
314.1291	314.1288	-0.87	1	36679.08	C20H15N3O	(M+H)+
315.1324	315.1319	-1.54	1	8223.14	C20H15N3O	(M+H)+
316.1358	316.1348	-3.34	1	1034.97	C20H15N3O	(M+H)+
317.1382	317.1376	-1.97	1	66	C20H15N3O	(M+H)+
336.1112	336.1107	-1.31	1	60.07	C20H15N3O	(M+Na)+

Compound-5a

EI MS (70 eV):



ESI-QTOF (positive ionization)

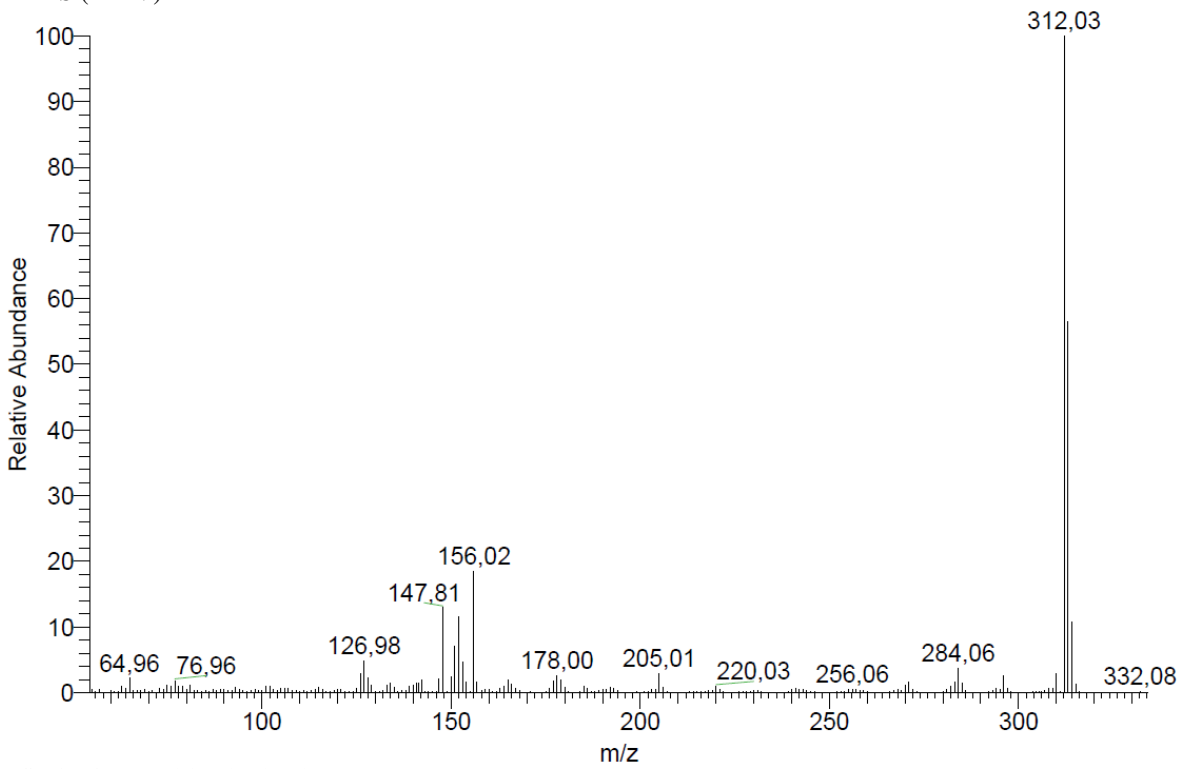


MS Spectrum Peak List

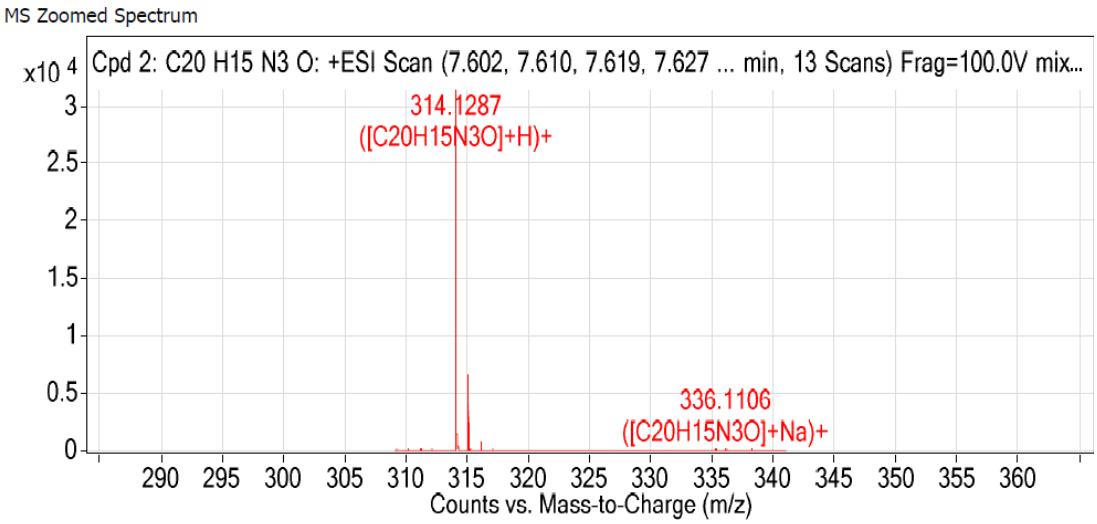
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
298.0743	298.0742	-0.53	1	22391.09	C16H12ClN3O	(M+H)+
299.077	299.0772	0.42	1	4070.67	C16H12ClN3O	(M+H)+
300.0717	300.0717	-0.18	1	7156.17	C16H12ClN3O	(M+H)+
301.0744	301.0744	-0.15	1	1221.69	C16H12ClN3O	(M+H)+
302.0734	302.0771	12.35	1	77.33	C16H12ClN3O	(M+H)+

Compound-5b

EI MS (70 eV):



ESI-QTOF (positive ionization)

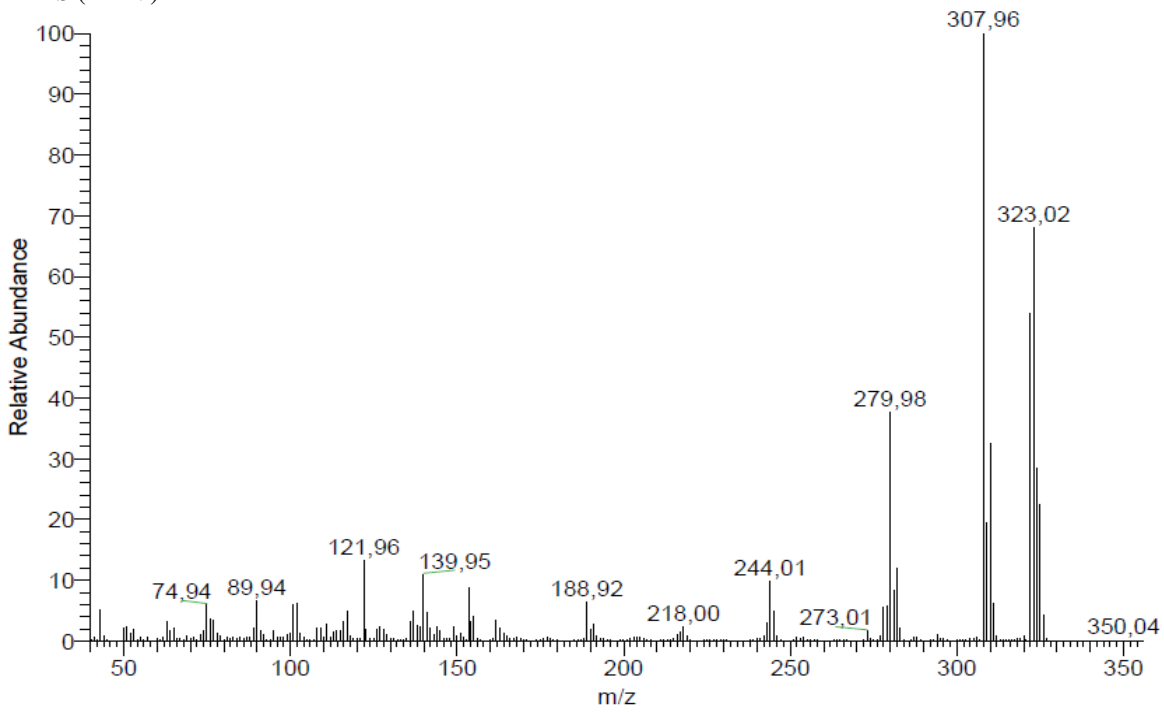


MS Spectrum Peak List

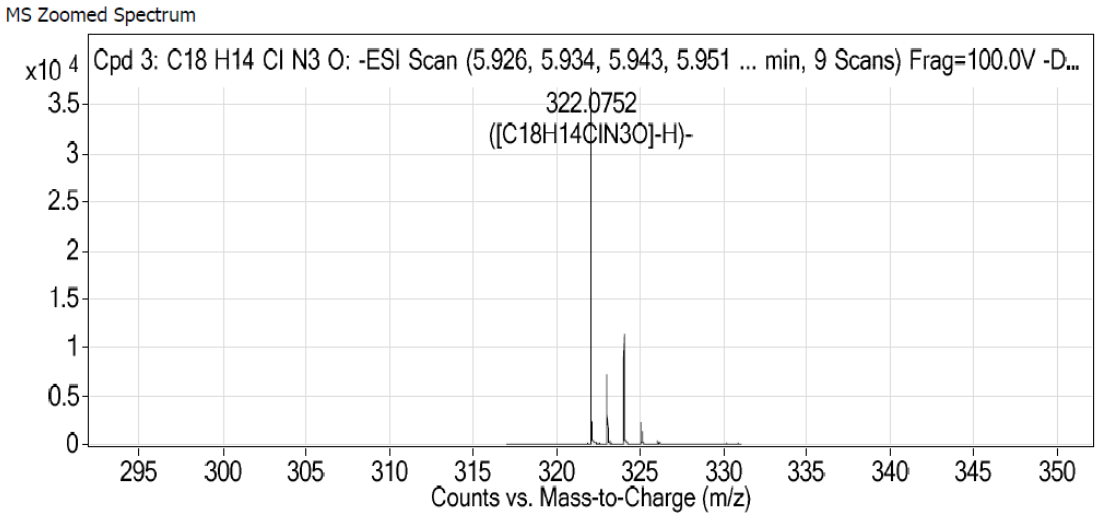
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
314.1287	314.1288	0.17	1	31500.21	C20H15N3O	(M+H)+
315.1323	315.1319	-1.38	1	6980.97	C20H15N3O	(M+H)+
316.1358	316.1348	-3.22	1	817.01	C20H15N3O	(M+H)+
317.1379	317.1376	-1.05	1	63.34	C20H15N3O	(M+H)+
336.1106	336.1107	0.33	1	108.92	C20H15N3O	(M+Na)+

Compound-6a

EI MS (70 eV):



ESI-QTOF (negative ionization)

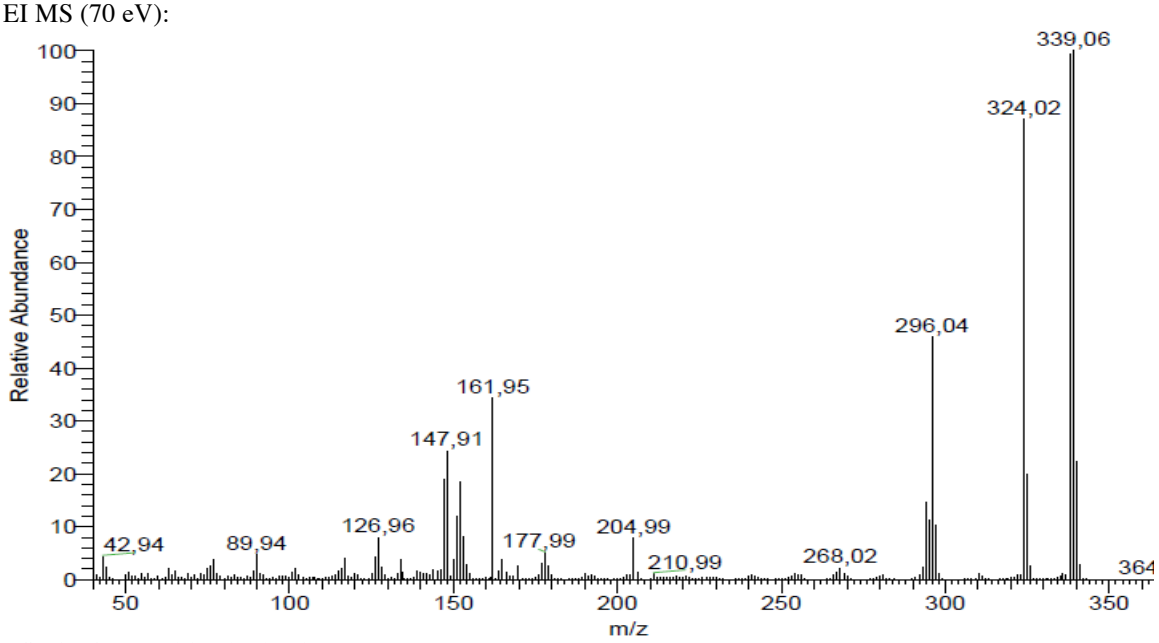


MS Spectrum Peak List

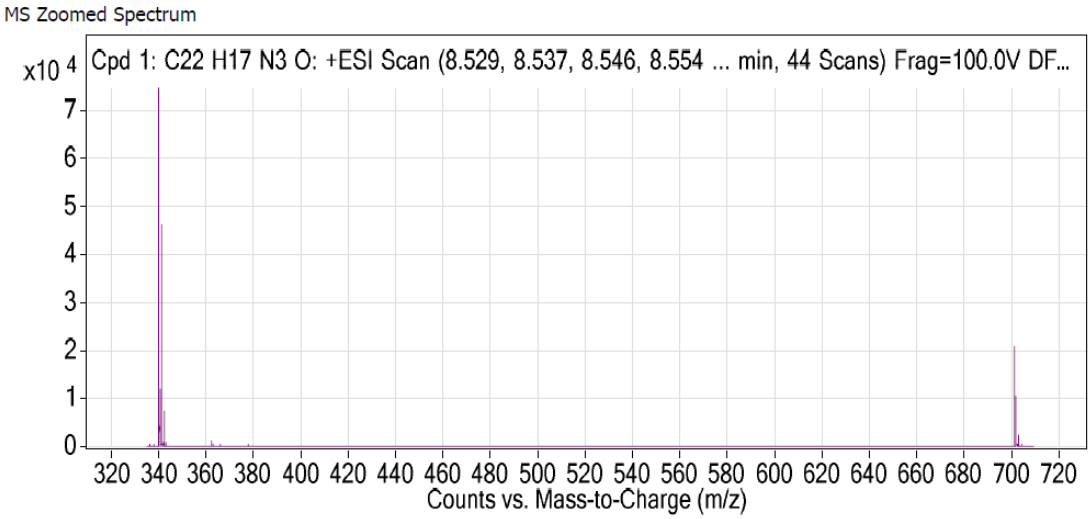
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
322.0752	322.0753	0.27	1	37574.44	C18H14ClN3O	(M-H)-
323.0785	323.0783	-0.73	1	7523.98	C18H14ClN3O	(M-H)-
324.0729	324.0729	0.03	1	11691.43	C18H14ClN3O	(M-H)-
325.0764	325.0756	-2.67	1	2384.38	C18H14ClN3O	(M-H)-
326.0773	326.0783	3.2	1	366.82	C18H14ClN3O	(M-H)-

Compound-6b

EI MS (70 eV):



ESI-QTOF (positive ionization)

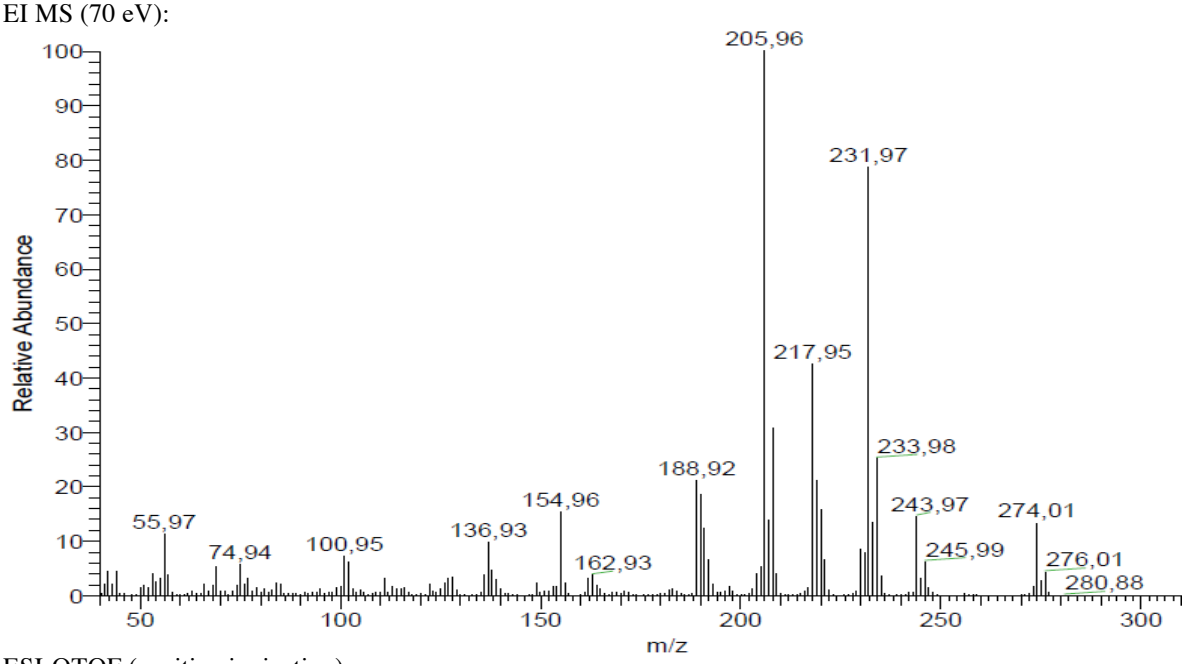


MS Spectrum Peak List

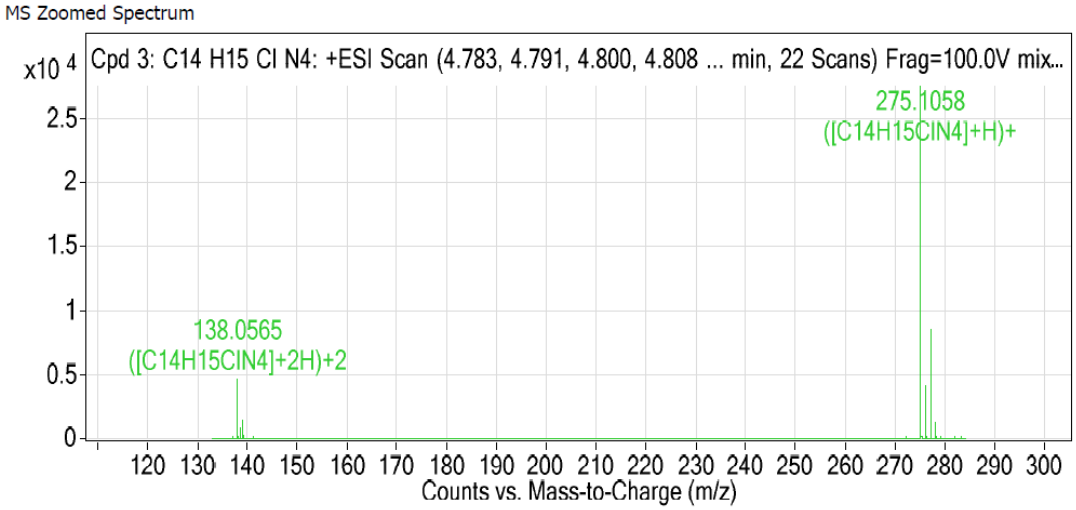
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
340.1442	340.1444	0.69	1	35868.74	C22H17N3O	(M+H)+
341.1473	341.1475	0.62	1	8573.41	C22H17N3O	(M+H)+
342.1506	342.1505	-0.2	1	1178.38	C22H17N3O	(M+H)+
343.1505	343.1534	8.28	1	108.88	C22H17N3O	(M+H)+
362.1256	362.1264	2.21	1	634.27	C22H17N3O	(M+Na)+
363.1308	363.1295	-3.67	1	147.79	C22H17N3O	(M+Na)+
378.1011	378.1003	-1.98	1	217.49	C22H17N3O	(M+K)+
701.2637	701.2635	-0.29	1	1954.56	C22H17N3O	(2M+Na)+
702.2665	702.2666	0.22	1	970.31	C22H17N3O	(2M+Na)+
703.2674	703.2697	3.24	1	227.78	C22H17N3O	(2M+Na)+

Compound-7a

EI MS (70 eV):



ESI-QTOF (positive ionization)

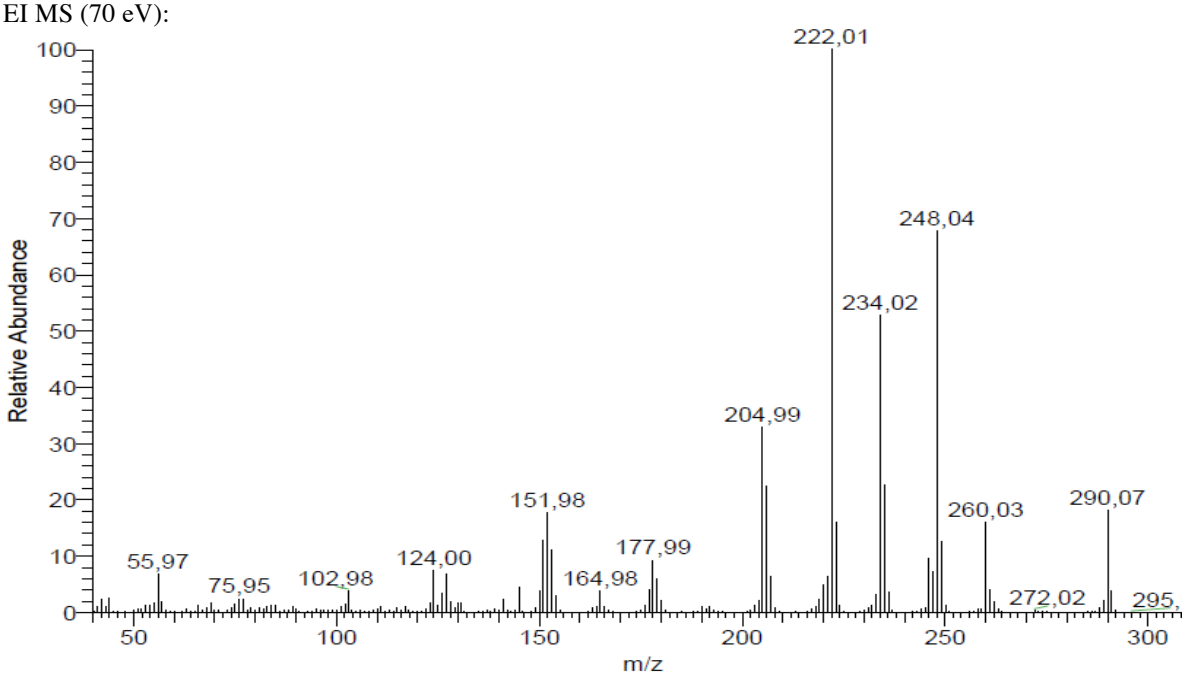


MS Spectrum Peak List

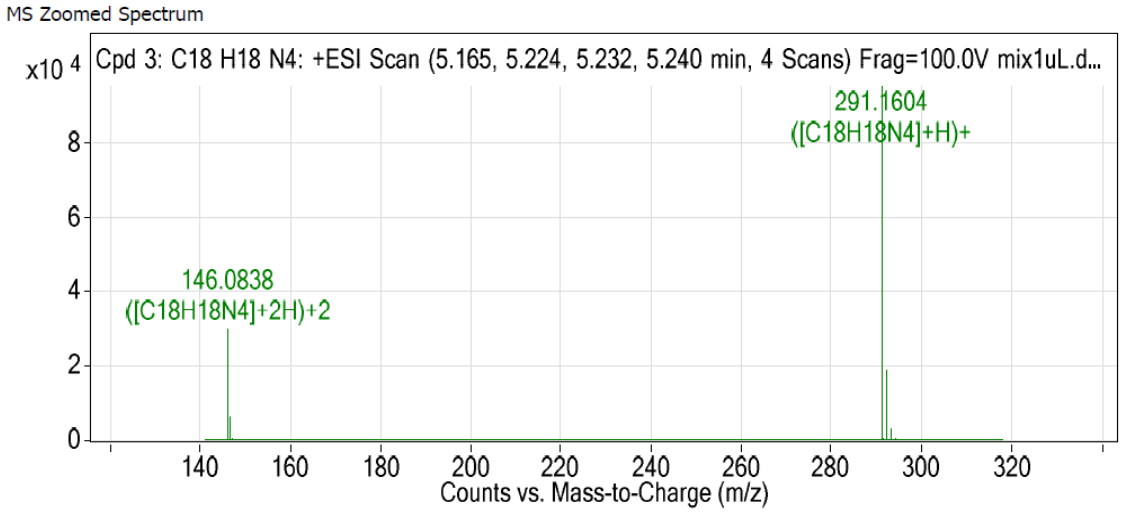
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
138.0565	138.0565	0.45	2	4721.31	C14H15ClN4	(M+2H)+2
138.5585	138.558	-3.78	2	838.95	C14H15ClN4	(M+2H)+2
139.055	139.0552	1.9	2	1536.71	C14H15ClN4	(M+2H)+2
139.5576	139.5565	-7.65	2	292.12	C14H15ClN4	(M+2H)+2
275.1058	275.1058	-0.15	1	27792.35	C14H15ClN4	(M+H)+
276.1088	276.1086	-0.66	1	4359.65	C14H15ClN4	(M+H)+
277.1027	277.1032	1.69	1	8458.56	C14H15ClN4	(M+H)+
278.106	278.1058	-0.79	1	1319.96	C14H15ClN4	(M+H)+
279.1075	279.1085	3.73	1	86.08	C14H15ClN4	(M+H)+

Compound-7b

EI MS (70 eV):



ESI-QTOF (positive ionization)

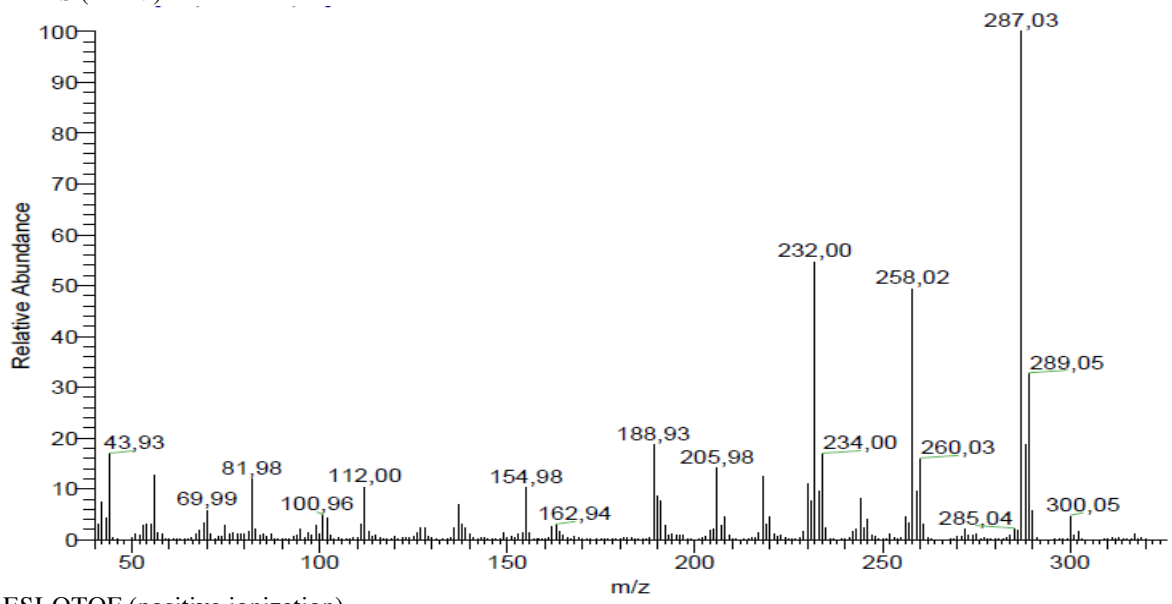


MS Spectrum Peak List

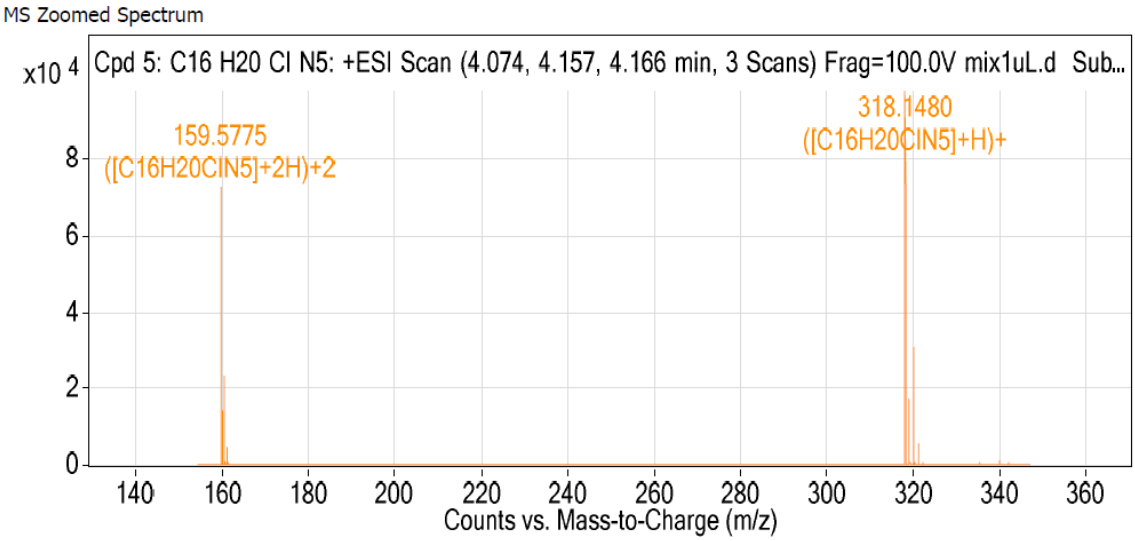
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
146.0838	146.0838	0.35	2	30000.28	C18H18N4	(M+2H)+2
146.5853	146.5853	-0.05	2	6574.1	C18H18N4	(M+2H)+2
147.0872	147.0868	-2.56	2	670.02	C18H18N4	(M+2H)+2
290.1529	290.1526	-0.94	1	72.01	C18H18N4	M+
291.1604	291.1604	0.07	1	95697.88	C18H18N4	(M+H)+
292.1636	292.1634	-0.64	1	18823.12	C18H18N4	(M+H)+
293.1743	293.1663	-27.33	1	2515.68	C18H18N4	(M+H)+
294.1788	294.1692	-32.66	1	533.79	C18H18N4	(M+H)+
313.1431	313.1424	-2.41	1	232.3	C18H18N4	(M+Na)+

Compound-8a

EI MS (70 eV):



ESI-QTOF (positive ionization)

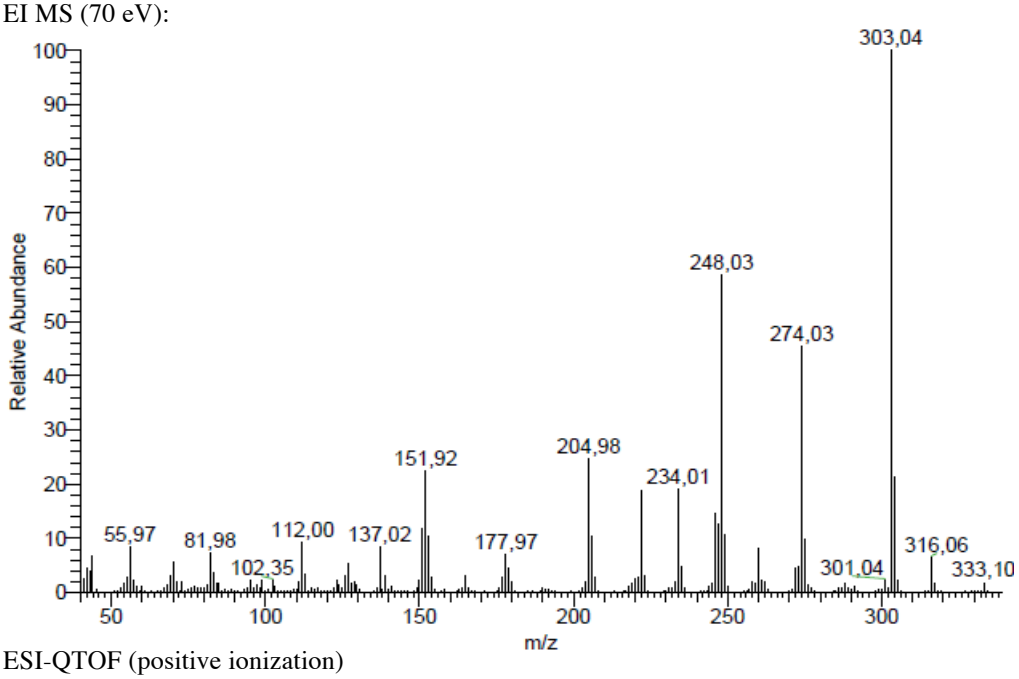


MS Spectrum Peak List

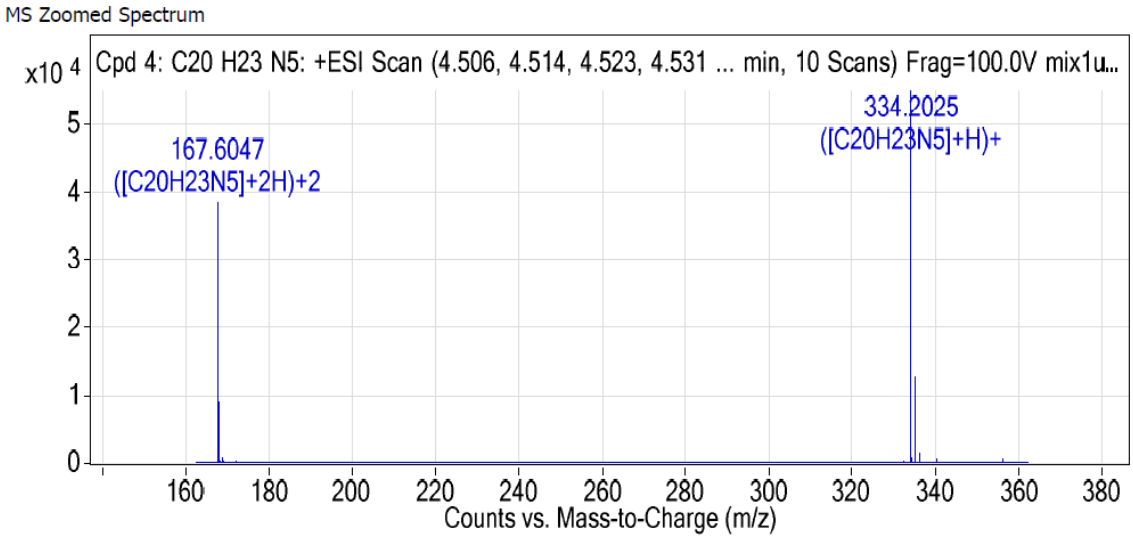
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
159.5775	159.5776	1.16	2	72814.99	C16H20ClN5	(M+2H)+2
160.0787	160.079	1.83	2	14321.99	C16H20ClN5	(M+2H)+2
160.5761	160.5764	1.83	2	23190.45	C16H20ClN5	(M+2H)+2
161.0772	161.0776	2.84	2	4904.01	C16H20ClN5	(M+2H)+2
318.148	318.148	0	1	98667.85	C16H20ClN5	(M+H)+
319.1509	319.1508	-0.18	1	17068.97	C16H20ClN5	(M+H)+
320.1453	320.1455	0.52	1	30788.87	C16H20ClN5	(M+H)+
321.1485	321.148	-1.5	1	5659.77	C16H20ClN5	(M+H)+
322.149	322.1507	5.3	1	574.63	C16H20ClN5	(M+H)+
340.1291	340.1299	2.55	1	980.45	C16H20ClN5	(M+Na)+

Compound-8b

EI MS (70 eV):



ESI-QTOF (positive ionization)

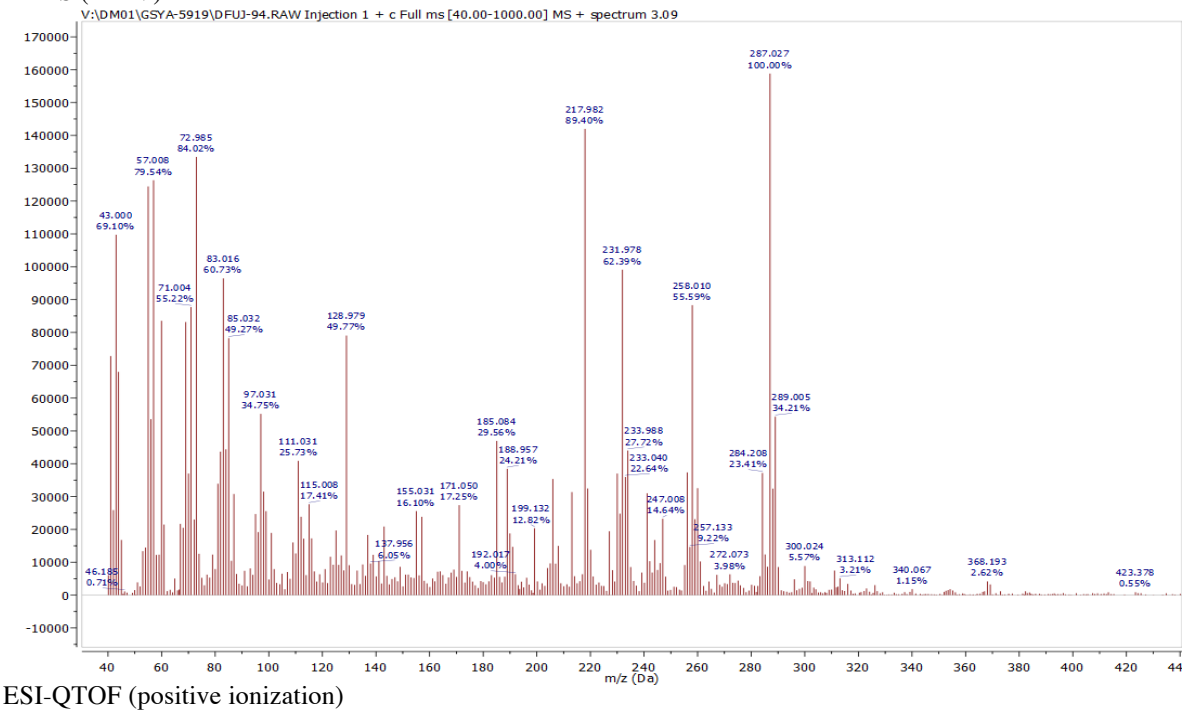


MS Spectrum Peak List

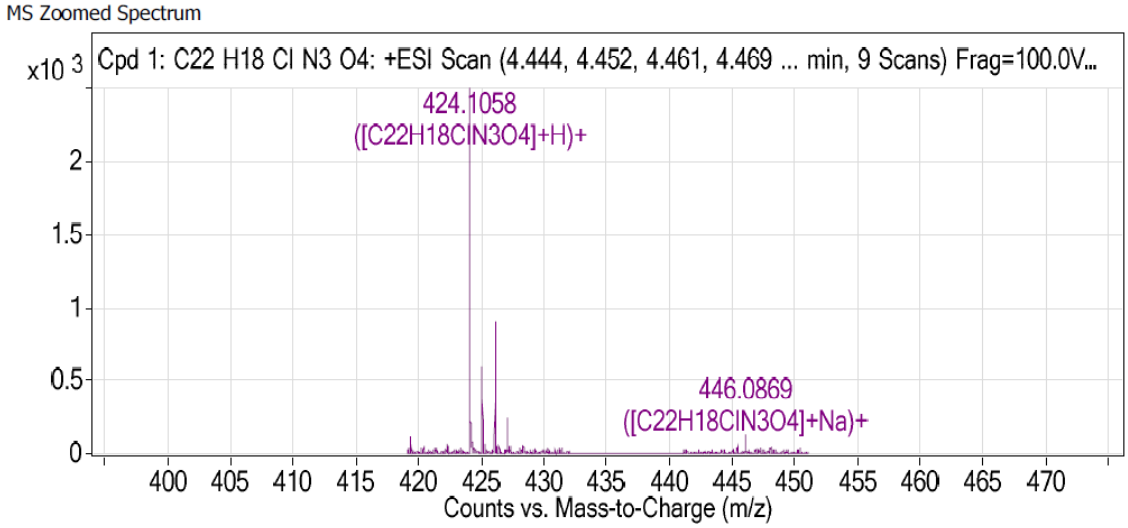
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
167.6047	167.6049	1.2	2	38757.25	C20H23N5	(M+2H)+2
168.1062	168.1064	1.35	2	9285.34	C20H23N5	(M+2H)+2
168.6081	168.6078	-1.31	2	1029.38	C20H23N5	(M+2H)+2
334.2025	334.2026	0.49	1	55875.35	C20H23N5	(M+H)+
335.2056	335.2055	-0.21	1	12647.92	C20H23N5	(M+H)+
336.2091	336.2084	-2.07	1	1419.51	C20H23N5	(M+H)+
337.2116	337.2113	-0.93	1	117.88	C20H23N5	(M+H)+
356.1838	356.1846	2.12	1	559.45	C20H23N5	(M+Na)+
357.1876	357.1875	-0.45	1	135.32	C20H23N5	(M+Na)+

Compound-9

EI MS (70 eV):



ESI-QTOF (positive ionization)

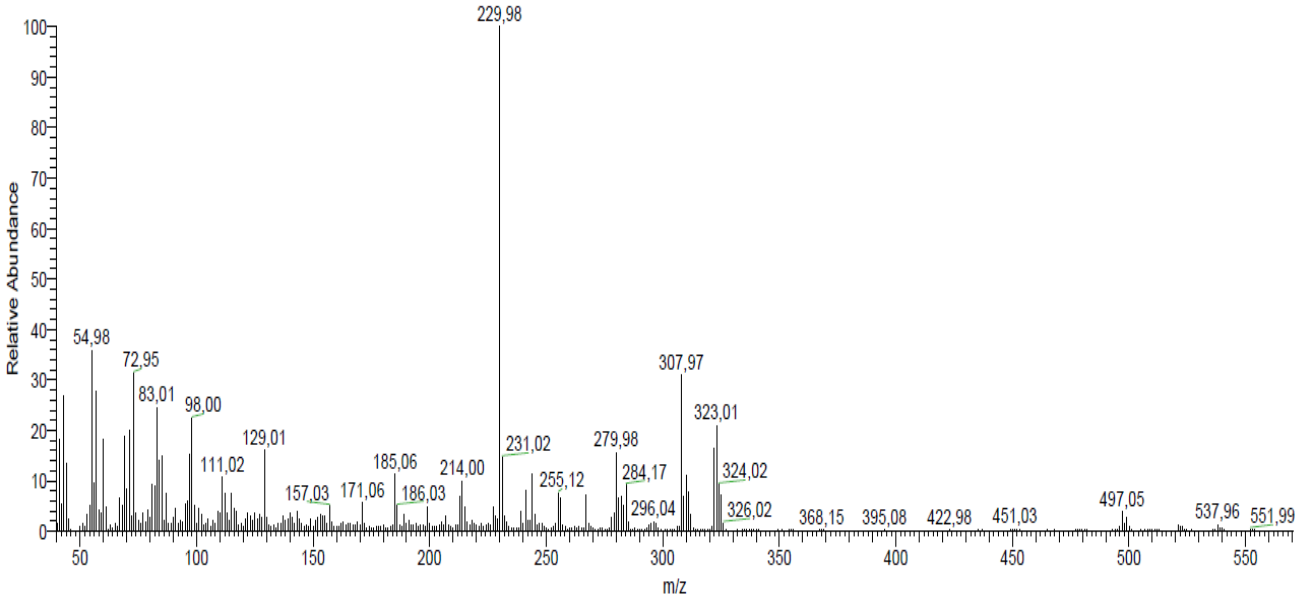


MS Spectrum Peak List

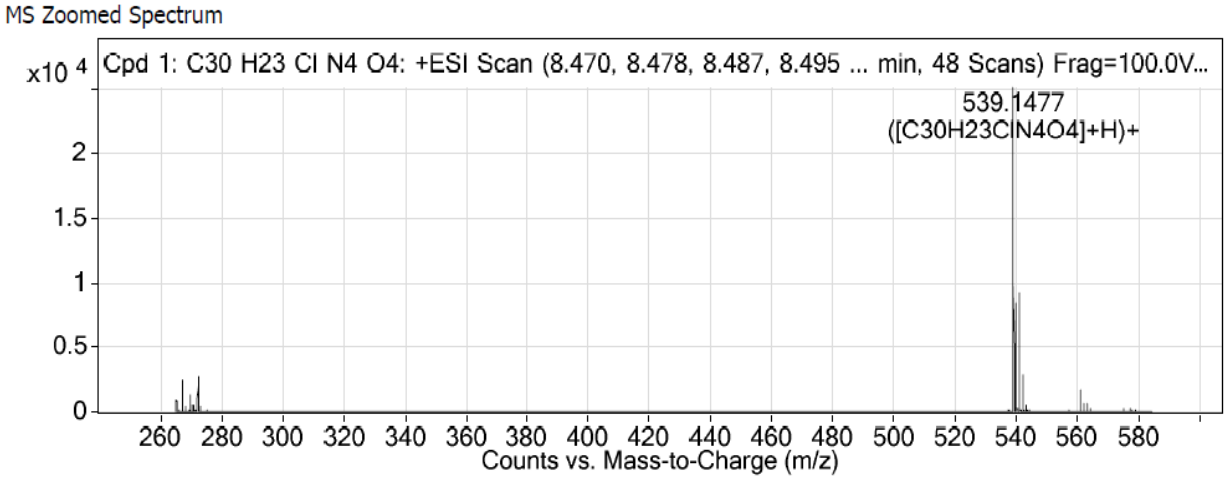
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
424.1058	424.1059	0.13	1	2546.19	C22H18ClN3O4	(M+H)+
425.1093	425.109	-0.79	1	624.55	C22H18ClN3O4	(M+H)+
426.1035	426.1039	0.89	1	960.85	C22H18ClN3O4	(M+H)+
427.1062	427.1064	0.62	1	254.52	C22H18ClN3O4	(M+H)+
446.0869	446.0878	2.01	1	96.91	C22H18ClN3O4	(M+Na)+

Compound-10a

EI MS (70 eV):



ESI-QTOF (negative ionization)

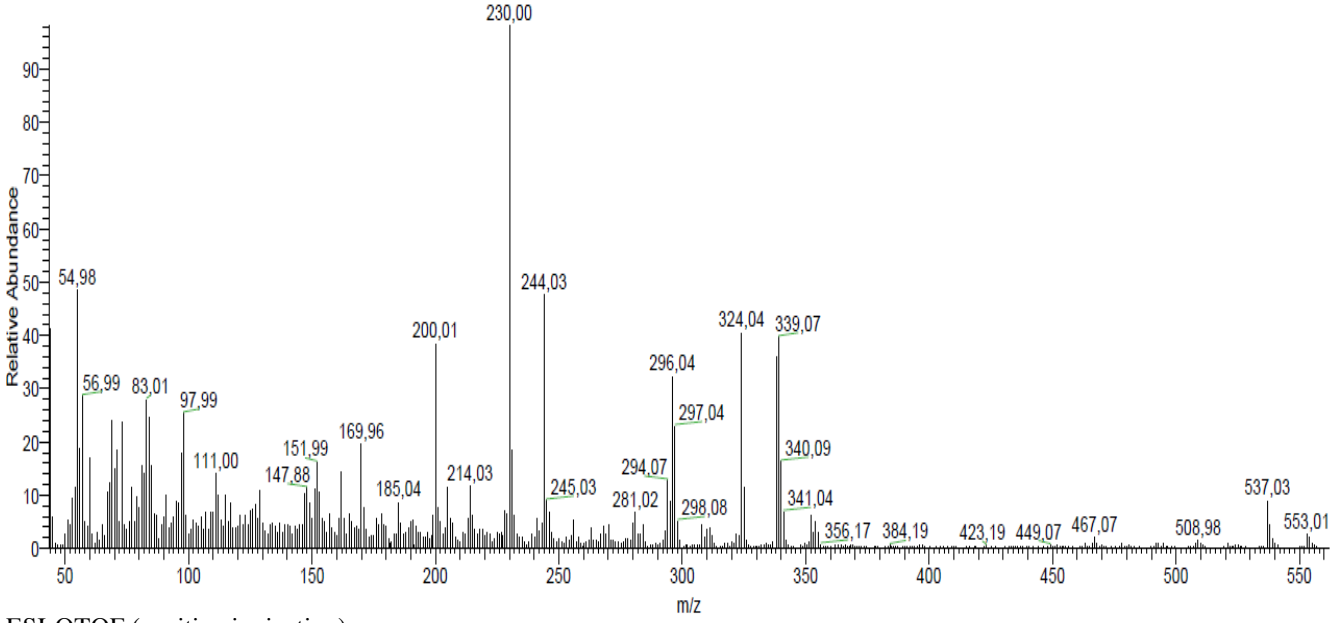


MS Spectrum Peak List

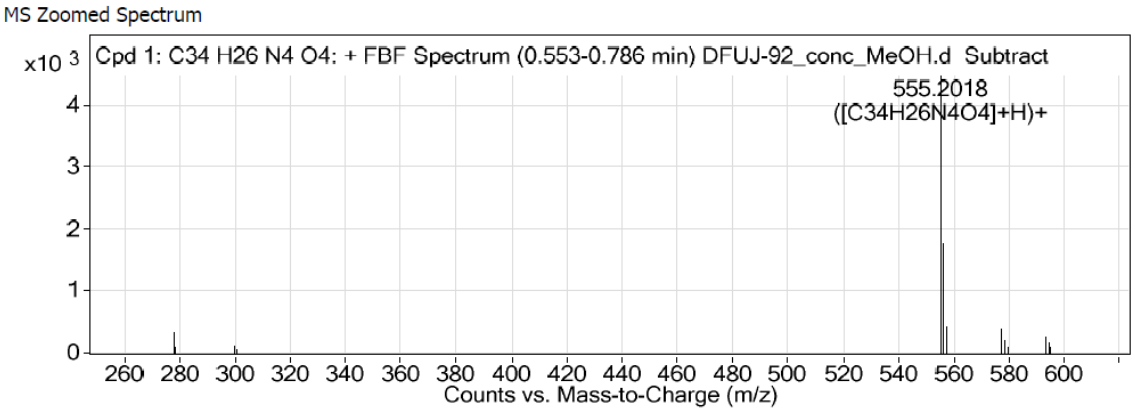
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
270.0778	270.0777	-0.47	2	1474.46	C30H23ClN4O4	(M+2H)+2
271.0774	271.077	-1.57	2	606.35	C30H23ClN4O4	(M+2H)+2
539.1477	539.1481	0.62	1	25868.74	C30H23ClN4O4	(M+H)+
540.1507	540.1512	0.82	1	8713.94	C30H23ClN4O4	(M+H)+
541.146	541.1466	1.1	1	9300.86	C30H23ClN4O4	(M+H)+
542.1482	542.1489	1.2	1	2934.69	C30H23ClN4O4	(M+H)+
561.1294	561.13	1.12	1	1807.6	C30H23ClN4O4	(M+Na)+
562.1325	562.1331	1.14	1	699.04	C30H23ClN4O4	(M+Na)+
563.1281	563.1286	0.9	1	703.34	C30H23ClN4O4	(M+Na)+
577.1029	577.1039	1.84	1	318.6	C30H23ClN4O4	(M+K)+

Compound-10b

EI MS (70 eV):



ESI-QTOF (positive ionization)

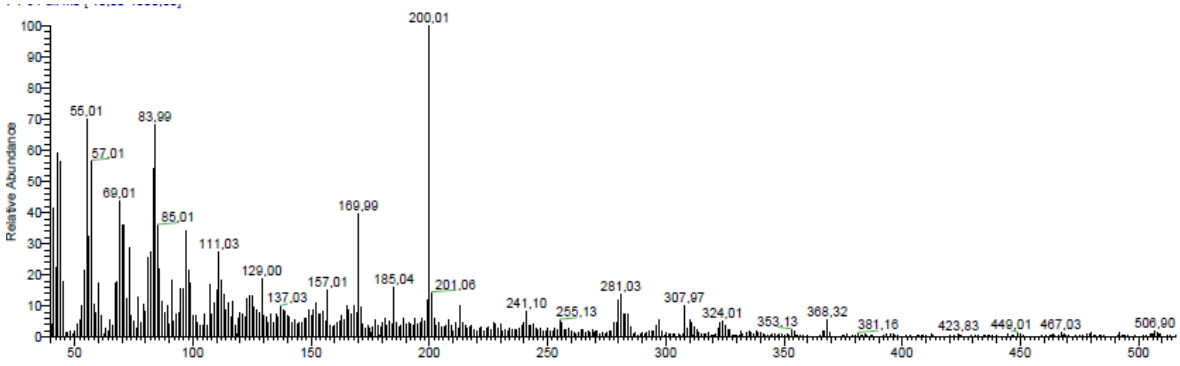


MS Spectrum Peak List

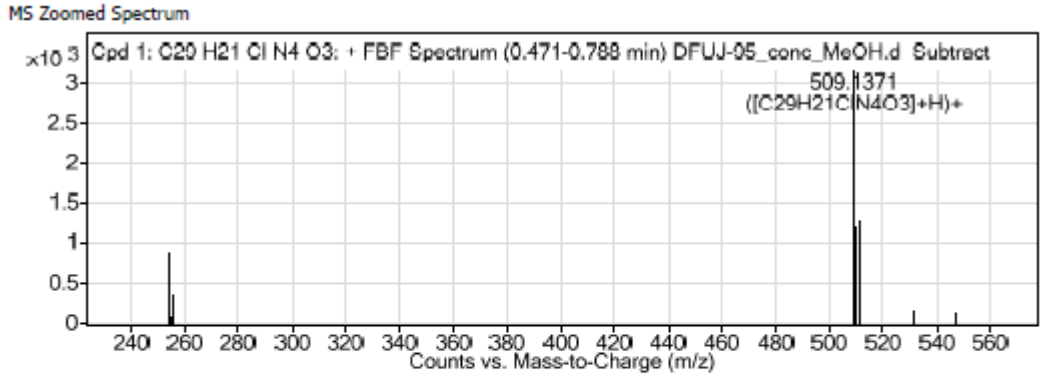
m/z	z	Abund	Formula	Ion
278.1064	2	320.45	C34H26N4O4	(M+2H)+2
300.0841	2	112.63	C34H26N4O4	(M+2Na)+2
555.2018	1	4457.28	C34H26N4O4	(M+H)+
556.2046	1	1769.82	C34H26N4O4	(M+H)+
557.2094	1	421.59	C34H26N4O4	(M+H)+
577.1854	1	382.99	C34H26N4O4	(M+Na)+
578.1877	1	198.02	C34H26N4O4	(M+Na)+
593.1562	1	257.12	C34H26N4O4	(M+K)+
594.1615	1	153.21	C34H26N4O4	(M+K)+
595.1695	1	100.41	C34H26N4O4	(M+K)+

Compound-11a

EI MS (70 eV):



ESI-QTOF (positive ionization)

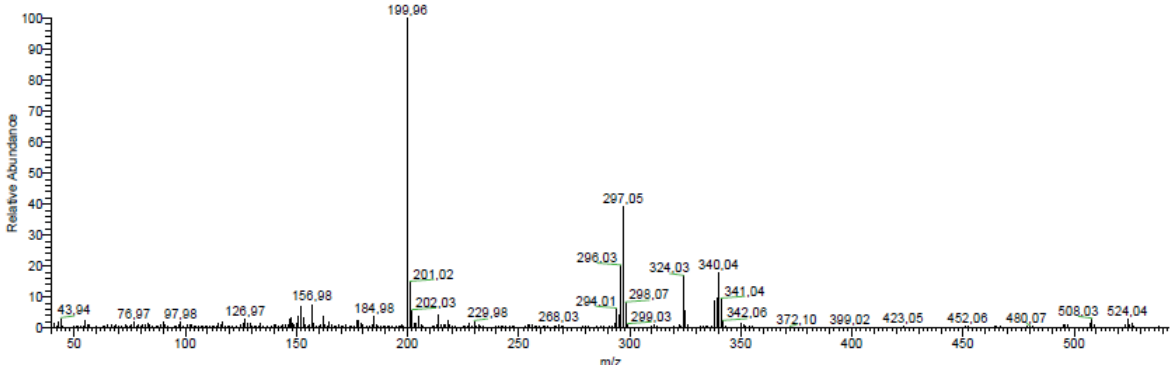


MS Spectrum Peak List

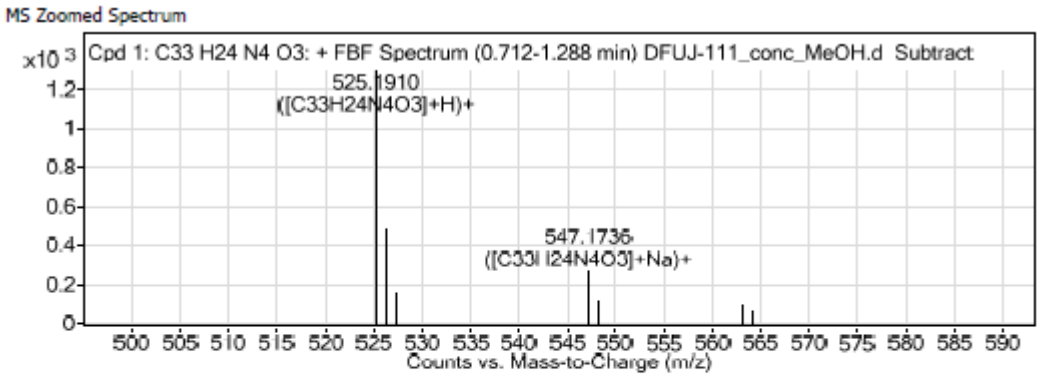
m/z	z	Abund	Formula	Ion
254.0698	2	854.26	C29H21ClN4O3	M+2
254.5794	2	58.61	C29H21ClN4O3	M+2
255.0737	2	351.97	C29H21ClN4O3	M+2
509.1371	1	3142.96	C29H21ClN4O3	(M+H)+
510.1383	1	1204.68	C29H21ClN4O3	(M+H)+
511.136	1	1259.48	C29H21ClN4O3	(M+H)+

Compound-11b

EI MS (70 eV):



ESI-QTOF (positive ionization)

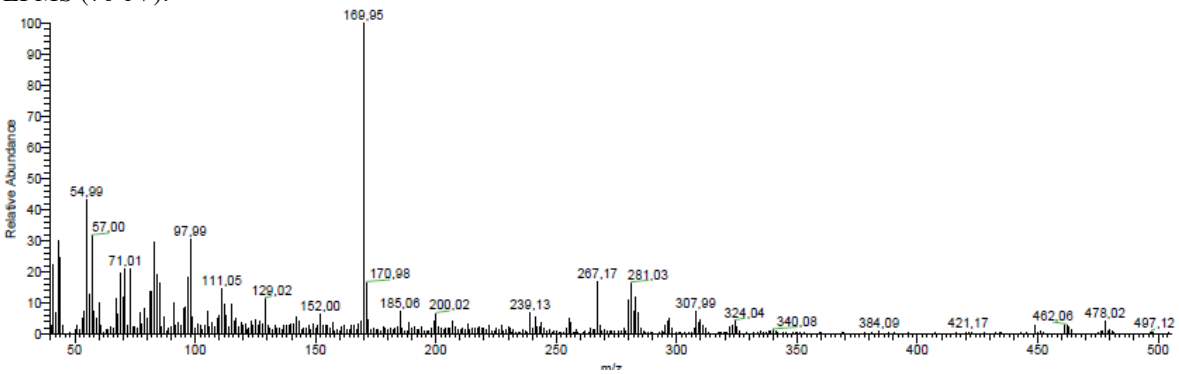


MS Spectrum Peak List

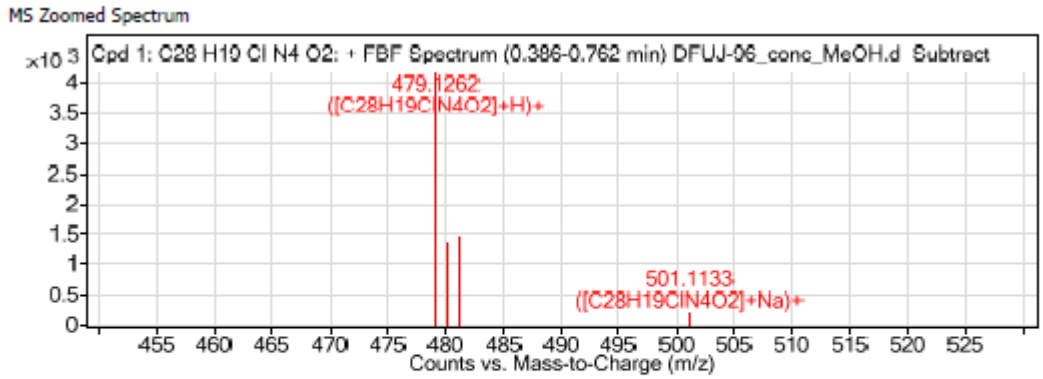
m/z	z	Abund	Formula	Ion
525.191	1	1290.9	C33H24N4O3	(M+H)+
526.1951	1	488.89	C33H24N4O3	(M+H)+
527.1965	1	152.15	C33H24N4O3	(M+H)+
547.1736	1	265.02	C33H24N4O3	(M+Na)+
548.1764	1	122.07	C33H24N4O3	(M+Na)+
563.1528	1	101.06	C33H24N4O3	(M+K)+
564.152	1	69.64	C33H24N4O3	(M+K)+

Compound-12a

EI MS (70 eV):



ESI-QTOF (positive ionization)



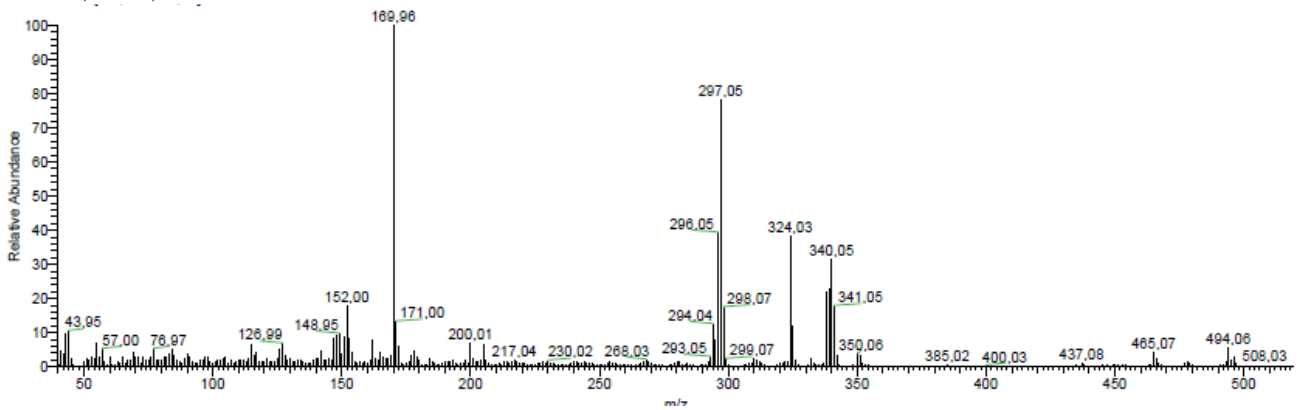
MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
479.1262	1	4169.07	C28H19ClN4O2	(M+H)+
480.1296	1	1345.63	C28H19ClN4O2	(M+H)+
481.1247	1	1461.19	C28H19ClN4O2	(M+H)+
501.1133	1	204.37	C28H19ClN4O2	(M+Na)+

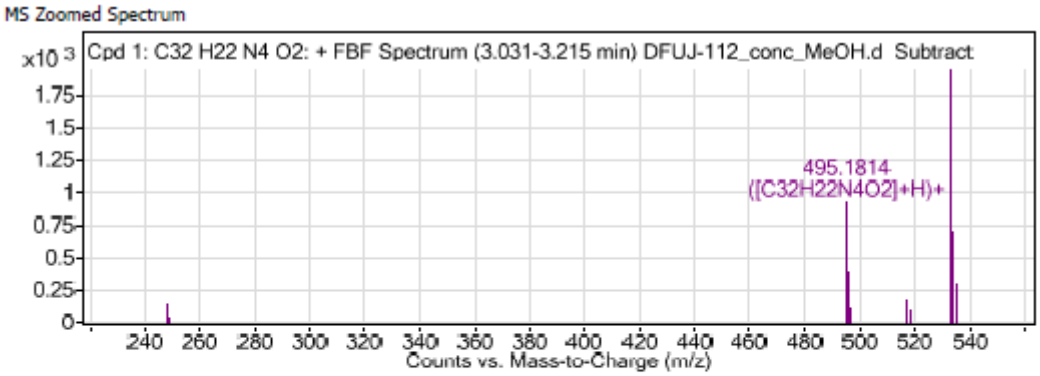
MS Spectrum

Compound-12b

EI MS (70 eV):



ESI-QTOF (positive ionization)

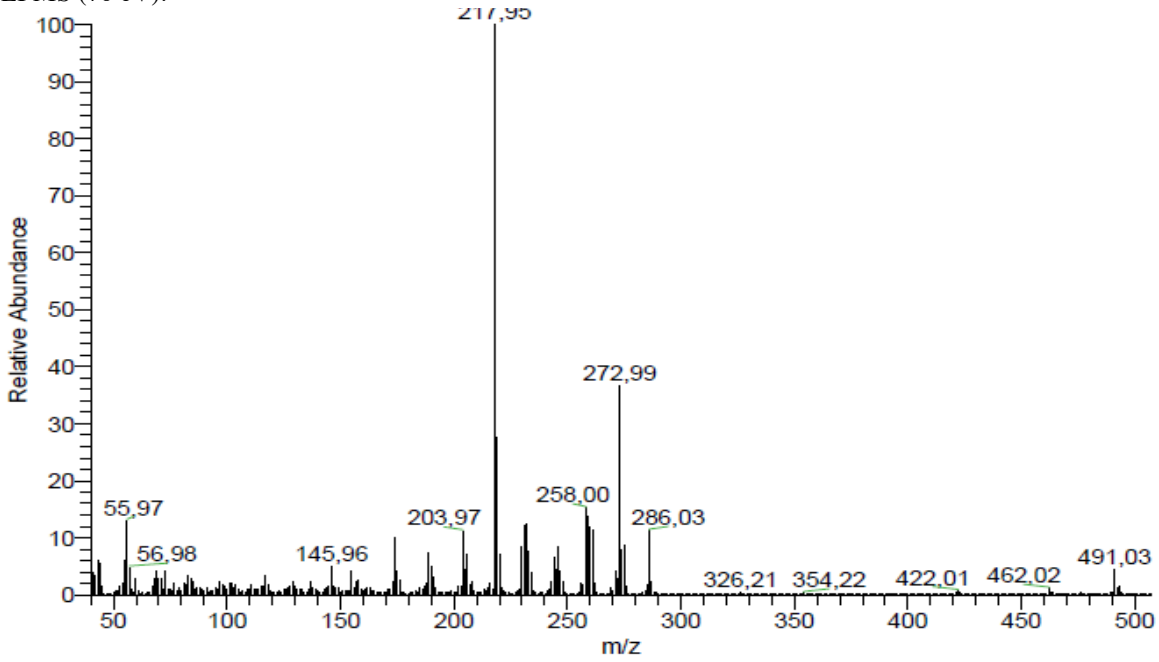


MS Spectrum Peak List

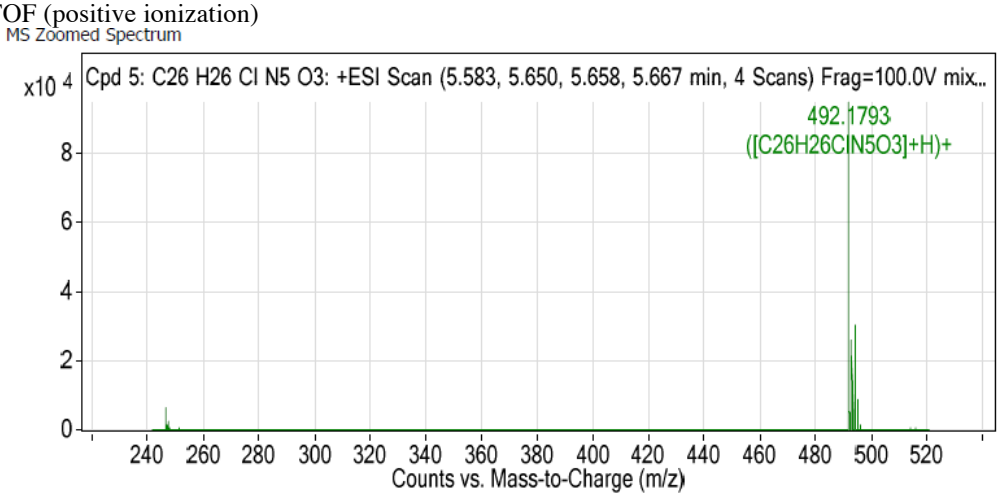
m/z	z	Abund	Formula	Ion
248.0902	2	150.18	C32H22N4O2	(M+2H)+2
248.5825	2	29.22	C32H22N4O2	(M+2H)+2
495.1814	1	931.92	C32H22N4O2	(M+H)+
496.1829	1	390.12	C32H22N4O2	(M+H)+
497.1828	1	107.43	C32H22N4O2	(M+H)+
517.1619	1	181.5	C32H22N4O2	(M+Na)+
518.1597	1	92.36	C32H22N4O2	(M+Na)+

Compound-13a

EI MS (70 eV):



ESI-QTOF (positive ionization)

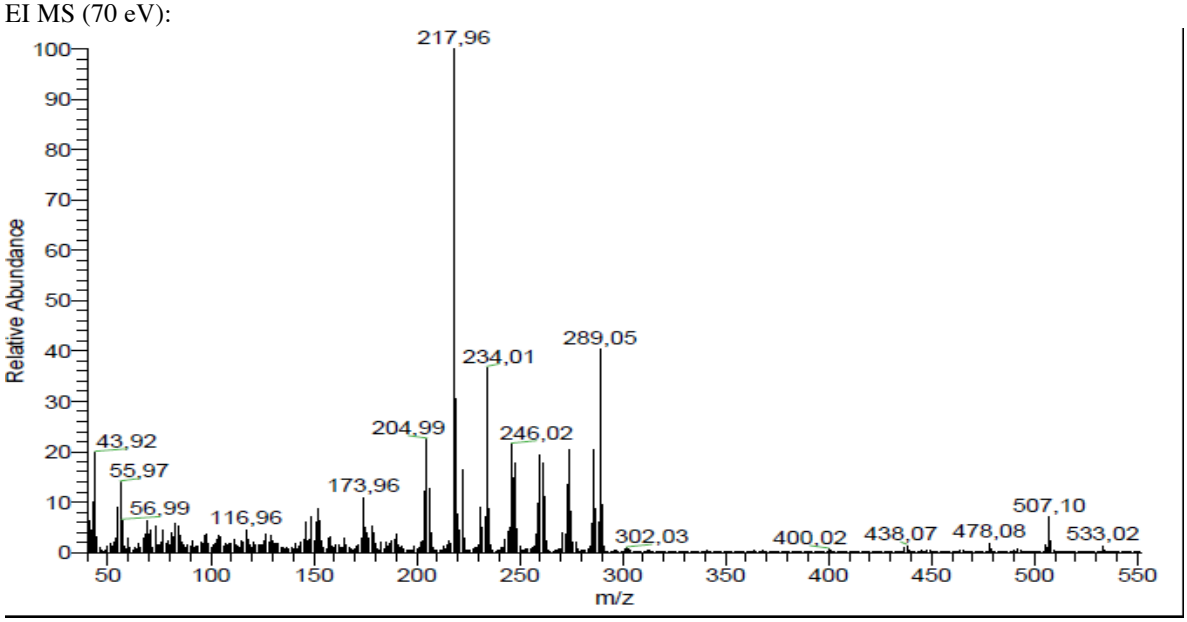


MS Spectrum Peak List

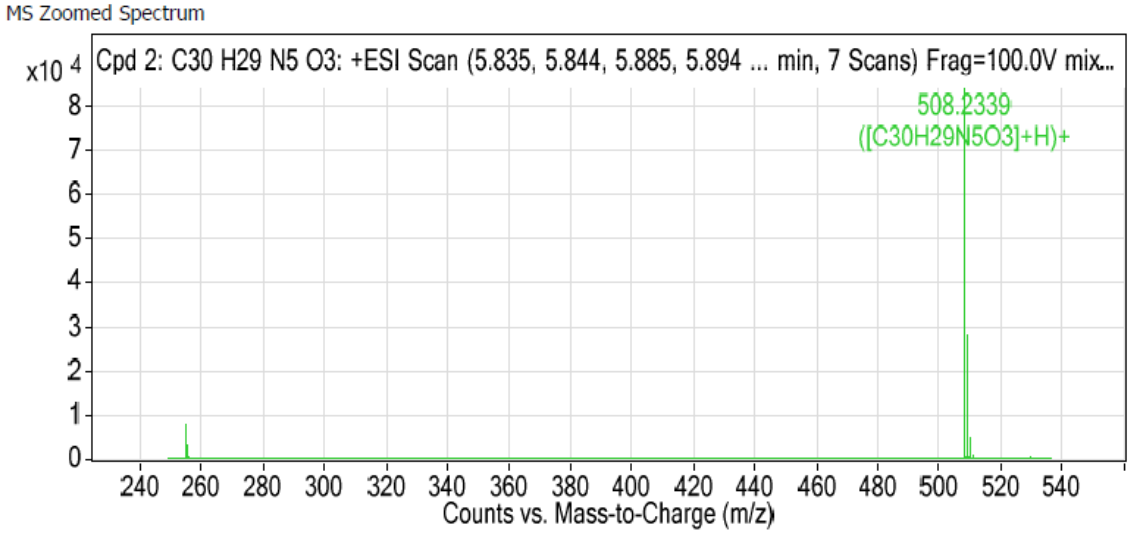
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
246.5934	246.5935	0.38	2	6541.92	C26H26ClN5O3	(M+2H)+2
247.0958	247.095	-3.43	2	1689.59	C26H26ClN5O3	(M+2H)+2
247.5926	247.5926	0.15	2	2421.77	C26H26ClN5O3	(M+2H)+2
248.0934	248.0938	1.37	2	643.27	C26H26ClN5O3	(M+2H)+2
492.1793	492.1797	0.8	1	94984.34	C26H26ClN5O3	(M+H)+
493.1825	493.1827	0.45	1	25904.63	C26H26ClN5O3	(M+H)+
494.1773	494.1779	1.28	1	31211.81	C26H26ClN5O3	(M+H)+
495.18	495.1802	0.41	1	8946.72	C26H26ClN5O3	(M+H)+
496.1825	496.1828	0.53	1	1634.62	C26H26ClN5O3	(M+H)+
514.1608	514.1616	1.6	1	751.62	C26H26ClN5O3	(M+Na)+

Compound-13b

EI MS (70 eV):



ESI-QTOF (positive ionization)

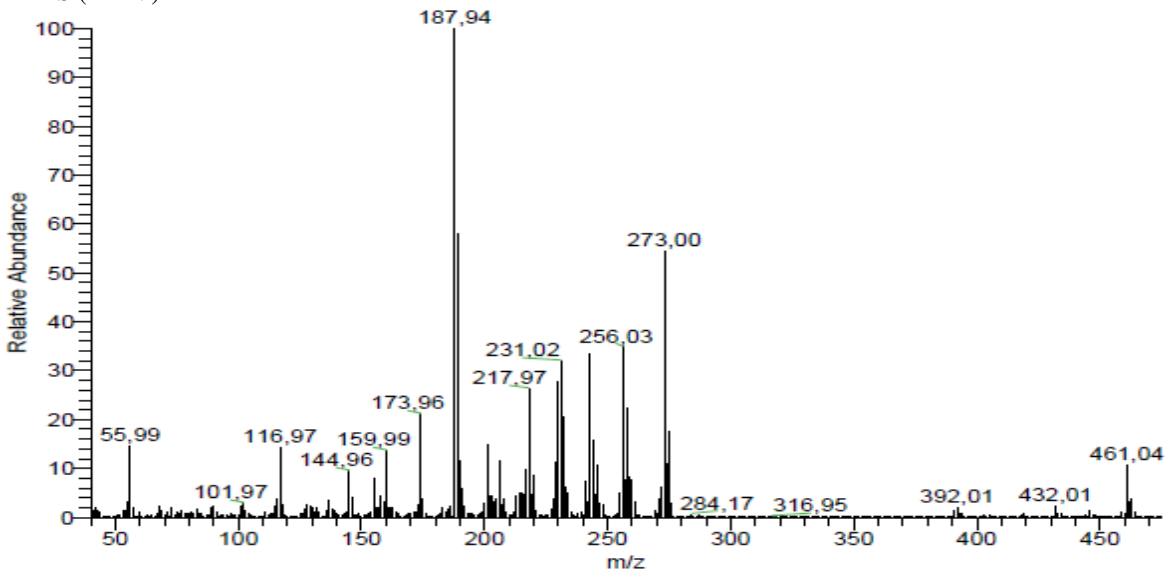


MS Spectrum Peak List

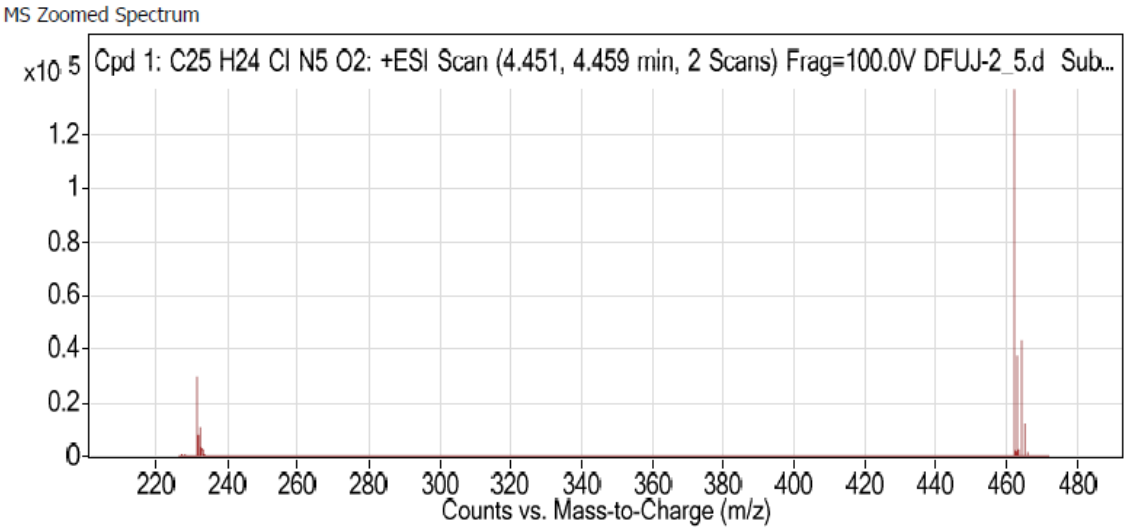
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
254.6207	254.6208	0.37	2	8068.13	C30H29N5O3	(M+2H)+2
255.1225	255.1223	-0.66	2	3158.09	C30H29N5O3	(M+2H)+2
255.624	255.6238	-1.07	2	620.52	C30H29N5O3	(M+2H)+2
508.2339	508.2343	0.91	1	86245.99	C30H29N5O3	(M+H)+
509.2369	509.2374	0.88	1	28085.54	C30H29N5O3	(M+H)+
510.2408	510.2402	-1.19	1	4868.47	C30H29N5O3	(M+H)+
511.2426	511.243	0.81	1	710.06	C30H29N5O3	(M+H)+
530.2161	530.2163	0.29	1	675.4	C30H29N5O3	(M+Na)+
531.2175	531.2193	3.36	1	174.87	C30H29N5O3	(M+Na)+

Compound-14a

EI MS (70 eV):



ESI-QTOF (positive ionization)

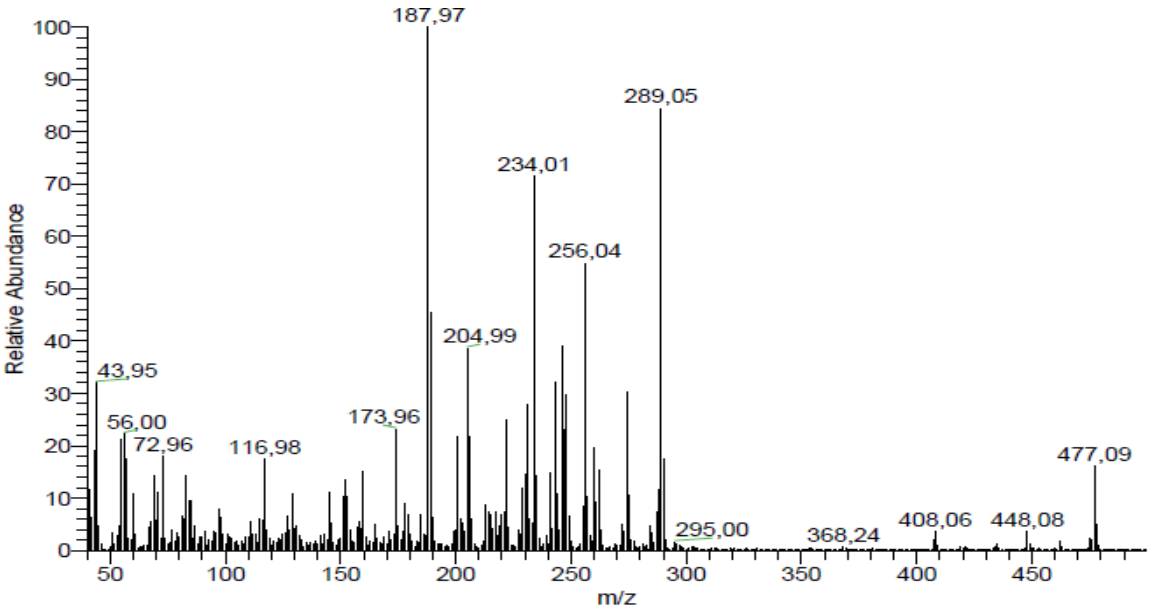


MS Spectrum Peak List

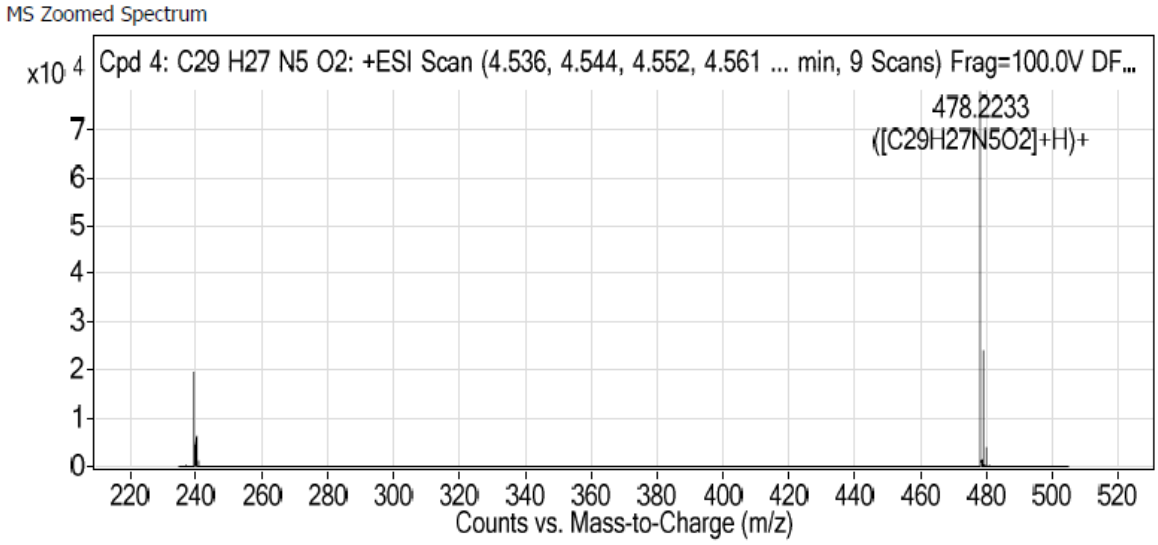
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
231.5875	231.5882	3.19	2	20447.81	C25H24ClN5O2	(M+2H)+2
232.089	232.0897	3.09	2	5735.47	C25H24ClN5O2	(M+2H)+2
232.5862	232.5873	4.77	2	6813.16	C25H24ClN5O2	(M+2H)+2
233.0884	233.0884	0.19	2	1998.8	C25H24ClN5O2	(M+2H)+2
233.5906	233.5898	-3.75	2	742.84	C25H24ClN5O2	(M+2H)+2
462.1687	462.1691	0.86	1	96951.16	C25H24ClN5O2	(M+H)+
463.1723	463.1721	-0.49	1	25742.32	C25H24ClN5O2	(M+H)+
464.1673	464.1673	0.03	1	31467.23	C25H24ClN5O2	(M+H)+
465.1689	465.1696	1.5	1	8536.45	C25H24ClN5O2	(M+H)+
466.1719	466.1722	0.72	1	819	C25H24ClN5O2	(M+H)+

Compound-14b

EI MS (70 eV):



ESI-QTOF (positive ionization)

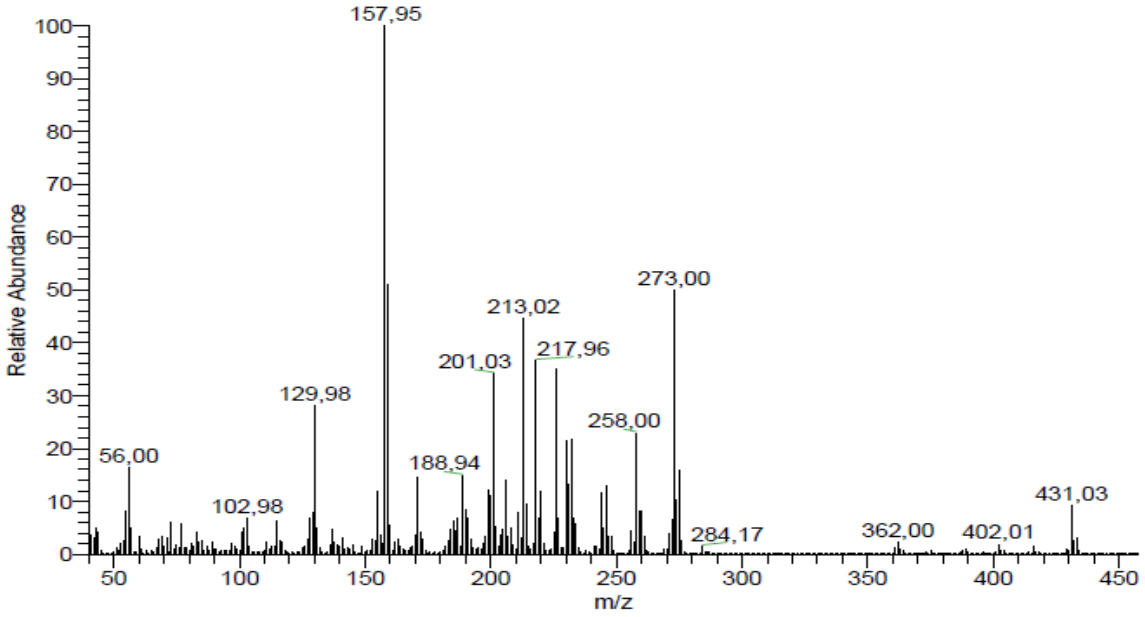


MS Spectrum Peak List

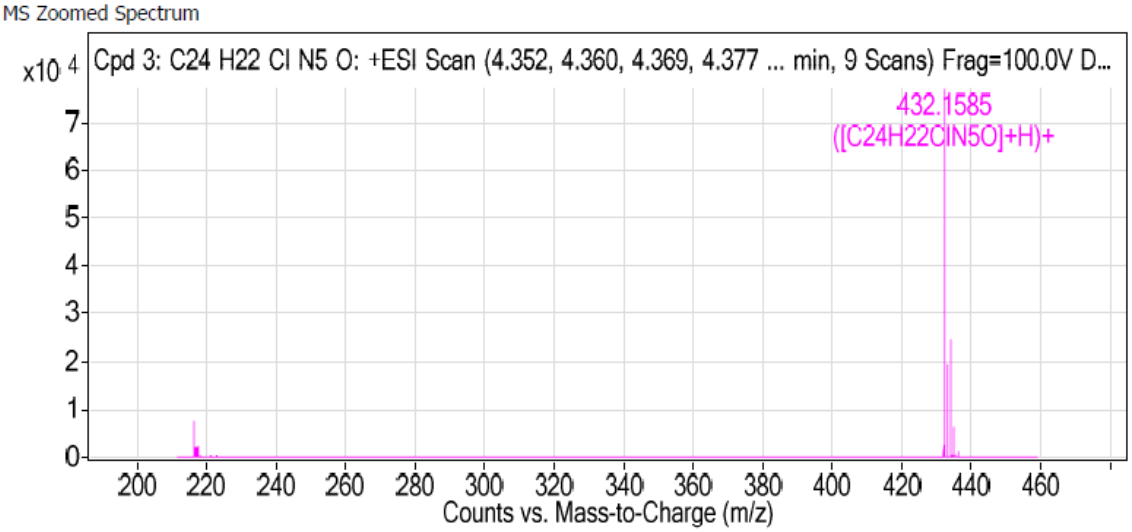
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
239.6151	239.6155	1.63	2	19635.67	C29H27N5O2	(M+2H)+2
240.1169	240.117	0.65	2	6780.67	C29H27N5O2	(M+2H)+2
240.6182	240.6185	1.04	2	1237.9	C29H27N5O2	(M+2H)+2
241.1197	241.1199	0.76	2	119.69	C29H27N5O2	(M+2H)+2
478.2233	478.2238	0.89	1	78136.55	C29H27N5O2	(M+H)+
479.2264	479.2268	0.85	1	24376.47	C29H27N5O2	(M+H)+
480.229	480.2297	1.48	1	4254.08	C29H27N5O2	(M+H)+
481.2317	481.2325	1.58	1	537.89	C29H27N5O2	(M+H)+
500.2069	500.2057	-2.42	1	225.96	C29H27N5O2	(M+Na)+

Compound-15a

EI MS (70 eV):



ESI-QTOF (positive ionization)

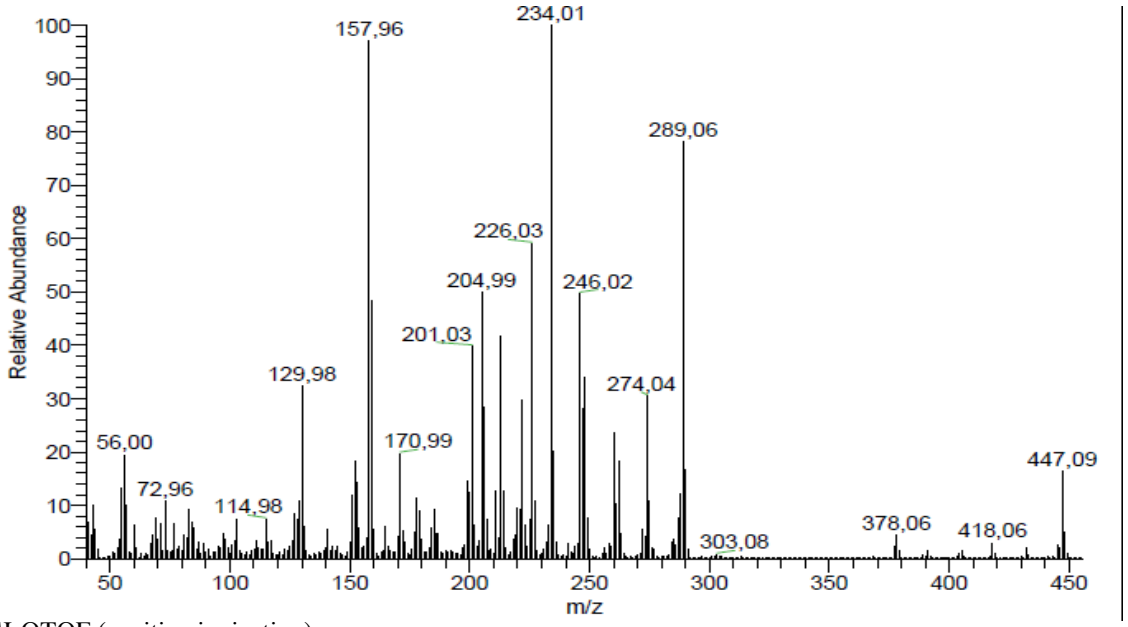


MS Spectrum Peak List

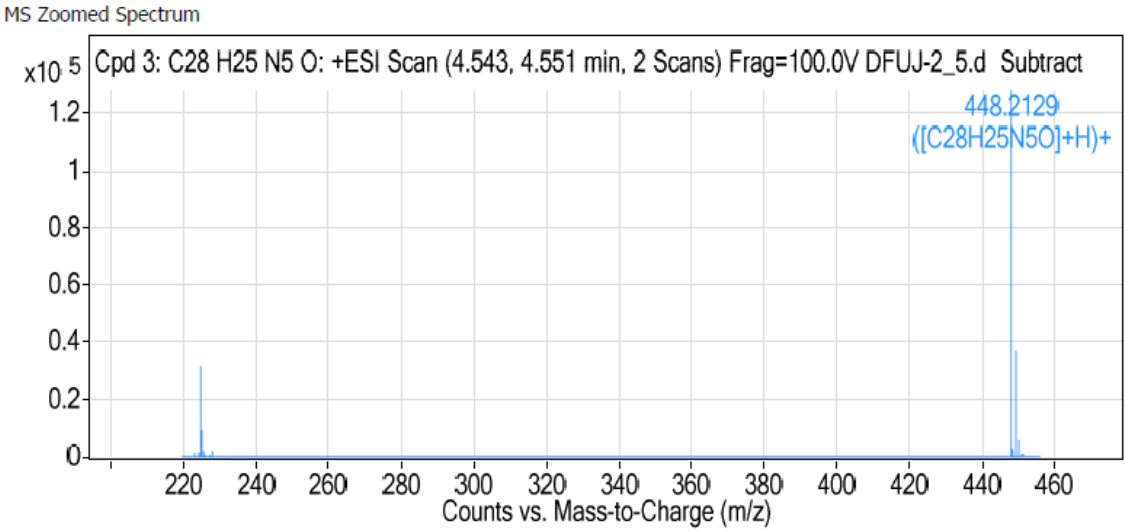
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
216.5825	216.5829	2.06	2	7646.09	C24H22ClN5O	(M+2H)+2
217.0847	217.0844	-1.24	2	2145.11	C24H22ClN5O	(M+2H)+2
217.581	217.5819	4.28	2	2654.04	C24H22ClN5O	(M+2H)+2
218.0813	218.0831	8.3	2	465.74	C24H22ClN5O	(M+2H)+2
432.1585	432.1586	0.15	1	77085.56	C24H22ClN5O	(M+H)+
433.1616	433.1615	-0.14	1	20337.61	C24H22ClN5O	(M+H)+
434.1561	434.1566	1.07	1	24839.15	C24H22ClN5O	(M+H)+
435.1589	435.1589	0.15	1	6283.17	C24H22ClN5O	(M+H)+
436.1605	436.1616	2.53	1	1047.51	C24H22ClN5O	(M+H)+
454.1398	454.1405	1.48	1	91.55	C24H22ClN5O	(M+Na)+

Compound-15b

EI MS (70 eV):



ESI-QTOF (positive ionization)

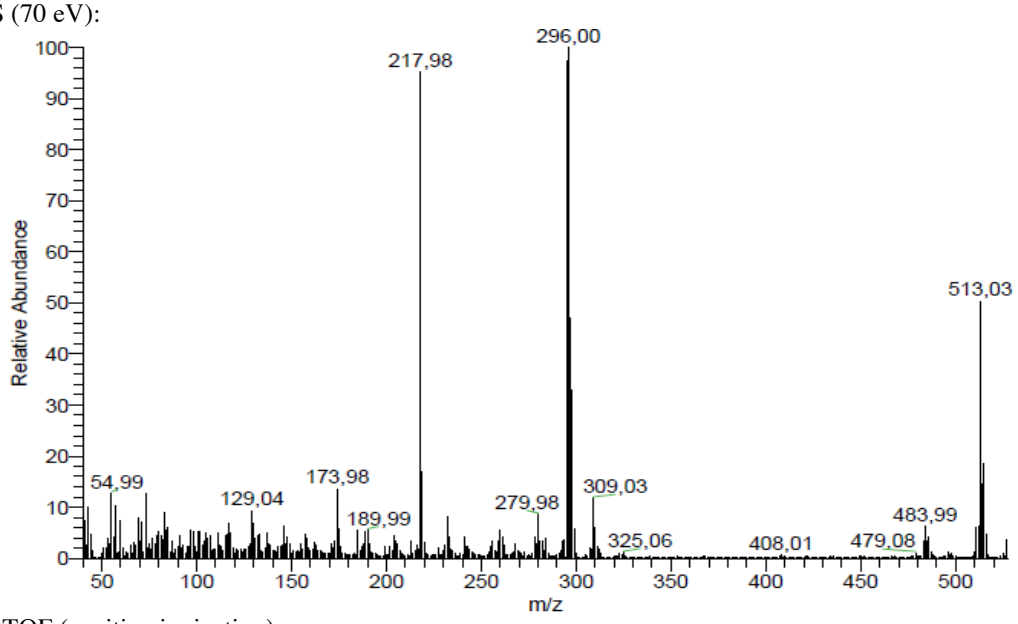


MS Spectrum Peak List

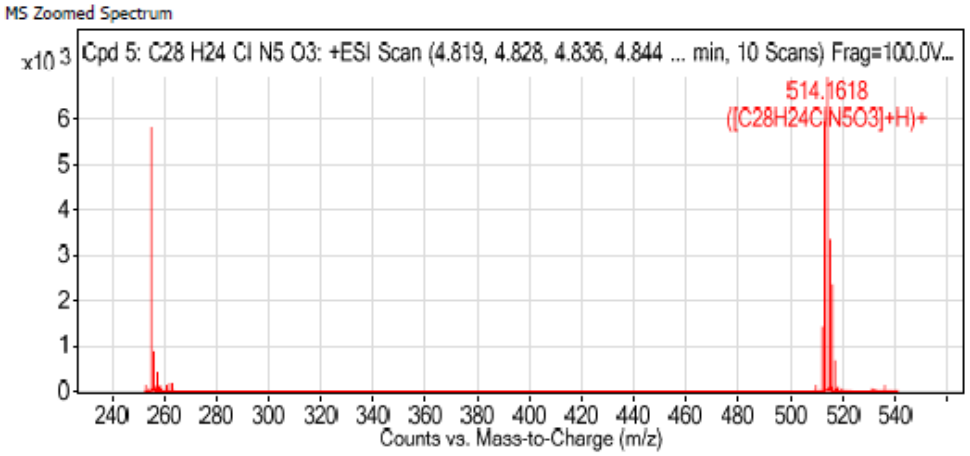
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
224.61	224.6102	1.18	2	31469.39	C28H25N5O	(M+2H)+2
225.1114	225.1117	1.42	2	9652.85	C28H25N5O	(M+2H)+2
225.6121	225.6132	4.81	2	1876.05	C28H25N5O	(M+2H)+2
226.1091	226.1147	24.49	2	137.28	C28H25N5O	(M+2H)+2
448.2129	448.2132	0.66	1	128534.05	C28H25N5O	(M+H)+
449.216	449.2162	0.5	1	38207.29	C28H25N5O	(M+H)+
450.219	450.2192	0.41	1	6056.7	C28H25N5O	(M+H)+
451.2235	451.222	-3.24	1	784.28	C28H25N5O	(M+H)+

Compound-16a

EI MS (70 eV):



ESI-QTOF (positive ionization)

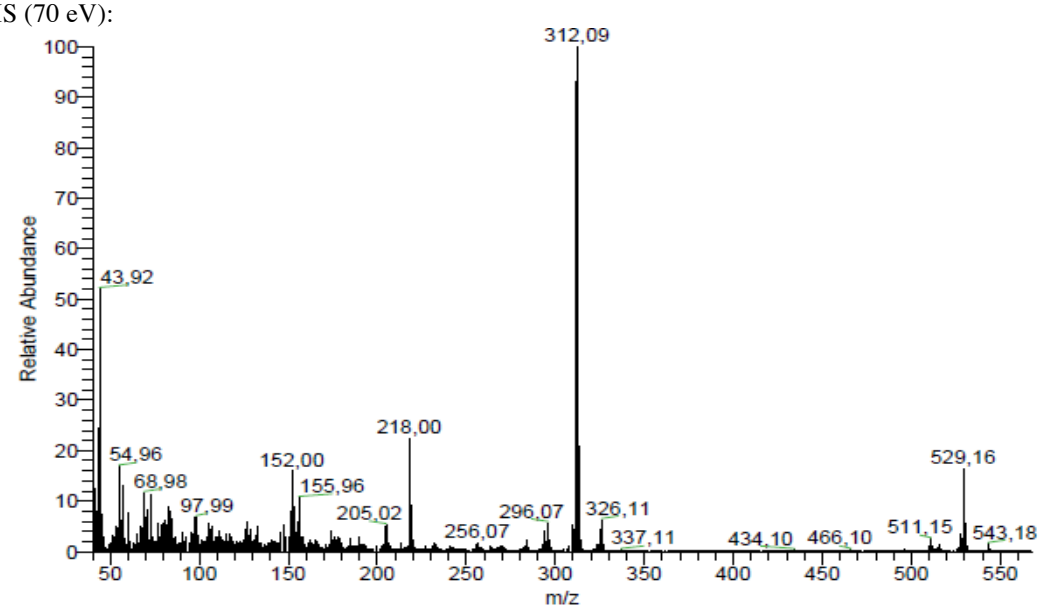


MS Spectrum Peak List

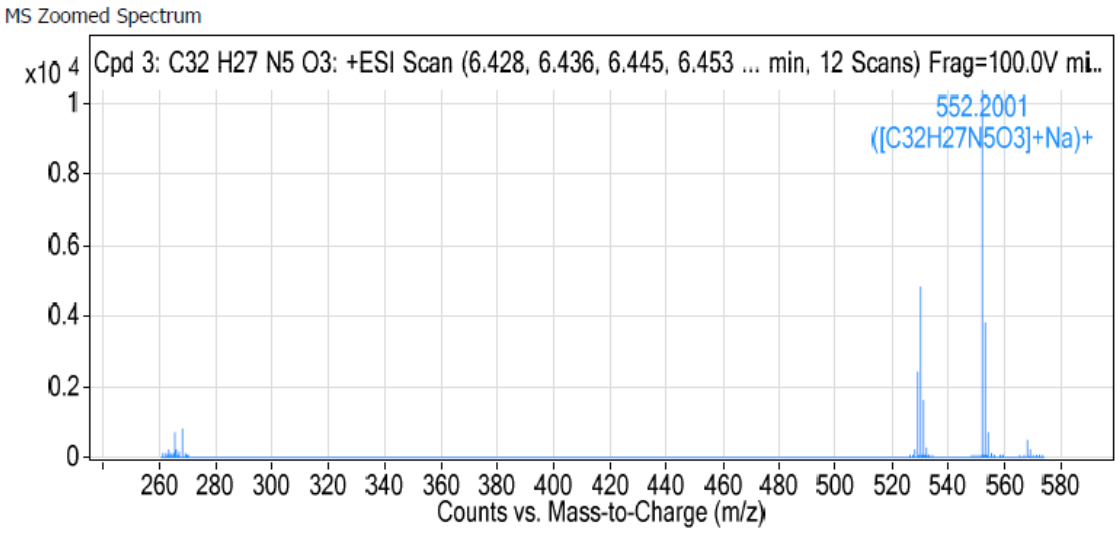
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
257.5854	257.5857	1.03	2	488.1	C28H24ClN5O3	(M+2H)+2
258.0876	258.0872	-1.79	2	123.01	C28H24ClN5O3	(M+2H)+2
258.5863	258.5849	-5.68	2	156.79	C28H24ClN5O3	(M+2H)+2
259.0836	259.086	9.26	2	26.1	C28H24ClN5O3	(M+2H)+2
514.1618	514.164	4.37	1	7041.11	C28H24ClN5O3	(M+H)+
515.1587	515.1671	16.29	1	3466.86	C28H24ClN5O3	(M+H)+
516.1605	516.1624	3.8	1	2486.46	C28H24ClN5O3	(M+H)+
517.1629	517.1647	3.37	1	707.97	C28H24ClN5O3	(M+H)+
518.1712	518.1673	-7.71	1	44.95	C28H24ClN5O3	(M+H)+
536.1466	536.146	-1.05	1	108.57	C28H24ClN5O3	(M+Na)+

Compound-16b

EI MS (70 eV):



ESI-QTOF (positive ionization)

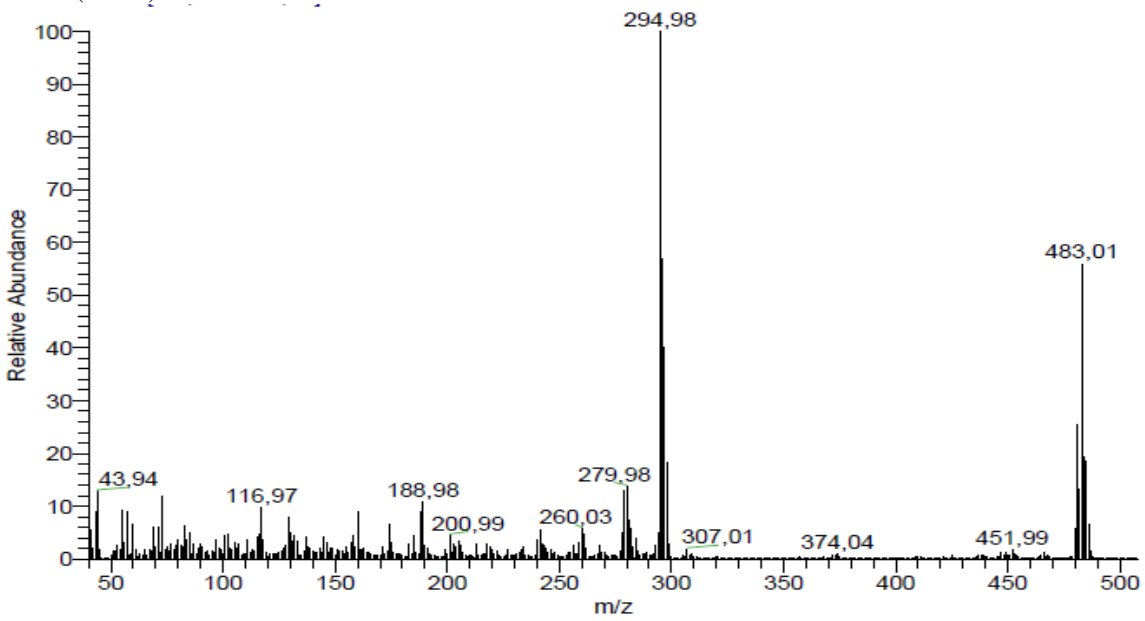


MS Spectrum Peak List

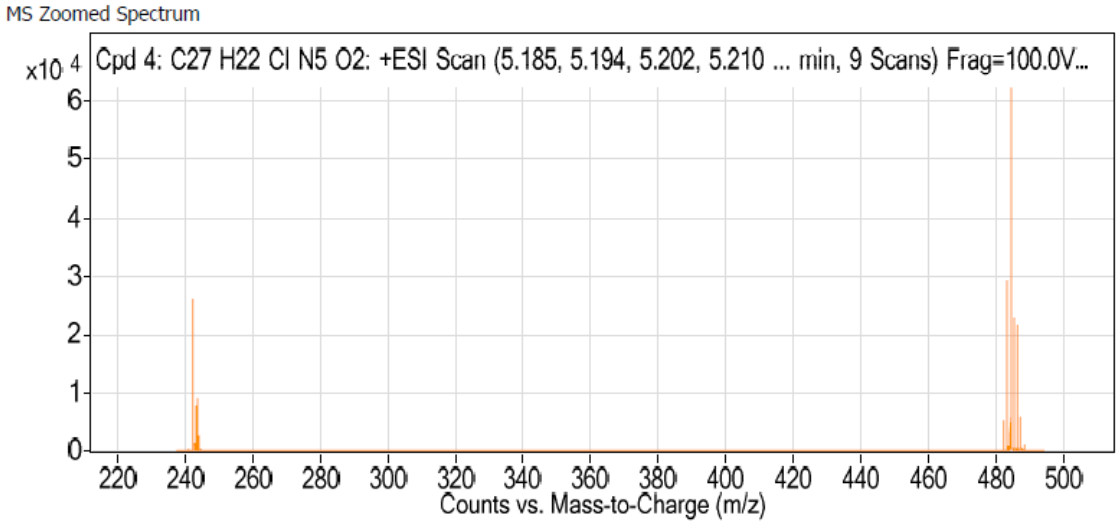
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
265.6133	265.613	-1.36	2	736.64	C32H27N5O3	(M+2H)+2
266.1153	266.1145	-3	2	226.95	C32H27N5O3	(M+2H)+2
530.2169	530.2187	3.32	1	4940	C32H27N5O3	(M+H)+
531.2209	531.2217	1.65	1	1682.09	C32H27N5O3	(M+H)+
532.2216	532.2246	5.64	1	264.44	C32H27N5O3	(M+H)+
552.2001	552.2006	0.89	1	10708.76	C32H27N5O3	(M+Na)+
553.2033	553.2037	0.76	1	3947.83	C32H27N5O3	(M+Na)+
554.2054	554.2066	2.14	1	731.08	C32H27N5O3	(M+Na)+
568.1728	568.1745	3.1	1	563.15	C32H27N5O3	(M+K)+
569.1781	569.1776	-0.83	1	198.83	C32H27N5O3	(M+K)+

Compound-17a

EI MS (70 eV):



ESI-QTOF (positive ionization)

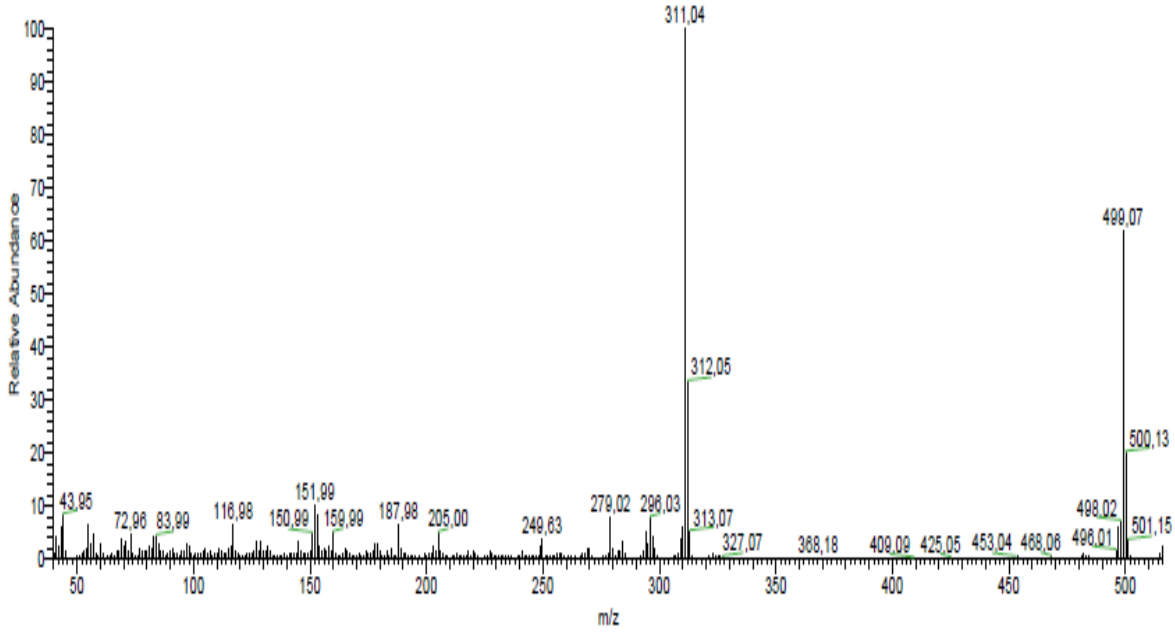


MS Spectrum Peak List

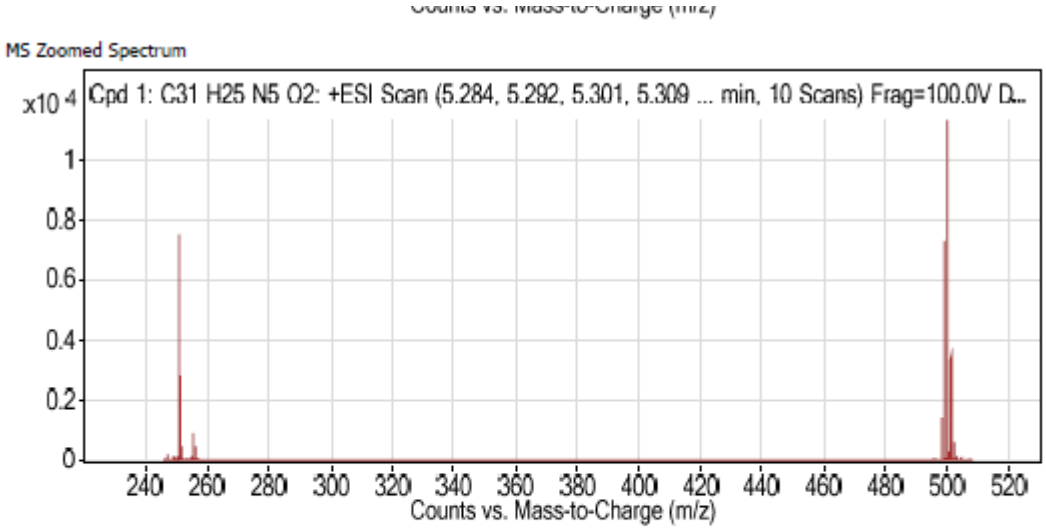
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
242.58	242.5804	1.63	2	26186.62	C27H22ClN5O2	(M+2H)+2
243.0817	243.0819	0.67	2	7805.67	C27H22ClN5O2	(M+2H)+2
243.5789	243.5795	2.35	2	9478.5	C27H22ClN5O2	(M+2H)+2
244.0799	244.0806	2.95	2	2537.79	C27H22ClN5O2	(M+2H)+2
244.5826	244.582	-2.39	2	494.36	C27H22ClN5O2	(M+2H)+2
484.1522	484.1535	2.71	1	63651.75	C27H22ClN5O2	(M+H)+
485.1517	485.1565	9.81	1	23329.83	C27H22ClN5O2	(M+H)+
486.1506	486.1518	2.43	1	21912.67	C27H22ClN5O2	(M+H)+
487.153	487.154	2.05	1	5904.65	C27H22ClN5O2	(M+H)+
488.1556	488.1567	2.13	1	977.71	C27H22ClN5O2	(M+H)+

Compound-17b

EI MS (70 eV):



ESI-QTOF (positive ionization)

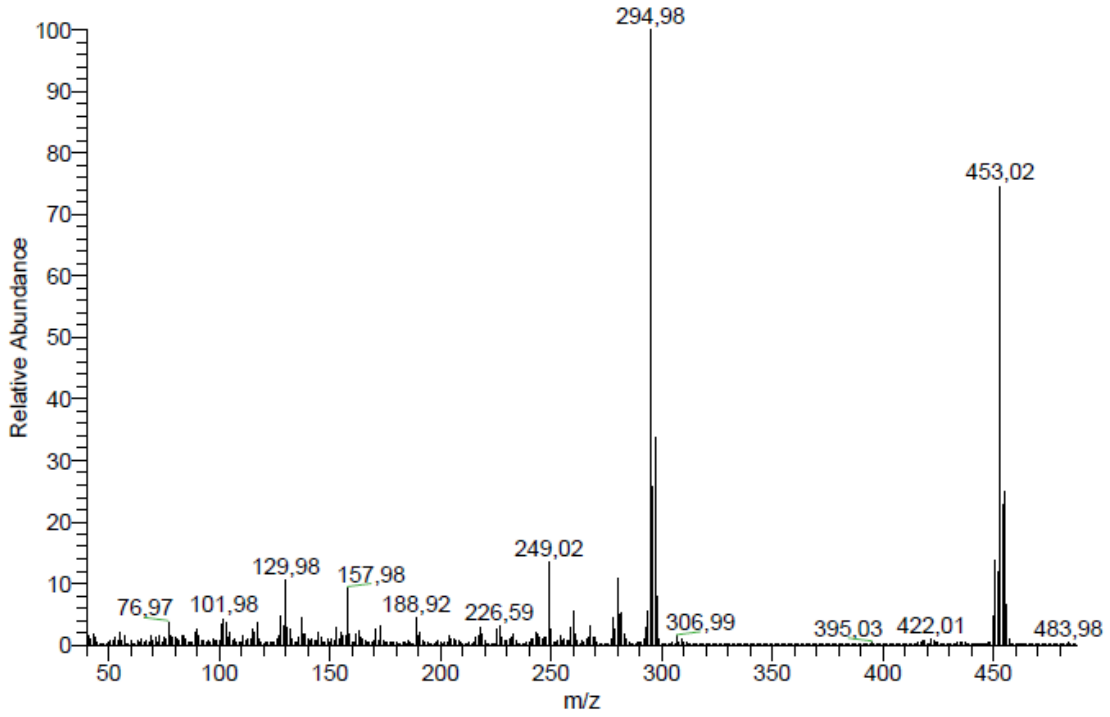


MS Spectrum Peak List

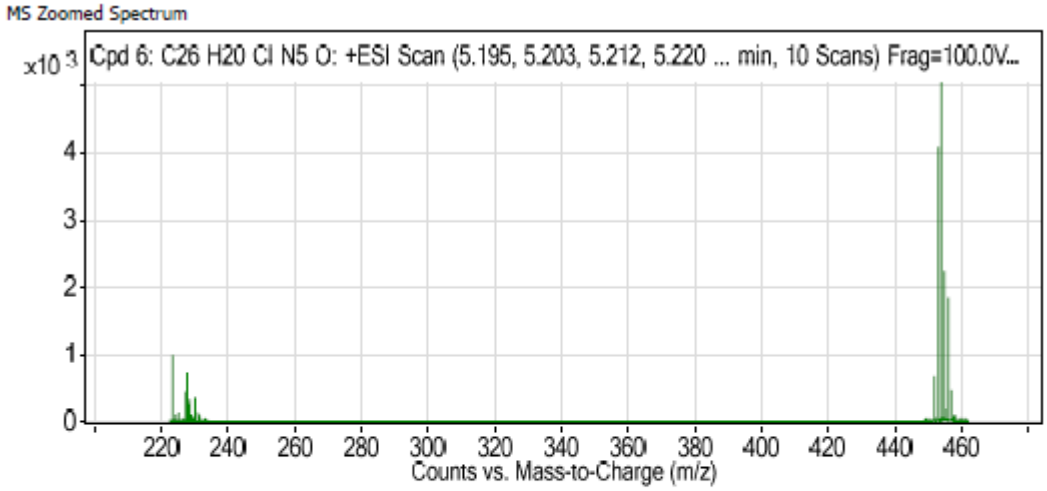
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
250.6074	250.6077	1.22	2	7619.07	C31H25N5O2	(M+2H)+2
251.1097	251.1092	-1.73	2	2814.04	C31H25N5O2	(M+2H)+2
251.6102	251.6107	2.09	2	544.7	C31H25N5O2	(M+2H)+2
252.1218	252.1121	-38.4	2	45.46	C31H25N5O2	(M+2H)+2
500.2065	500.2081	3.25	1	11325.85	C31H25N5O2	(M+H)+
501.2104	501.2112	1.54	1	3617.13	C31H25N5O2	(M+H)+
502.214	502.2141	0.19	1	679.17	C31H25N5O2	(M+H)+

Compound-18a

EI MS (70 eV):



ESI-QTOF (positive ionization)

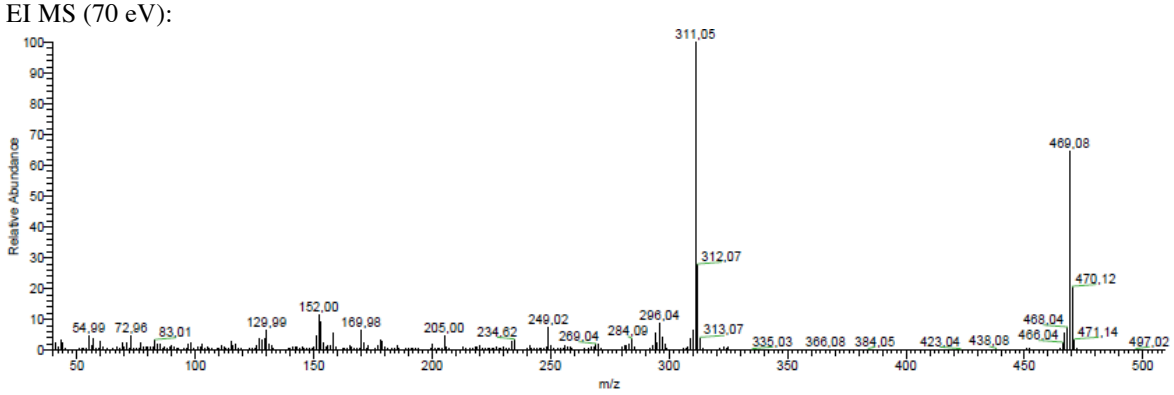


MS Spectrum Peak List

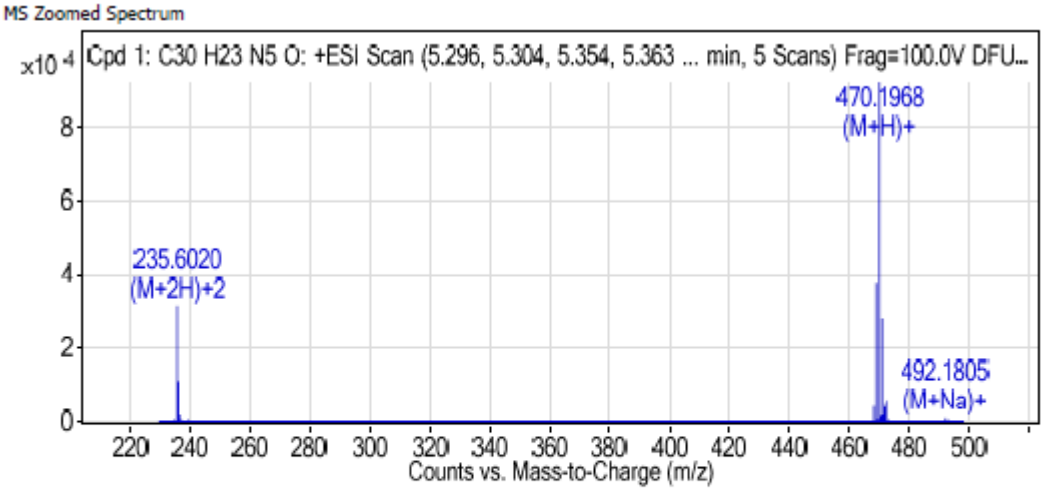
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
227.5748	227.5751	1.13	2	863.57	C26H20ClN5O	(M+2H)+2
228.0771	228.0766	-2.22	2	271.41	C26H20ClN5O	(M+2H)+2
228.5732	228.5742	4.26	2	383.04	C26H20ClN5O	(M+2H)+2
229.0781	229.0753	-12.31	2	103.67	C26H20ClN5O	(M+2H)+2
454.1412	454.1429	3.77	1	5046.45	C26H20ClN5O	(M+H)+
455.1391	455.1459	15.03	1	2342.88	C26H20ClN5O	(M+H)+
456.1391	456.1411	4.45	1	1917.91	C26H20ClN5O	(M+H)+
457.1422	457.1434	2.63	1	539.57	C26H20ClN5O	(M+H)+

Compound-18b

EI MS (70 eV):



ESI-QTOF (positive ionization)

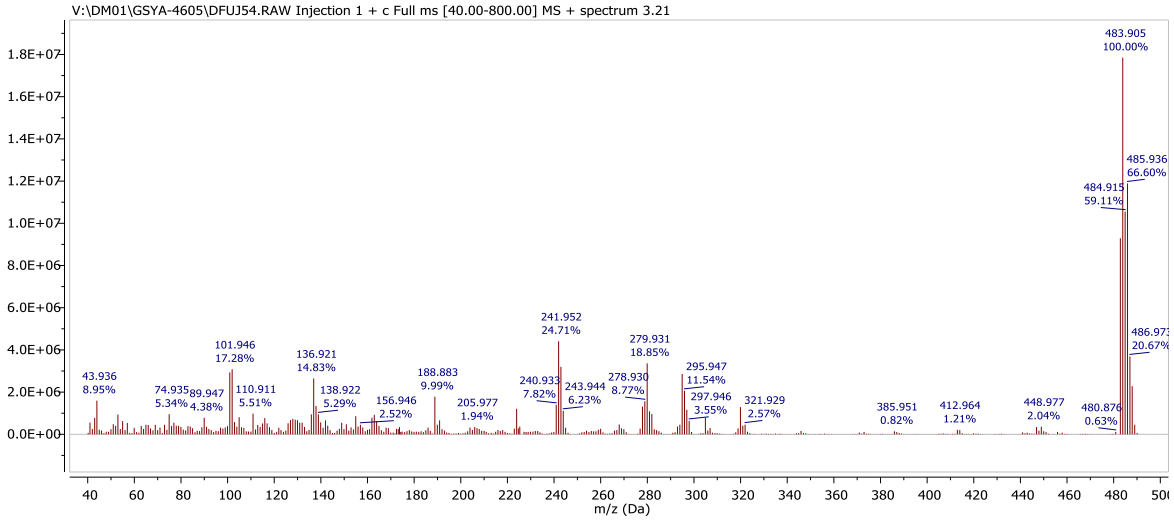


MS Spectrum Peak List

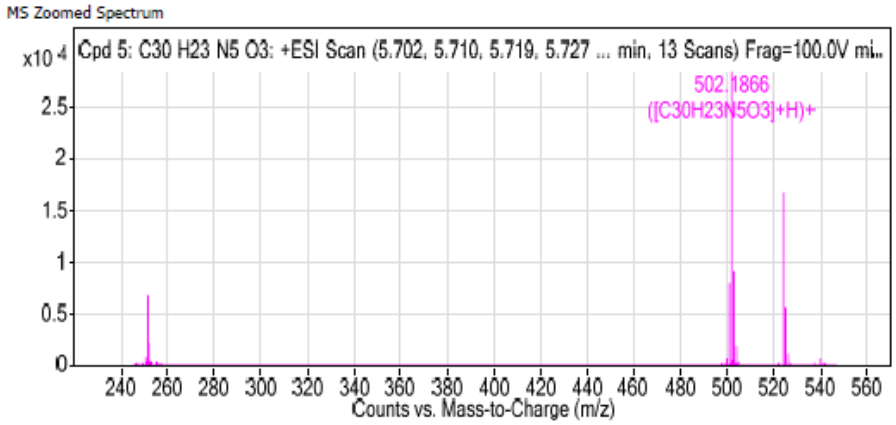
m/z	*Calc m/z*	Diff(ppm)	z	Abund	Ion
234.5943	234.5946	1.07	2	363.33	M+2
235.602	235.6024	1.64	2	31448.77	(M+2H)+2
236.1036	236.1039	1.19	2	11158.63	(M+2H)+2
236.6047	236.6054	2.99	2	2063.11	(M+2H)+2
470.1968	470.1975	1.61	1	92411.3	(M+H)+
471.2002	471.2006	0.82	1	28401.02	(M+H)+
472.2033	472.2036	0.54	1	4631.83	(M+H)+
473.206	473.2065	0.9	1	597.6	(M+H)+
492.1805	492.1795	-2.05	1	1141.9	(M+Na)+
493.1834	493.1825	-1.69	1	485.93	(M+Na)+

Compound-19b

EI MS (70 eV):



ESI-QTOF (positive ionization)



MS Spectrum Peak List

m/z	*Calc m/z*	Diff(ppm)	z	Abund	Formula	Ion
250.5893	250.5895	0.91	2	692.13	C30H23N5O3	M+2
251.5972	251.5973	0.31	2	6822.78	C30H23N5O3	(M+2H)+2
252.0989	252.0988	-0.37	2	2267.47	C30H23N5O3	(M+2H)+2
502.1866	502.1874	1.45	1	28737.94	C30H23N5O3	(M+H)+
503.1897	503.1904	1.38	1	9412.55	C30H23N5O3	(M+H)+
504.1921	504.1933	2.42	1	1859.4	C30H23N5O3	(M+H)+
524.169	524.1693	0.6	1	16903.03	C30H23N5O3	(M+Na)+
525.172	525.1724	0.67	1	5703.55	C30H23N5O3	(M+Na)+
526.1744	526.1752	1.55	1	1078.7	C30H23N5O3	(M+Na)+
540.143	540.1432	0.37	1	684.74	C30H23N5O3	(M+K)+