

Supplementary Materials

Design and Synthesis of New Pyrimidine- Quinolone Hybrids as Novel *h*LDHA Inhibitors

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1. *In-silico* studies

Table S1. Affinity and energy values (kcal/mol) involved in the interaction of the screening compounds (**10–21**) and reference **W31** when docked in the LDHA active site.

Compound	S	Arg ¹⁶⁸	His ¹⁹²	Asn ¹³⁷	Asp ¹⁹⁴
W31	-10,444	-8,7	-6	-3,6	-3,5
10	-9,950	-10,3	0	0	-7,7
11	-9,301	0	-2,7	-4,5	0
12	-7,467	0	0	0	-10.1
13	-9,601	-7.1	0	0	-4.7
14	-9,983	-5.7	-3.2	0	-3.5
15	-9,231	-1,6	0	0	-5
16	-9,372	0	-2,6	-4,4	0
17	-9,463	-6,5	0	0	0
18	-9,917	-6	0	0	-3,4
19	-8,130	0	0	0	0
20	-8,70	0	0	0	-2,5
21	-8,399	0	-2,5	-4,5	0

Table S2. Affinity and energy values (kcal/mol) involved in the interaction of the screening compounds (**10–21**) and reference **NAD** when docked in the NAD site.

Compound	S	Asp ⁵¹	Val ¹³⁵	Arg ⁹⁸	Val ³⁰
NAD	-13,280	-7,7	-3,7	-16,9	-5,6
10	-9,847	0	-3,9	-4,3	0
11	-8,446	0	-3,3	-5,9	0
12	-8,668	0	0	0	0
13	-9,782	0	0	0	0
14	-8,431	-3.4	0	0	0
15	-8,001	0	0	-2,4	0
16	-8,499	-0,7	0	0	0
17	-8,597	-0,6	0	0	0
18	-8,588	0	0	0	0
19	-8,486	0	0	0	0
20	-8,829	0	0	0	0
21	-9,073	0	0	0	0

Table S3. Affinity and energy values (kcal/mol) involved in the interaction of the screening compounds (**10–21**) when docked in the extended site.

Compound	S	Arg ¹⁶⁸	His ¹⁹²	Asn ¹³⁷	Asp ¹⁹⁴	Asp ⁵¹	Val ¹³⁵	Arg ⁹⁸	Val ³⁰
10	-8,652	-3,1	0	-1,3	0	0	0	0	0
11	-7,608	-9,3	-7	-3,4	-3,4	0	0	0	0
12	-8,727	-0,7	0	0	0	0	0	0	0
13	-8,239	0	0	0	0	0	0	0	0
14	-8,121	0	-5,8	0	-4,8	0	0	0	0
15	-8,098	0	0	-0,7	0	0	0	0	0
16	-7,857	0	-3,1	-4,9	0	0	0	0	0
17	-8,172	0	0	0	-1,6	0	0	0	0
18	-8,658	0	0	0	0	0	0	0	0
19	-8,341	-2,9	0	-3,5	0	0	0	0	0
20	-7,826	0	-4,4	-0,5	0	0	0	0	0
21	-7,385	-3,7	0	-8,1	0	0	0	0	0

Table S4. Affinity and energy values (kcal/mol) involved in the interaction of compounds **24–31(a–c)** with the main aminoacid residues. If empty, that compound did not pass some of the filtering stages.

Quinolone	Aryl	Comp.	Arg ¹⁶⁸	His ¹⁹²	Asn ¹³⁷	Asp ¹⁹⁴	Affinity
6-H	4-ClPh	24a	-7,8	0	0	-4,8	-9,240
	4-CF ₃ Ph	25a	-4,5	0	-0,5	-2	-9,781
	Naphthalene-2-yl	26a	-5,1	0	-0,7	-3,1	-10,254
	3,4-(OCH ₂ O)Ph	27a					
6-Cl	4-ClPh	24b	-4,7	0	-0,5	-5,1	-9,971
	4-CF ₃ Ph	25b	-4,3	0	-0,6	-4	-10,115
	Naphthalene-2-yl	26b	-5,9	0	0	-3,1	-10,355
	3,4-(OCH ₂ O)Ph	27b	-5,8	-2	-4,2	0	-10,066
6-OCH ₃	4-ClPh	24c	-8,2	-0,6	-0,6	0	-9,215
	4-CF ₃ Ph	25c	-2,2	0	0	0	-9,442
	Naphthalene-2-yl	26c	-6,6	0	0	-3,2	-10,765
	3,4-(OCH ₂ O)Ph	27c	-3,7	0	0	0	-9,353
6-H	4-ClPh	28a					
	4-CF ₃ Ph	29a	-11,1	0	0	0	-9,217
	Naphthalene-2-yl	30a					
	3,4-(OCH ₂ O)Ph	31a					
6-Cl	4-ClPh	28b	-8,7	0	0	0	-9,145
	4-CF ₃ Ph	29b	-4,4	0	0	0	-9,506
	Naphthalene-2-yl	30b					
	3,4-(OCH ₂ O)Ph	31b	-2,5	-0,8	0	0	-9,024
6-OCH ₃	4-ClPh	28c					
	4-CF ₃ Ph	29c					
	Naphthalene-2-yl	30c	-5,9	0	0	0	-9,357
	3,4-(OCH ₂ O)Ph	31c	-4,8	0	0	0	-9,268

Table S5. Affinity and energy values (kcal/mol) involved in the interaction of the different pyrimidine-quinolone hybrids **24–31(a–c)** and **33–36(a–c)** with the main aminoacid residues. If empty, that compound did not pass some of the filtering stages.

Quinolone	Aryl	Comp.	Arg ¹⁶⁸	His ¹⁹²	Asn ¹³⁷	Asp ¹⁹⁴	Affinity
6-H	4-ClPh	24a	-7,8	0	0	-4,8	-9,240
	4-CF ₃ Ph	25a	-4,5	0	-0,5	-2	-9,781
	Naphthalene-2-yl	26a	-5,1	0	-0,7	-3,1	-10,254
	3,4-(OCH ₂ O)Ph	27a					
6-Cl	4-ClPh	24b	-4,7	0	-0,5	-5,1	-9,971
	4-CF ₃ Ph	25b	-4,3	0	-0,6	-4	-10,115
	Naphthalene-2-yl	26b	-5,9	0	0	-3,1	-10,355
	3,4-(OCH ₂ O)Ph	27b	-5,8	-2	-4,2	0	-10,066
6-OCH ₃	4-ClPh	24c	-8,2	-0,6	-0,6	0	-9,215
	4-CF ₃ Ph	25c	-2,2	0	0	0	-9,442
	Naphthalene-2-yl	26c	-6,6	0	0	-3,2	-10,765
	3,4-(OCH ₂ O)Ph	27c	-3,7	0	0	0	-9,353
6-H	4-ClPh	28a					
	4-CF ₃ Ph	29a	-11,1	0	0	0	-9,217
	Naphthalene-2-yl	30a					
	3,4-(OCH ₂ O)Ph	31a					
6-Cl	4-ClPh	28b	-8,7	0	0	0	-9,145
	4-CF ₃ Ph	29b	-4,4	0	0	0	-9,506
	Naphthalene-2-yl	30b					
	3,4-(OCH ₂ O)Ph	31b	-2,5	-0,8	0	0	-9,024
6-OCH ₃	4-ClPh	28c					
	4-CF ₃ Ph	29c					
	Naphthalene-2-yl	30c	-5,9	0	0	0	-9,357
	3,4-(OCH ₂ O)Ph	31c	-4,8	0	0	0	-9,268
6-H	4-ClPh	33a	-6,5	0	0	0	-9,278
	4-CF ₃ Ph	34a	-6,1	0	0	-0,9	-10,134
	Naphthalene-2-yl	35a	-6	0	0	-0,9	-10,324
	3,4-(OCH ₂ O)Ph	36a					
6-Cl	4-ClPh	33b	-2,8	0	0	-0,7	-9,616
	4-CF ₃ Ph	34b	-5,6	0	0	-6	-10,218
	Naphthalene-2-yl	35b	-5,4	-1,5	0	-0,5	-9,693
	3,4-(OCH ₂ O)Ph	36b	-5,2	0	0	-5,3	-9,820
6-OCH ₃	4-ClPh	33c	-6,6	0	0	0	-9,386
	4-CF ₃ Ph	34c	-11,2	0	-1,5	0	-9,251
	Naphthalene-2-yl	35c	-6,7	0	0	0	-9,329
	3,4-(OCH ₂ O)Ph	36c					

Table S6. Mean energy values (kcal/mol) involved in the interaction of hybrids **24–31(a–c)** and **33–36(a–c)** with the main aminoacid residues

Substitution	Compounds	Arg ¹⁶⁸	Asp ¹⁹⁴	His ¹⁹²	Asn ¹³⁷	Affinity
<i>Ortho</i>	24-27(a-c)	-5,3	-3,6	-1,3	-1,2	-9,869
<i>Para</i>	28-31(a-c)	-6,2	0,0	-0,8	0,0	-9,253
<i>Meta</i>	33-36(a-c)	-6,2	-2,4	-1,5	-1,5	-9,705

2. Chemistry

Table S7. Conditions used in different trials for reaction between intermediates **24–25** and **1–4**.

Solvent	Acid	Base	Catalyst	Heating
EtOH				MW (120°C)
EtOH		Et ₃ N		MW (120°C)
EtOH		K ₂ CO ₃		MW (120°C)
EtOH		K ₂ CO ₃	KI	MW (120°C)
EtOH	pTSA			MW (120°C)
EtOH	HCl			MW (120°C)
DMF		K ₂ CO ₃	KI	MW (160°C)
DMF		K ₂ CO ₃	KI	MW (180°C)
DMF		K ₂ CO ₃	Pd(OAc) ₂ + BINAP	80°C
DMSO		K ₂ CO ₃	AgNO ₃	80°C → 100°C
CH ₃ CN				MW (120°C)
CH ₃ CN		Et ₃ N		MW (120°C)
CH ₃ CN		K ₂ CO ₃	Pd(OAc) ₂	MW (120°C)

3. LDHA biological assays.

3.1 Dose-response inhibition curves

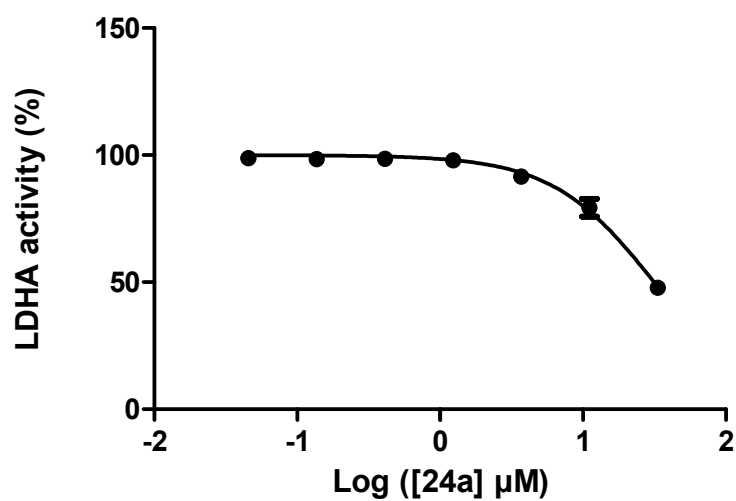


Figure S1. LDHA inhibition curve of compound **24a** (mean \pm SD of $n = 3$ replicates)

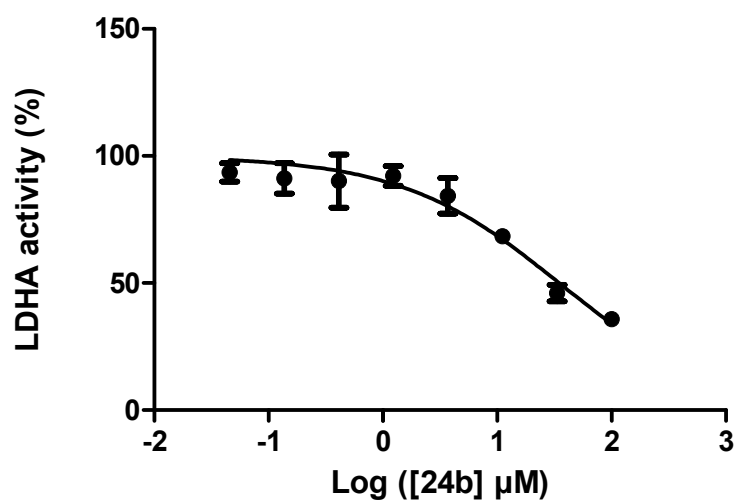


Figure S2. LDHA inhibition curve of compound **24b** (mean \pm SD of $n = 3$ replicates)

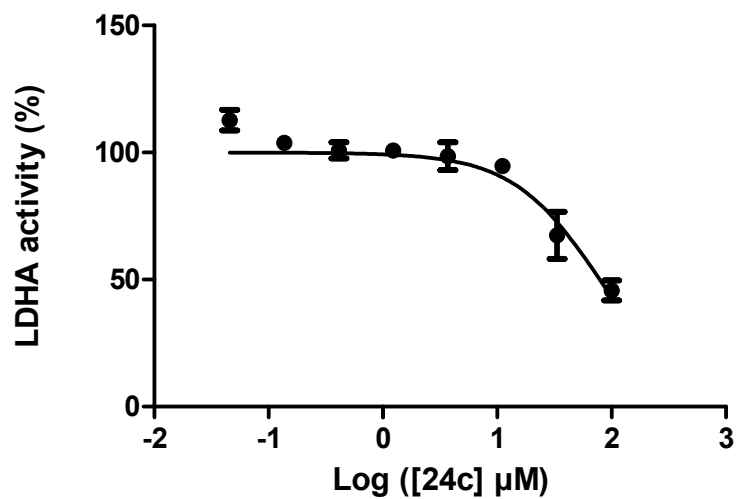


Figure S3. LDHA inhibition curve of compound **24c** (mean \pm SD of $n = 3$ replicates)

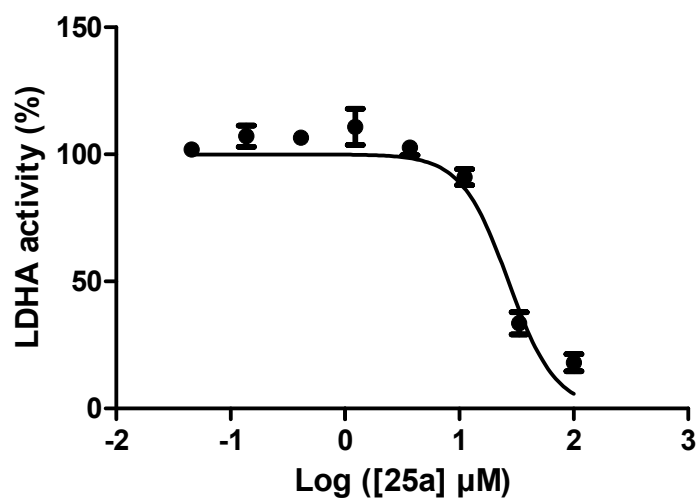


Figure S4. LDHA inhibition curve of compound **25a** (mean \pm SD of $n = 3$ replicates)

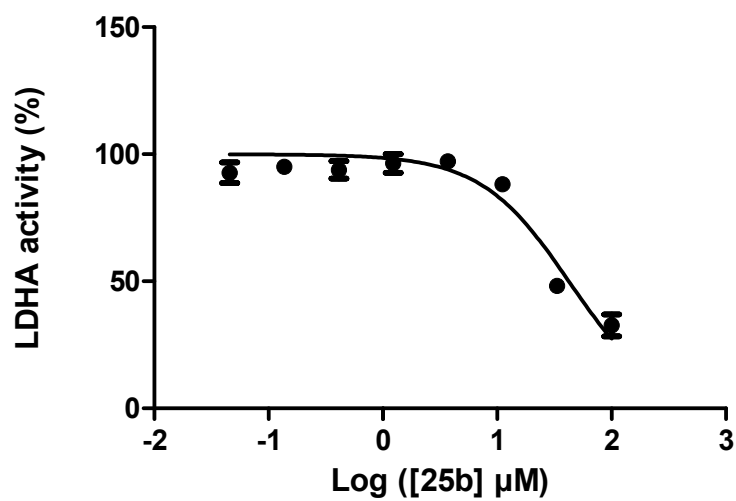


Figure S5. LDHA inhibition curve of compound **25b** (mean \pm SD of $n = 3$ replicates)

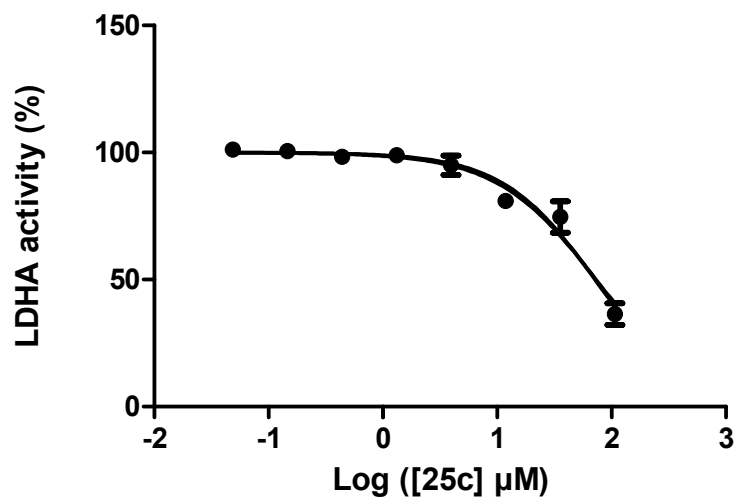


Figure S6. LDHA inhibition curve of compound **25c** (mean \pm SD of $n = 3$ replicates)

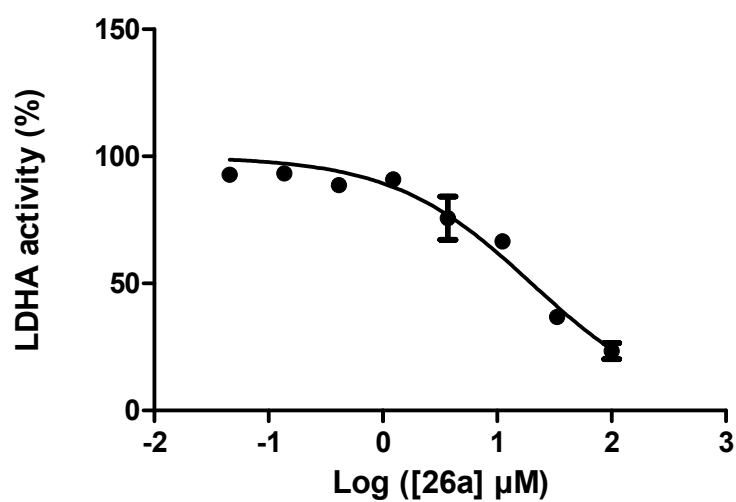


Figure S7. LDHA inhibition curve of compound **26a** (mean \pm SD of $n = 3$ replicates)

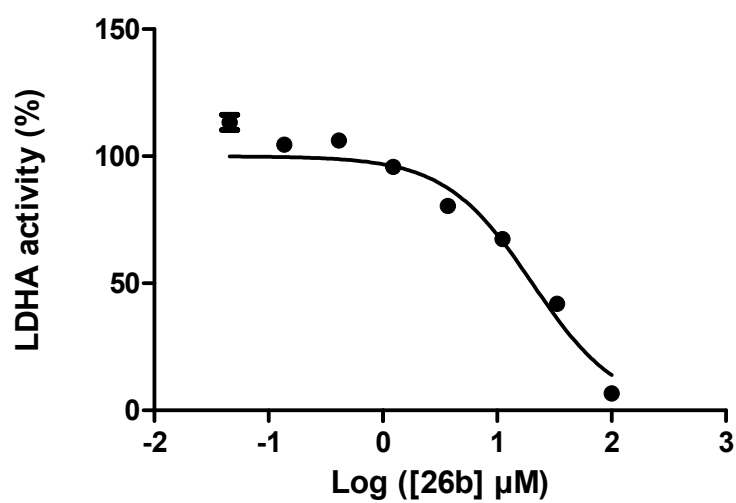


Figure S8. LDHA inhibition curve of compound **26b** (mean \pm SD of $n = 3$ replicates)

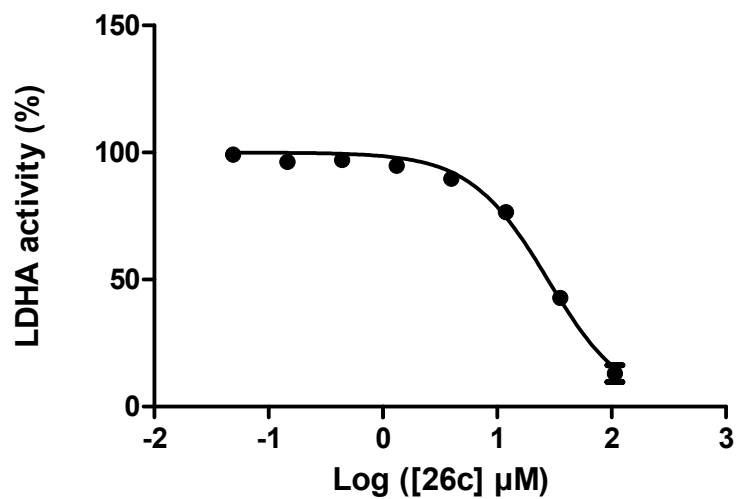


Figure S9. LDHA inhibition curve of compound **26c** (mean \pm SD of $n = 3$ replicates)

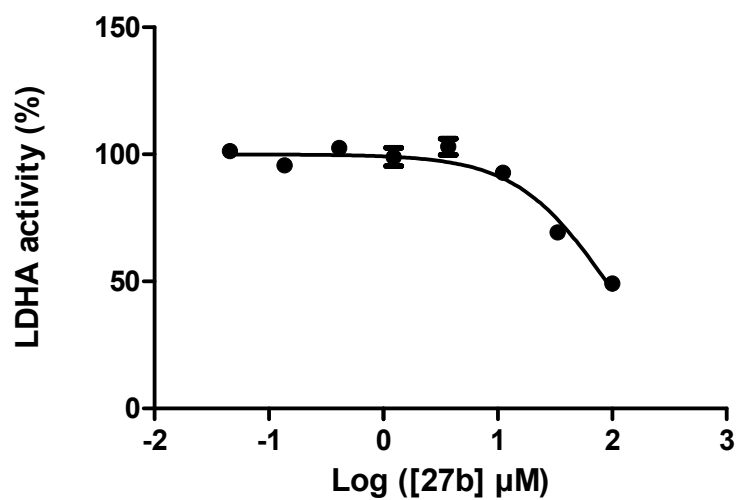


Figure S10. LDHA inhibition curve of compound **27b** (mean \pm SD of $n = 3$ replicates)

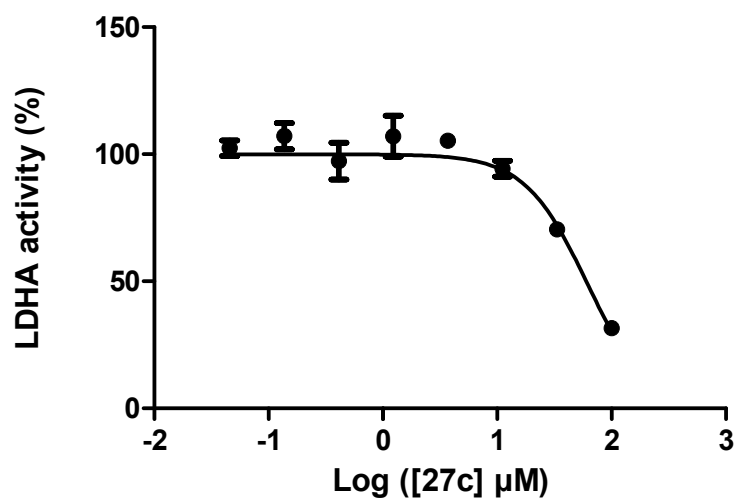


Figure S11. LDHA inhibition curve of compound **27c** (mean \pm SD of $n = 3$ replicates)

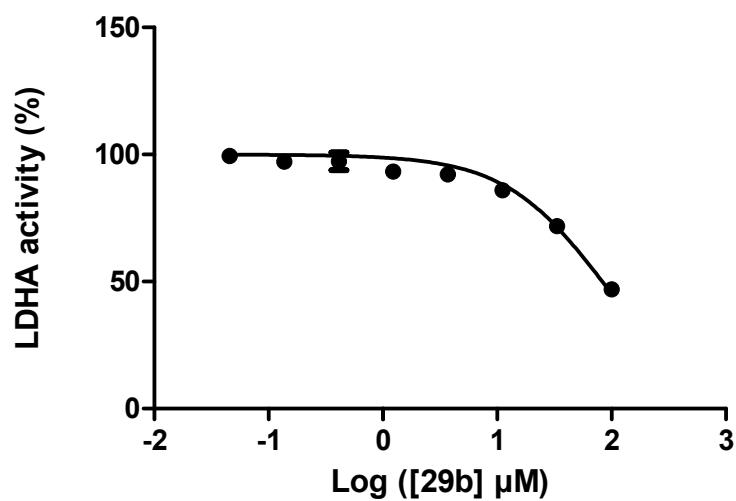


Figure S12. LDHA inhibition curve of compound **29b** (mean \pm SD of $n = 3$ replicates)

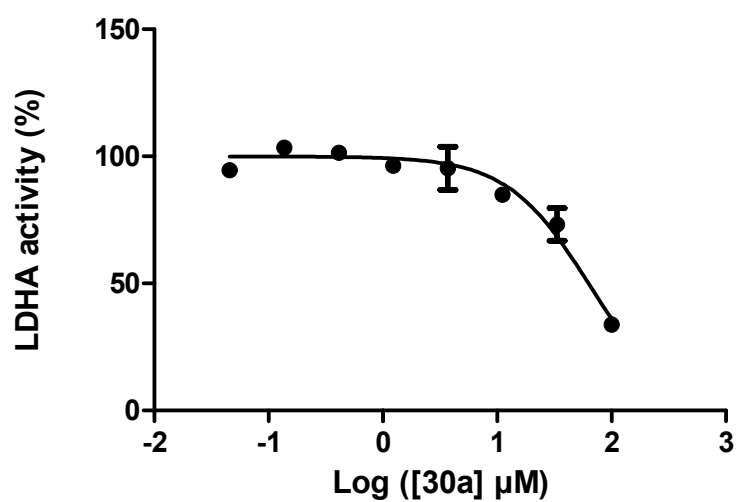


Figure S13. LDHA inhibition curve of compound **30a** (mean \pm SD of $n = 3$ replicates)

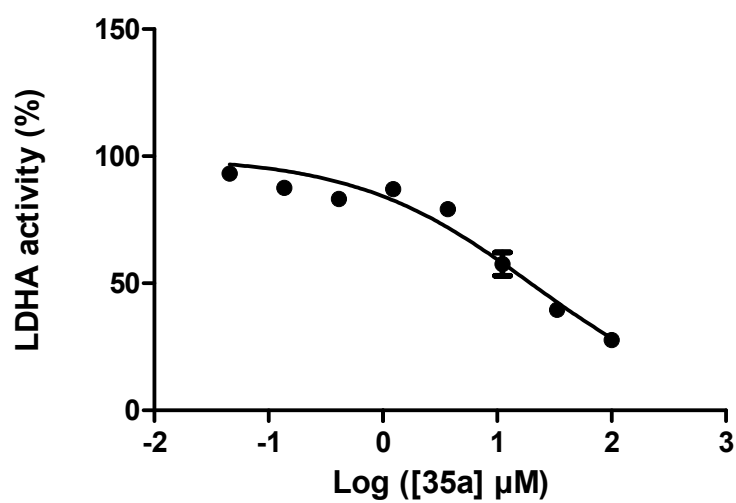


Figure S14. LDHA inhibition curve of compound **35a** (mean \pm SD of $n = 3$ replicates)

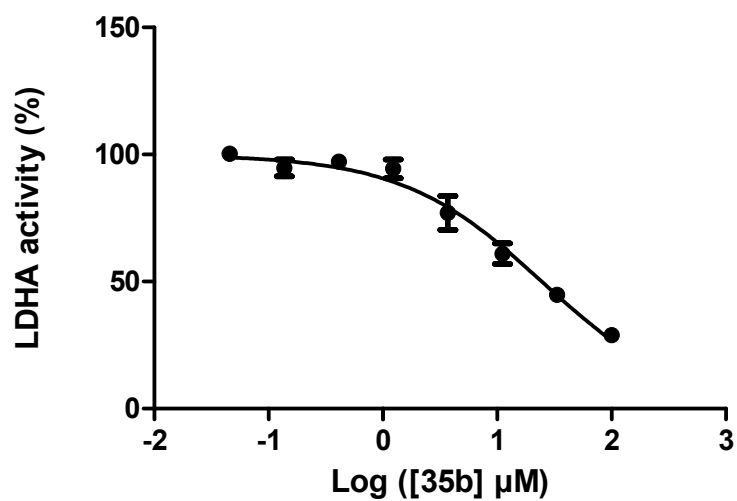


Figure S15. LDHA inhibition curve of compound **35b** (mean \pm SD of $n = 3$ replicates)

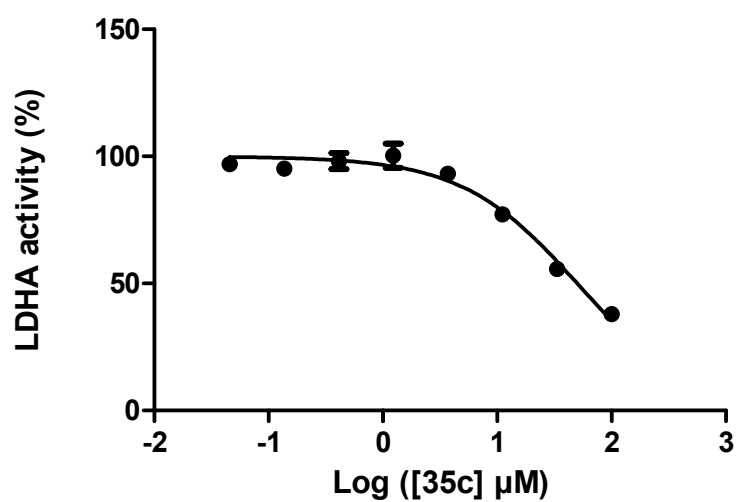
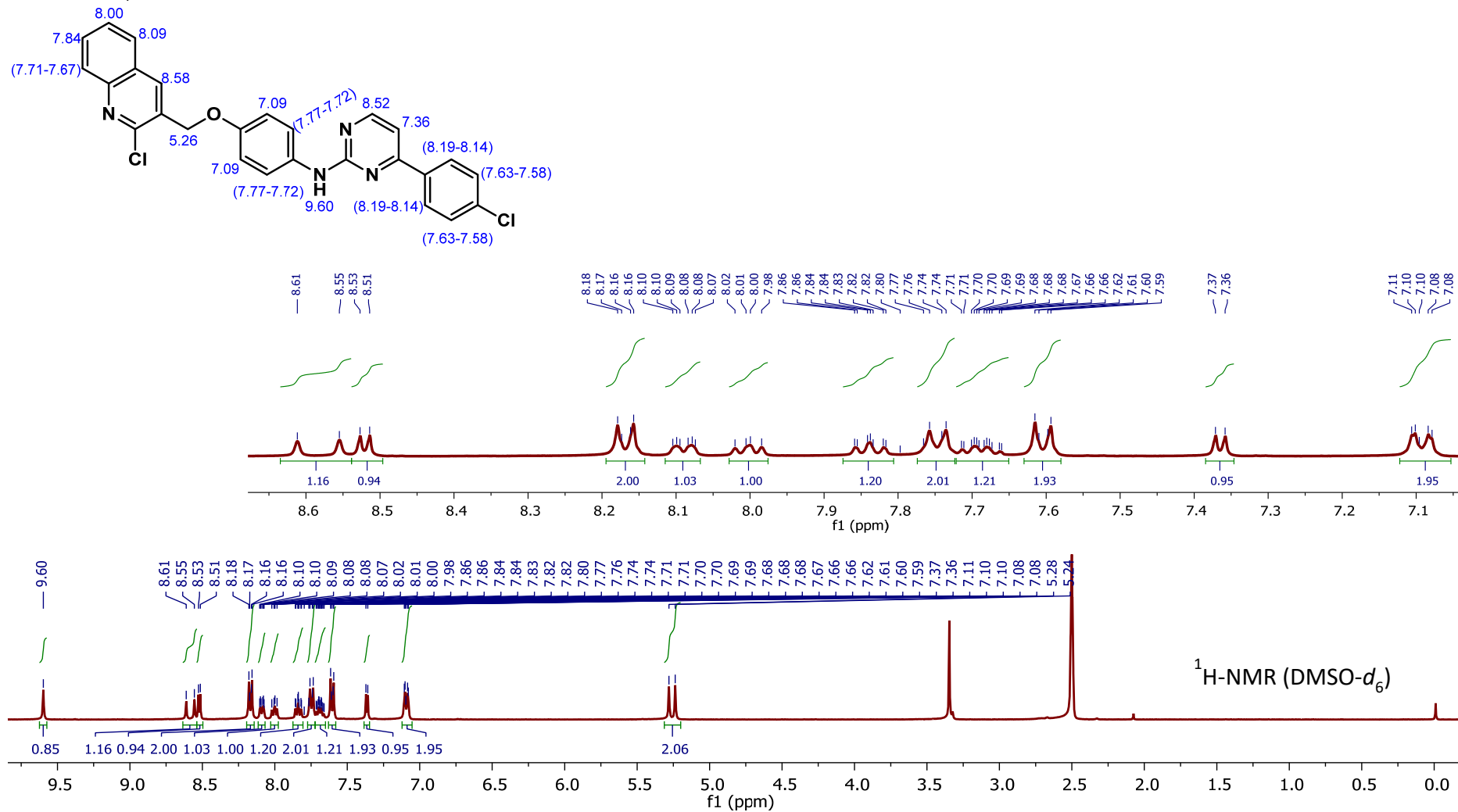
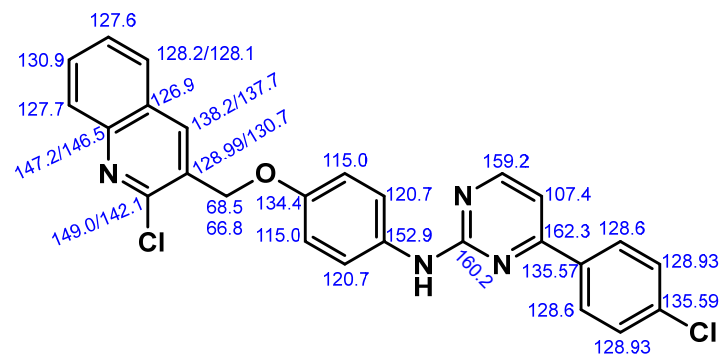


Figure S16. LDHA inhibition curve of compound **35c** (mean \pm SD of $n = 3$ replicates)

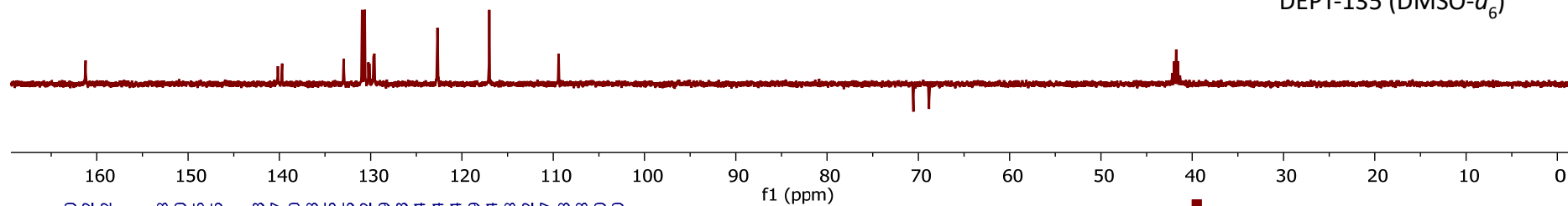
4. NMR, MS and HRMS spectra.

4.1 Compound 8

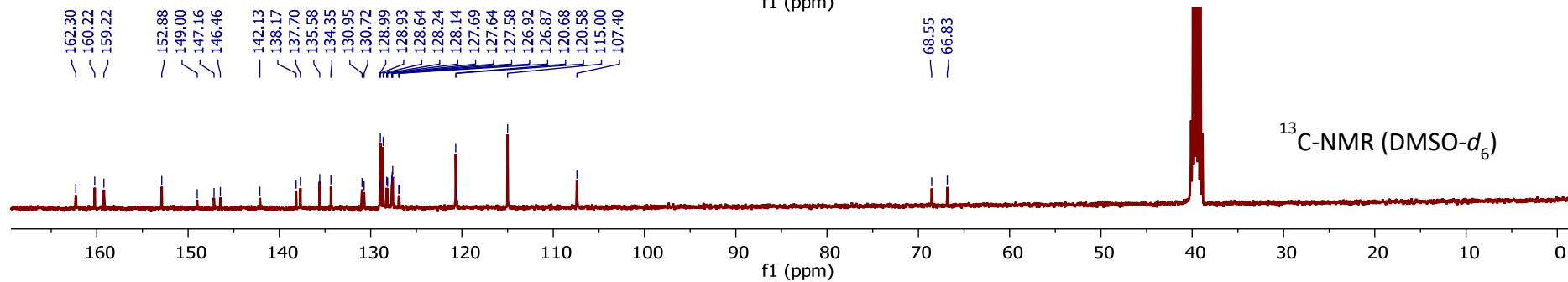




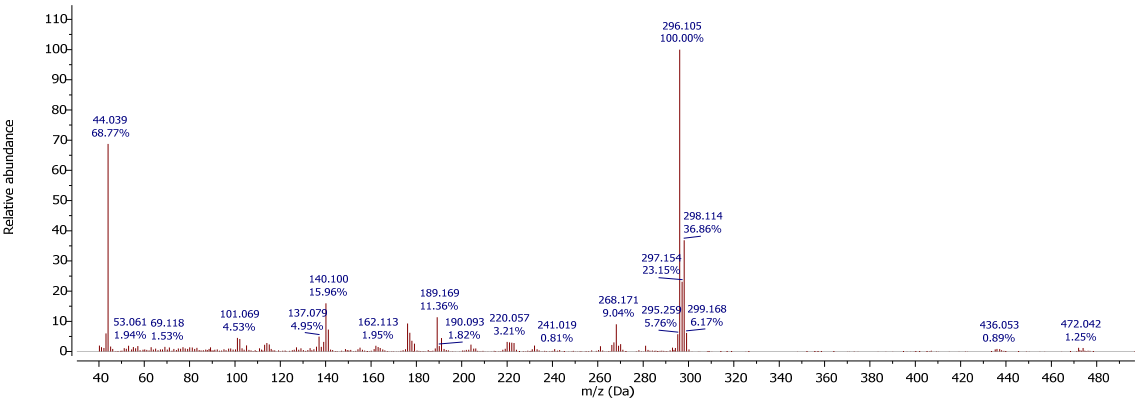
DEPT-135 (DMSO- d_6)



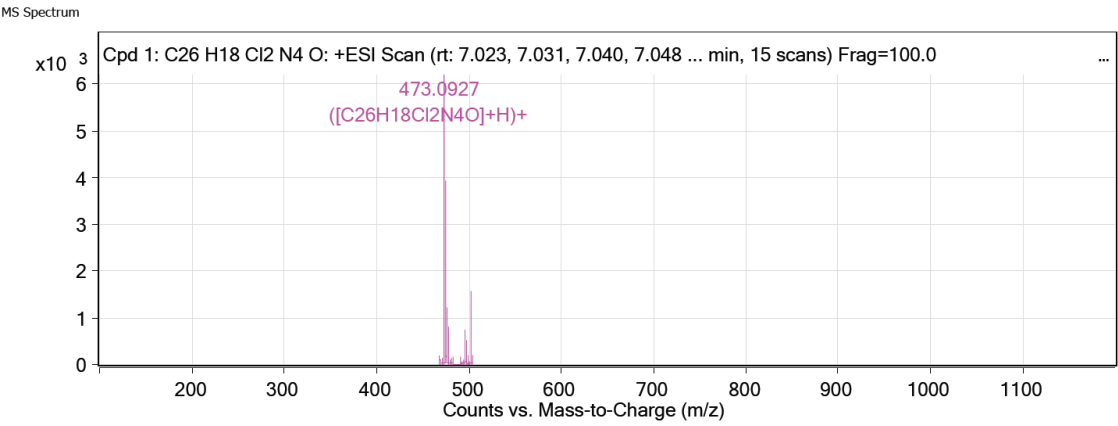
^{13}C -NMR (DMSO- d_6)



EI MS (70eV)



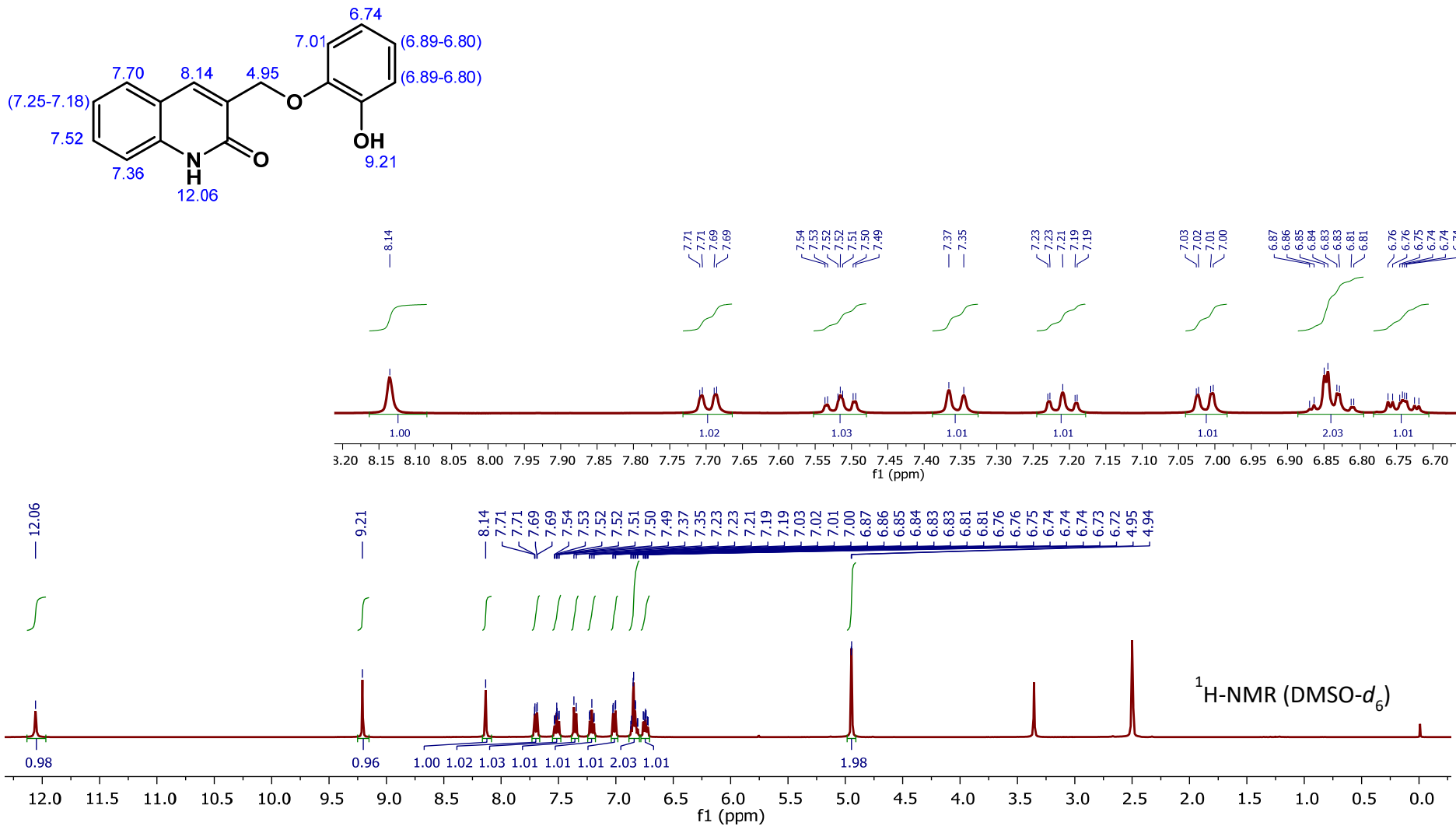
ESI-QTOF (positive ionization)

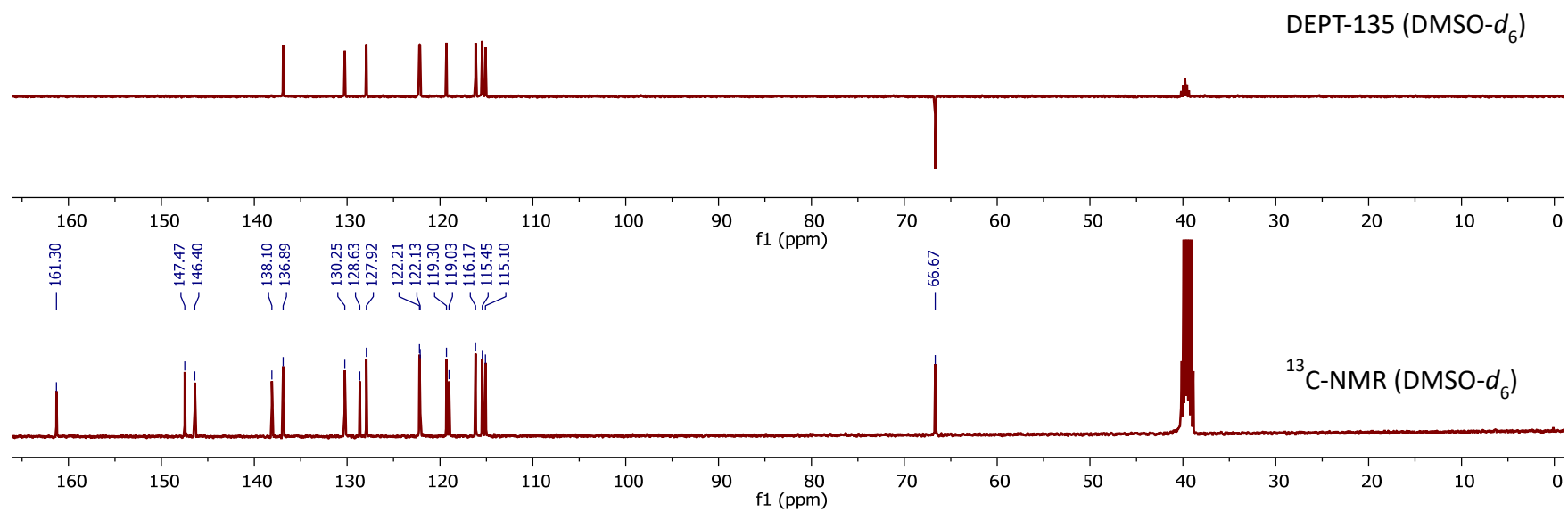
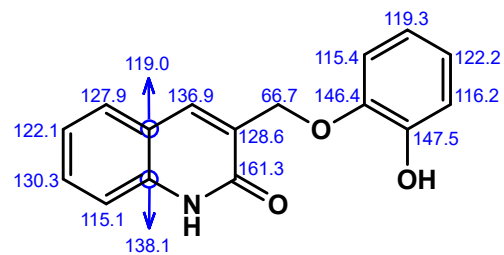


MS Spectrum Peak List

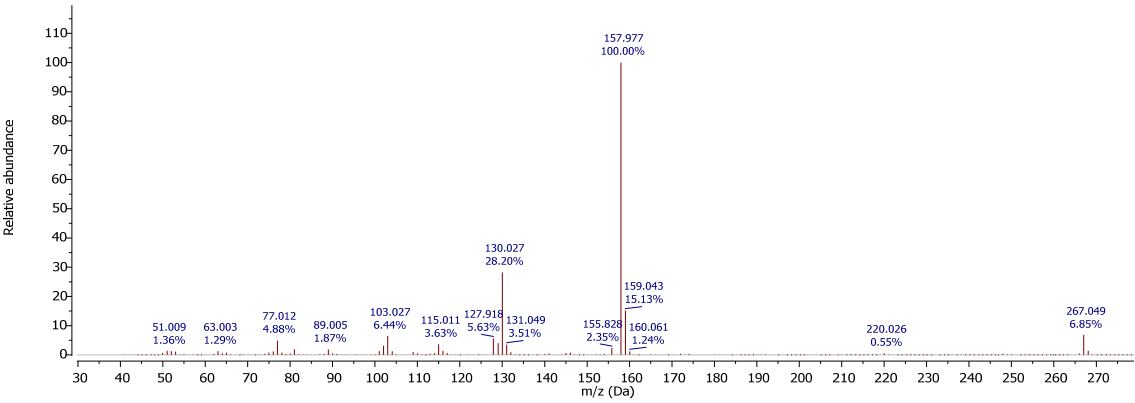
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
473.0927	473.093	0.76	1	6219.32	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
474.0961	474.0961	0.12	1	1828.22	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
475.0904	475.0907	0.57	1	4097	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
476.0932	476.0934	0.26	1	1239.43	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
477.09	477.0892	-1.84	1	857.27	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
478.0927	478.091	-3.67	1	181.88	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+H) ⁺
495.0751	495.075	-0.15	1	756.54	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+Na) ⁺
496.0769	496.0781	2.29	1	195.74	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+Na) ⁺
497.0737	497.0726	-2.1	1	510.59	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+Na) ⁺
499.0814	499.0711	-20.67	1	153.04	C ₂₆ H ₁₈ Cl ₂ N ₄ O	(M+Na) ⁺

4.2 Compound 9

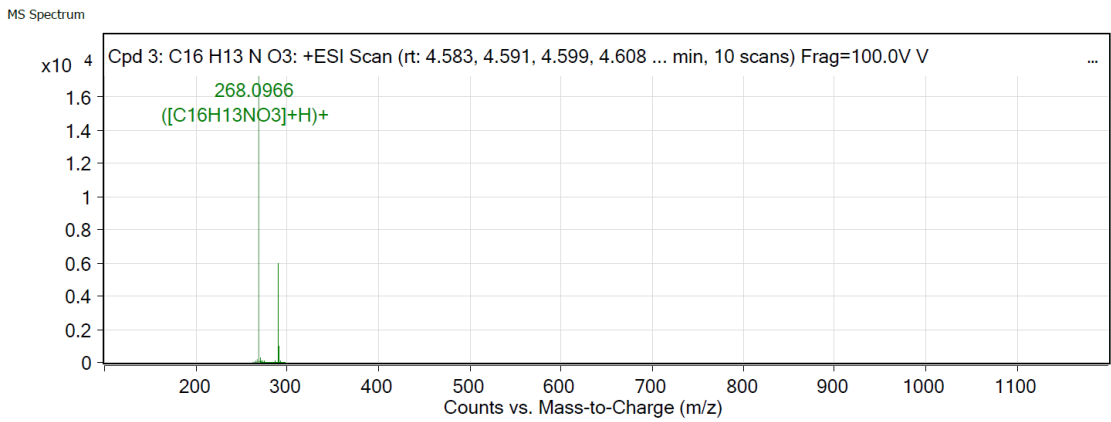




EI MS (70eV)



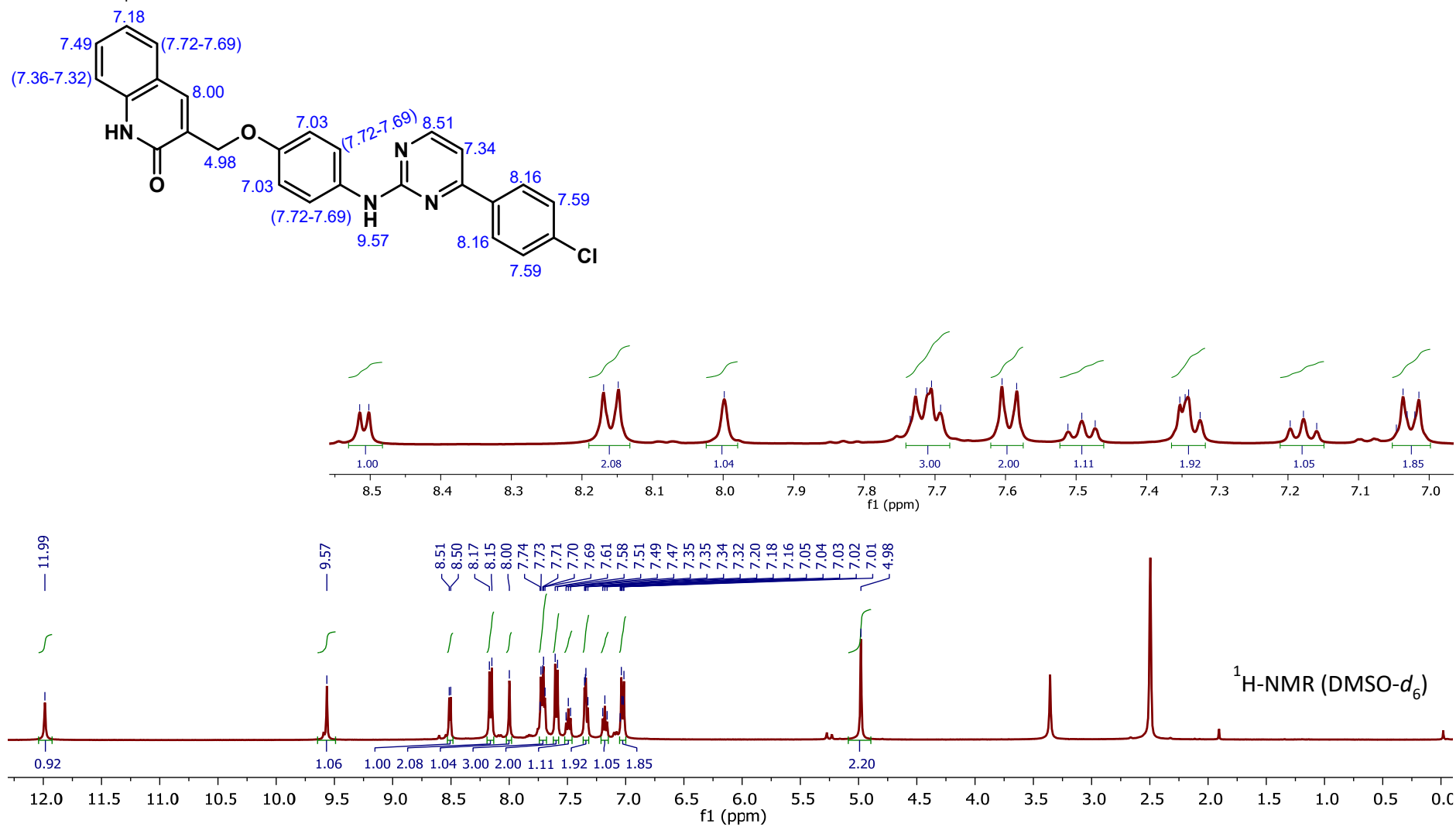
ESI-QTOF (positive ionization)

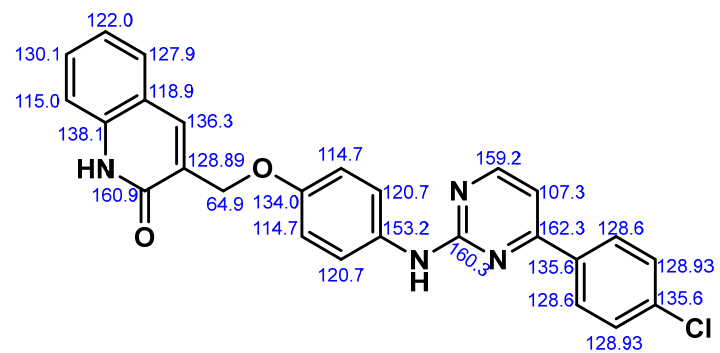


MS Spectrum Peak List

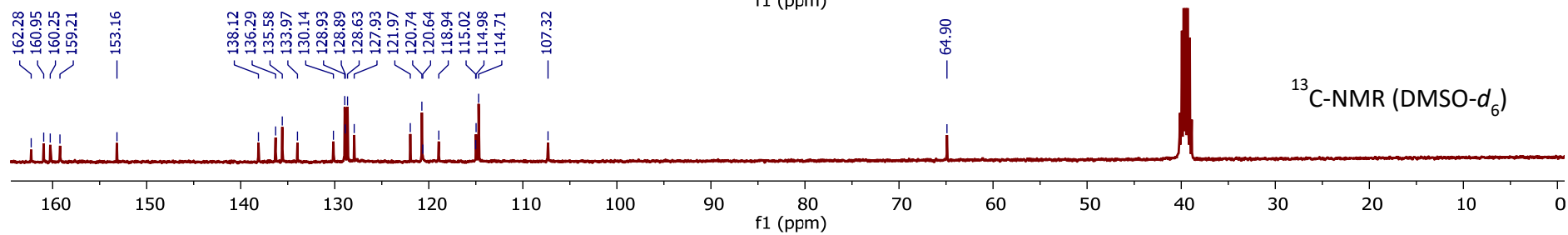
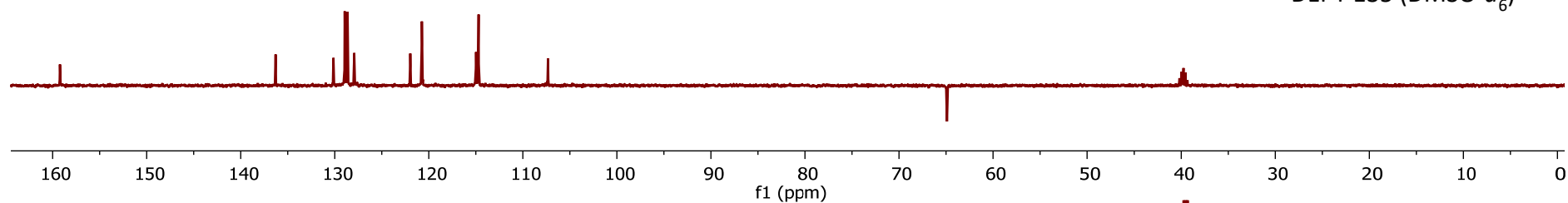
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
267.088	267.089	3.55	1	127.47	C ₁₆ H ₁₃ NO ₃	M+
268.0966	268.0968	0.73	1	17277.36	C ₁₆ H ₁₃ NO ₃	(M+H)+
269.1	269.1001	0.37	1	3074.52	C ₁₆ H ₁₃ NO ₃	(M+H)+
270.1029	270.1027	-0.75	1	357.6	C ₁₆ H ₁₃ NO ₃	(M+H)+
290.0779	290.0788	2.93	1	6088.36	C ₁₆ H ₁₃ NO ₃	(M+Na)+
291.0816	291.082	1.48	1	1041.68	C ₁₆ H ₁₃ NO ₃	(M+Na)+
292.082	292.0846	9.11	1	89.78	C ₁₆ H ₁₃ NO ₃	(M+Na)+

4.3 Compound 15

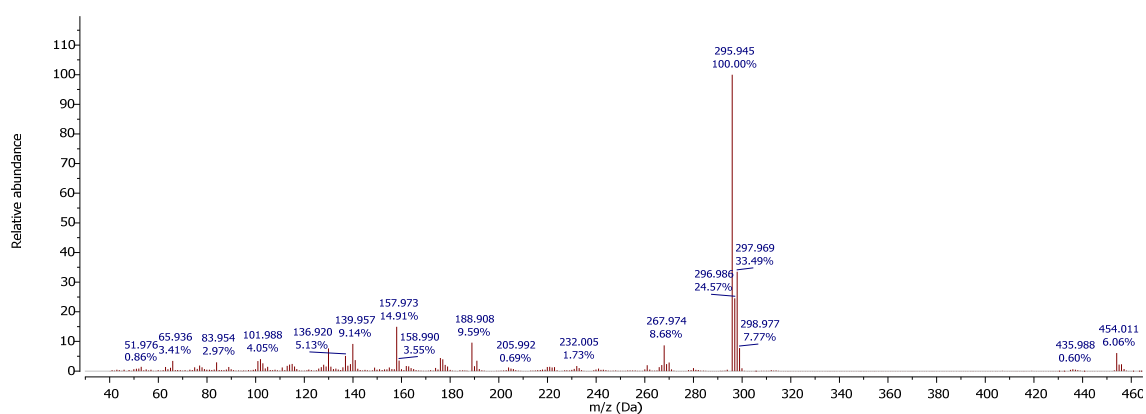




DEPT-135 (DMSO- d_6)

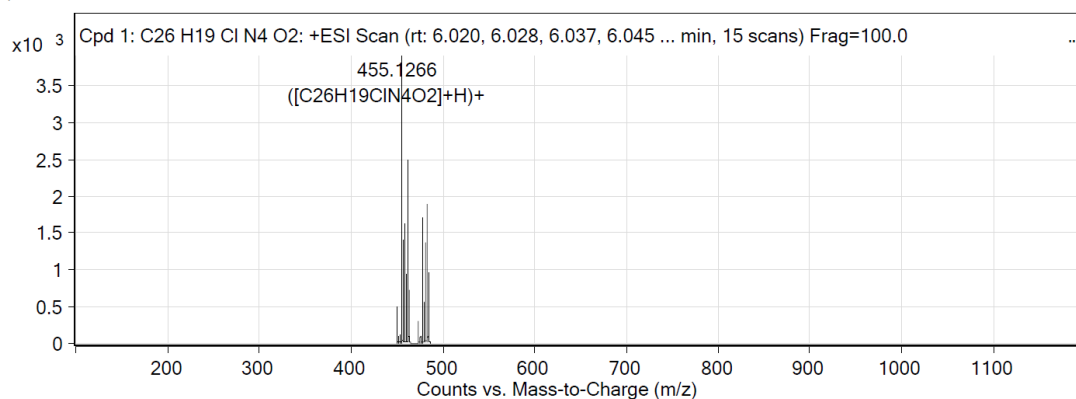


EI MS (70eV)



ESI-QTOF (positive ionization)

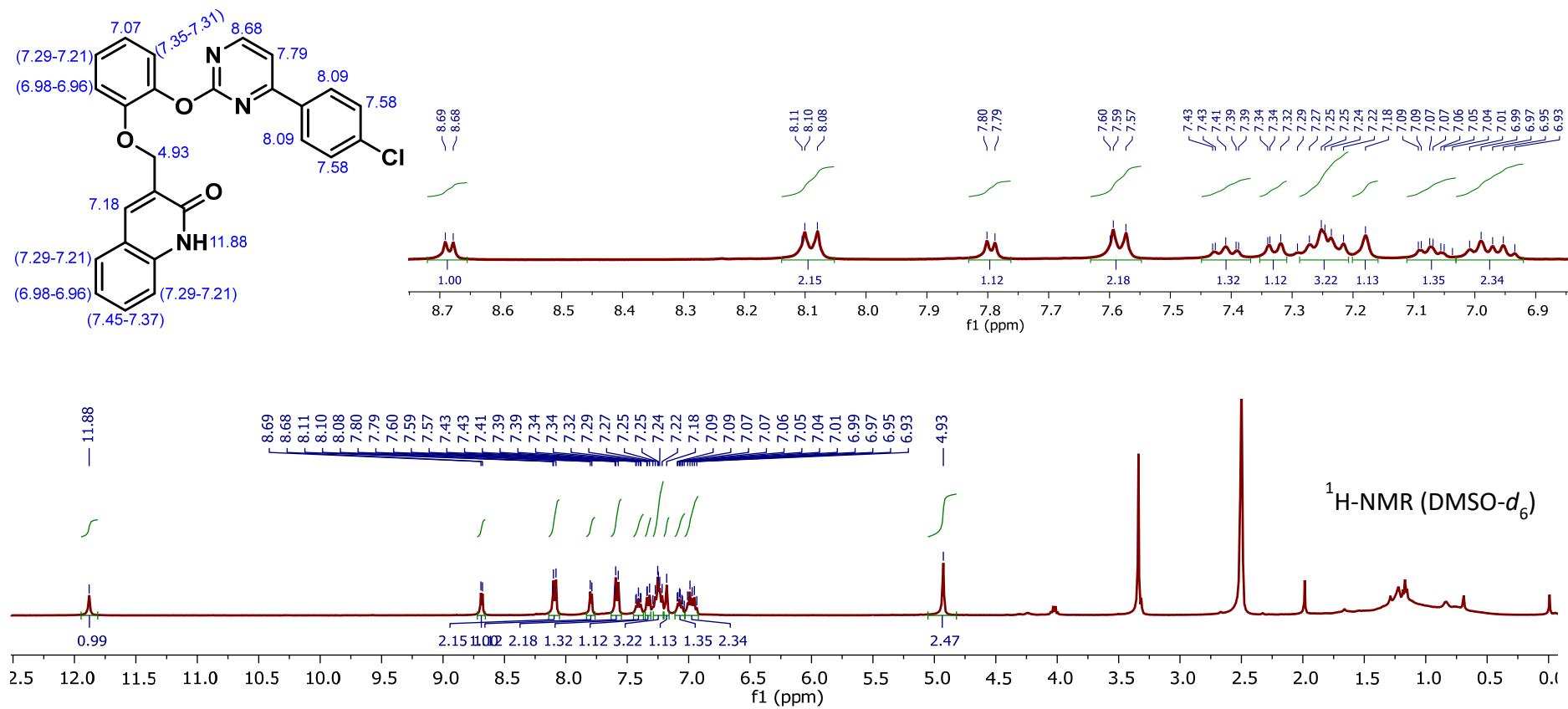
MS Spectrum

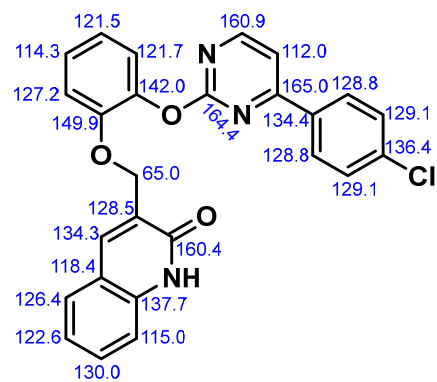


MS Spectrum Peak List

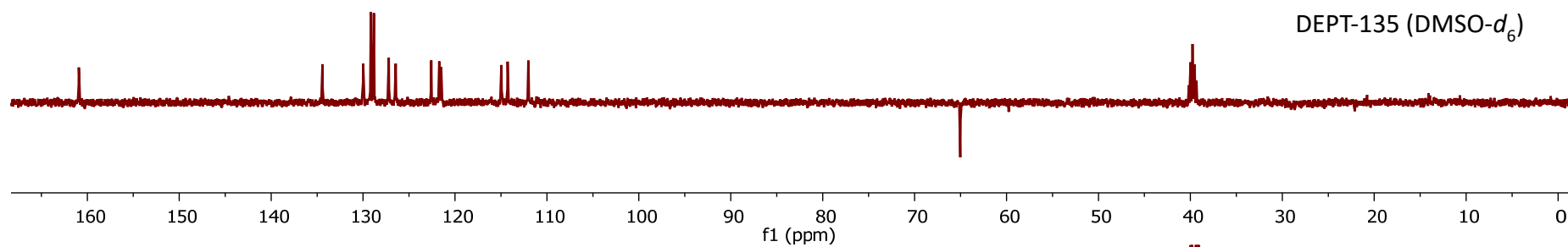
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
455.1266	455.1269	0.7	1	3951.15	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+H) ⁺
456.1289	456.13	2.41	1	1176.77	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+H) ⁺
457.1247	457.1251	0.9	1	1488.47	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+H) ⁺
458.1277	458.1275	-0.53	1	395.03	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+H) ⁺
459.1327	459.1302	-5.56	1	40.66	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+H) ⁺
477.1082	477.1089	1.34	1	1772.62	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+Na) ⁺
478.1116	478.1119	0.66	1	450.63	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+Na) ⁺
479.1066	479.1071	1.08	1	540.46	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+Na) ⁺
480.109	480.1094	0.9	1	127.29	C ₂₆ H ₁₉ ClN ₄ O ₂	(M+Na) ⁺

4.4 Compound 19

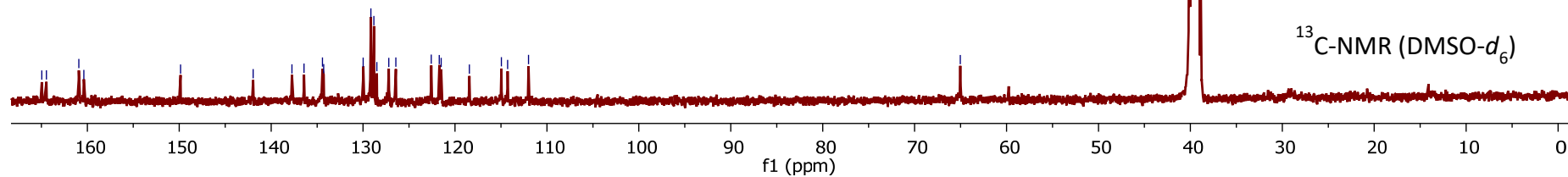




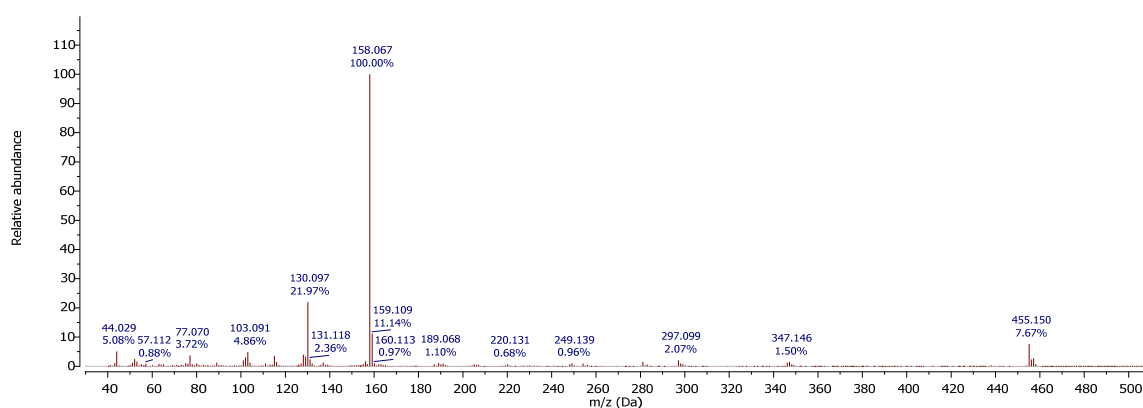
DEPT-135 (DMSO- d_6)



^{13}C -NMR (DMSO- d_6)

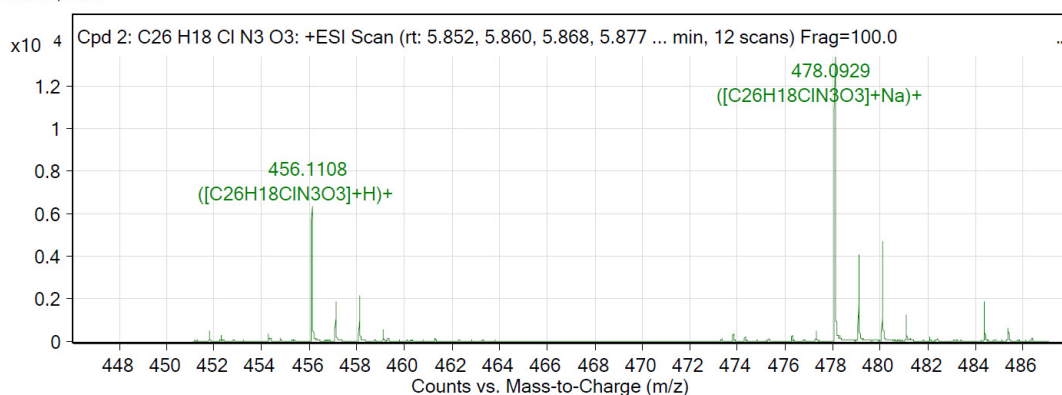


EI MS (70eV)



ESI-QTOF (positive ionization)

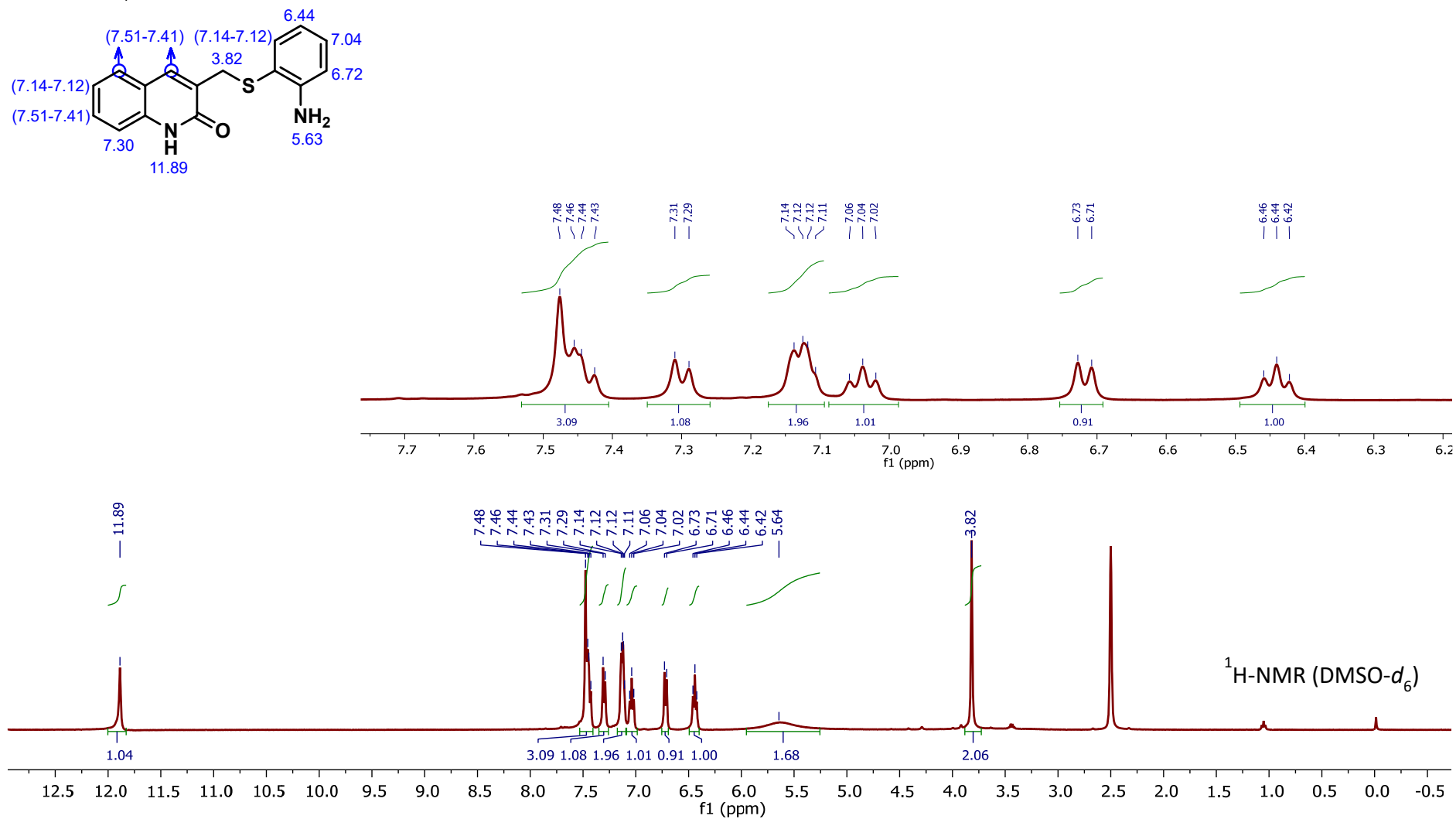
MS Zoomed Spectrum

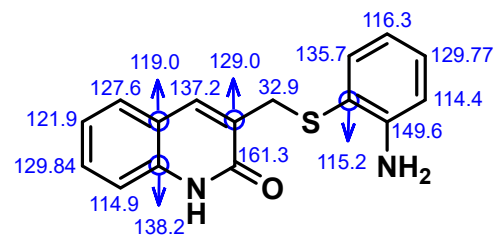


MS Spectrum Peak List

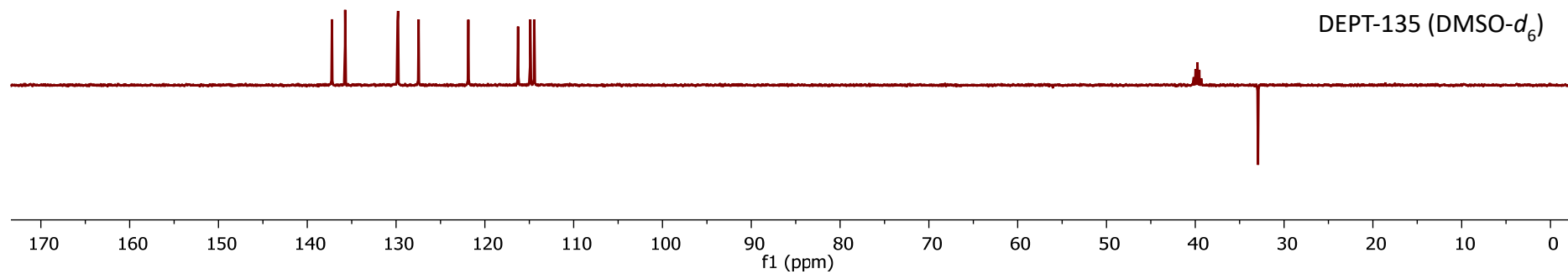
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
456.1108	456.1109	0.21	1	6375.96	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+H)+
457.1138	457.1141	0.65	1	1920.26	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+H)+
458.1088	458.1092	0.86	1	2208.63	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+H)+
459.1117	459.1116	-0.2	1	576.29	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+H)+
460.1171	460.1143	-6.16	1	20.83	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+H)+
478.0929	478.0929	-0.05	1	13461.33	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+Na)+
479.0956	479.096	0.83	1	4169.89	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+Na)+
480.091	480.0911	0.23	1	4700.13	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+Na)+
481.0925	481.0936	2.24	1	1299.51	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+Na)+
482.0944	482.0962	3.73	1	194.51	C ₂₆ H ₁₈ CIN ₃ O ₃	(M+Na)+

4.5 Compound 22a

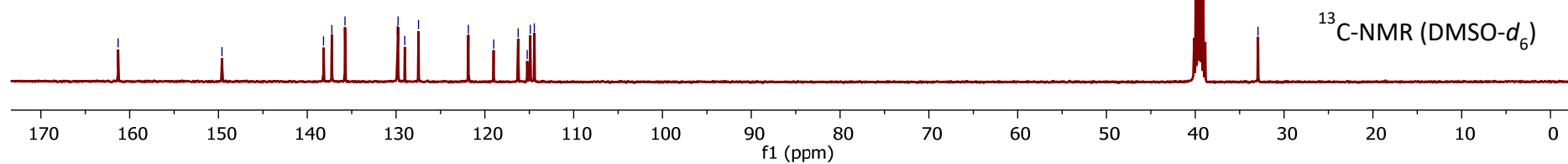




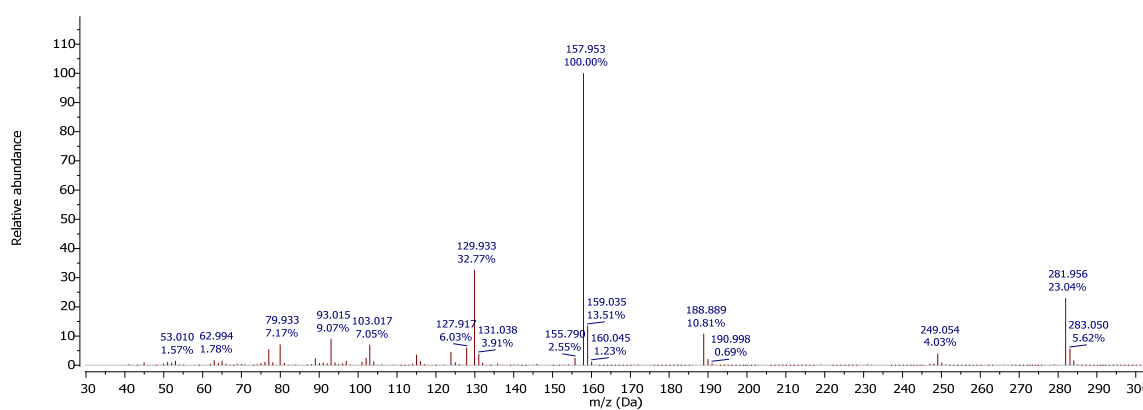
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

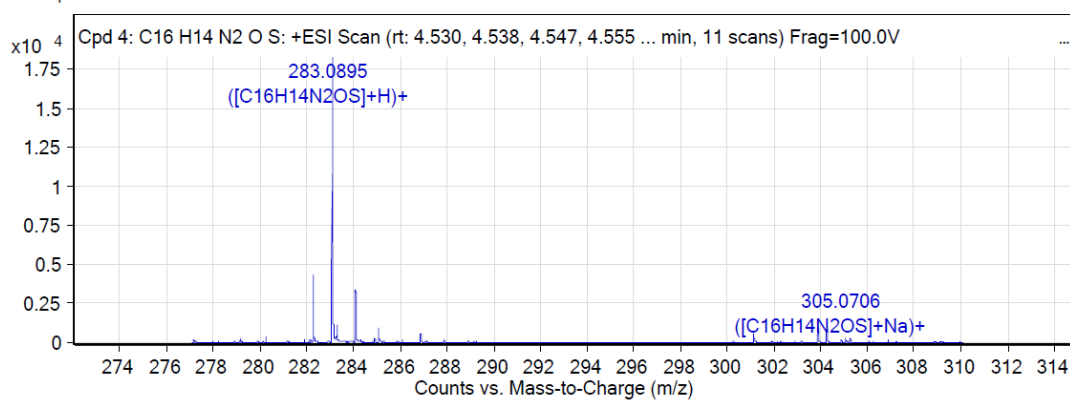


EI MS (70eV)



ESI-QTOF (positive ionization)

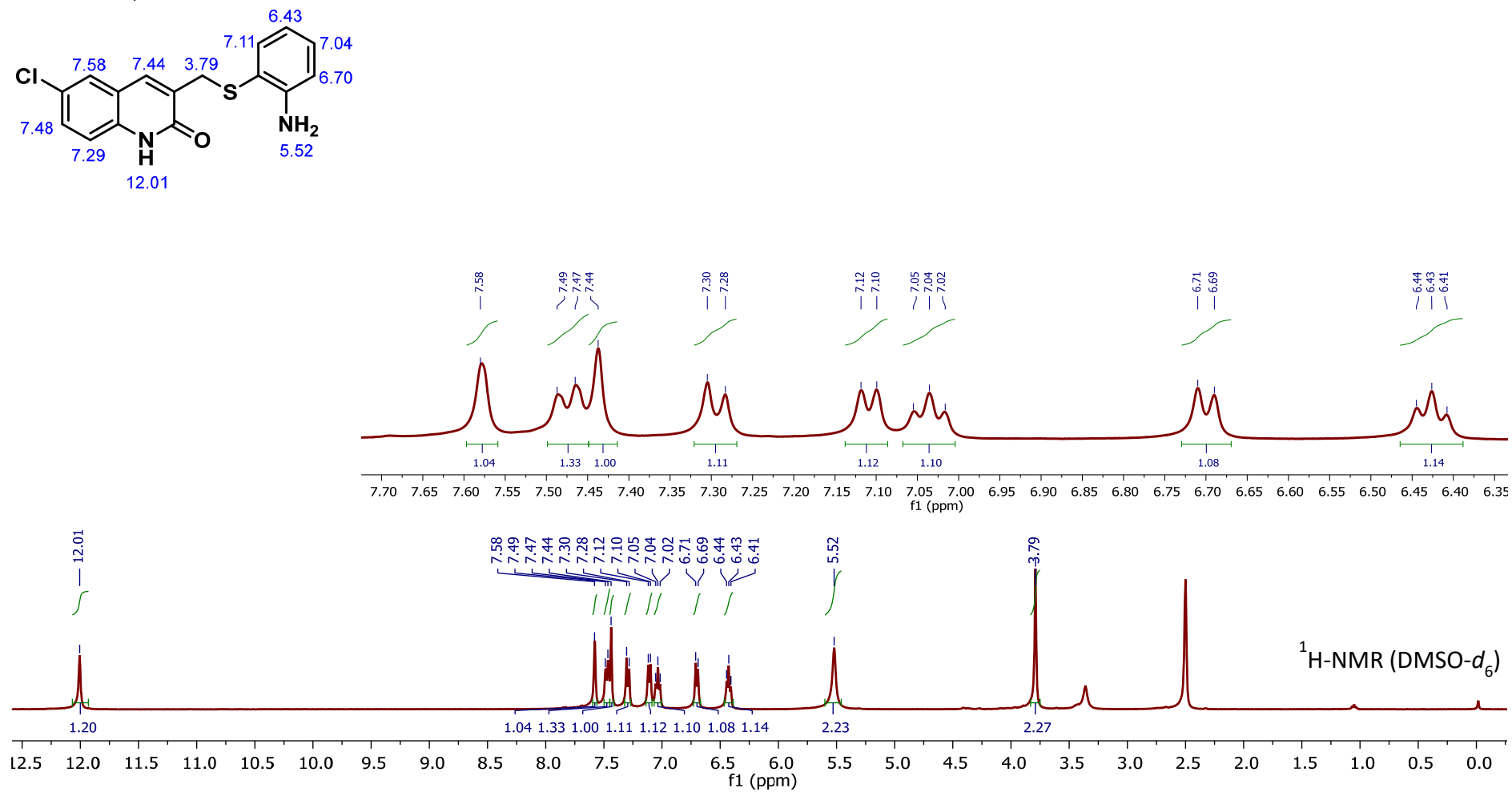
MS Zoomed Spectrum

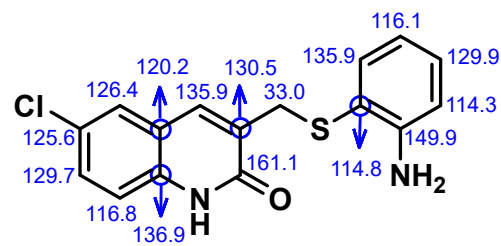


MS Spectrum Peak List

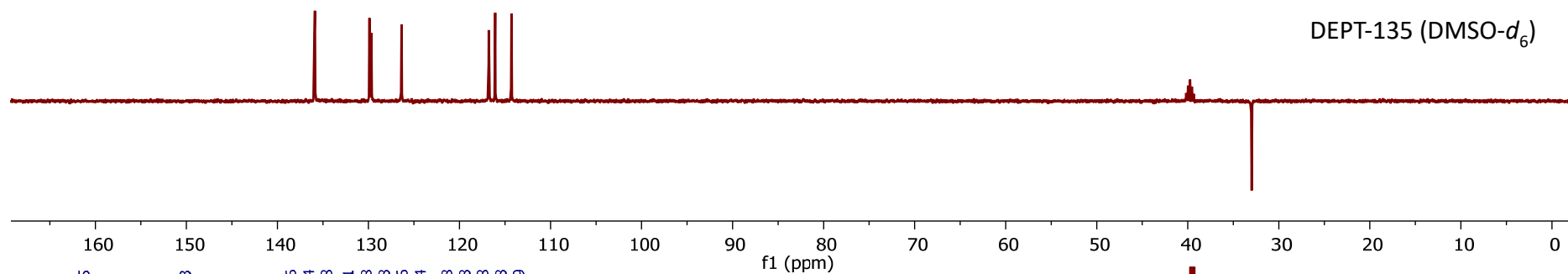
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
282.0818	282.0821	1.11	1	137.98	C16H14N2OS	M+
283.0895	283.09	1.54	1	18691.6	C16H14N2OS	(M+H)+
284.0925	284.0929	1.36	1	3518.1	C16H14N2OS	(M+H)+
285.0894	285.0887	-2.3	1	1059.53	C16H14N2OS	(M+H)+
305.0706	305.0719	4.29	1	309.66	C16H14N2OS	(M+Na)+

4.6 Compound 22b

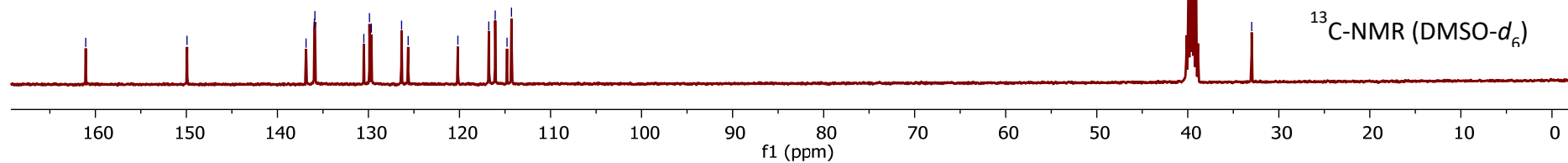




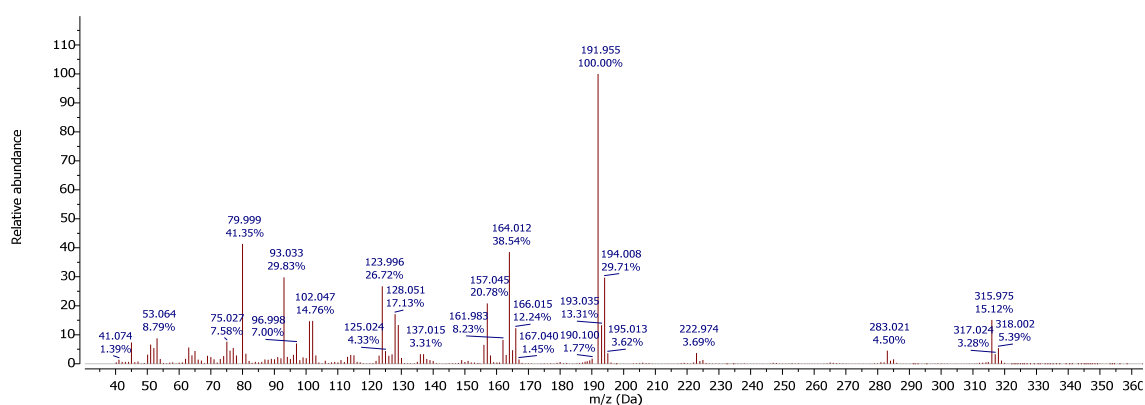
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

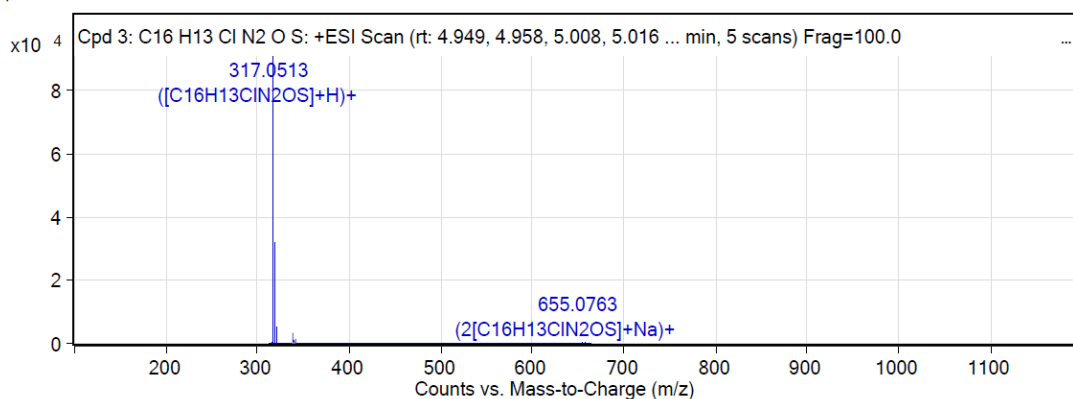


EI MS (70eV)



ESI-QTOF (positive ionization)

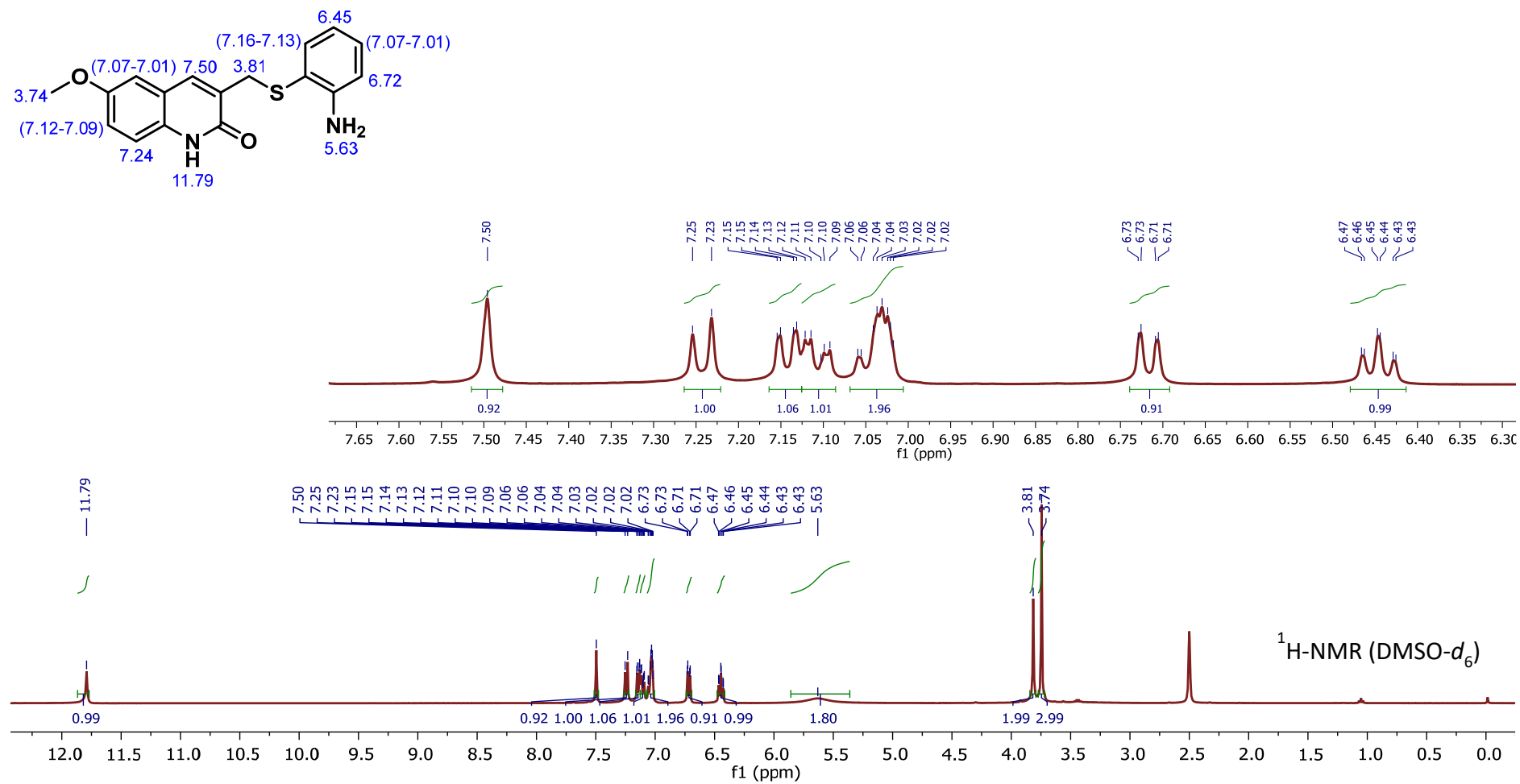
MS Spectrum

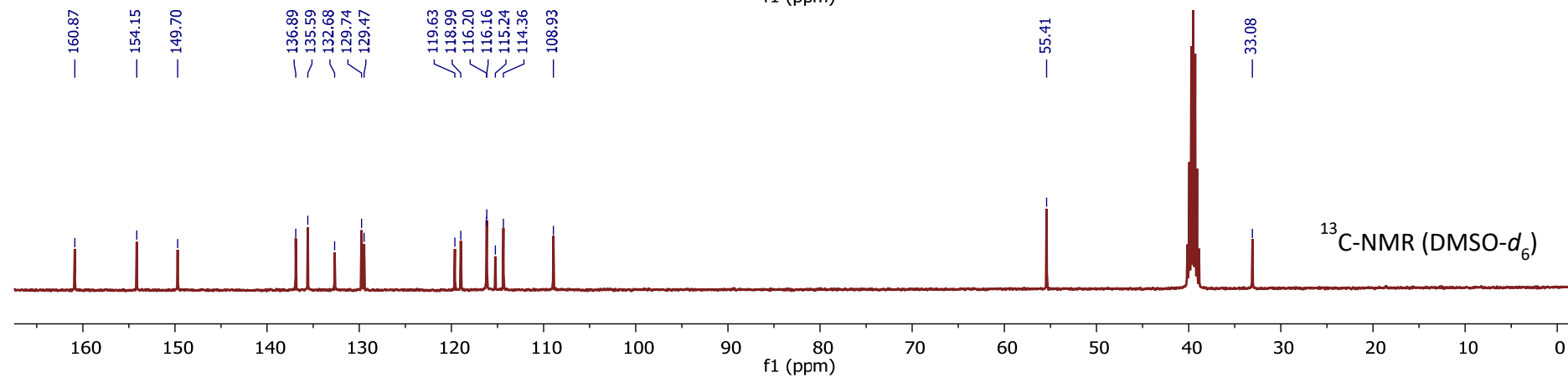
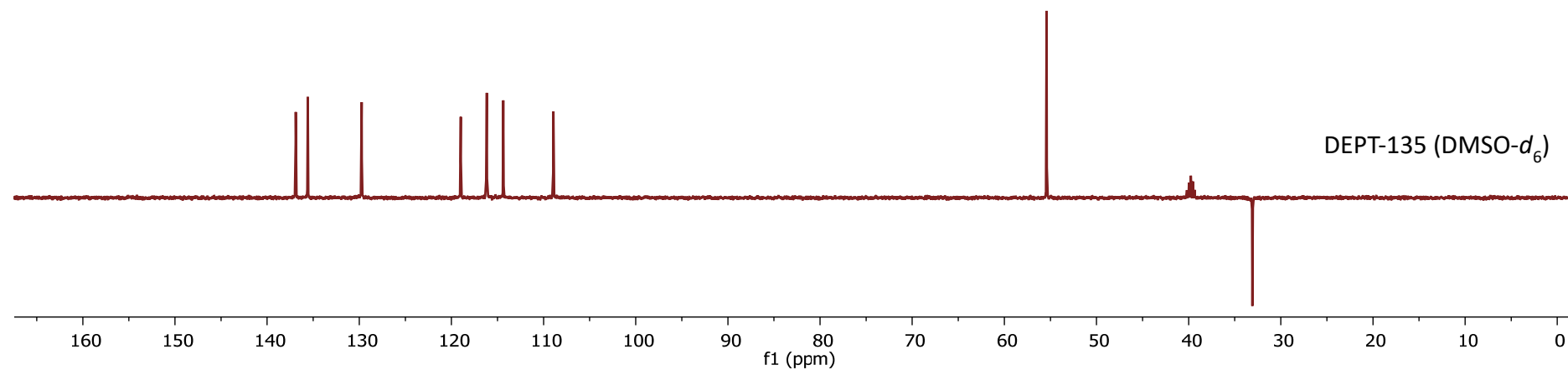
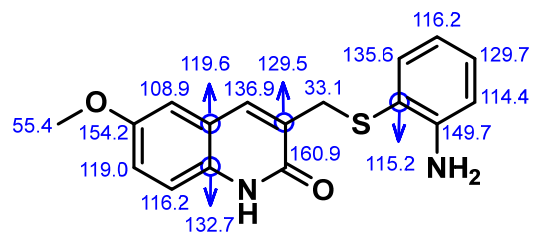


MS Spectrum Peak List

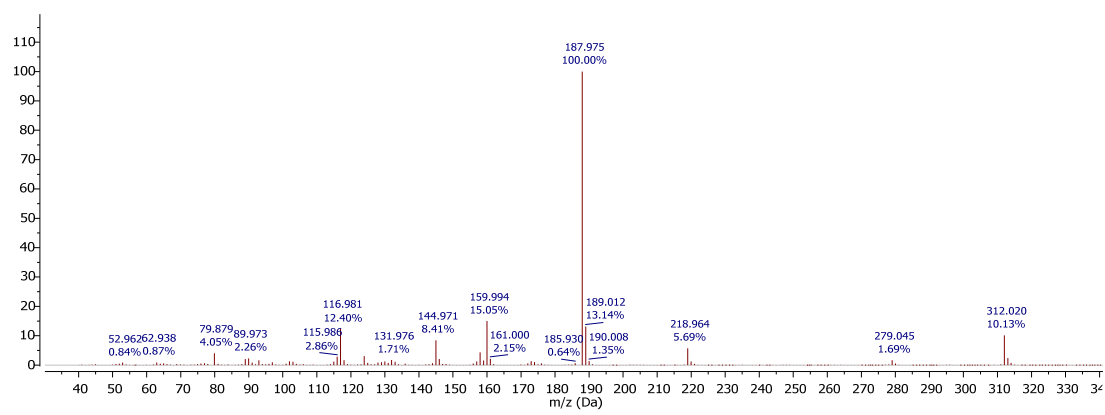
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
317.0513	317.051	-1.12	1	91054.87	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
318.0546	318.054	-1.99	1	15869.8	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
319.0487	319.0483	-1.11	1	31865.69	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
320.051	320.051	0.26	1	5519.68	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
321.0472	321.0471	-0.25	1	1600.66	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
339.0331	339.0329	-0.36	1	3268.07	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
340.035	340.0359	2.52	1	831.13	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
341.0312	341.0303	-2.87	1	1435.39	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
655.0763	655.0766	0.5	1	451.57	C ₁₆ H ₁₃ ClN ₂ OS	(2M+Na) ⁺
657.0732	657.0744	1.72	1	361.43	C ₁₆ H ₁₃ ClN ₂ OS	(2M+Na) ⁺

4.7 Compound 22c

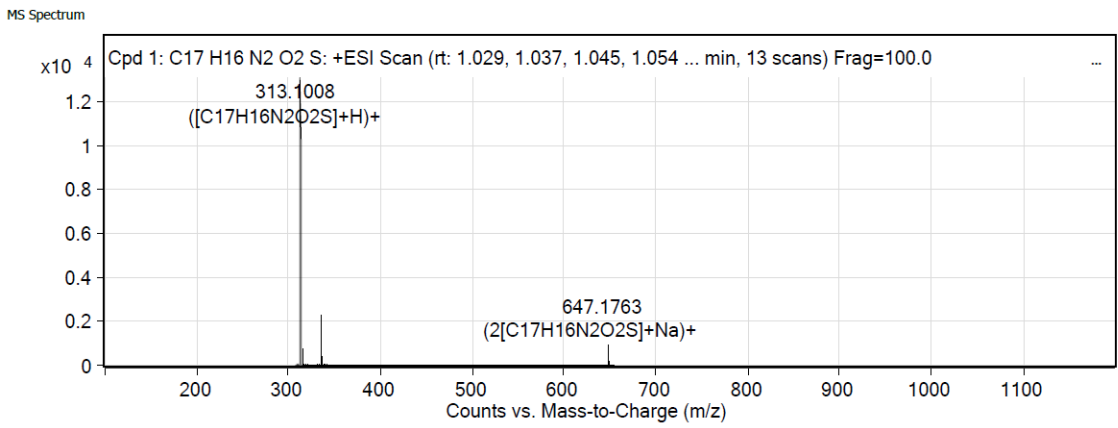




EI MS (70eV)



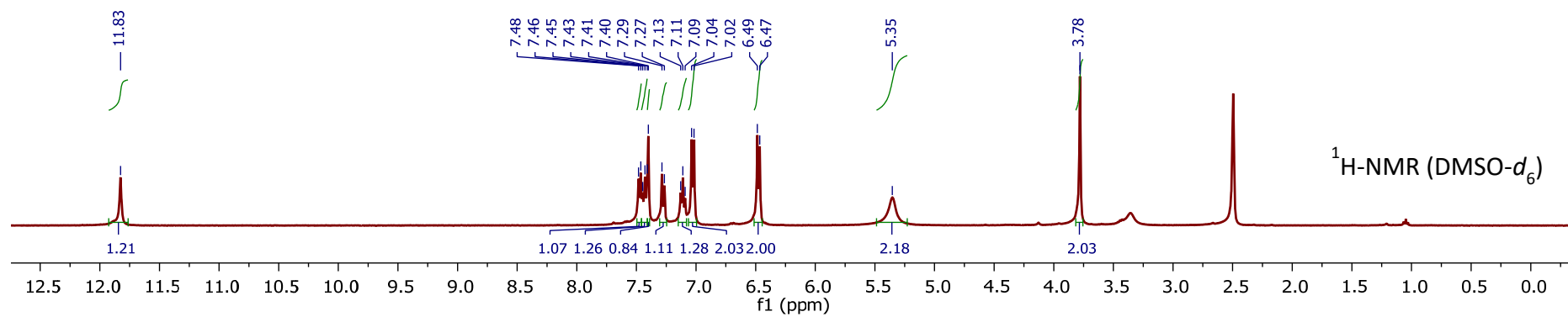
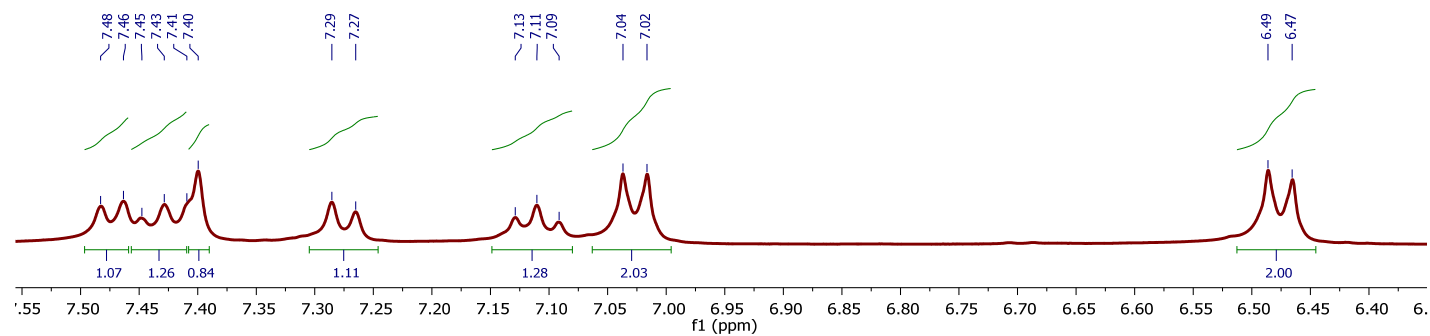
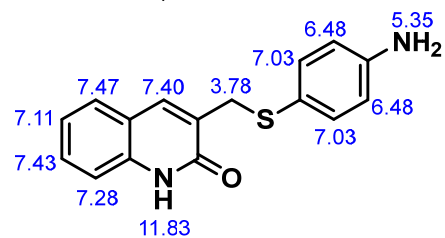
ESI-QTOF (positive ionization)

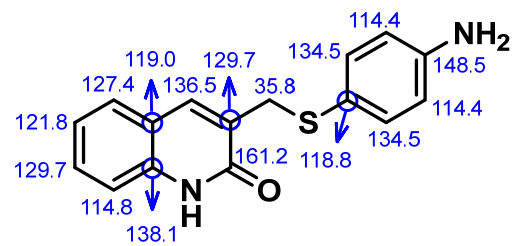


MS Spectrum Peak List

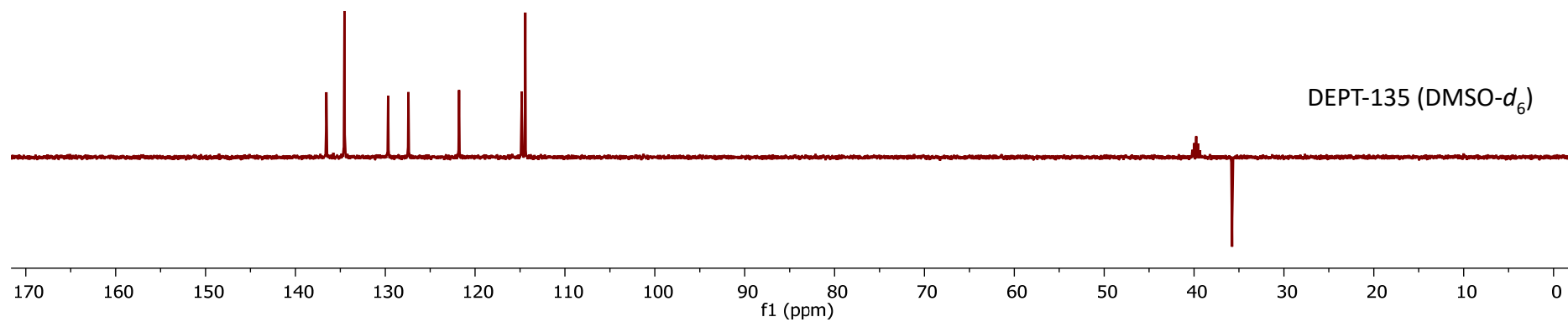
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
313.1008	313.1005	-1.02	1	13382.66	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H) ⁺
314.1039	314.1035	-1.22	1	2447.19	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H) ⁺
315.0996	315.0997	0.44	1	729.27	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H) ⁺
316.0981	316.1012	9.69	1	89.5	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H) ⁺
335.0826	335.0825	-0.45	1	2424.13	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+Na) ⁺
336.085	336.0855	1.39	1	462.95	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+Na) ⁺
337.0844	337.0817	-8.1	1	175.52	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+Na) ⁺
647.1763	647.1757	-0.84	1	988.01	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na) ⁺
648.1807	648.1787	-3.08	1	355.91	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na) ⁺
649.1746	649.1765	2.89	1	205.42	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na) ⁺

4.8 Compound 23a

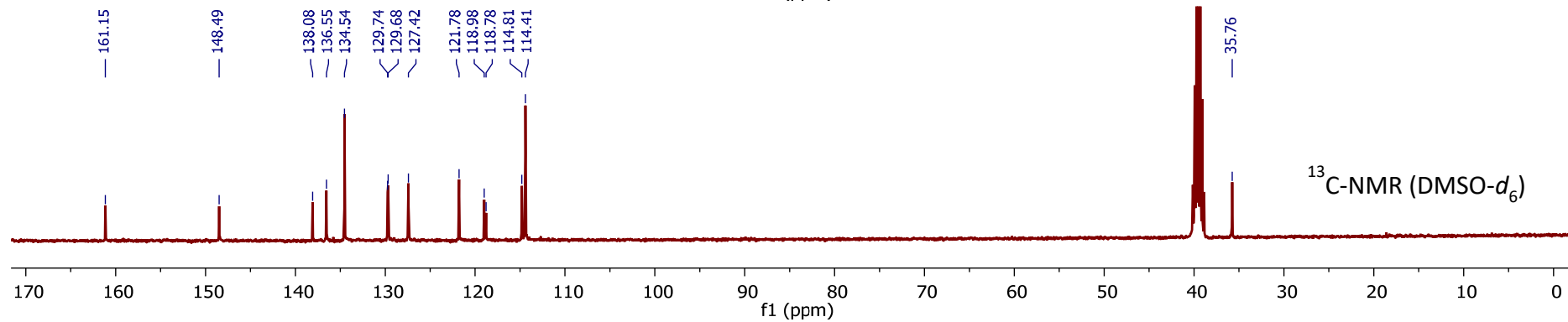




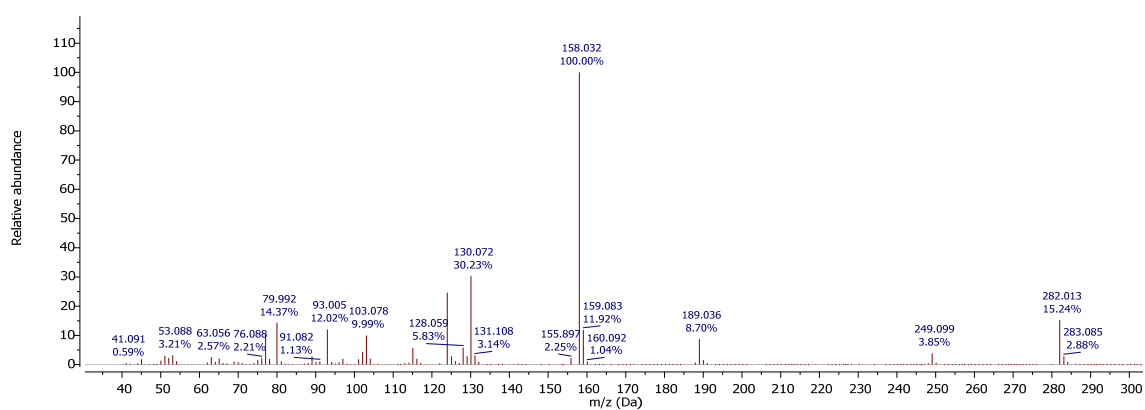
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

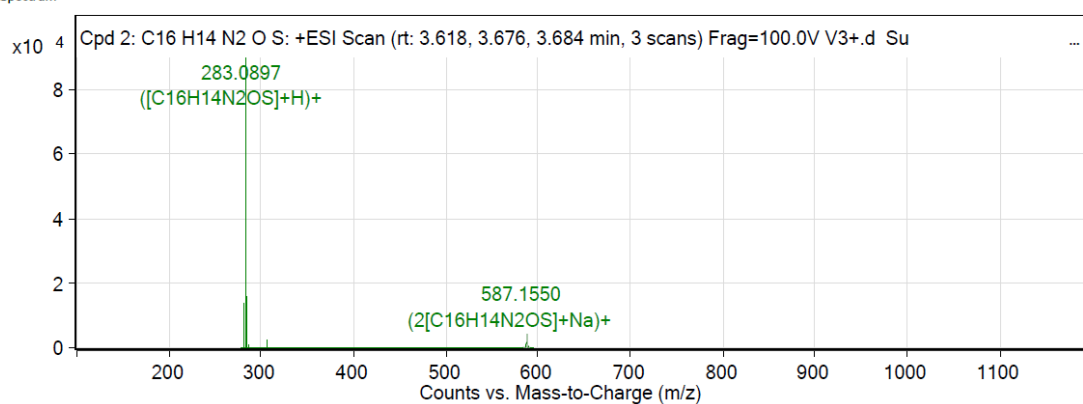


EI MS (70eV)



ESI-QTOF (positive ionization)

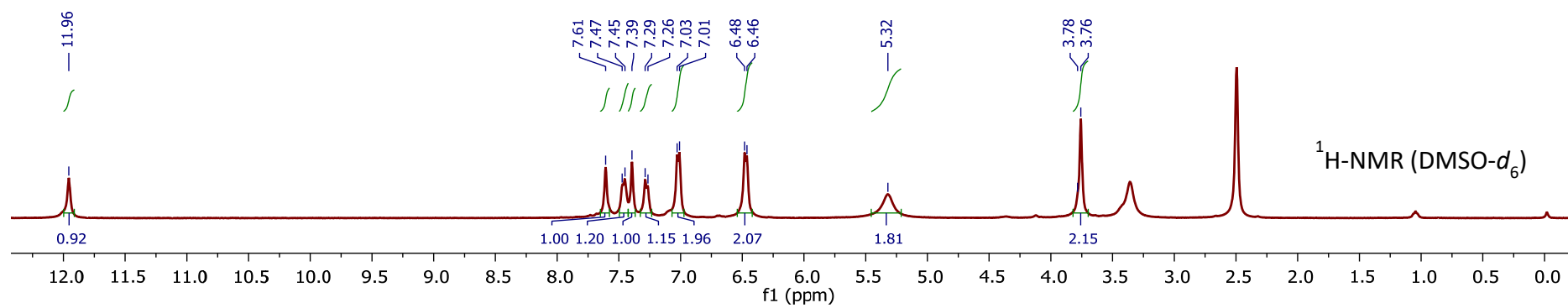
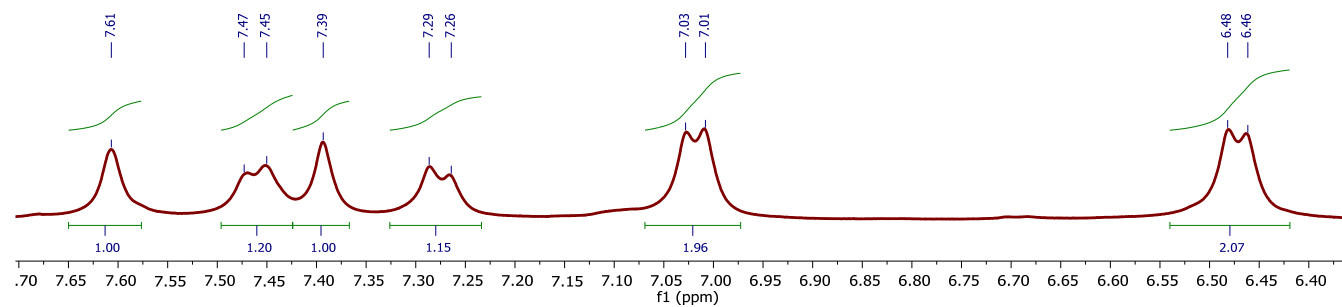
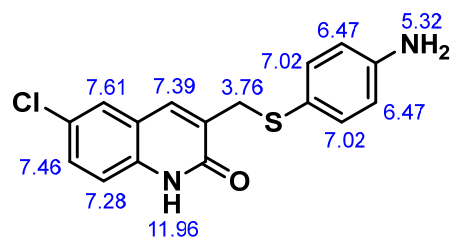
MS Spectrum

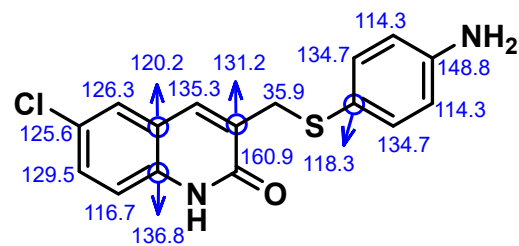


MS Spectrum Peak List

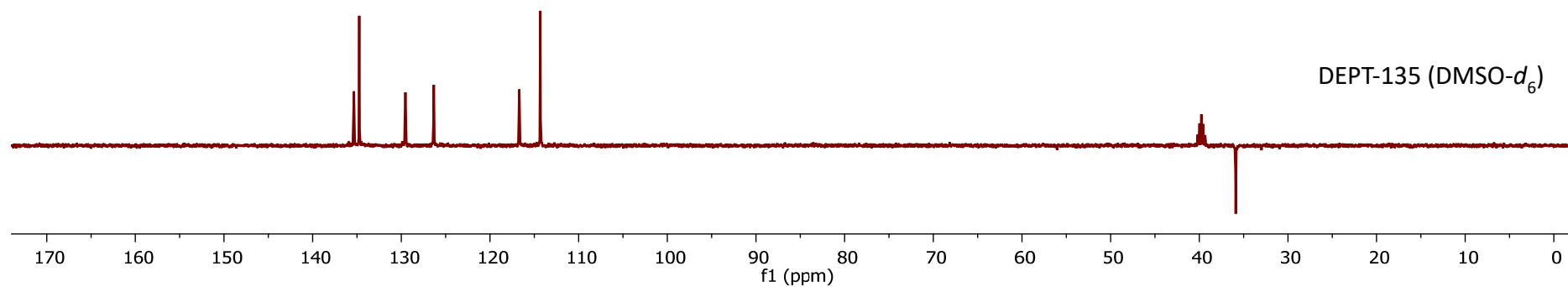
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
283.0897	283.09	0.78	1	90184.47	C16H14N2OS	(M+H)+
284.0929	284.0929	0.17	1	15839.54	C16H14N2OS	(M+H)+
285.0884	285.0887	1.25	1	4394.17	C16H14N2OS	(M+H)+
305.0717	305.0719	0.82	1	2215.43	C16H14N2OS	(M+Na)+
306.0746	306.0749	0.94	1	412.94	C16H14N2OS	(M+Na)+
307.0649	307.0707	18.86	1	152.5	C16H14N2OS	(M+Na)+
587.155	587.1546	-0.65	1	4516.79	C16H14N2OS	(2M+Na)+
588.1582	588.1576	-1.16	1	1762.98	C16H14N2OS	(2M+Na)+
589.1559	589.155	-1.66	1	727.91	C16H14N2OS	(2M+Na)+

4.9 Compound 23b

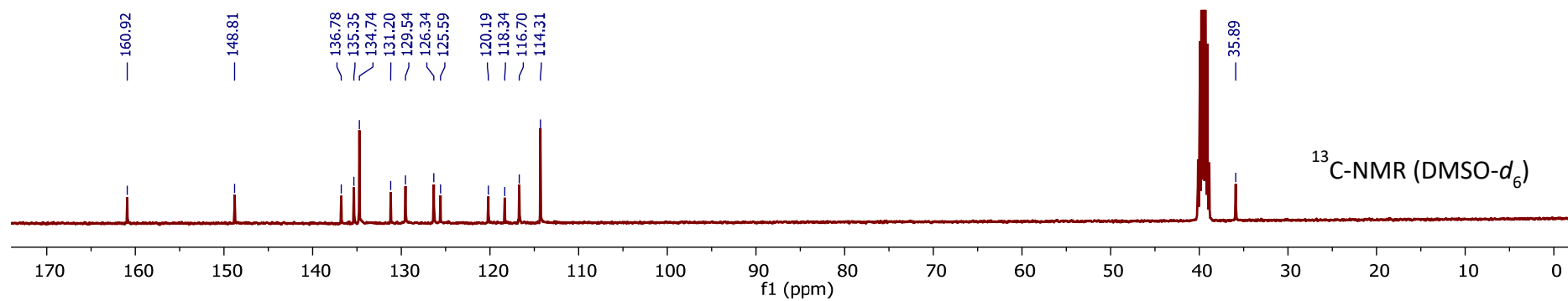




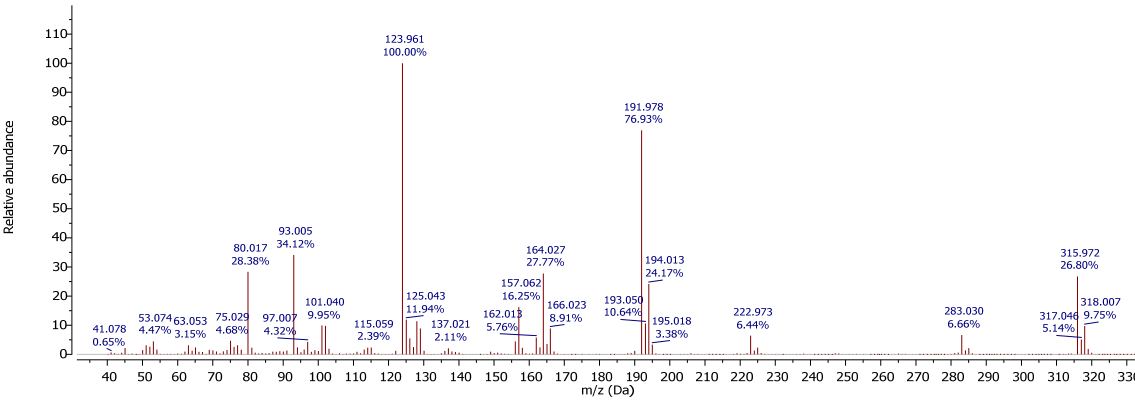
DEPT-135 (DMSO- d_6)



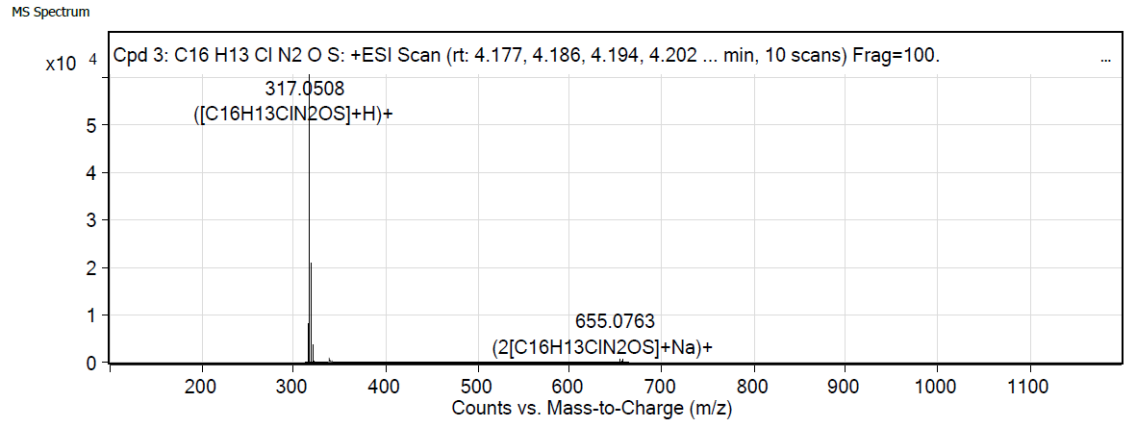
^{13}C -NMR (DMSO- d_6)



EI MS (70eV)



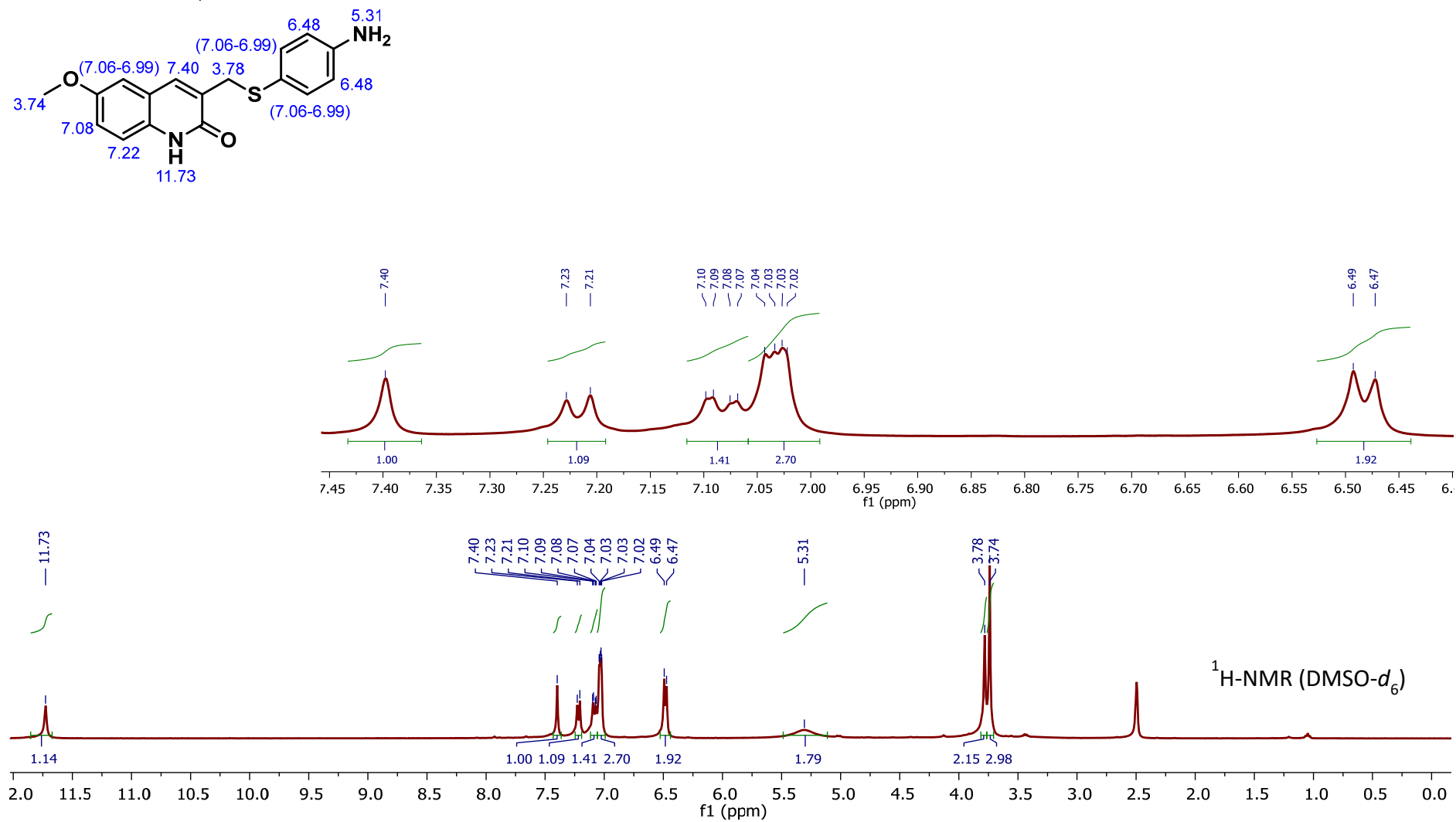
ESI-QTOF (positive ionization)

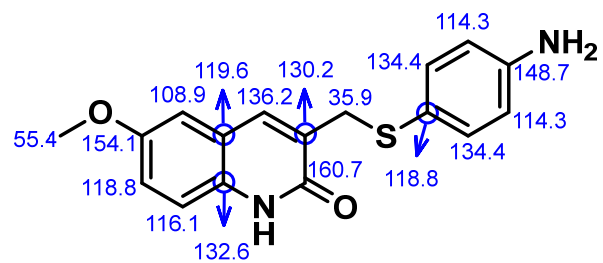


MS Spectrum Peak List

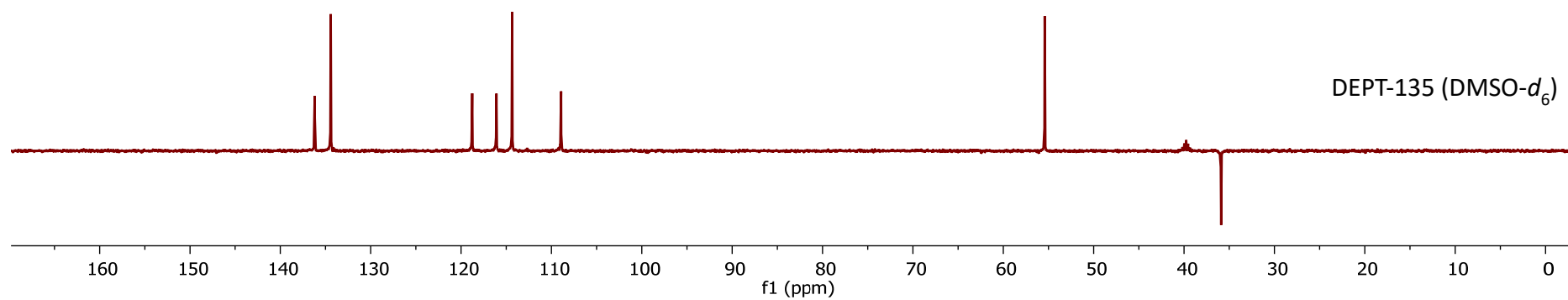
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
317.0508	317.051	0.45	1	60594.69	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+H) ⁺
318.0519	318.054	6.5	1	11698.33	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+H) ⁺
319.048	319.0483	1.08	1	21302.87	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+H) ⁺
320.0507	320.051	1.13	1	3894.05	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+H) ⁺
321.0456	321.0471	4.49	1	1189.33	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+H) ⁺
339.0321	339.0329	2.45	1	937.9	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+Na) ⁺
341.0301	341.0303	0.58	1	342.45	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(M+Na) ⁺
655.0763	655.0766	0.55	1	663.34	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(2M+Na) ⁺
657.0749	657.0744	-0.84	1	508.51	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(2M+Na) ⁺
658.0775	658.0768	-1.07	1	251.62	C ₁₆ H ₁₃ ClN ₂ O ₂ S	(2M+Na) ⁺

4.10 Compound 23c

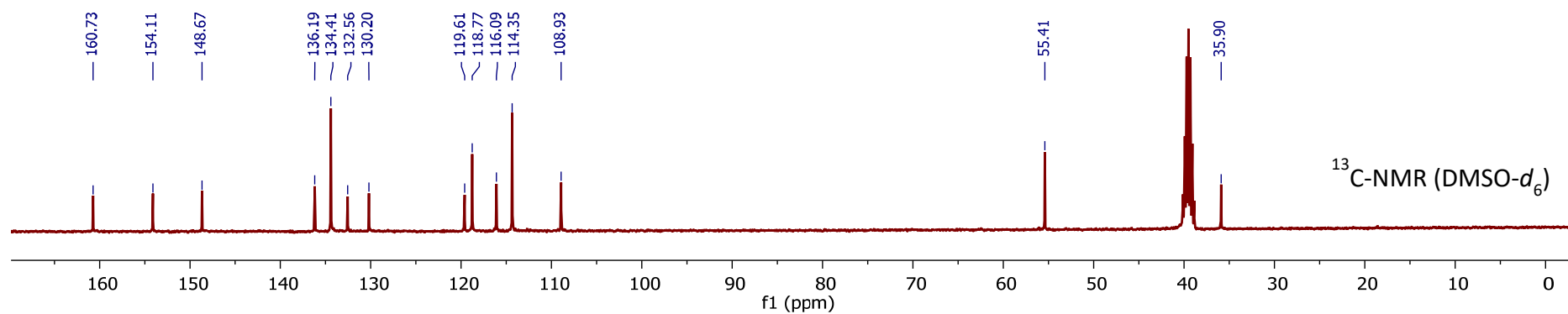




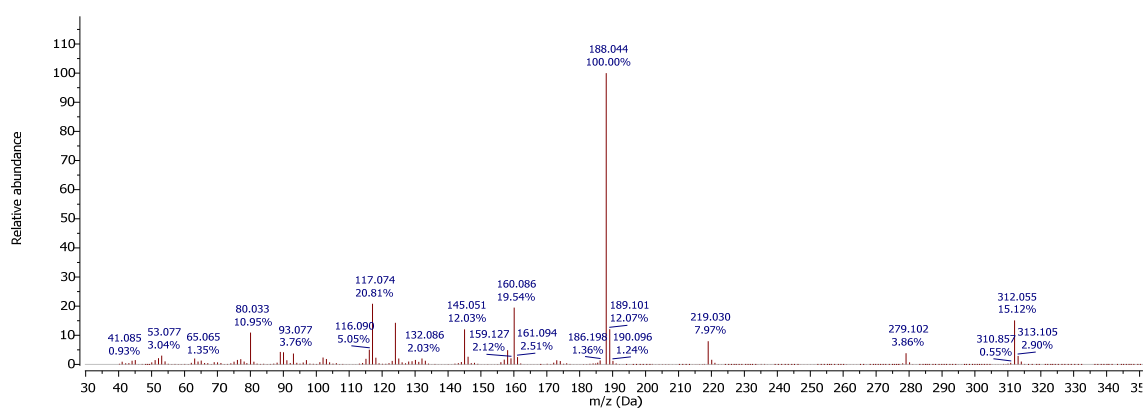
DEPT-135 (DMSO-*d*₆)



¹³C-NMR (DMSO-*d*₆)

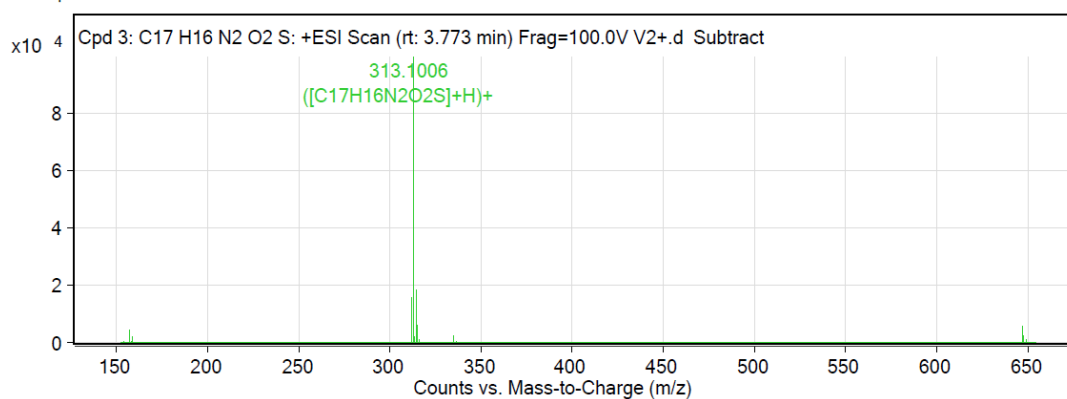


EI MS (70eV)



ESI-QTOF (positive ionization)

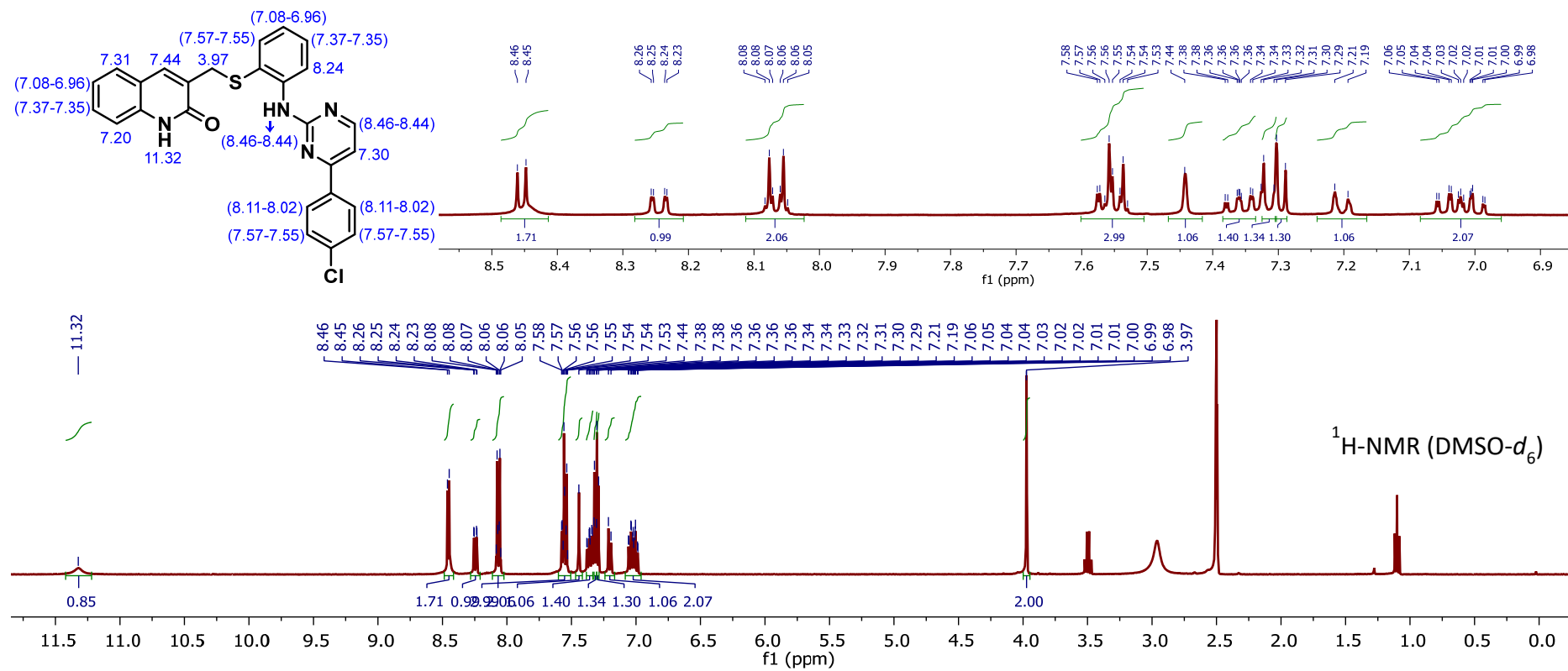
MS Zoomed Spectrum

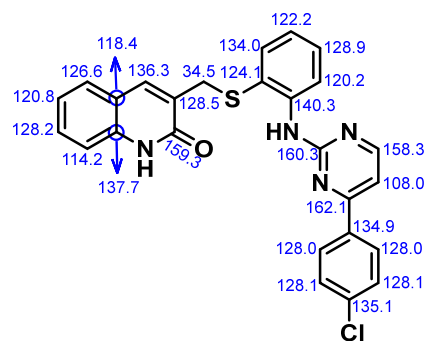


MS Spectrum Peak List

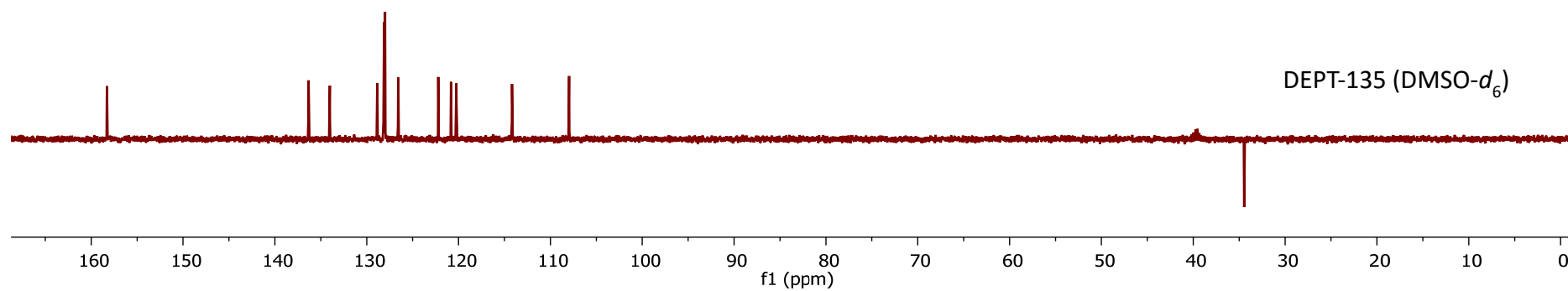
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
157.0524	157.0539	9.51	2	4559.77	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+2H)+2
157.5549	157.5554	3.06	2	765.06	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+2H)+2
313.1006	313.1005	-0.33	1	102166.45	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H)+
314.1042	314.1035	-2	1	18677.32	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H)+
315.0997	315.0997	-0.02	1	6155.71	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+H)+
335.0829	335.0825	-1.31	1	2635.22	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+Na)+
336.0885	336.0855	-9.12	1	518.64	C ₁₇ H ₁₆ N ₂ O ₂ S	(M+Na)+
647.177	647.1757	-2.05	1	5555	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na)+
648.1801	648.1787	-2.06	1	2482.27	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na)+
649.1823	649.1765	-8.92	1	842.61	C ₁₇ H ₁₆ N ₂ O ₂ S	(2M+Na)+

4.11 Compound 24a

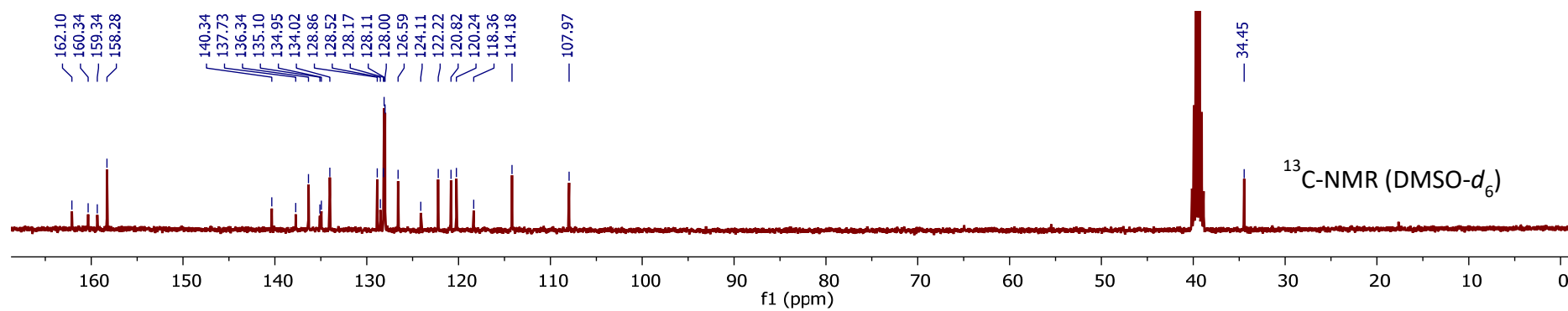




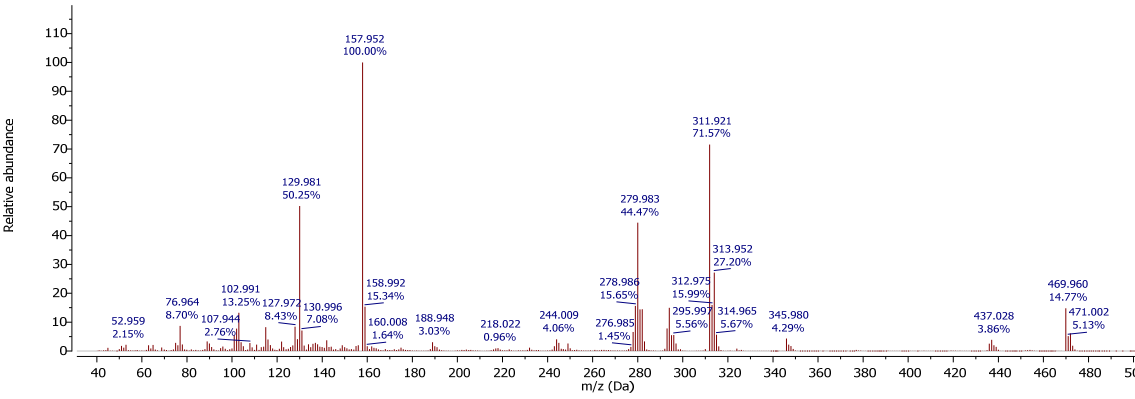
DEPT-135 ($\text{DMSO}-d_6$)



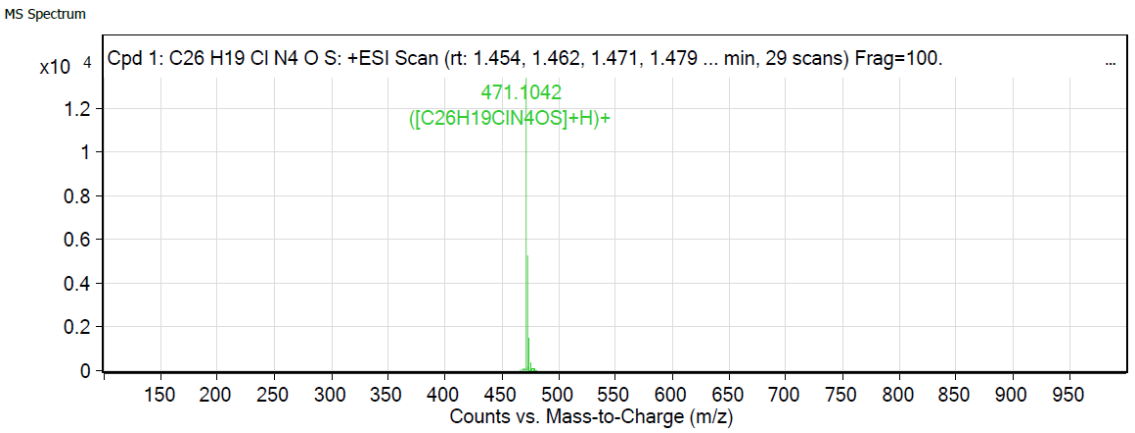
^{13}C -NMR ($\text{DMSO}-d_6$)



EI MS (70eV)



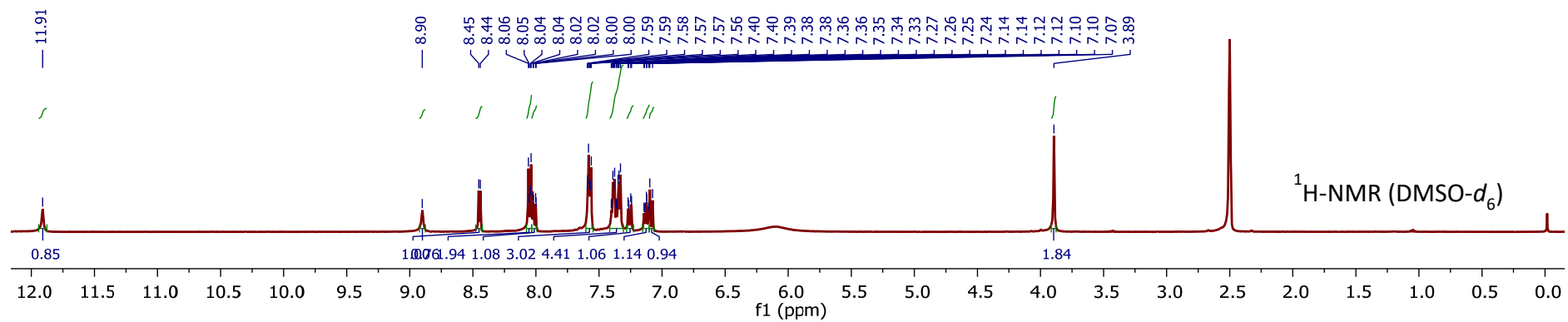
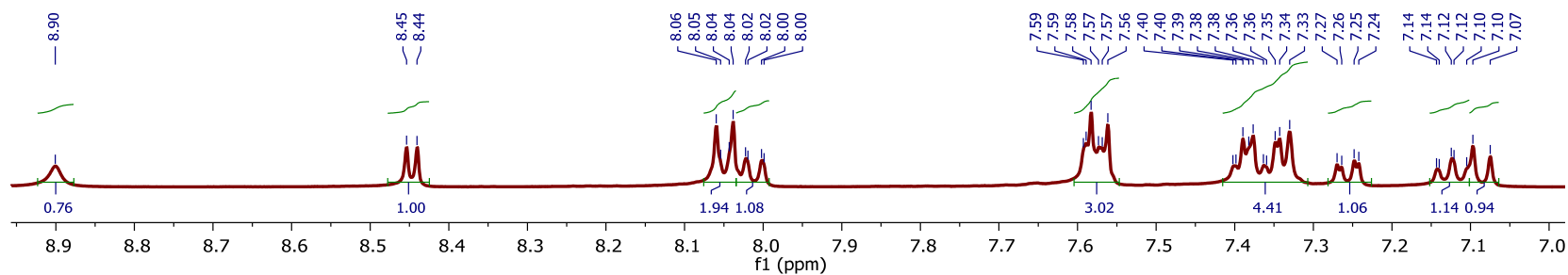
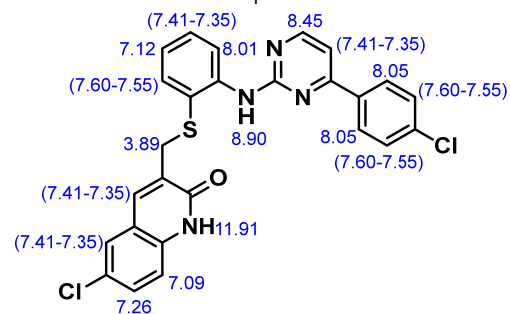
ESI-QTOF (positive ionization)

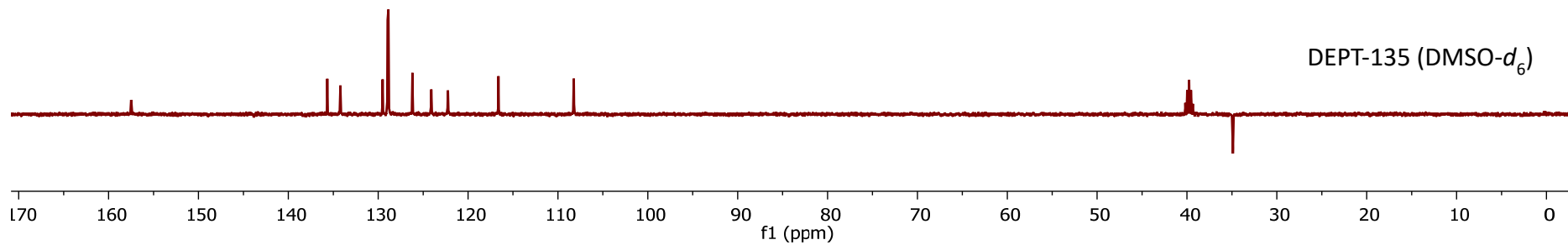


MS Spectrum Peak List

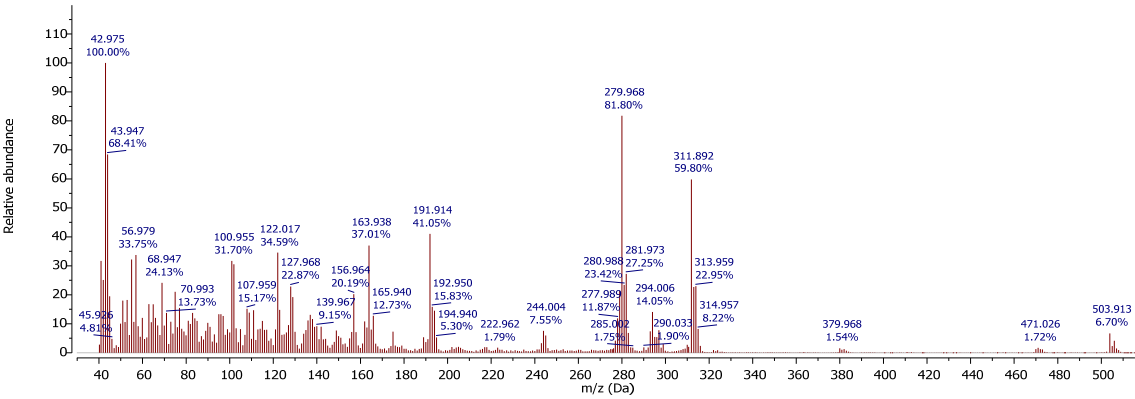
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
471.1042	471.1041	-0.14	1	13681.64	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺
472.1075	472.1071	-0.84	1	3982.72	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺
473.1018	473.102	0.35	1	5511.6	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺
474.1039	474.1043	0.85	1	1595.88	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺
475.1025	475.1025	-0.09	1	360.43	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺
476.1051	476.1029	-4.52	1	47.53	C ₂₆ H ₁₉ ClN ₄ O ₅	(M+H) ⁺

4.12 Compound 24b

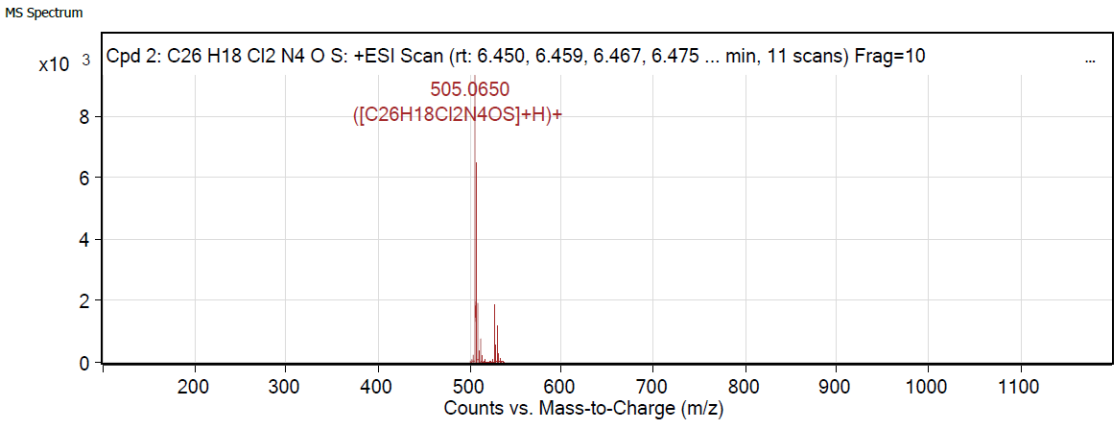




EI MS (70eV)

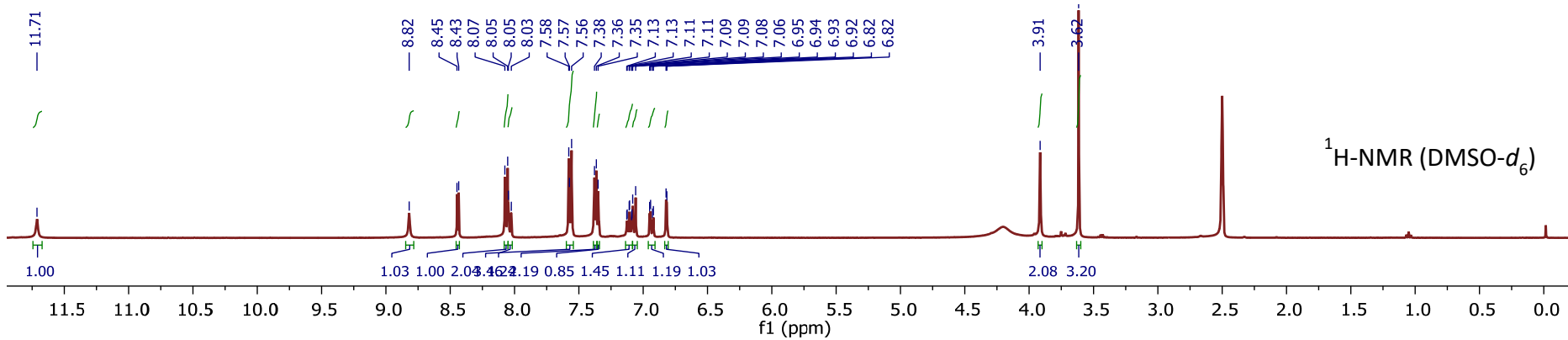
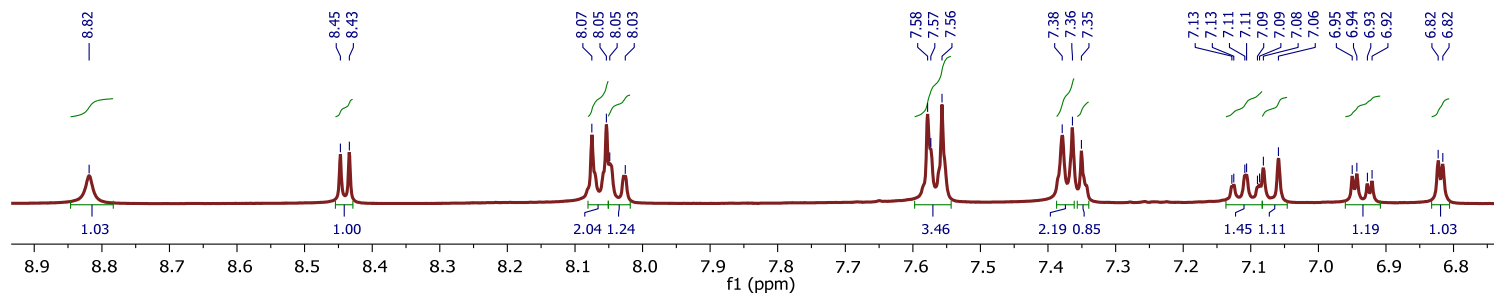
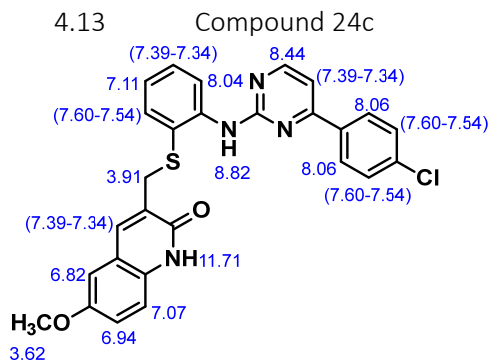


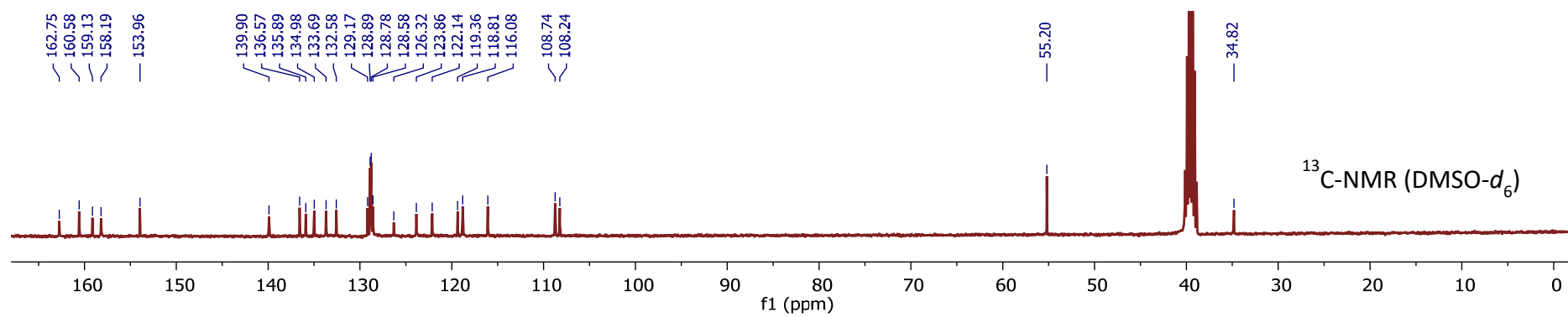
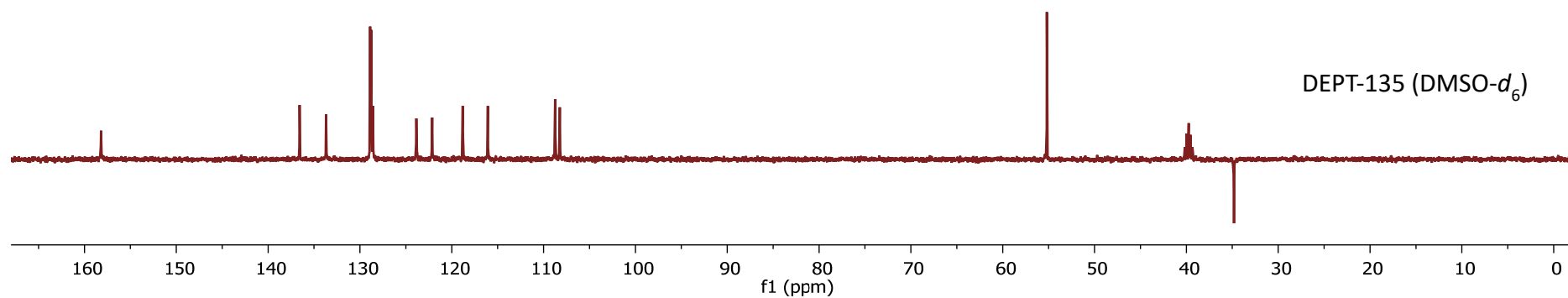
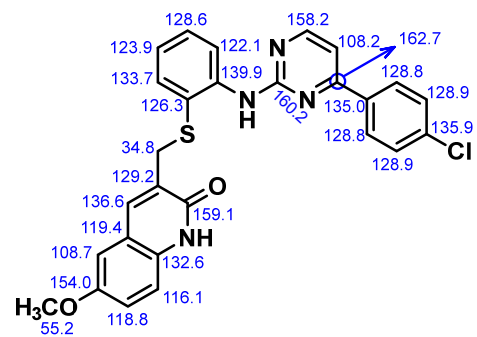
ESI-QTOF (positive ionization)



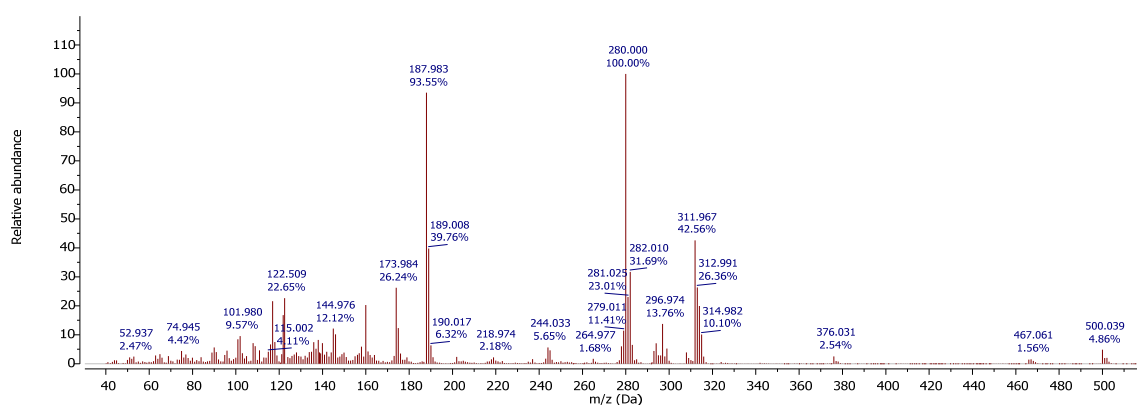
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
505.065	505.0651	0.24	1	9495.01	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
506.0685	506.0681	-0.87	1	3037.56	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
507.0624	507.0627	0.55	1	6658.38	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
508.0651	508.0653	0.41	1	1980.76	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
509.0605	509.0608	0.52	1	1507.94	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
510.0626	510.0626	0.07	1	423.29	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+H)+
527.0473	527.0471	-0.55	1	1897.1	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+Na)+
528.0515	528.05	-2.84	1	538.21	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+Na)+
529.0448	529.0446	-0.36	1	1290.64	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+Na)+
530.0491	530.0472	-3.54	1	371.94	C ₂₆ H ₁₈ Cl ₂ N ₄ OS	(M+Na)+



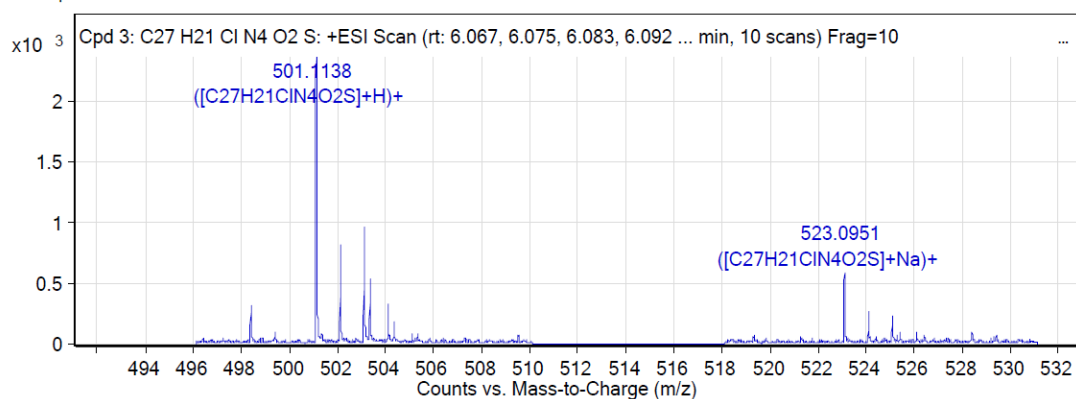


EI MS (70eV)



ESI-QTOF (positive ionization)

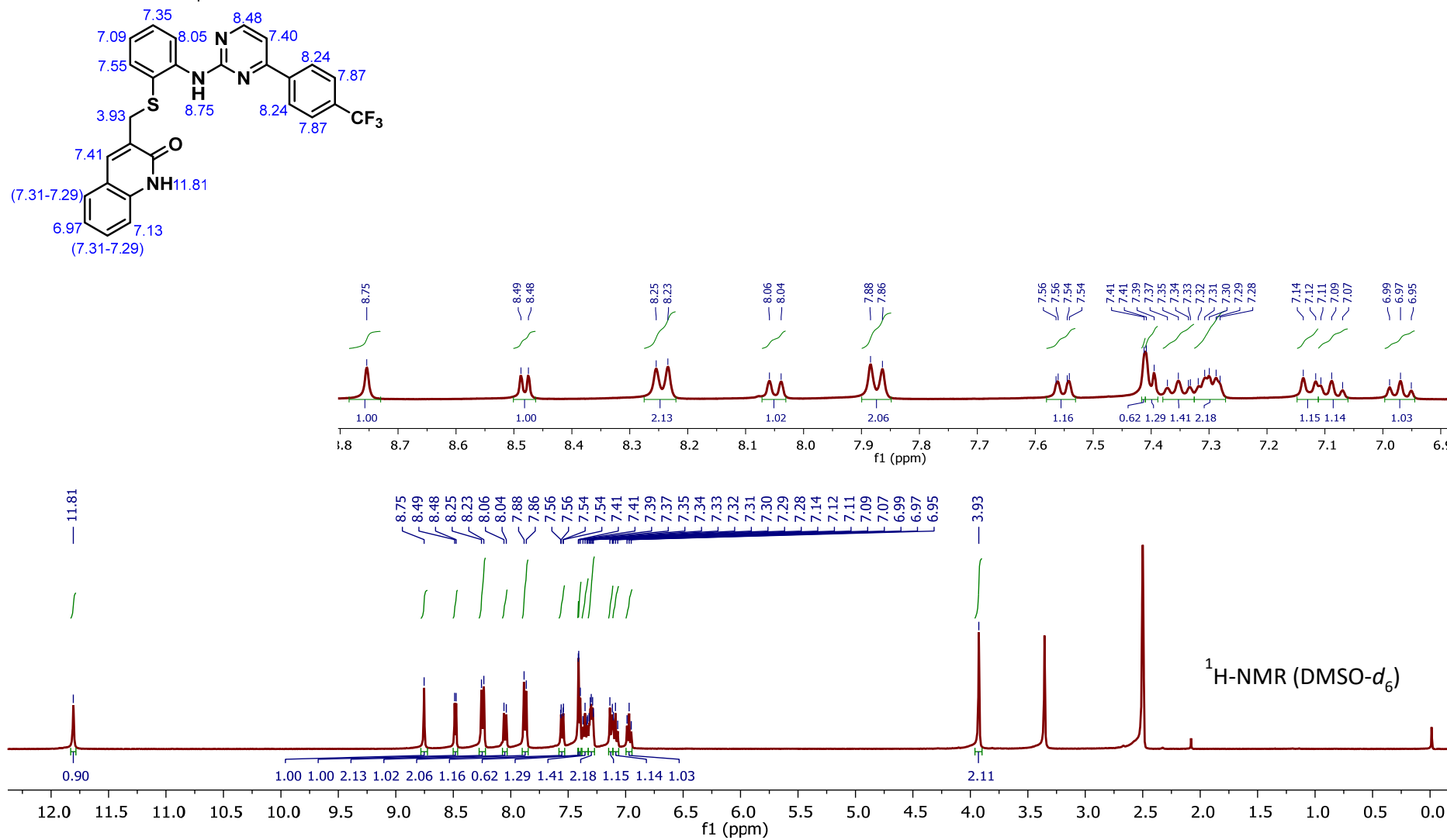
MS Zoomed Spectrum

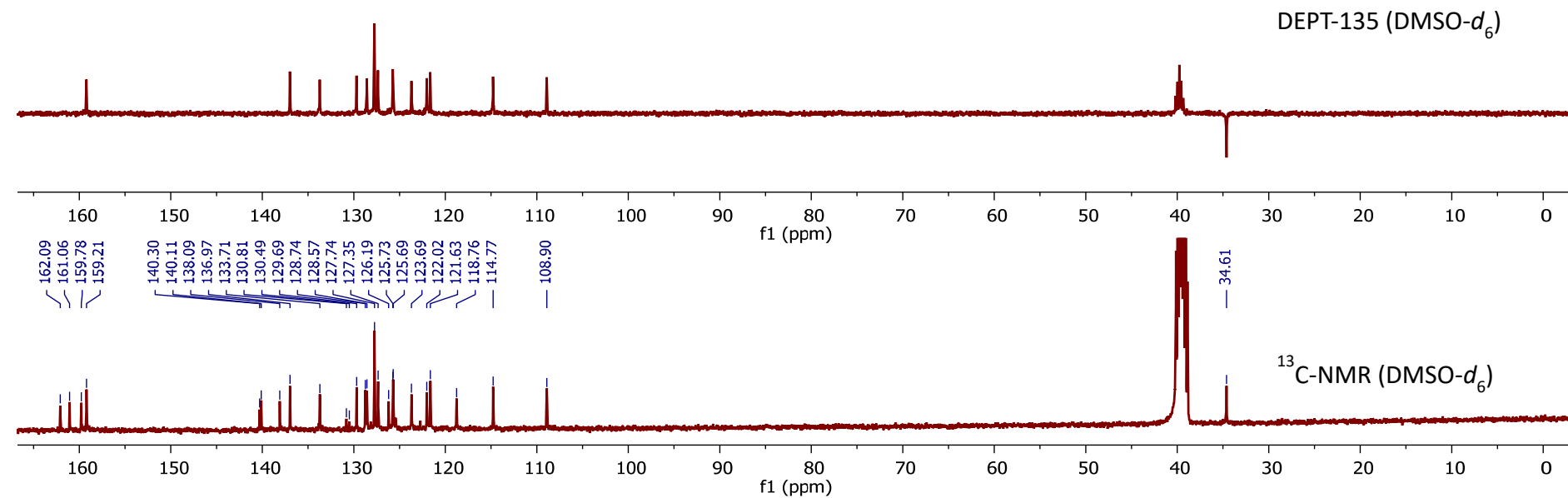


MS Spectrum Peak List

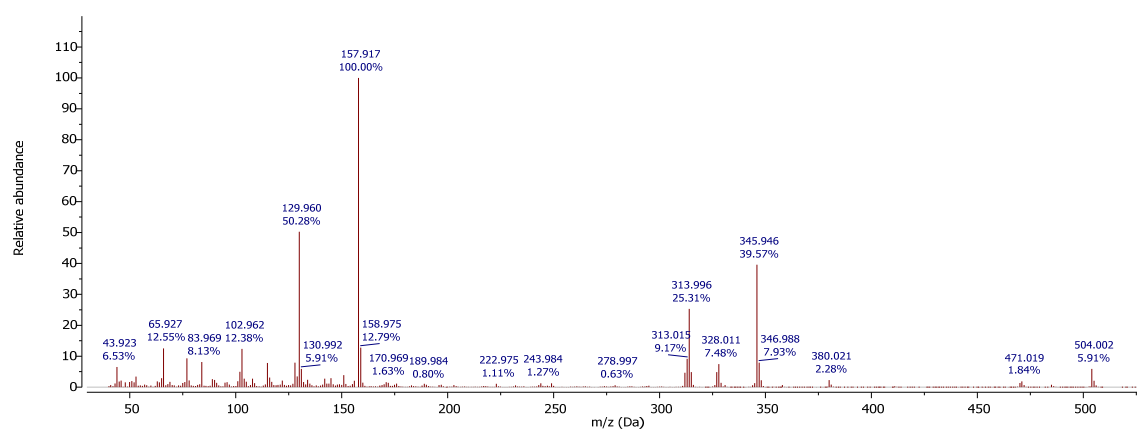
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
501.1138	501.1147	1.65	1	2387.34	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+H) ⁺
502.1158	502.1176	3.64	1	821.95	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+H) ⁺
503.1118	503.1127	1.77	1	1048.47	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+H) ⁺
504.1132	504.1115	3.65	1	374.25	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+H) ⁺
505.1054	505.1134	15.72	1	25.44	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+H) ⁺
523.0951	523.0966	2.88	1	604.97	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+Na) ⁺
524.099	524.0996	1.06	1	291.17	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+Na) ⁺
525.0945	525.0946	0.31	1	265.23	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+Na) ⁺
526.0955	526.0969	2.63	1	46.9	C ₂₇ H ₂₁ ClN ₄ O ₂ S	(M+Na) ⁺

4.14 Compound 25a

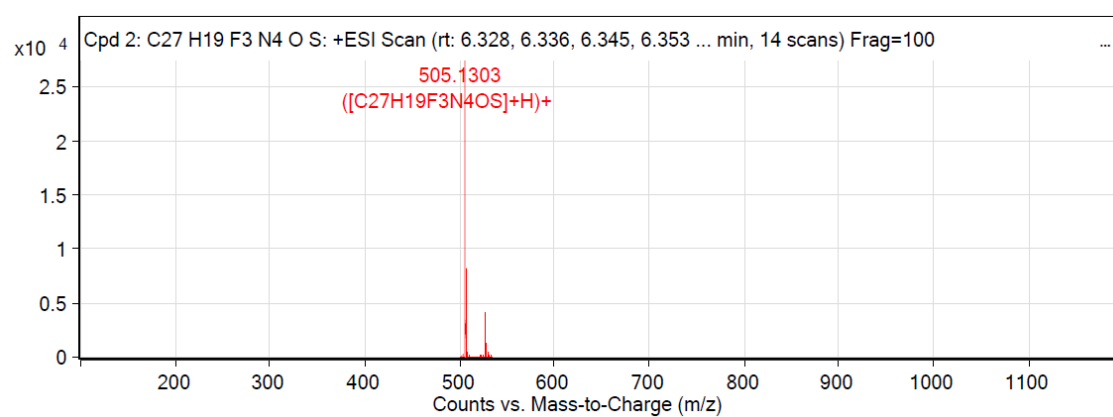




EI MS (70eV)

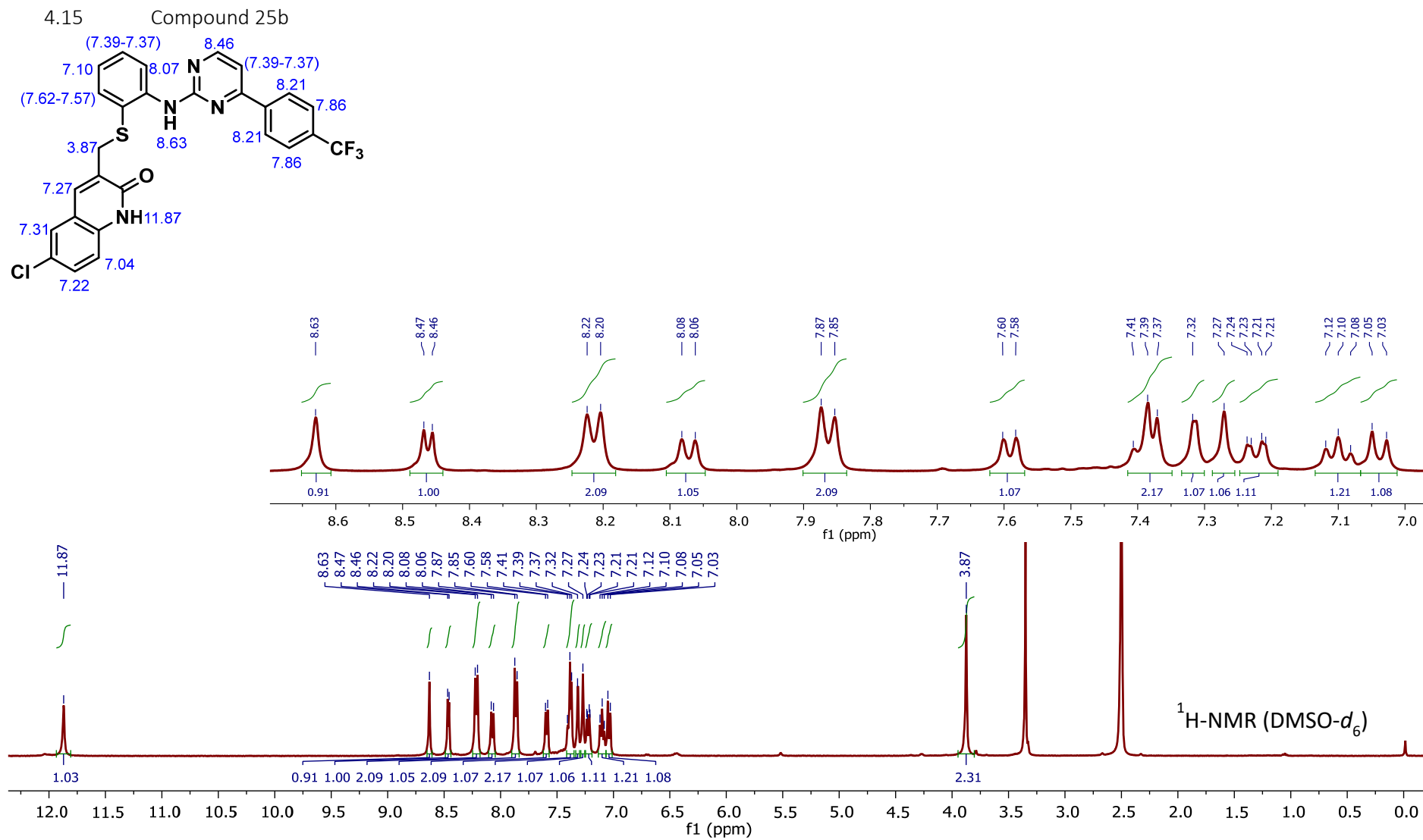


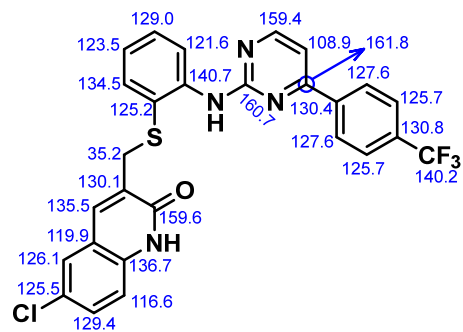
ESI-QTOF (positive ionization)



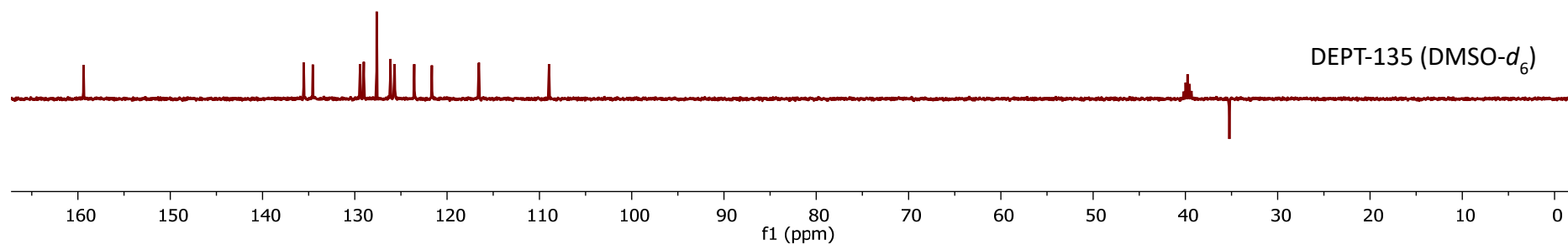
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
505.1303	505.1304	0.2	1	27882.64	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H) ⁺
506.1333	506.1334	0.34	1	8461.88	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H) ⁺
507.1315	507.1316	0.29	1	2272.03	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H) ⁺
527.1121	527.1124	0.55	1	4178.53	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na) ⁺
528.1155	528.1154	-0.25	1	1381.58	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na) ⁺
529.1131	529.1135	0.86	1	367.8	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na) ⁺

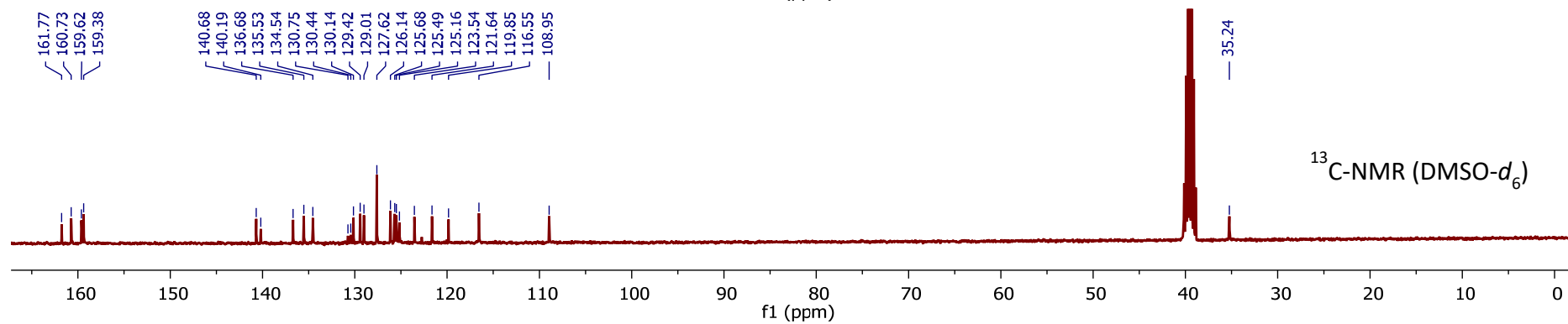




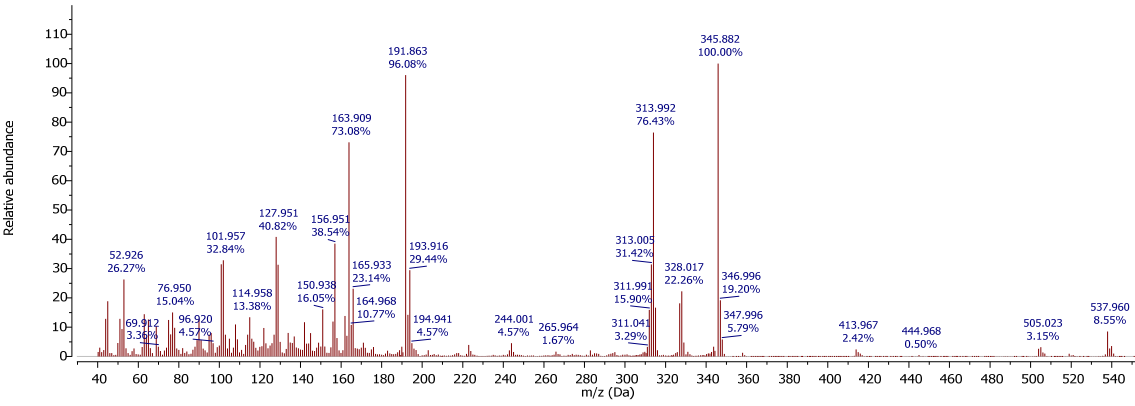
DEPT-135 ($\text{DMSO}-d_6$)



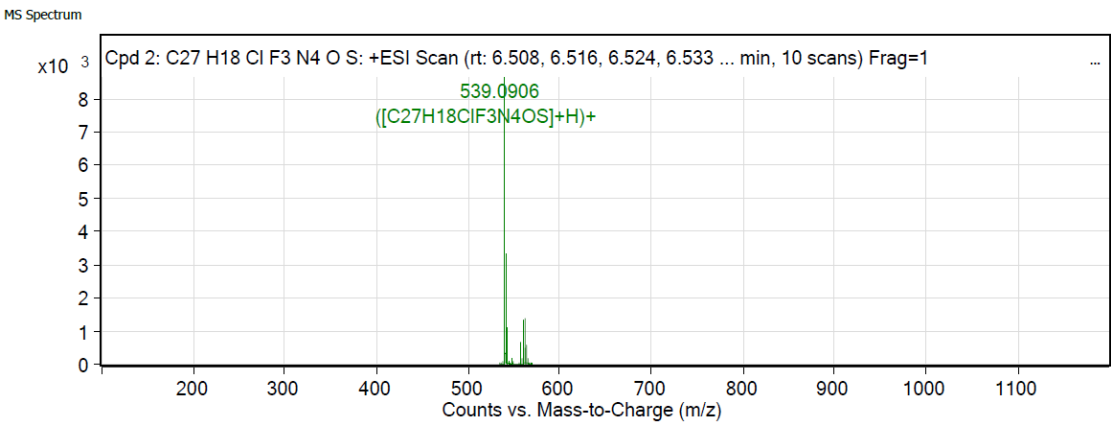
^{13}C -NMR ($\text{DMSO}-d_6$)



EI MS (70eV)

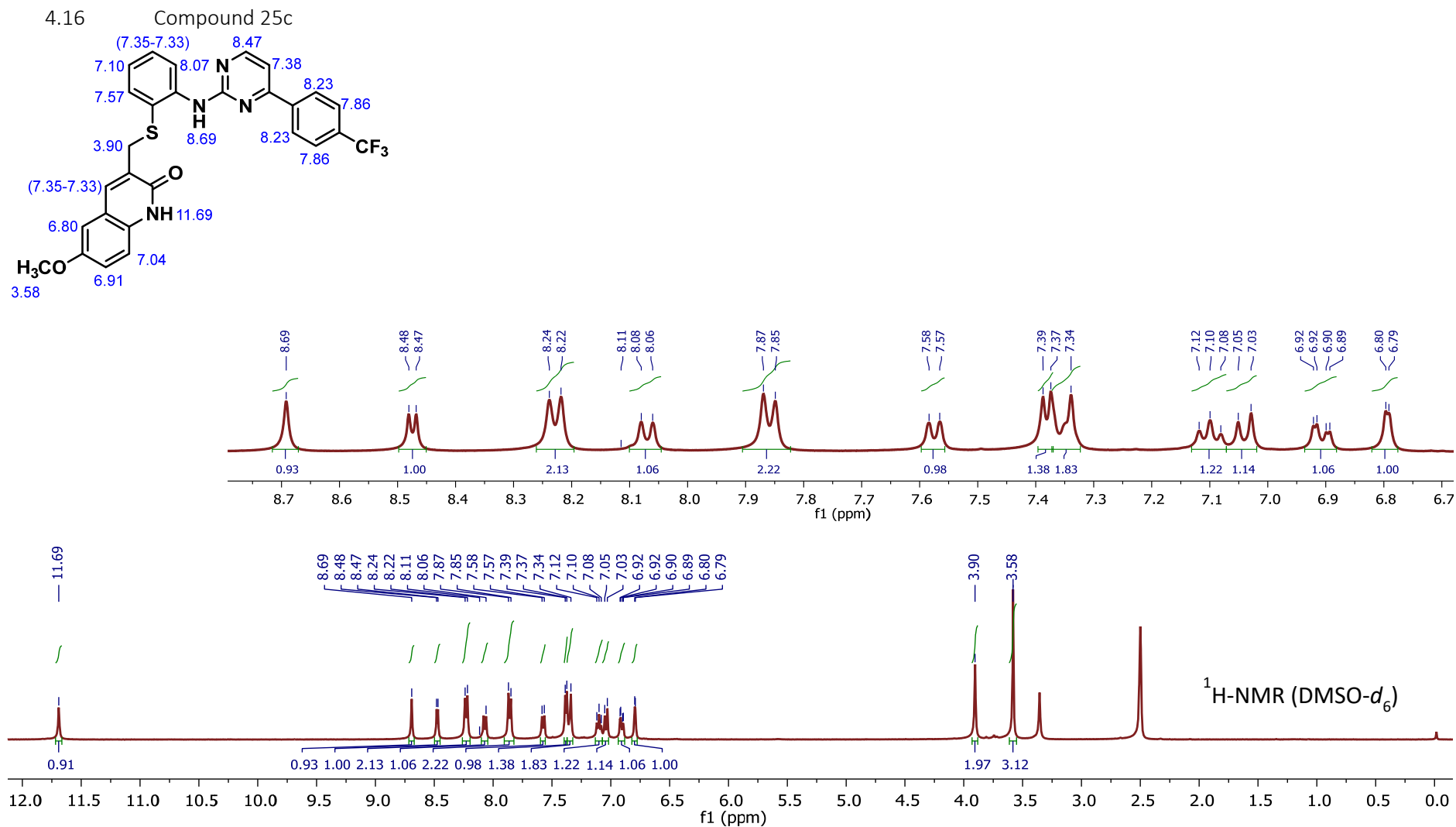


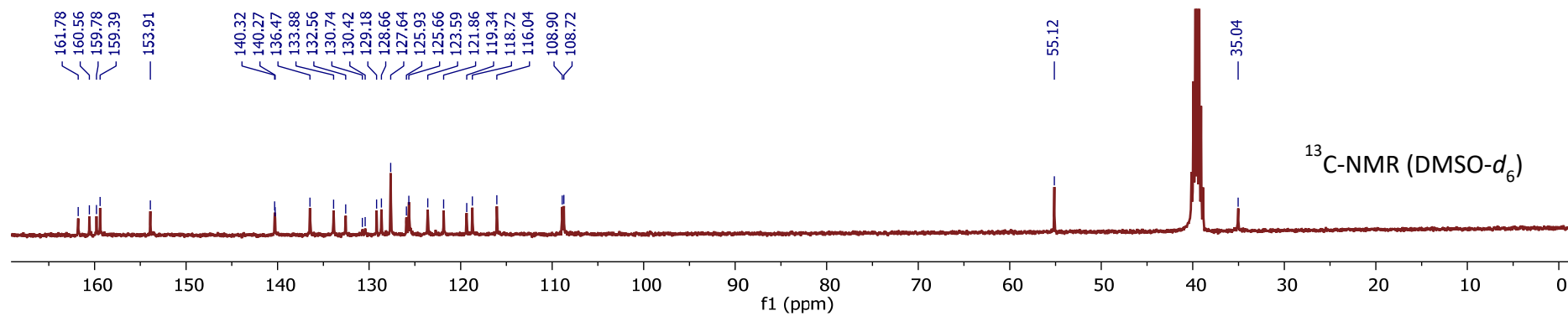
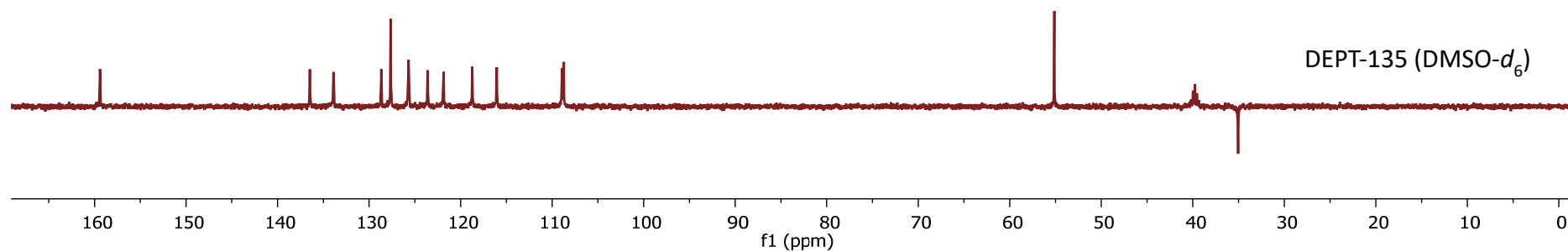
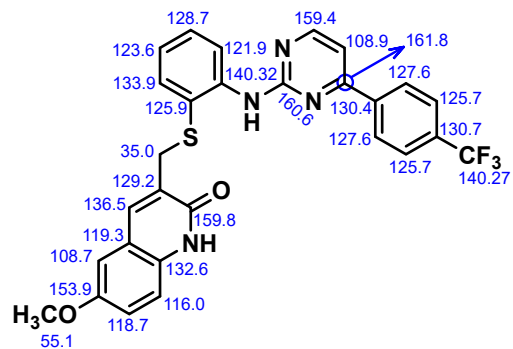
ESI-QTOF (positive ionization)



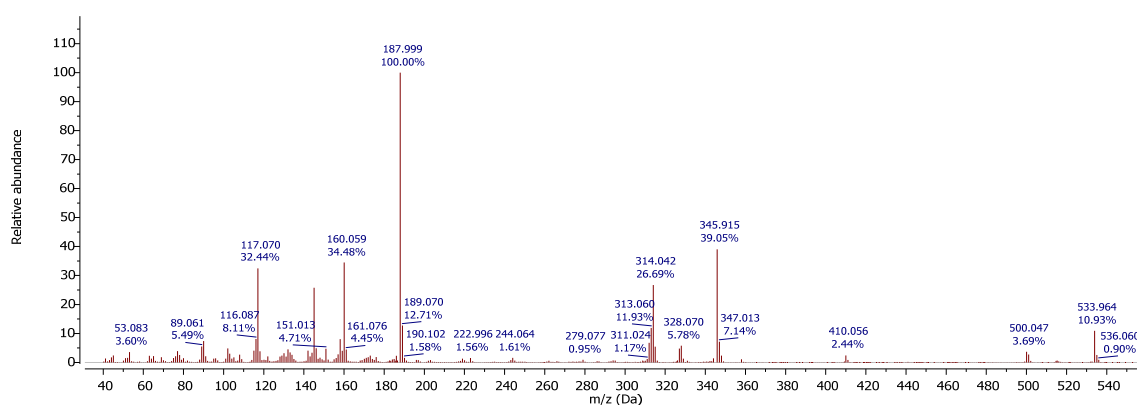
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
539.0906	539.0915	1.56	1	8896.48	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+H) ⁺
540.093	540.0945	2.7	1	2820.27	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+H) ⁺
541.0885	541.0895	1.72	1	3407.42	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+H) ⁺
542.0903	542.0918	2.72	1	1135.08	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+H) ⁺
543.0903	543.0901	-0.48	1	221.11	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+H) ⁺
561.0729	561.0734	0.87	1	1409.61	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+Na) ⁺
562.0749	562.0764	2.71	1	497.96	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+Na) ⁺
563.071	563.0714	0.77	1	598.91	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+Na) ⁺
564.0688	564.0737	8.76	1	130.54	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+Na) ⁺
565.0657	565.072	11.26	1	21.71	C ₂₇ H ₁₈ ClF ₃ N ₄ OS	(M+Na) ⁺



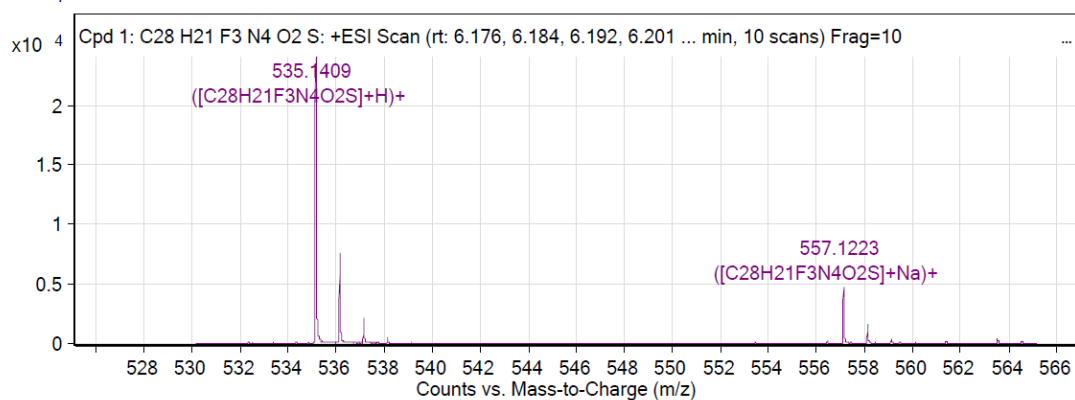


EI MS (70eV)



ESI-QTOF (positive ionization)

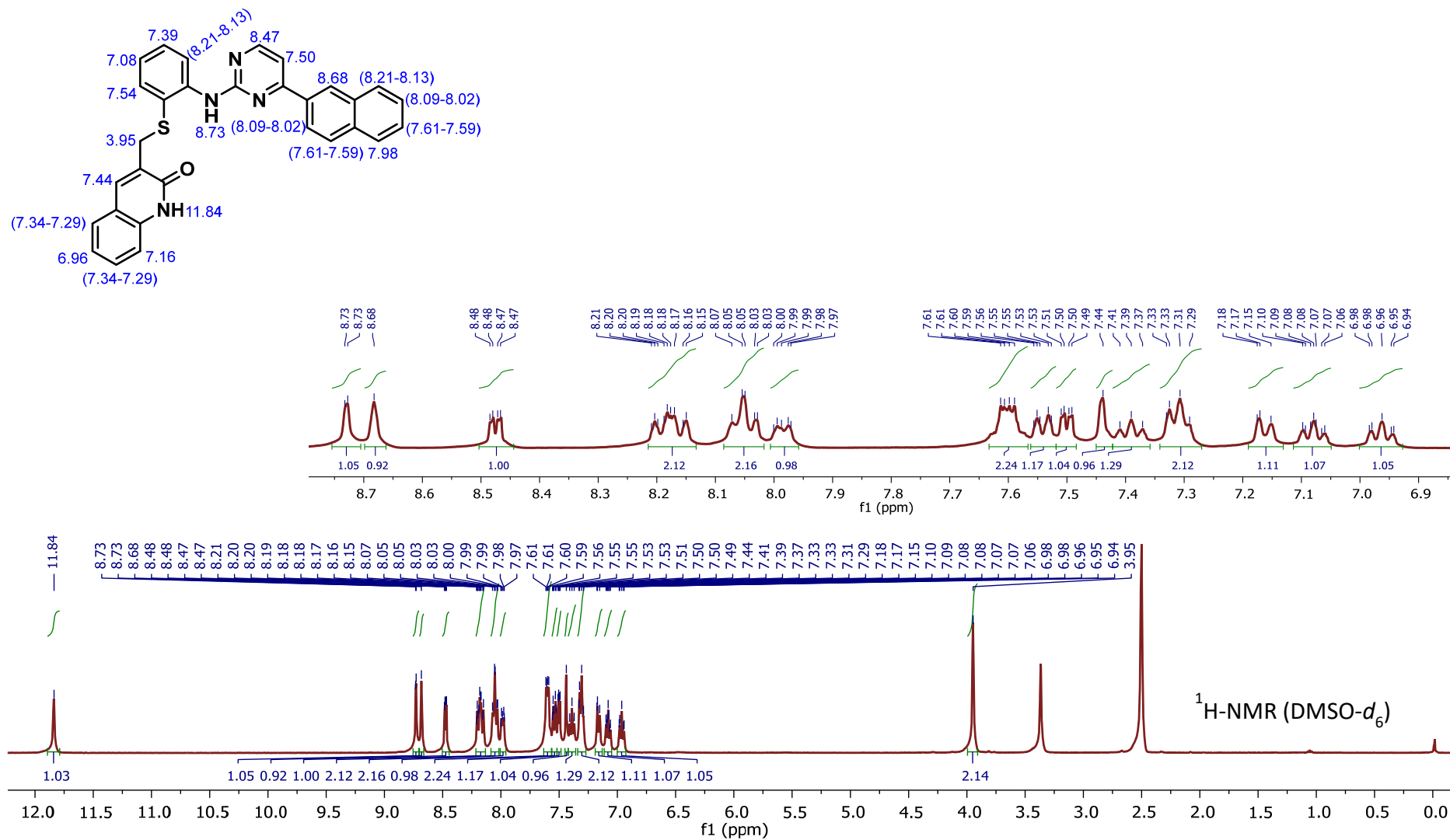
MS Zoomed Spectrum

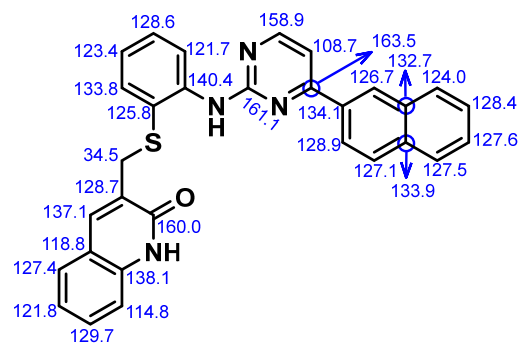


MS Spectrum Peak List

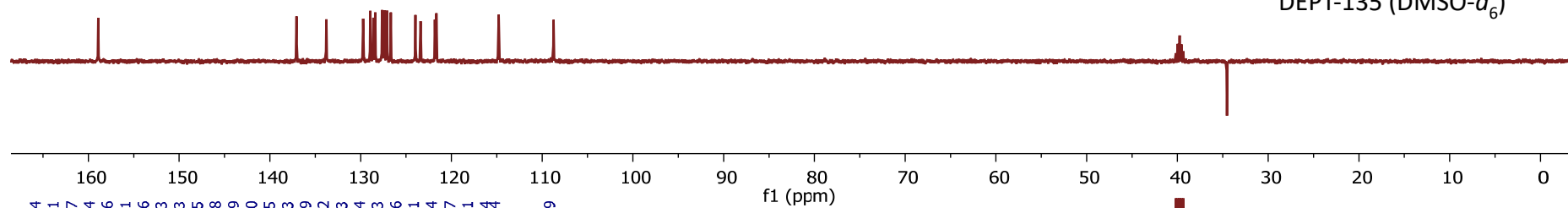
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
535.1409	535.141	0.18	1	24069.29	C28H21F3N4O2S	(M+H)+
536.1441	536.144	-0.1	1	7805.41	C28H21F3N4O2S	(M+H)+
537.1434	537.1424	-1.76	1	2137.66	C28H21F3N4O2S	(M+H)+
557.1223	557.123	1.13	1	4818.09	C28H21F3N4O2S	(M+Na)+
558.1259	558.126	0.08	1	1598.05	C28H21F3N4O2S	(M+Na)+
559.1254	559.1244	-1.85	1	469.72	C28H21F3N4O2S	(M+Na)+
560.1218	560.1249	5.6	1	46.38	C28H21F3N4O2S	(M+Na)+

4.17 Compound 26a

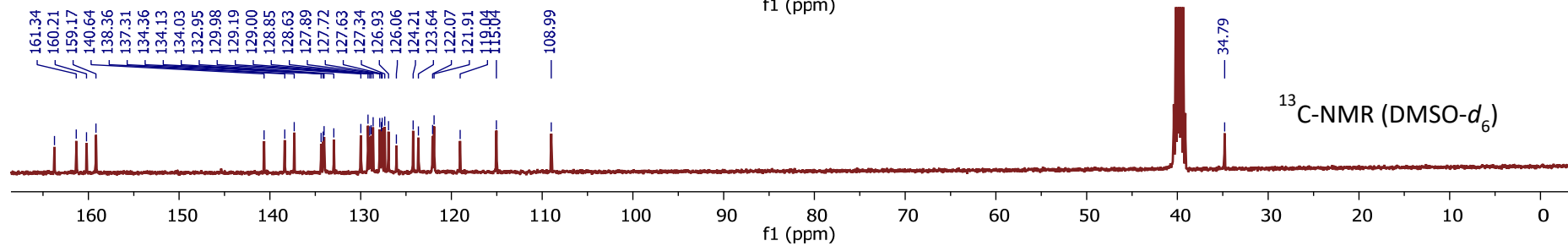




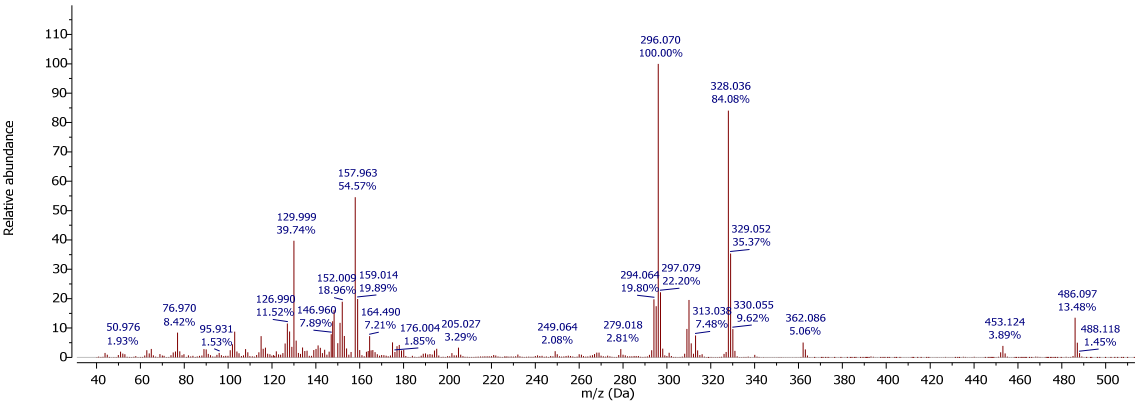
DEPT-135 ($\text{DMSO}-d_6$)



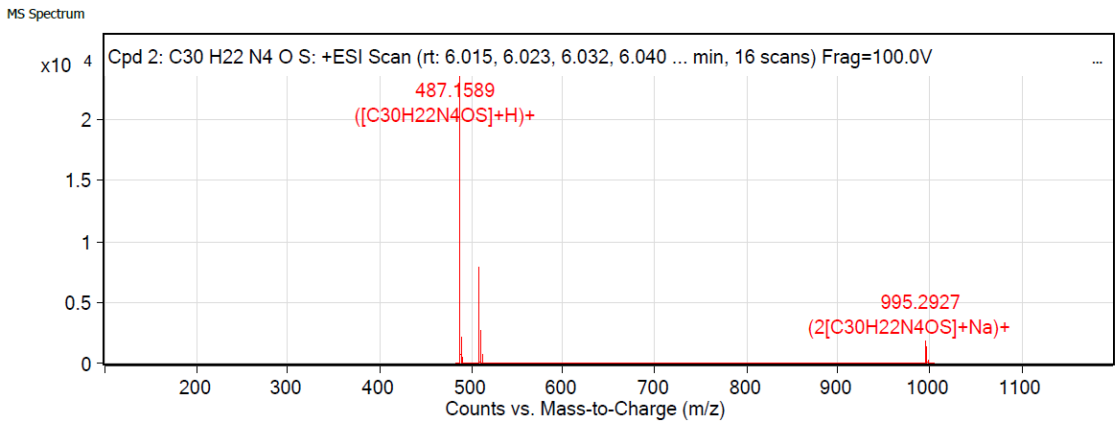
^{13}C -NMR ($\text{DMSO}-d_6$)



EI MS (70eV)



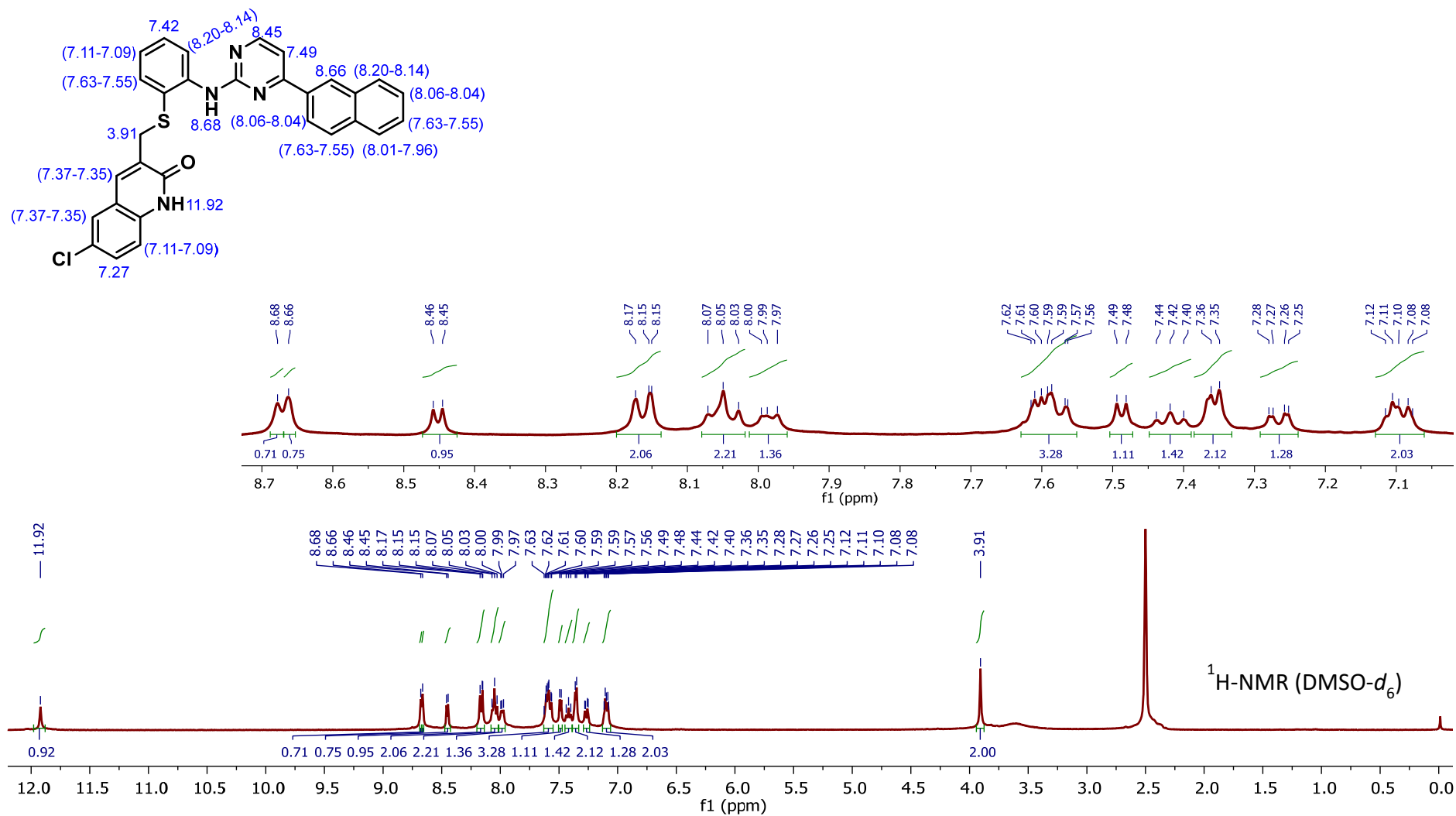
ESI-QTOF (positive ionization)

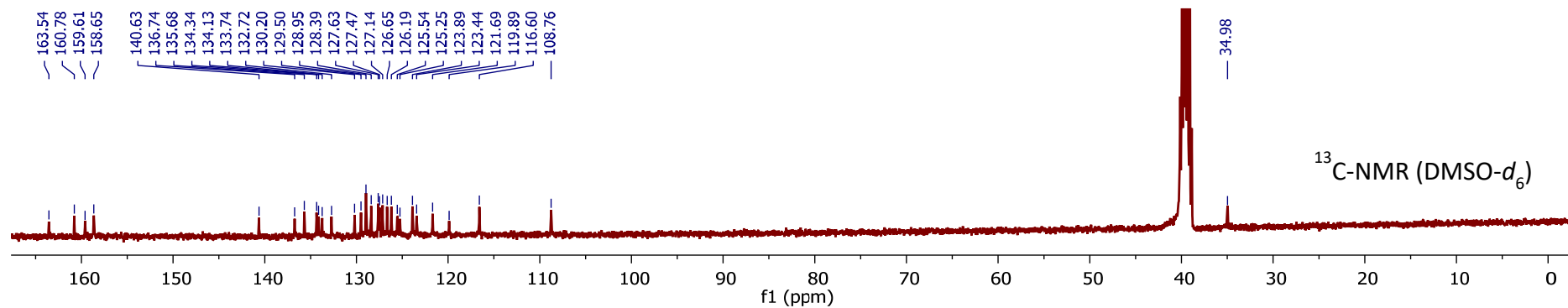
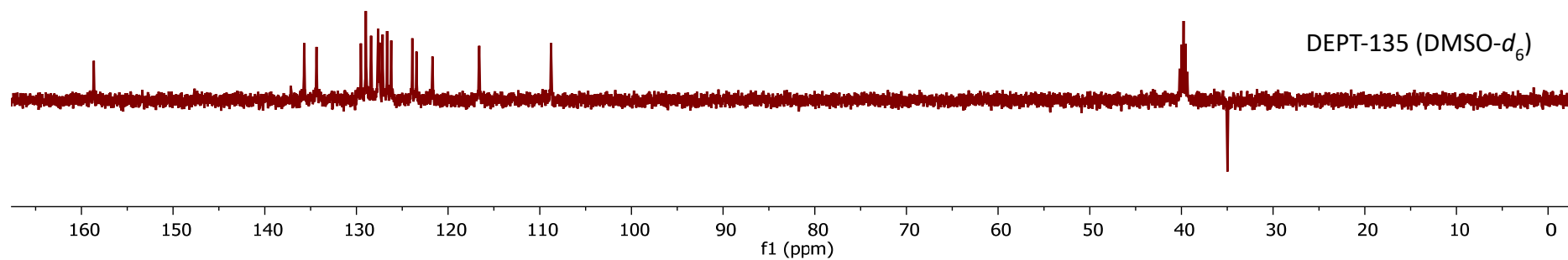
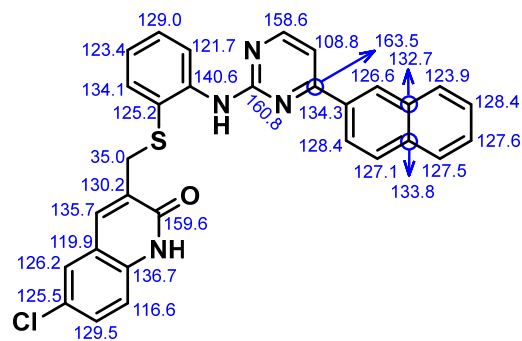


MS Spectrum Peak List

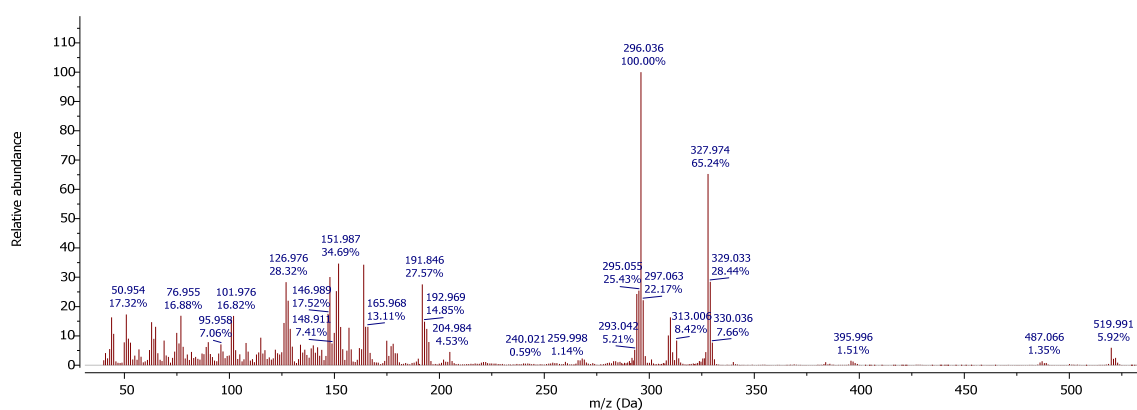
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
487.1589	487.1587	-0.29	1	23642.65	C ₃₀ H ₂₂ N ₄ OS	(M+H)+
488.162	488.1617	-0.58	1	8337.6	C ₃₀ H ₂₂ N ₄ OS	(M+H)+
489.1609	489.1604	-1.05	1	2287.91	C ₃₀ H ₂₂ N ₄ OS	(M+H)+
509.1406	509.1407	0.17	1	7921.39	C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
510.1437	510.1437	-0.14	1	2736.4	C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
511.1429	511.1423	-1.19	1	797.99	C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
995.2927	995.2921	-0.6	1	1972.33	C ₃₀ H ₂₂ N ₄ OS	(2M+Na)+
996.2959	996.2951	-0.79	1	1423.17	C ₃₀ H ₂₂ N ₄ OS	(2M+Na)+
997.2974	997.2954	-2.07	1	597.2	C ₃₀ H ₂₂ N ₄ OS	(2M+Na)+
998.2967	998.2958	-0.88	1	239.26	C ₃₀ H ₂₂ N ₄ OS	(2M+Na)+

4.18 Compound 26b



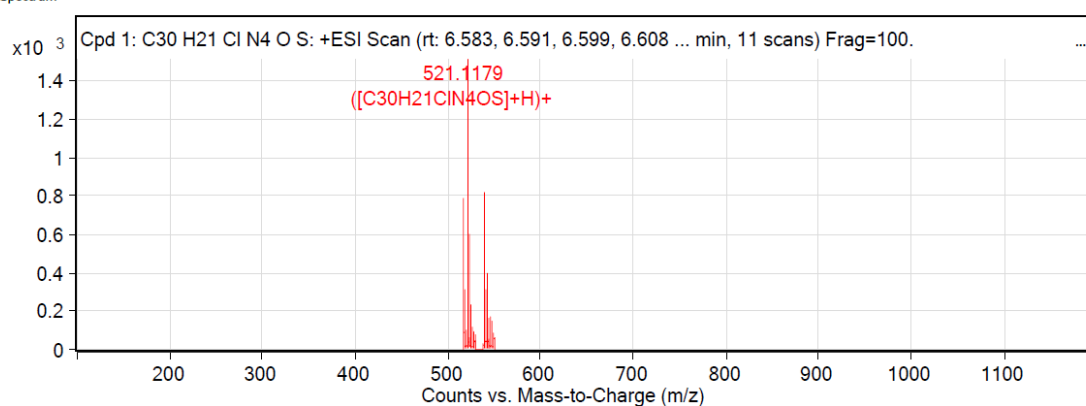


EI MS (70eV)



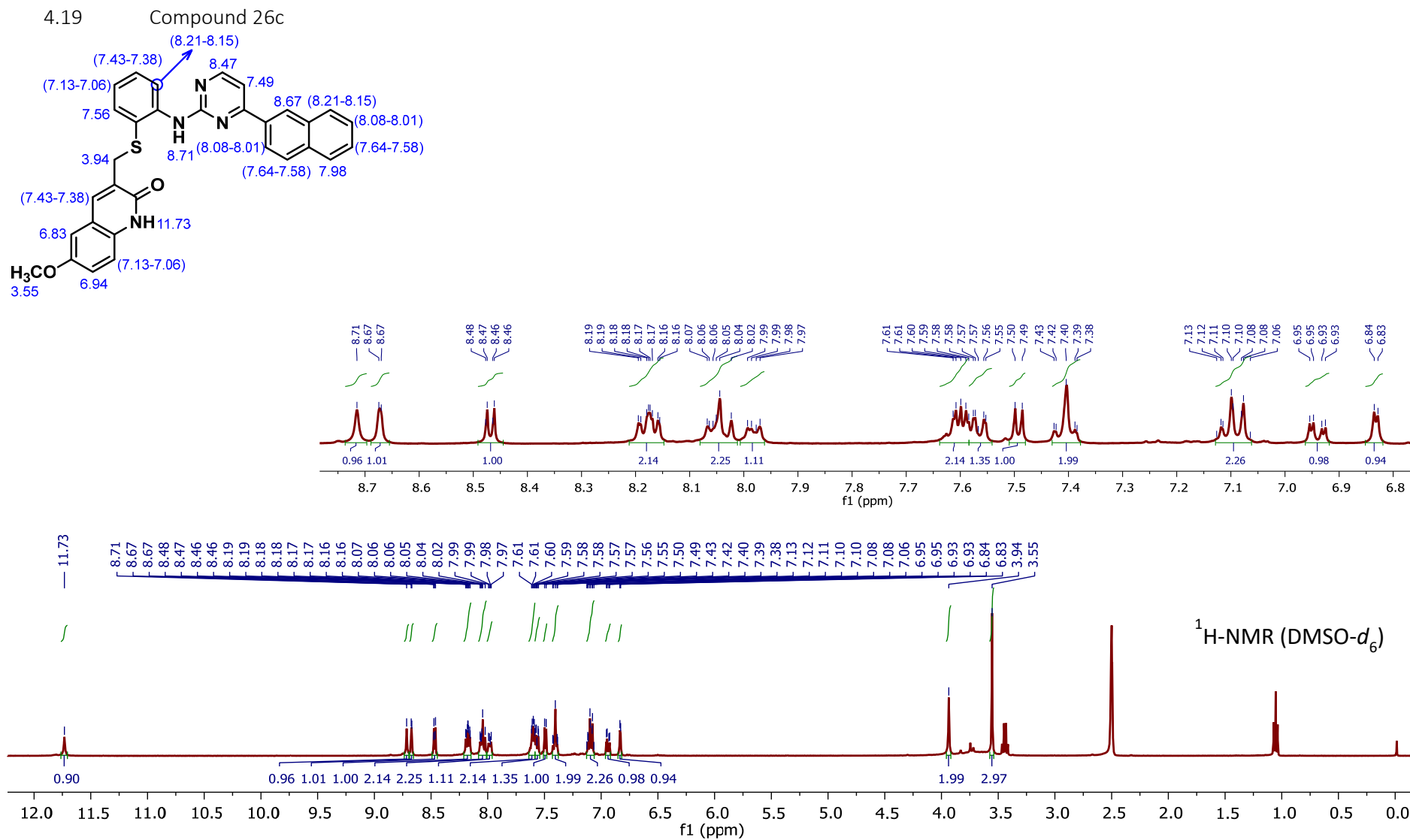
ESI-QTOF (positive ionization)

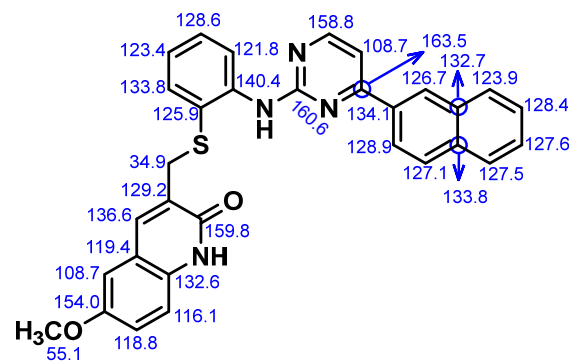
MS Spectrum



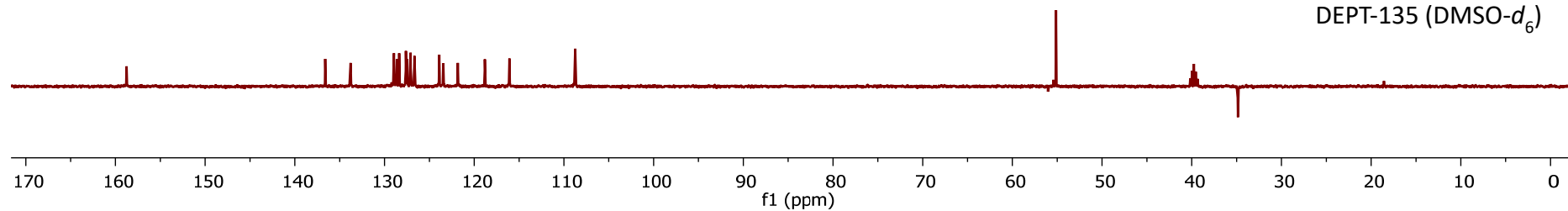
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
521.1179	521.1197	3.47	1	1600.01	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+H) ⁺
522.1209	522.1228	3.62	1	533.33	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+H) ⁺
523.1181	523.1179	-0.37	1	610.94	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+H) ⁺
524.1182	524.1201	3.75	1	212.57	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+H) ⁺
525.1234	525.1189	-8.57	1	48.47	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+H) ⁺
543.1007	543.1017	1.8	1	407.77	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+Na) ⁺
544.1089	544.1047	-7.63	1	128.08	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+Na) ⁺
545.0977	545.0999	4.04	1	142.36	C ₃₀ H ₂₁ ClN ₄ O ₅	(M+Na) ⁺

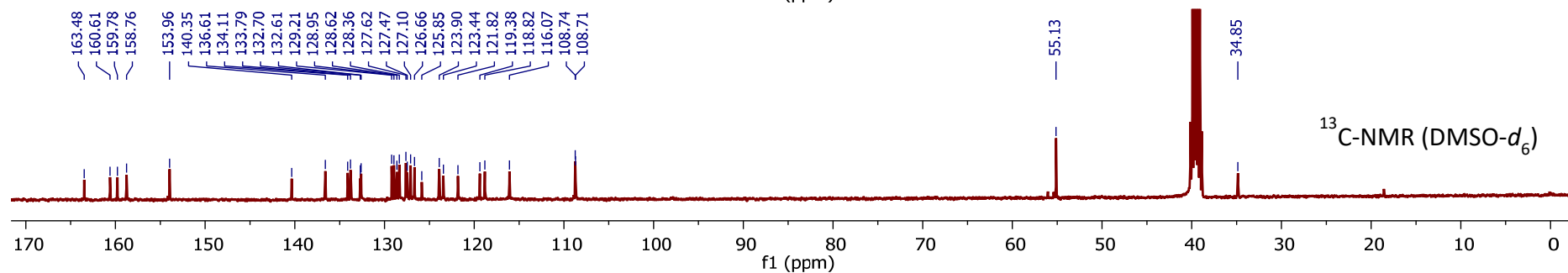




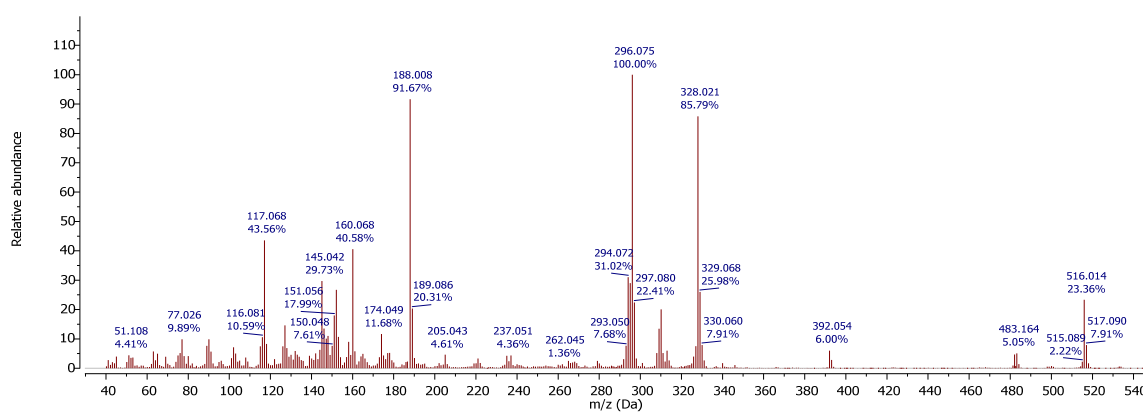
DEPT-135 (DMSO- d_6)



^{13}C -NMR (DMSO- d_6)

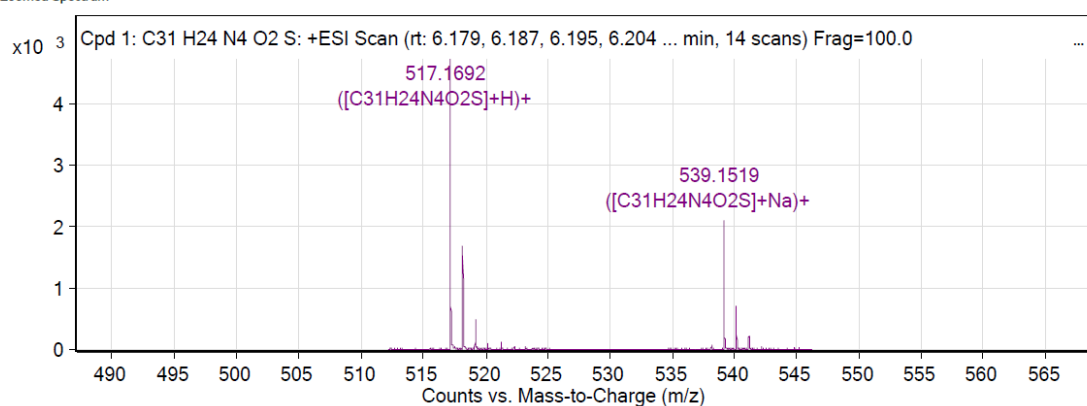


EI MS (70eV)



ESI-QTOF (positive ionization)

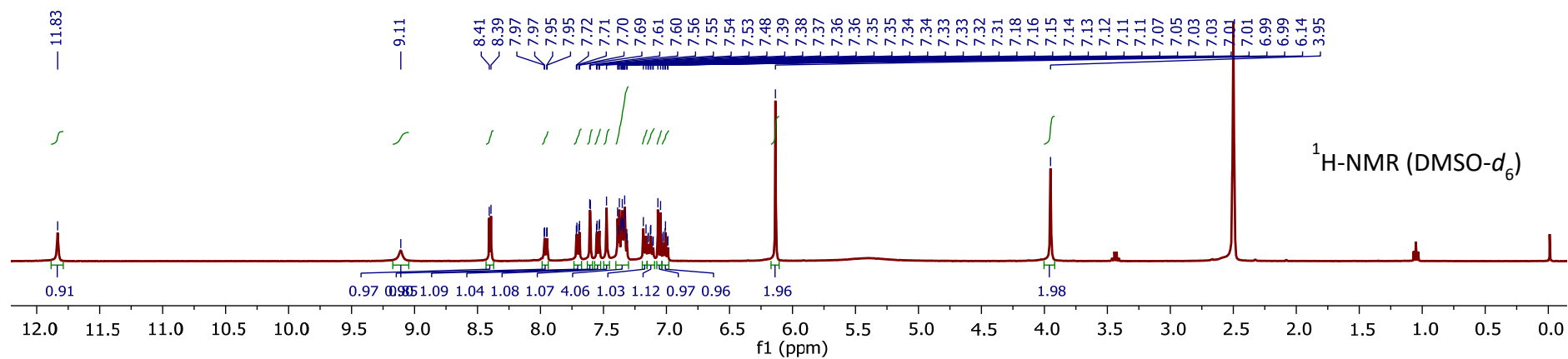
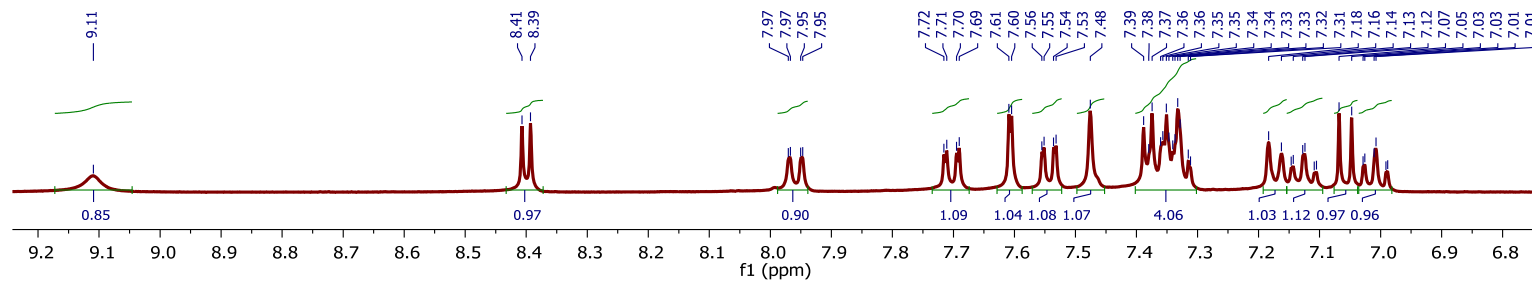
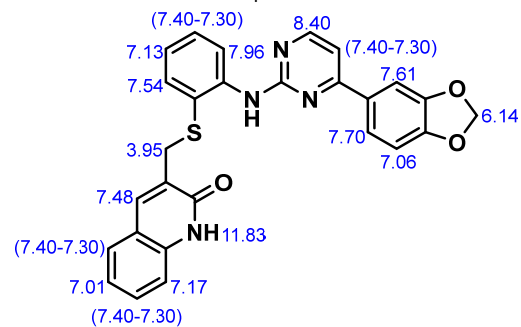
MS Zoomed Spectrum

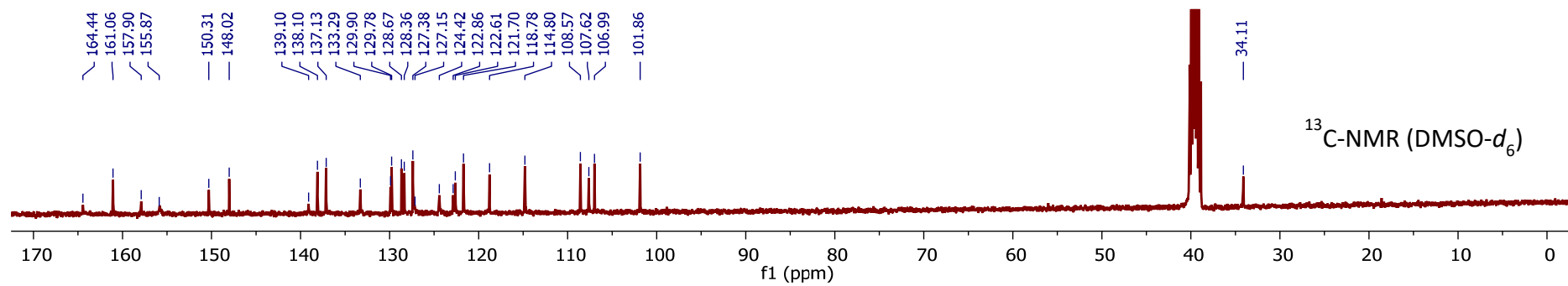
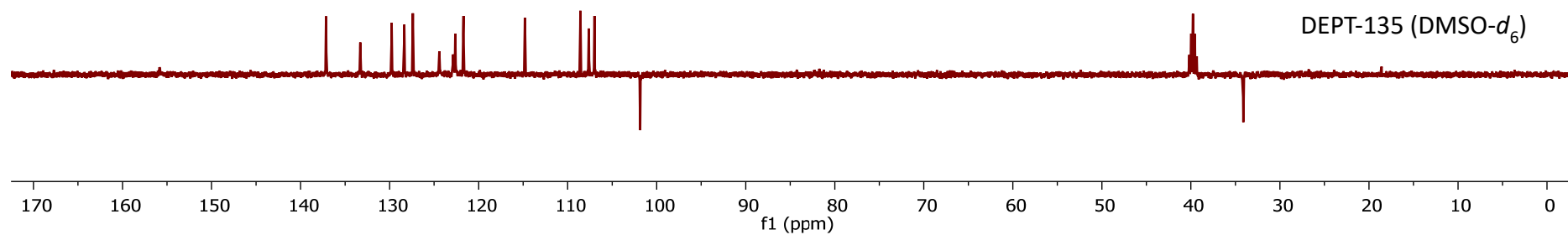
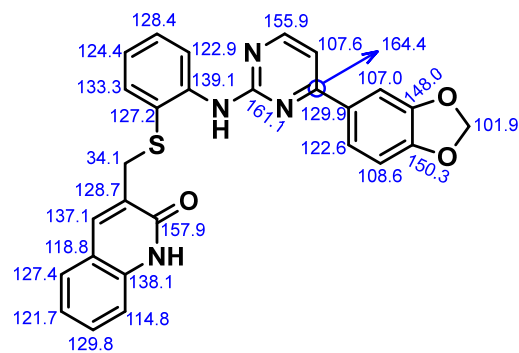


MS Spectrum Peak List

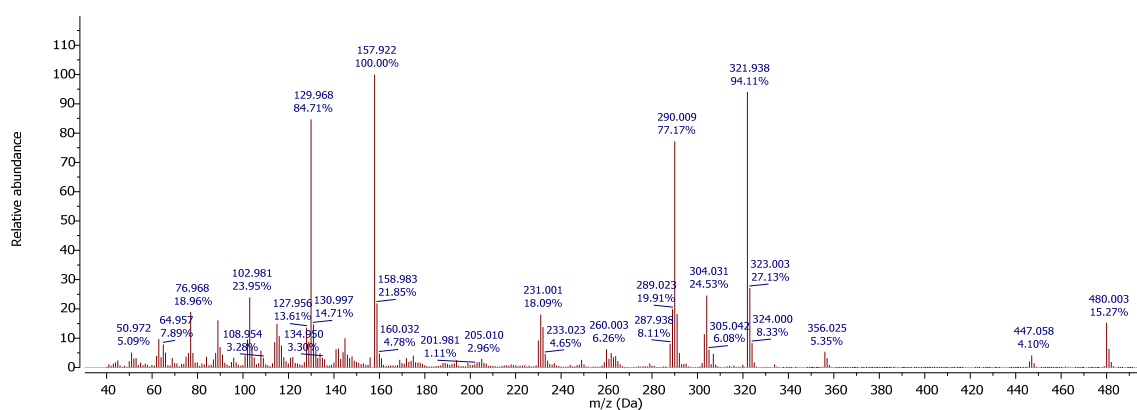
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
517.1692	517.1693	0.18	1	4806.15	C31H24N4O2S	(M+H)+
518.1721	518.1723	0.37	1	1741.63	C31H24N4O2S	(M+H)+
519.1722	519.1712	-1.67	1	551.25	C31H24N4O2S	(M+H)+
520.1747	520.1717	-5.78	1	59.42	C31H24N4O2S	(M+H)+
539.1519	539.1512	-1.17	1	2227.44	C31H24N4O2S	(M+Na)+
540.1547	540.1543	-0.79	1	725.25	C31H24N4O2S	(M+Na)+
541.1539	541.1531	-1.47	1	174.48	C31H24N4O2S	(M+Na)+

4.20 Compound 27a



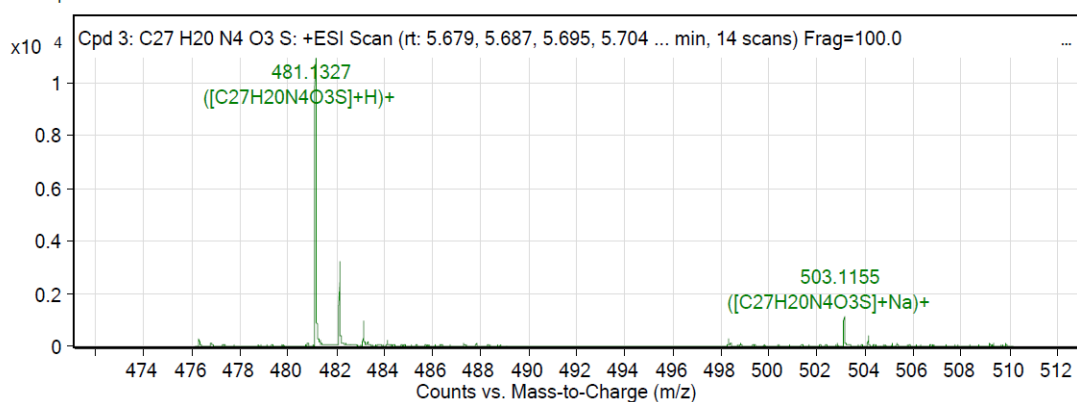


EI MS (70eV)



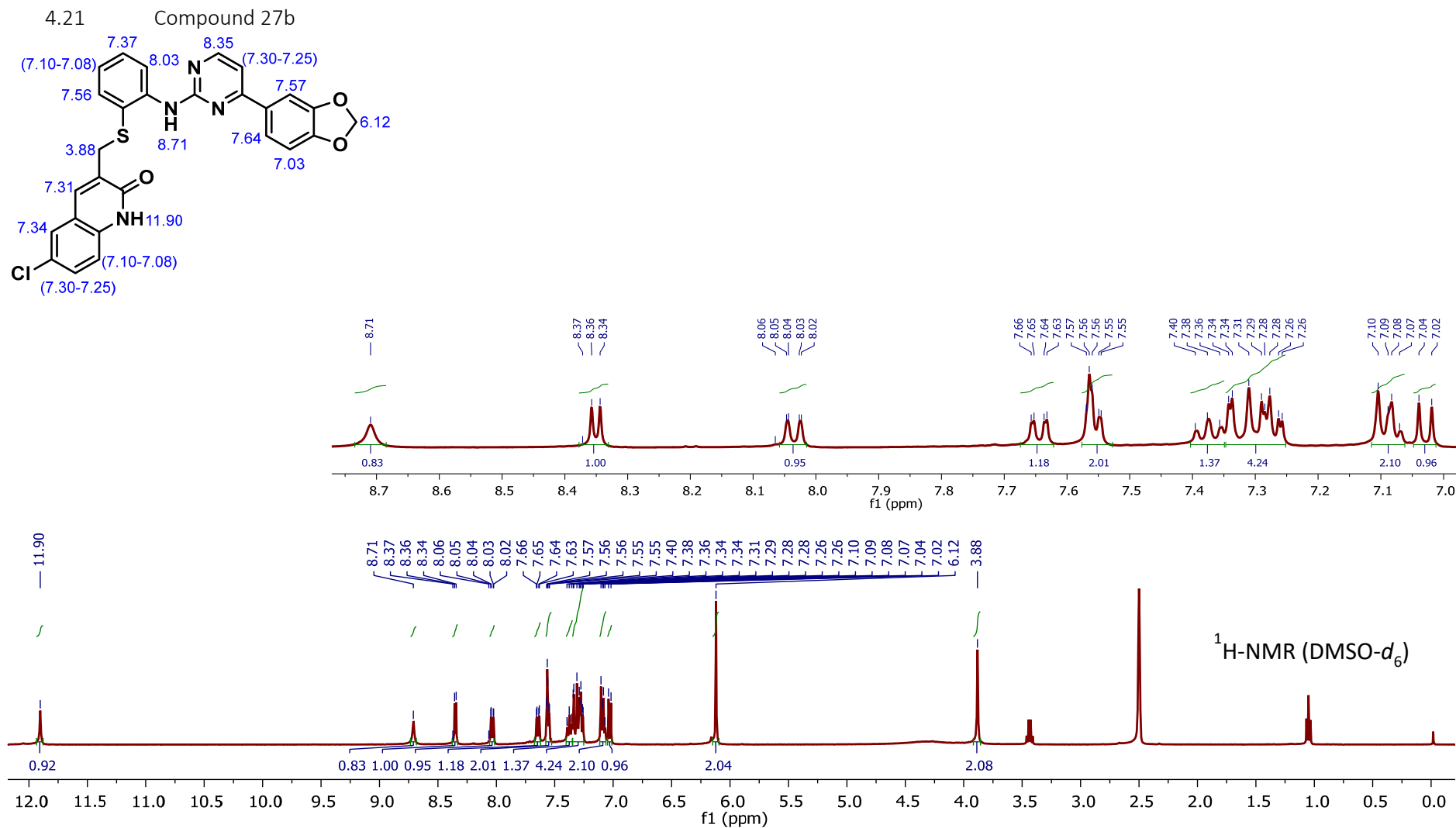
ESI-QTOF (positive ionization)

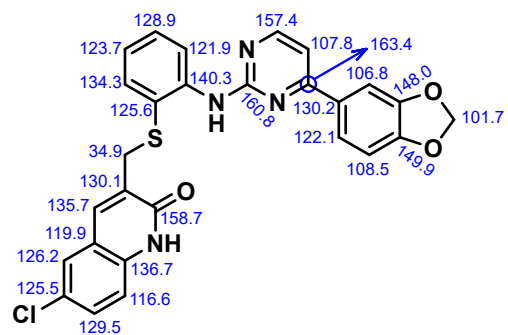
MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
481.1327	481.1329	0.32	1	10997.75	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H) ⁺
482.1356	482.1359	0.5	1	3385.77	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H) ⁺
483.1344	483.1342	-0.48	1	1002.74	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H) ⁺
484.1349	484.1349	0.03	1	191.21	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H) ⁺
503.1155	503.1148	-1.41	1	1172.9	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na) ⁺
504.1165	504.1178	2.71	1	371.69	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na) ⁺
505.1164	505.1161	-0.45	1	64.05	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na) ⁺

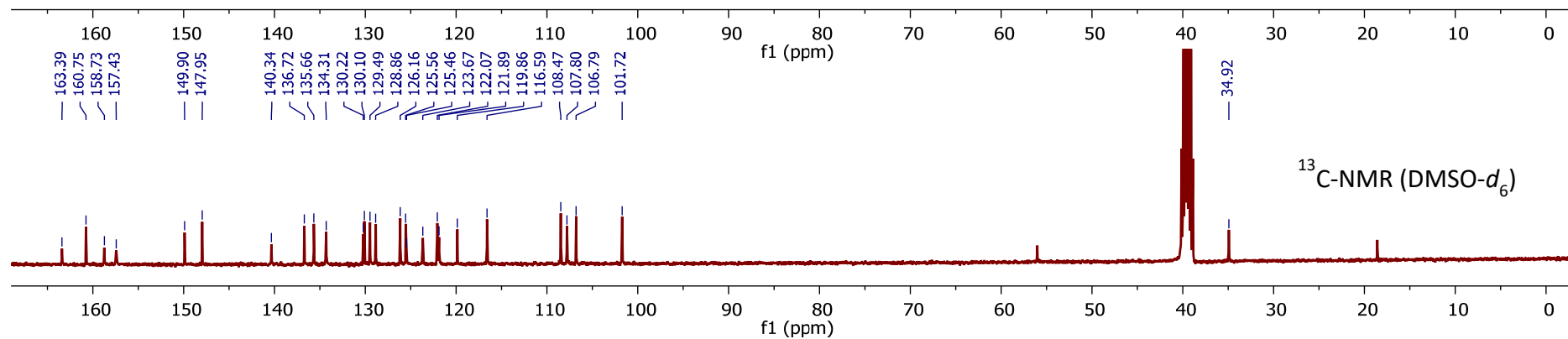




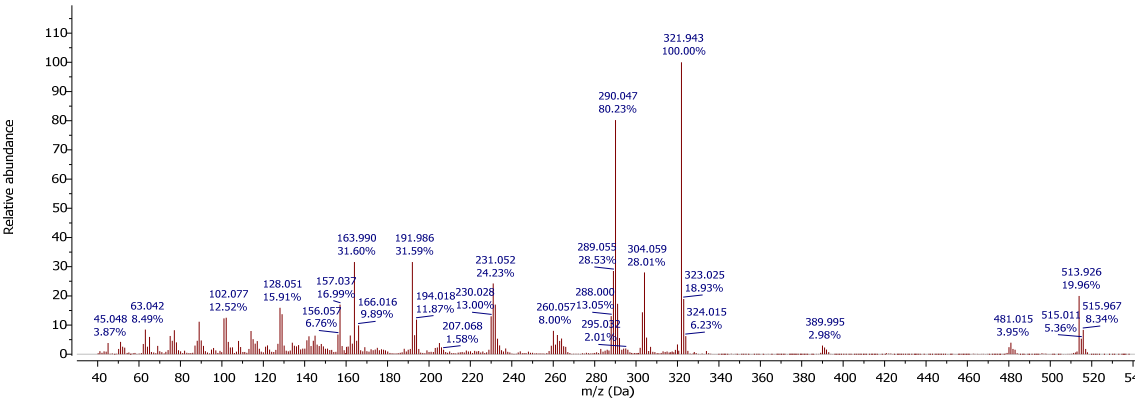
DEPT-135 ($\text{DMSO}-d_6$)



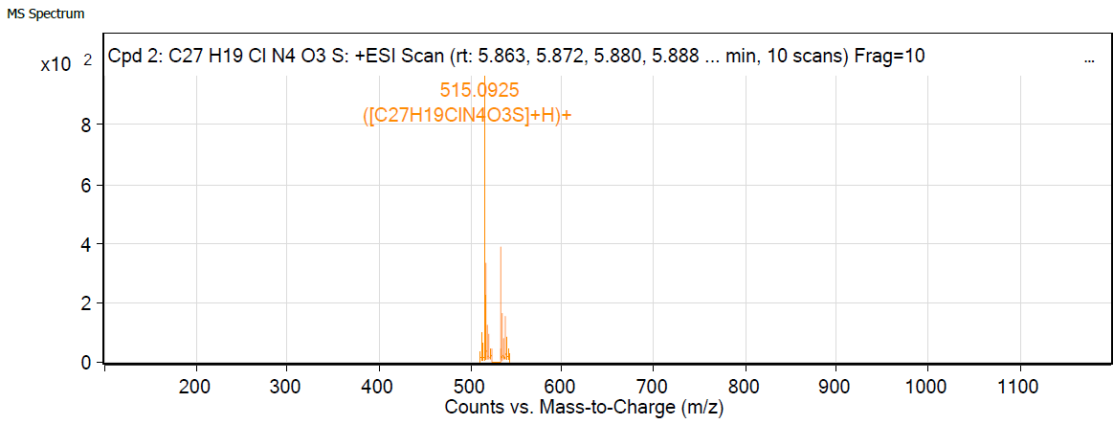
^{13}C -NMR ($\text{DMSO}-d_6$)



EI MS (70eV)



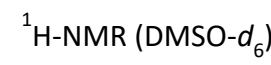
ESI-QTOF (positive ionization)

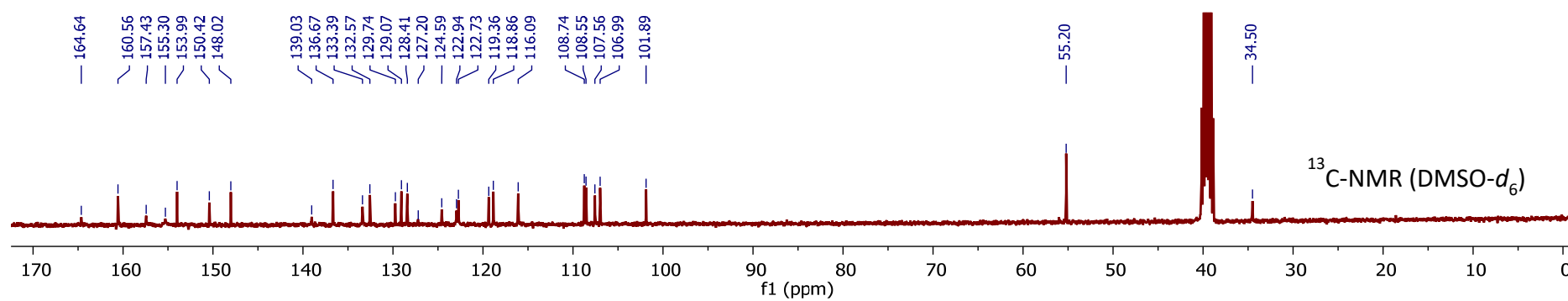
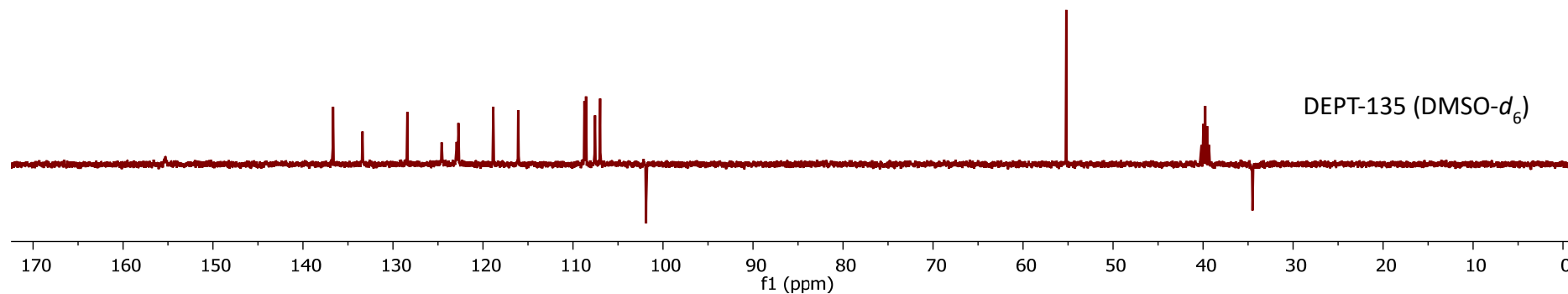
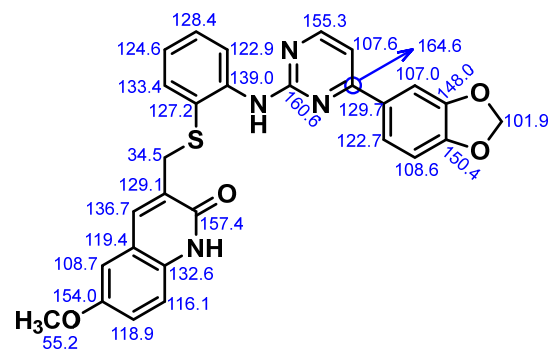


MS Spectrum Peak List

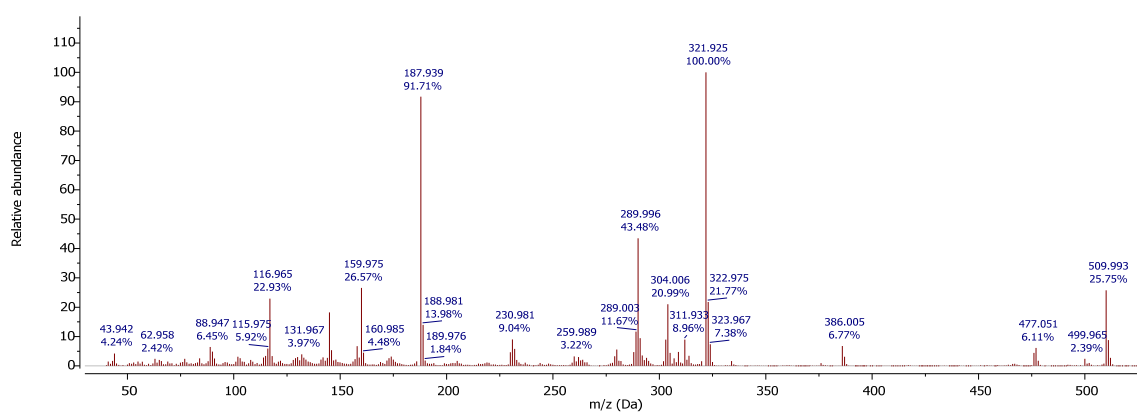
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
515.0925	515.0939	2.66	1	991.42	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H) ⁺
516.0936	516.0969	6.48	1	197.51	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H) ⁺
517.0902	517.092	3.48	1	309.58	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H) ⁺
518.0905	518.0943	7.26	1	47.33	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H) ⁺
519.0911	519.0949	7.51	1	0.00	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H) ⁺

Chemical structure of compound 10, 2-(2-(4-(benzo[d][1,3]oxazol-2-yl)phenyl)-1H-imidazol-5-yl)benzenethiol, with ¹³C NMR peaks labeled: 7.43-7.34, 7.15, 7.95, 8.40, 7.61-7.54, 7.43-7.34, 7.61-7.54, 7.69, 6.13, 7.08-7.06, 9.14, and 3.94.



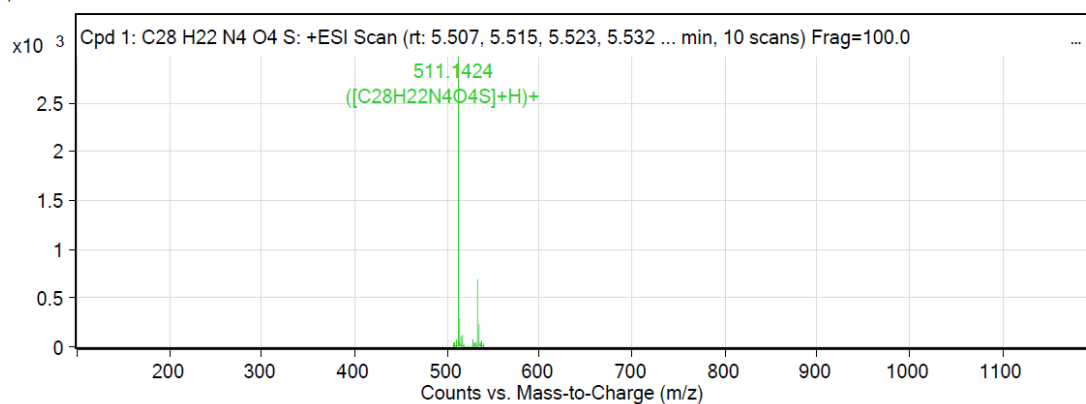


EI MS (70eV)



ESI-QTOF (positive ionization)

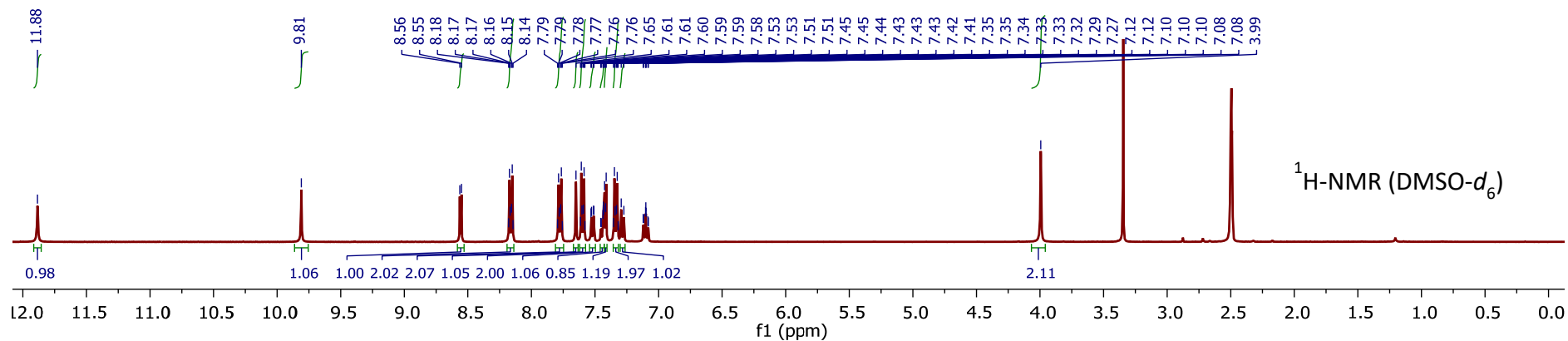
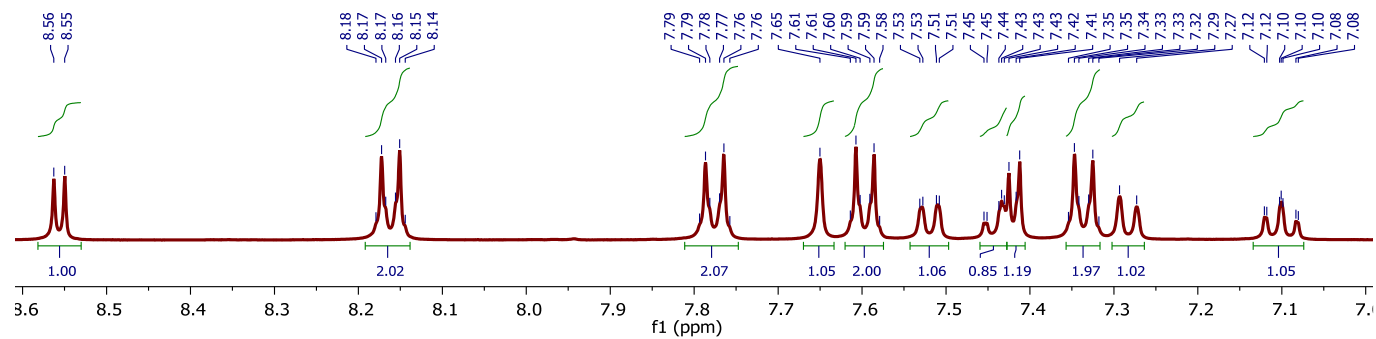
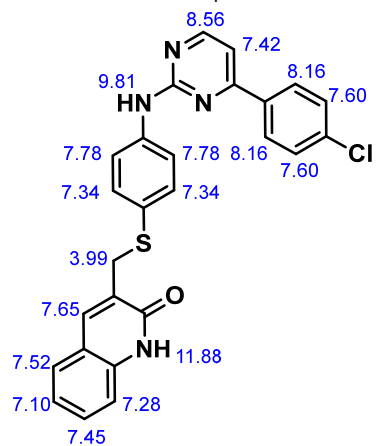
MS Spectrum

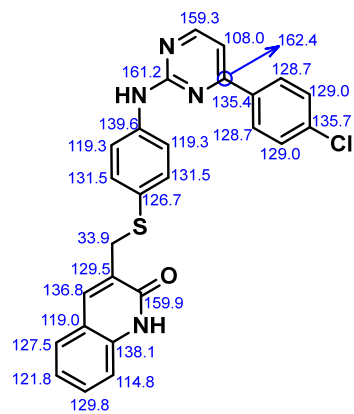


MS Spectrum Peak List

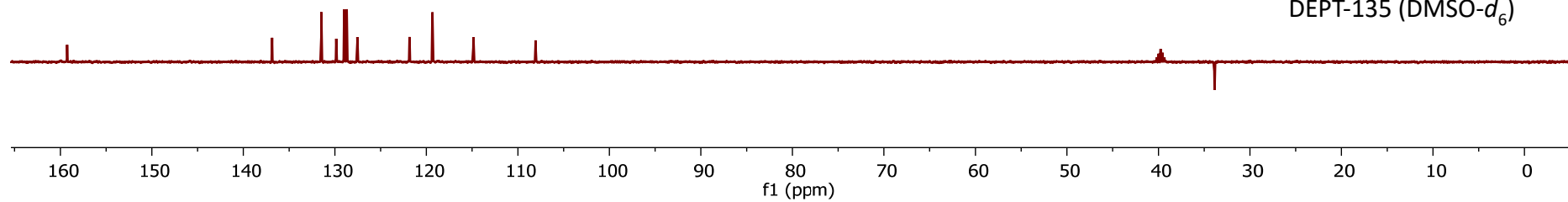
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
511.1424	511.1435	2.08	1	3015.56	C28H22N4O4S	(M+H)+
512.1468	512.1465	-0.68	1	976.06	C28H22N4O4S	(M+H)+
513.1478	513.145	-5.53	1	260.68	C28H22N4O4S	(M+H)+
533.1244	533.1254	-2.63	1	706.64	C28H22N4O4S	(M+Na)+
534.1277	534.1284	-1.32	1	240.8	C28H22N4O4S	(M+Na)+
535.1246	535.1269	-4.35	1	21.18	C28H22N4O4S	(M+Na)+

4.23 Compound 28a

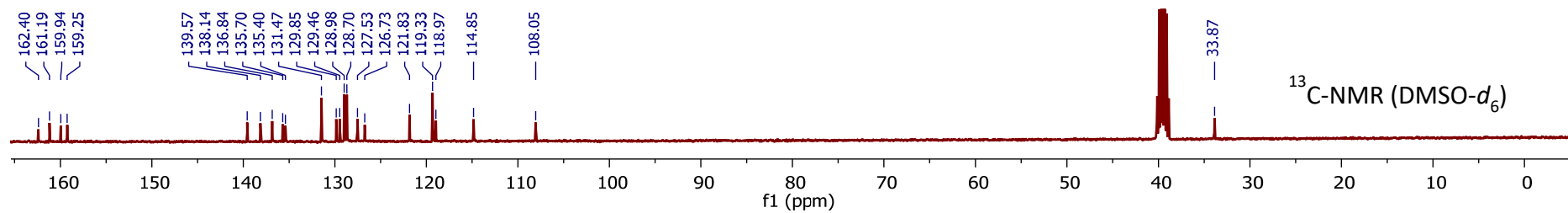




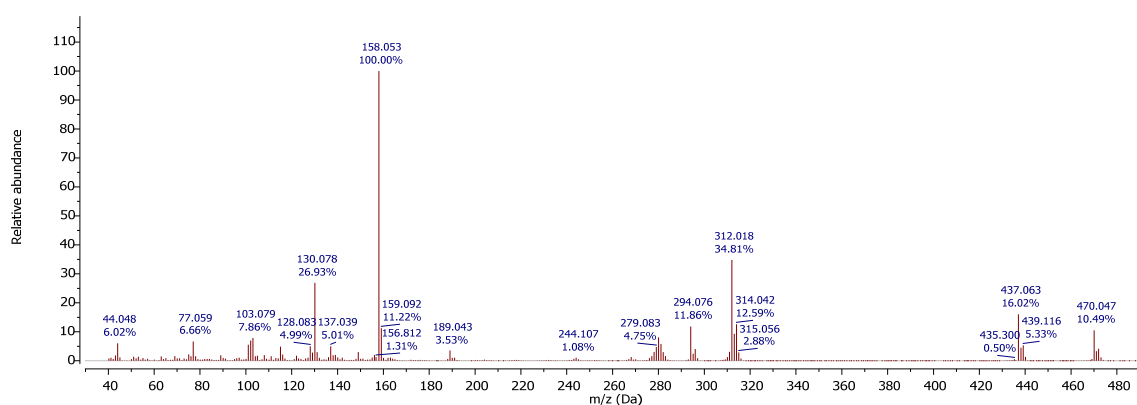
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

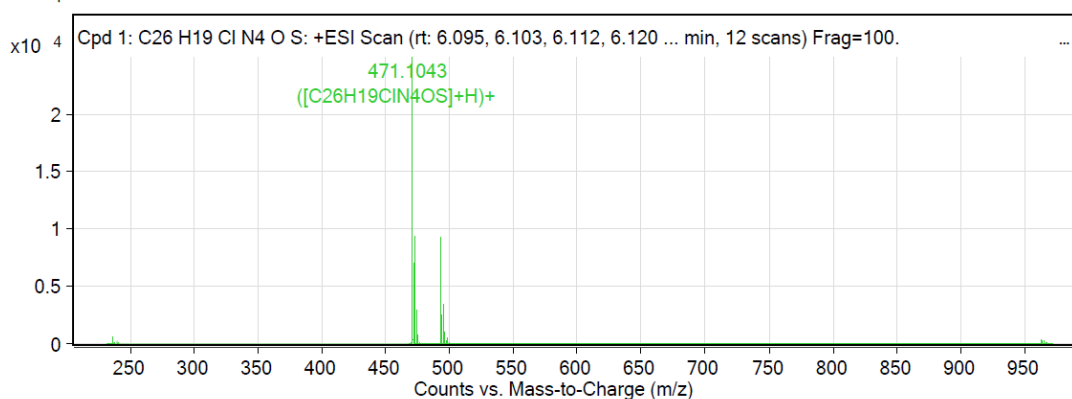


EI MS (70eV)



ESI-QTOF (positive ionization)

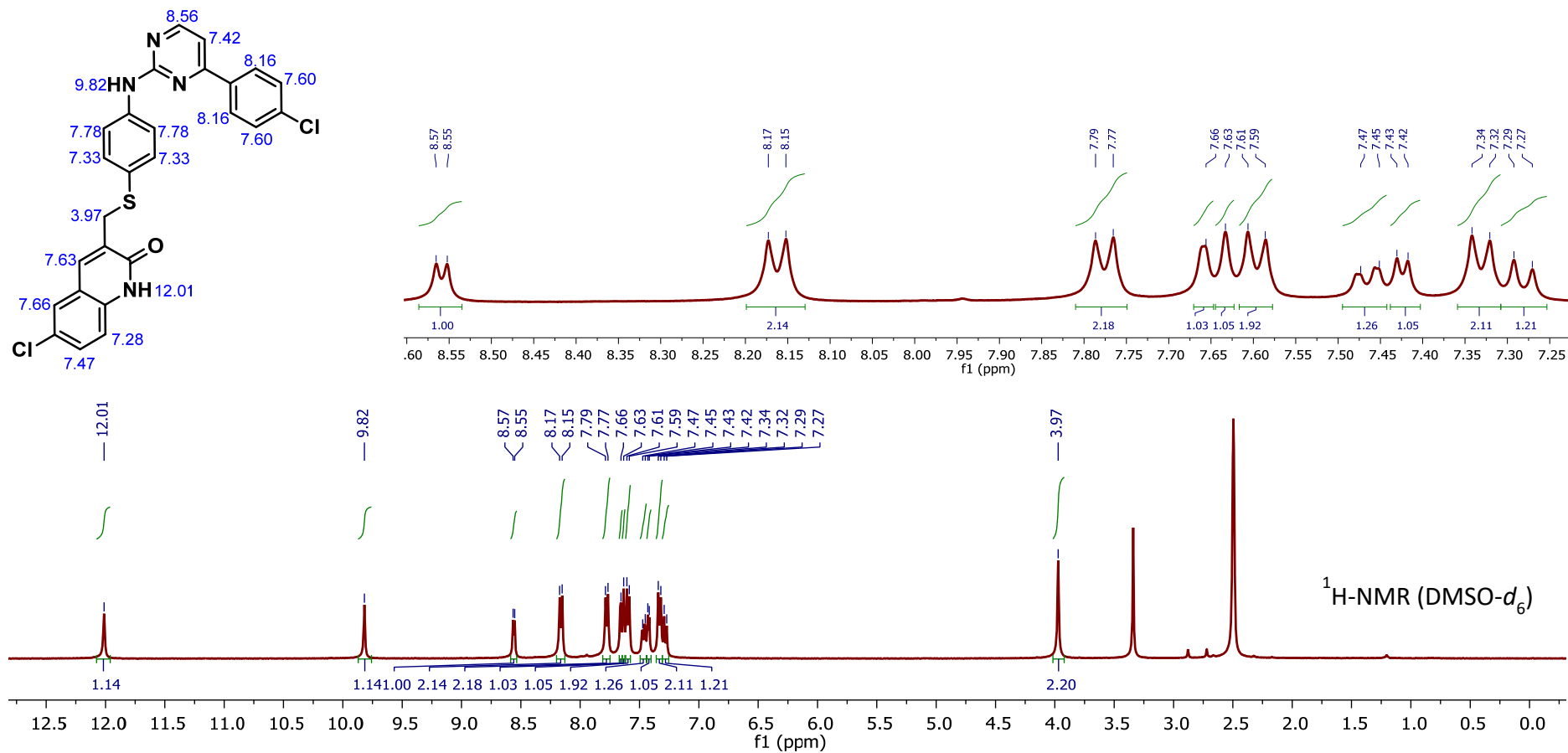
MS Zoomed Spectrum

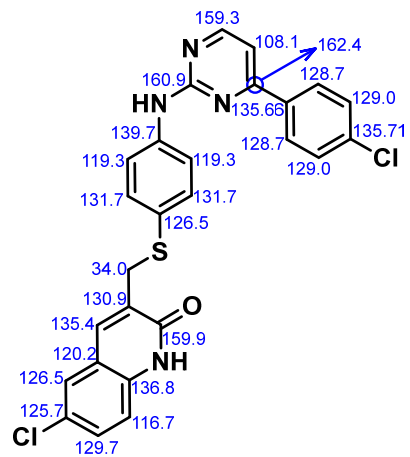


MS Spectrum Peak List

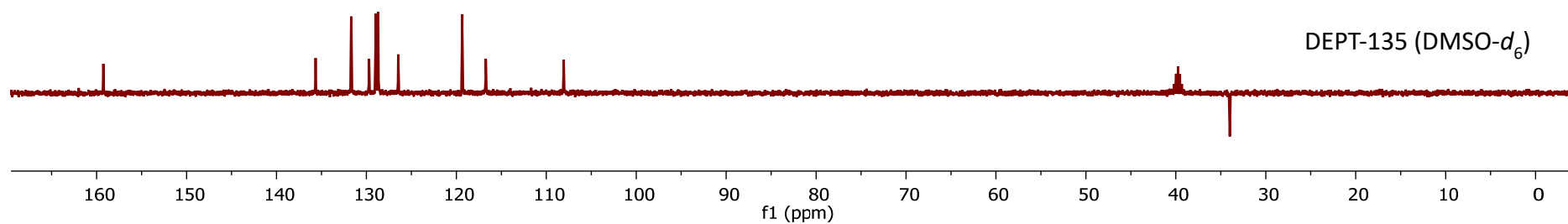
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
236.0563	236.0557	-2.45	2	703.69	C ₂₆ H ₁₉ ClN ₄ OS	(M+2H)+2
471.1043	471.1041	-0.42	1	25044.35	C ₂₆ H ₁₉ ClN ₄ OS	(M+H)+
472.107	472.1071	0.09	1	7196.44	C ₂₆ H ₁₉ ClN ₄ OS	(M+H)+
473.1022	473.102	-0.36	1	9531.86	C ₂₆ H ₁₉ ClN ₄ OS	(M+H)+
474.1047	474.1043	-0.84	1	3006.96	C ₂₆ H ₁₉ ClN ₄ OS	(M+H)+
493.086	493.086	0.09	1	9473.16	C ₂₆ H ₁₉ ClN ₄ OS	(M+Na)+
494.0895	494.089	-0.97	1	2629.7	C ₂₆ H ₁₉ ClN ₄ OS	(M+Na)+
495.0836	495.084	0.67	1	3647.4	C ₂₆ H ₁₉ ClN ₄ OS	(M+Na)+
496.0859	496.0863	0.7	1	1086.21	C ₂₆ H ₁₉ ClN ₄ OS	(M+Na)+
963.1817	963.1828	1.18	1	354.06	C ₂₆ H ₁₉ ClN ₄ OS	(2M+Na)+

4.24 Compound 28b

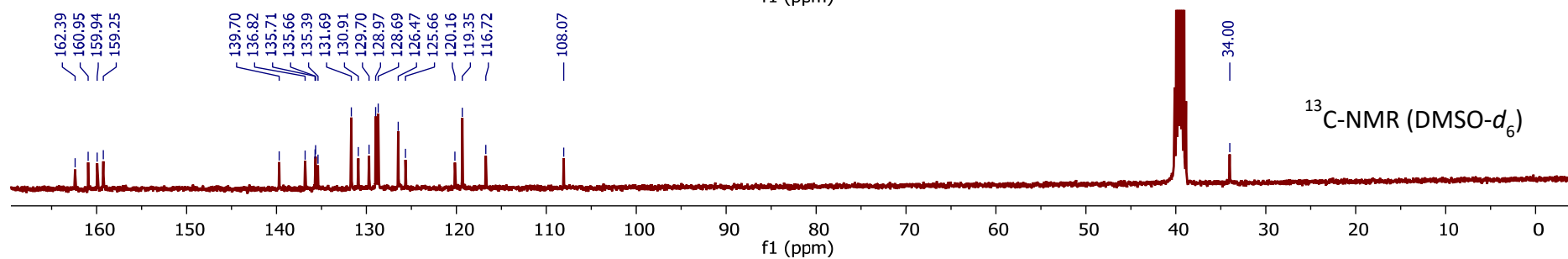




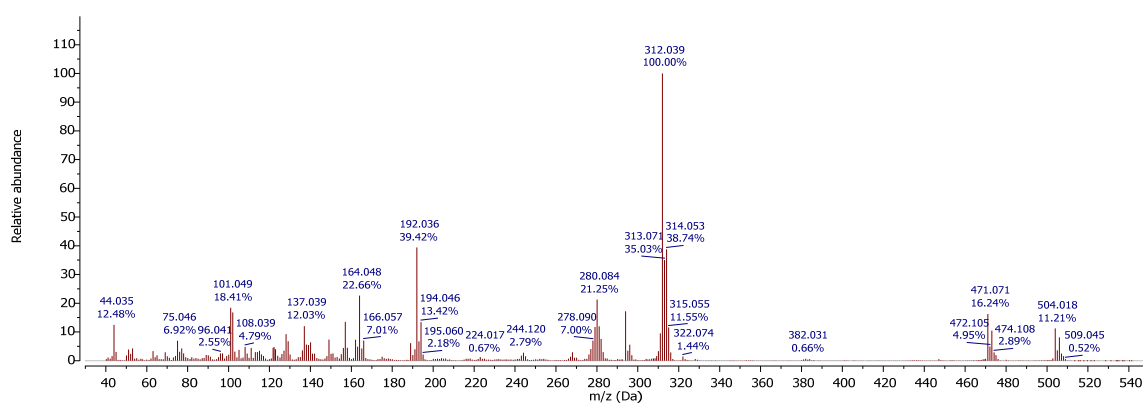
DEPT-135 (DMSO- d_6)



^{13}C -NMR (DMSO- d_6)

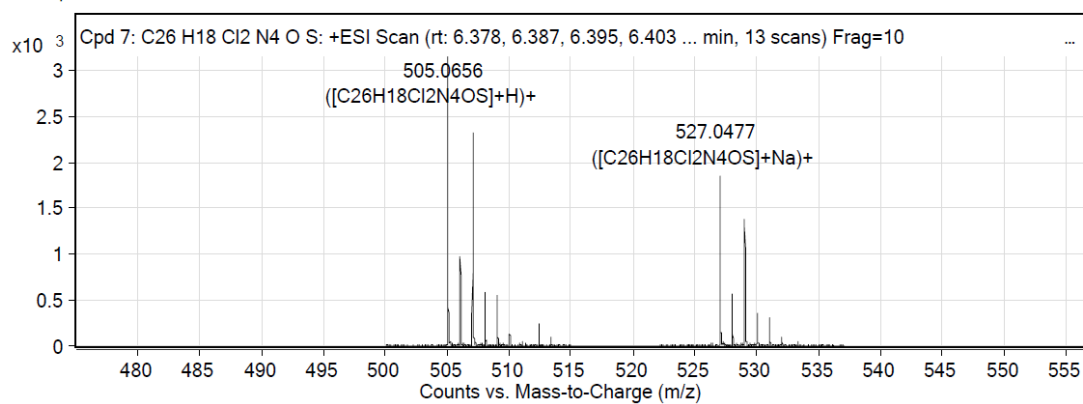


EI MS (70eV)



ESI-QTOF (positive ionization)

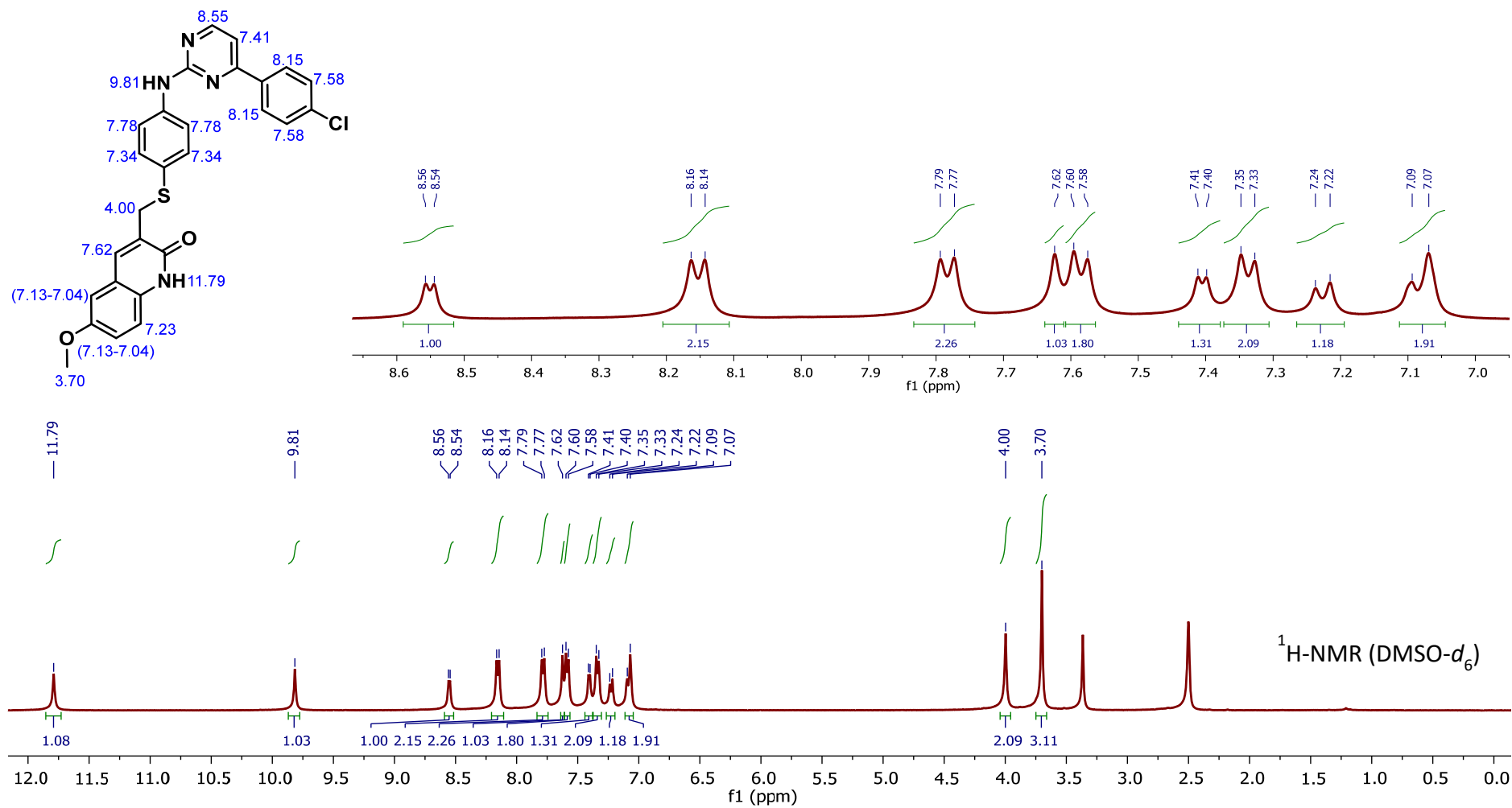
MS Zoomed Spectrum

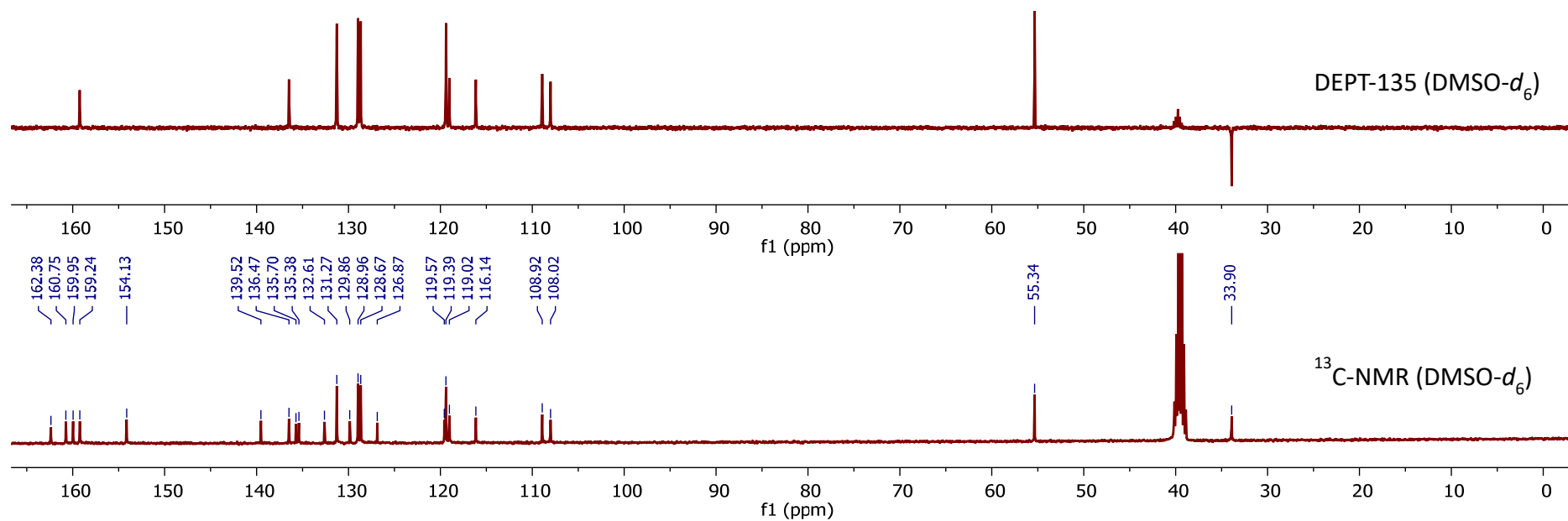
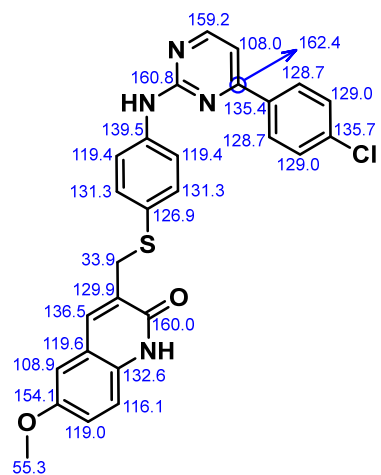


MS Spectrum Peak List

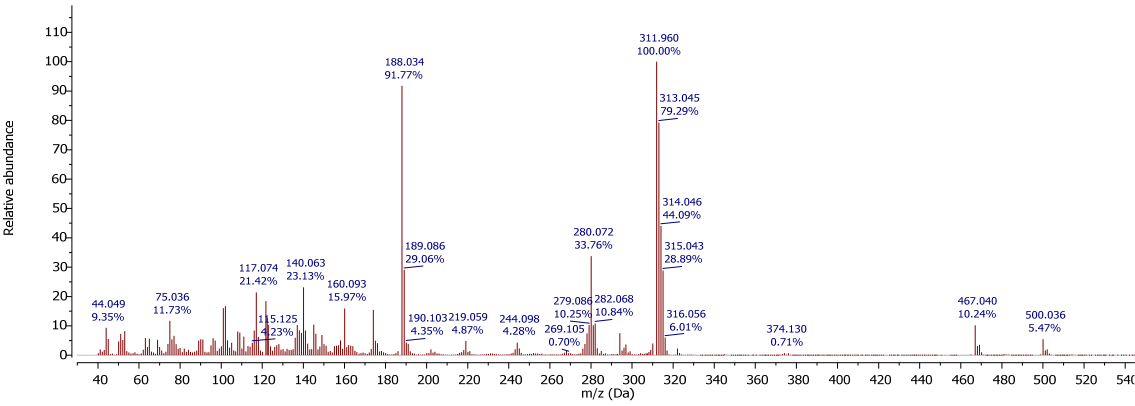
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
505.0656	505.0651	-0.89	1	3256.15	C26H18Cl2N4OS	(M+H)+
506.0683	506.0681	-0.35	1	1040.6	C26H18Cl2N4OS	(M+H)+
507.0631	507.0627	-0.92	1	2374.85	C26H18Cl2N4OS	(M+H)+
508.0668	508.0653	-3	1	635.36	C26H18Cl2N4OS	(M+H)+
509.0606	509.0608	0.34	1	581.17	C26H18Cl2N4OS	(M+H)+
527.0477	527.0471	-1.2	1	1915.42	C26H18Cl2N4OS	(M+Na)+
528.0503	528.05	-0.5	1	572.96	C26H18Cl2N4OS	(M+Na)+
529.0442	529.0446	0.76	1	1465.6	C26H18Cl2N4OS	(M+Na)+
530.0473	530.0472	-0.16	1	357.7	C26H18Cl2N4OS	(M+Na)+
531.0453	531.0427	-4.88	1	308.78	C26H18Cl2N4OS	(M+Na)+

4.25 Compound 28c



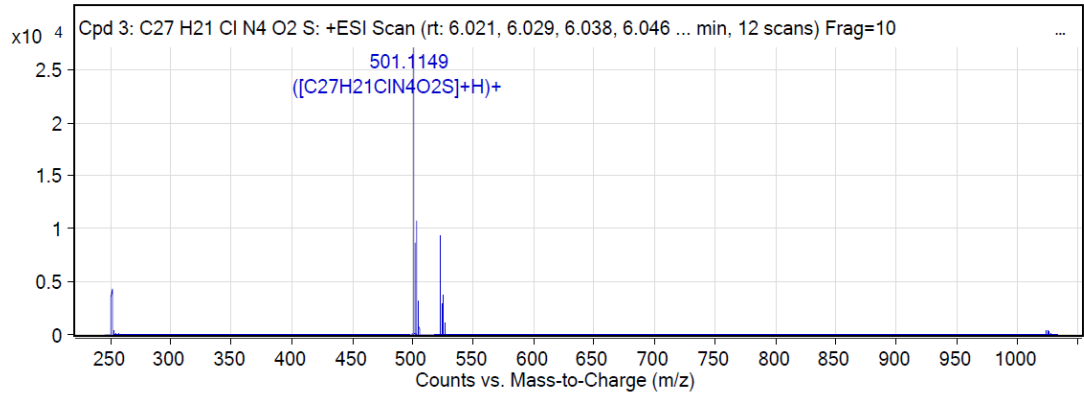


EI MS (70eV)



ESI-QTOF (positive ionization)

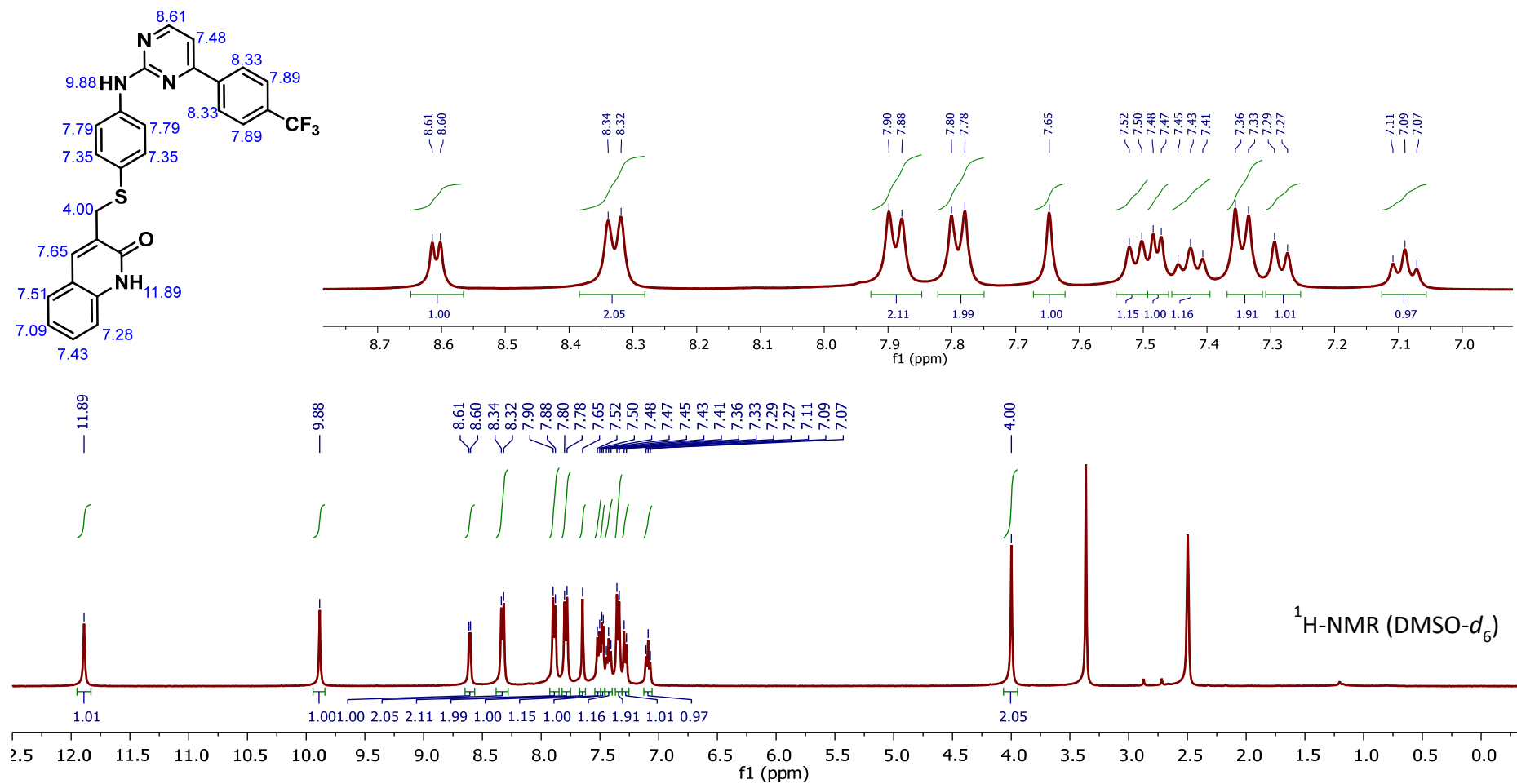
MS Zoomed Spectrum

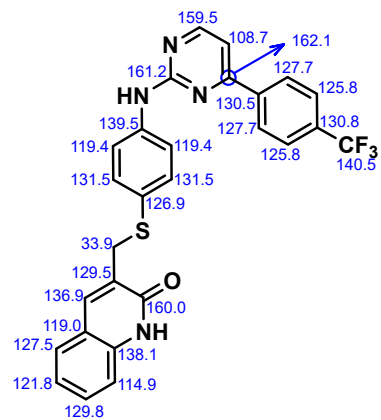


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
251.0607	251.061	0.87	2	4426.26	C27H21ClN4O2S	(M+2H)+2
252.0598	252.06	0.68	2	1891.7	C27H21ClN4O2S	(M+2H)+2
501.1149	501.1147	-0.58	1	27915.04	C27H21ClN4O2S	(M+H)+
502.1182	502.1176	-1.03	1	8698.28	C27H21ClN4O2S	(M+H)+
503.113	503.1127	-0.71	1	10863.01	C27H21ClN4O2S	(M+H)+
504.1153	504.115	-0.68	1	3341.83	C27H21ClN4O2S	(M+H)+
523.0968	523.0966	-0.44	1	9575.11	C27H21ClN4O2S	(M+Na)+
524.0994	524.0996	0.33	1	3051.01	C27H21ClN4O2S	(M+Na)+
525.0949	525.0946	-0.46	1	3856.37	C27H21ClN4O2S	(M+Na)+
1023.2084	1023.204	-4.34	1	341.57	C27H21ClN4O2S	(2M+Na)+

4.26 Compound 29a

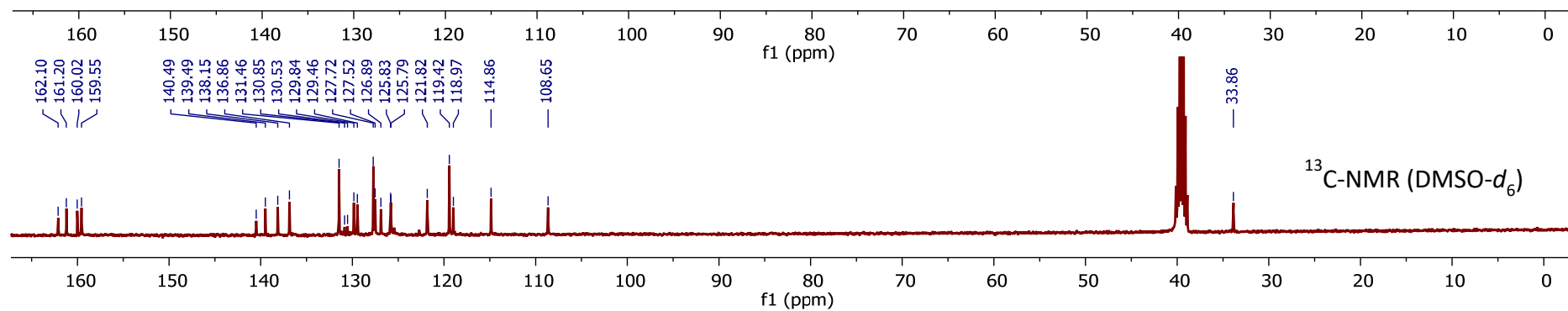




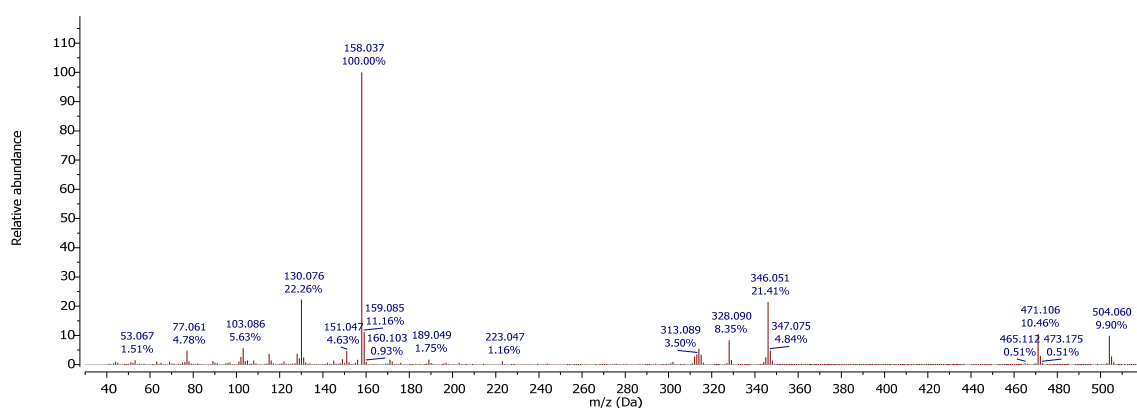
DEPT-135 (DMSO- d_6)



^{13}C -NMR (DMSO- d_6)

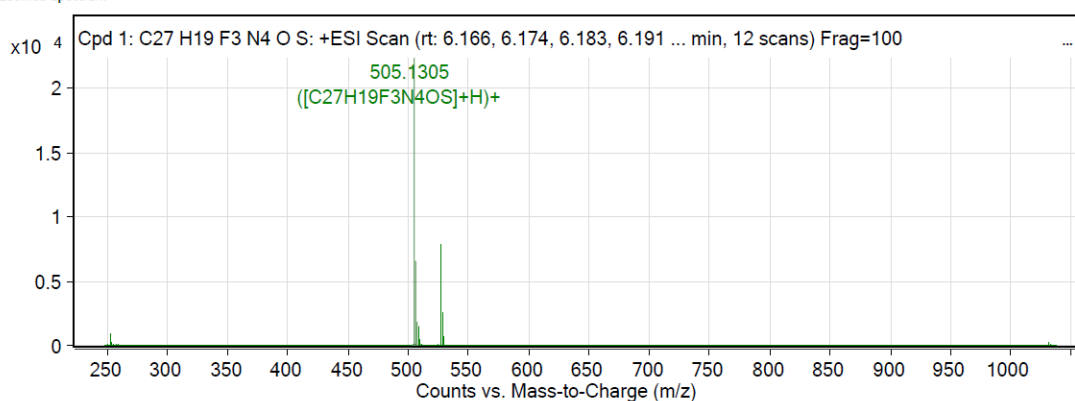


EI MS (70eV)



ESI-QTOF (positive ionization)

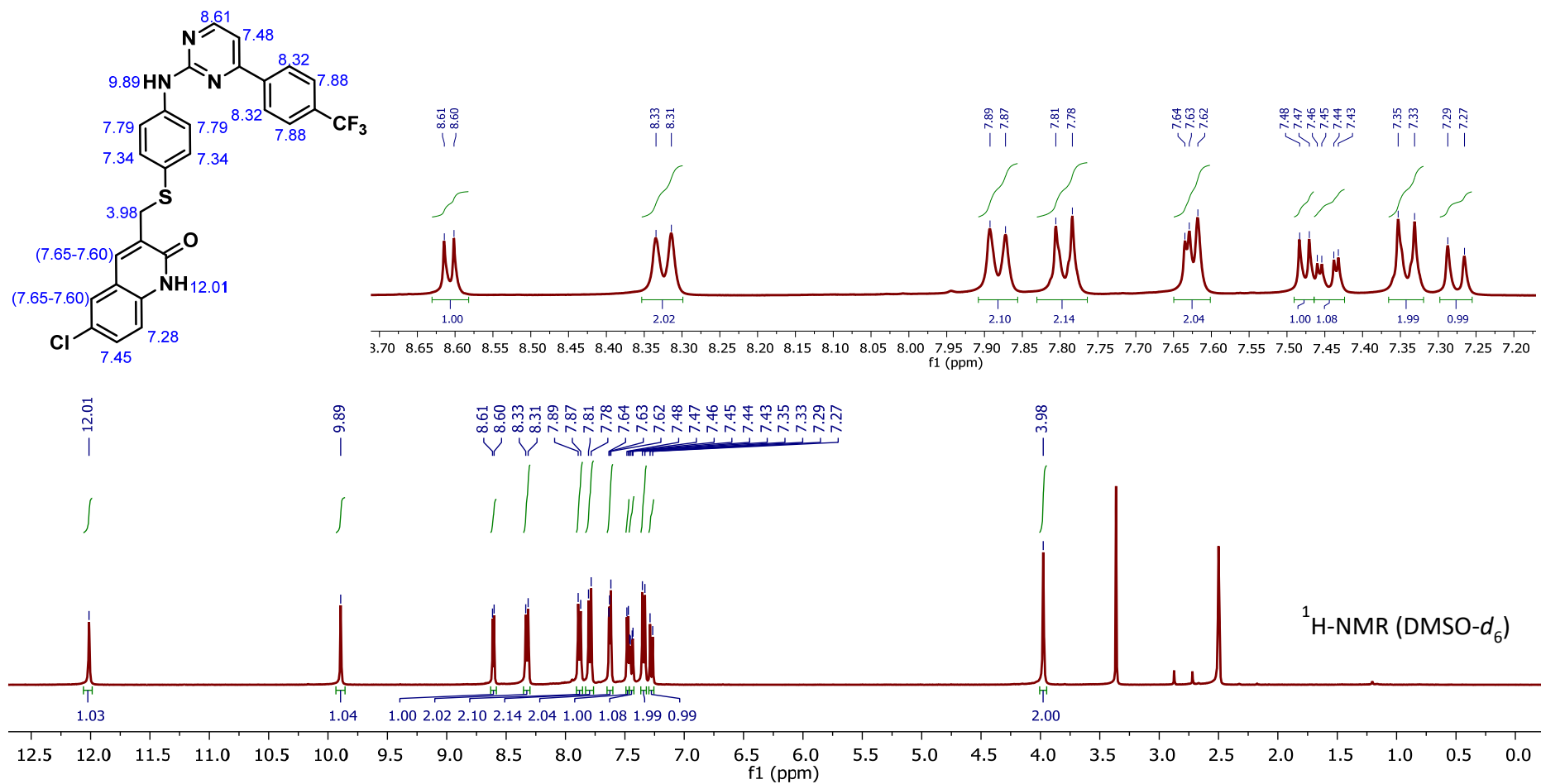
MS Zoomed Spectrum

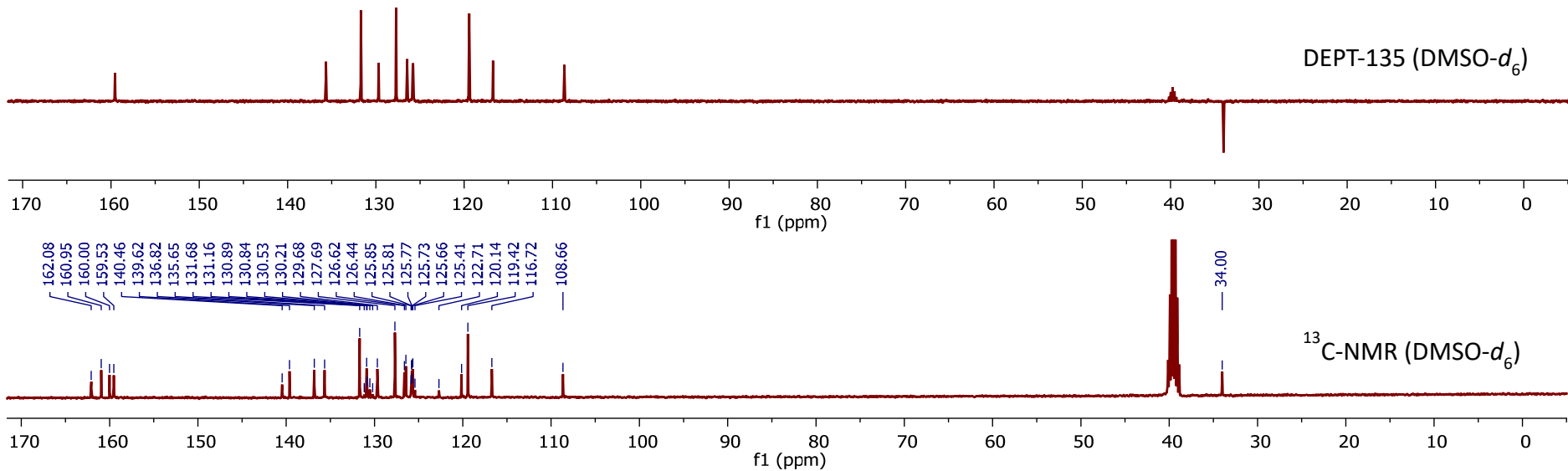


MS Spectrum Peak List

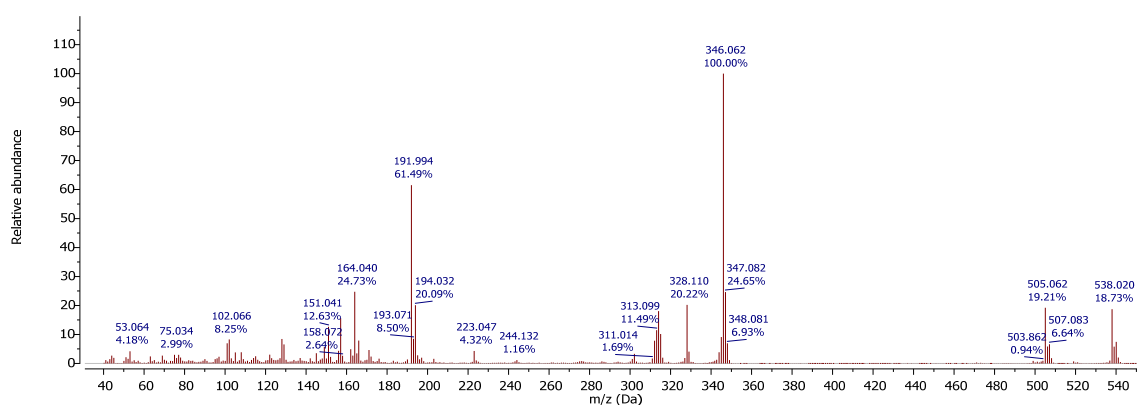
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
253.0686	253.0689	0.93	2	999.09	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+2H)+2
253.5731	253.5704	-10.91	2	251.84	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+2H)+2
505.1305	505.1304	-0.15	1	22389.96	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H)+
506.1334	506.1334	0.06	1	6679.36	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H)+
507.132	507.1316	-0.69	1	1904.2	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H)+
508.1332	508.1321	-2.15	1	355.41	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+H)+
527.1125	527.1124	-0.2	1	7999.77	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na)+
528.1149	528.1154	0.85	1	2662.99	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na)+
529.113	529.1135	0.99	1	829.77	C ₂₇ H ₁₉ F ₃ N ₄ O S	(M+Na)+
1031.2355	1031.2356	0.09	1	264.18	C ₂₇ H ₁₉ F ₃ N ₄ O S	(2M+Na)+

4.27 Compound 29b



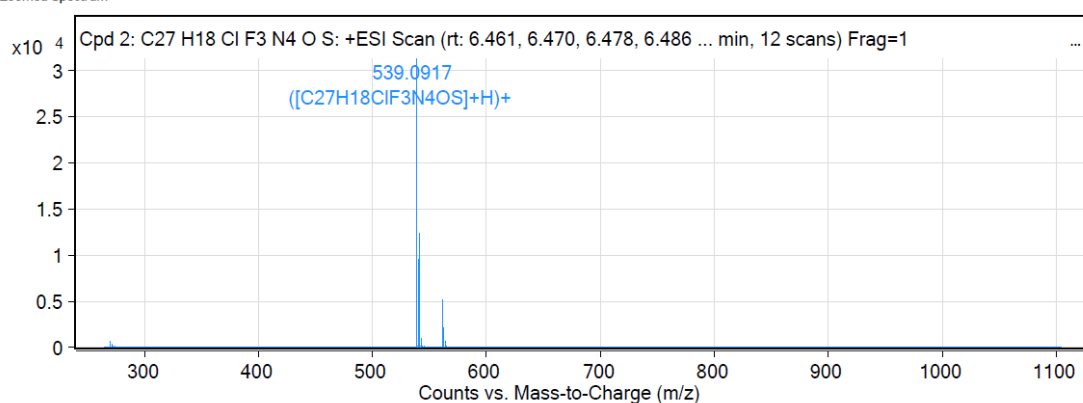


EI MS (70eV)



ESI-QTOF (positive ionization)

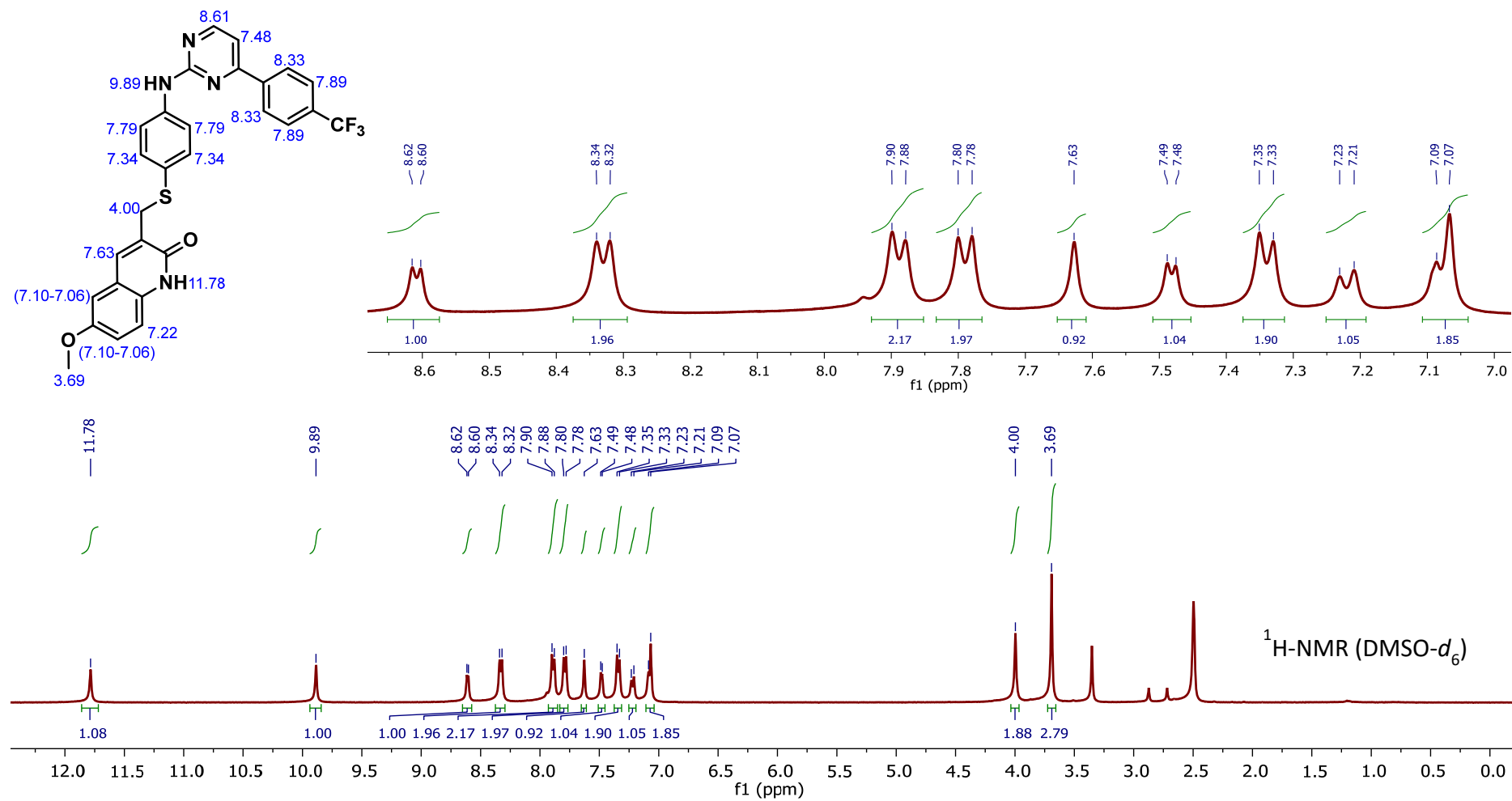
MS Zoomed Spectrum

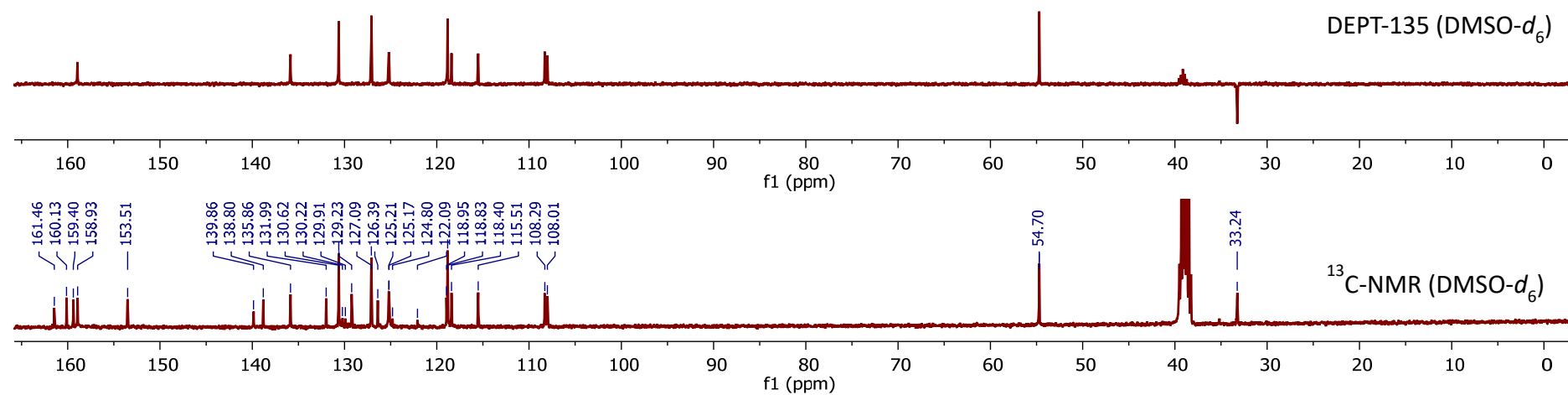
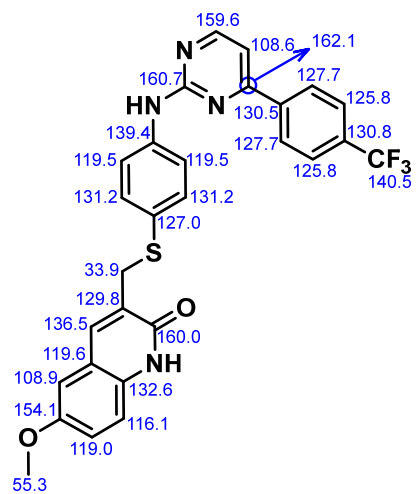


MS Spectrum Peak List

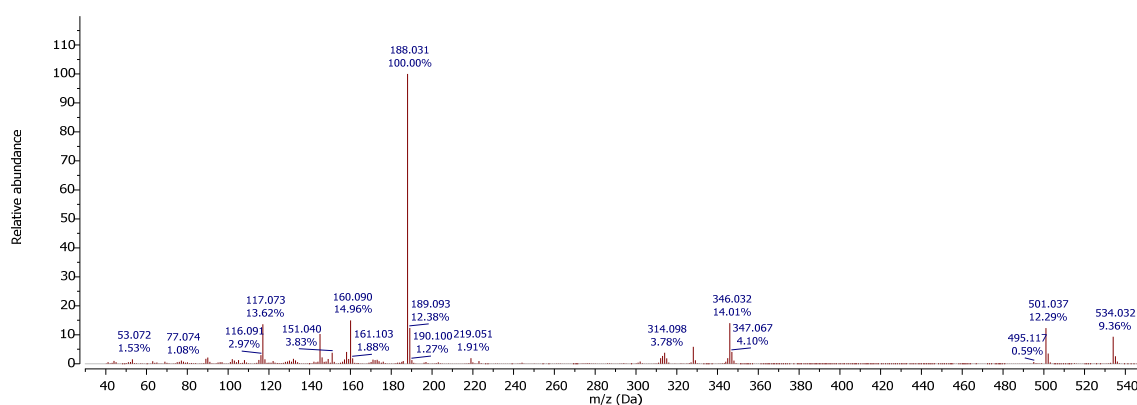
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
270.0488	270.0494	1.95	2	644.48	C27H18ClF3N4OS	(M+2H)+2
539.0917	539.0915	-0.46	1	31643.5	C27H18ClF3N4OS	(M+H)+
540.0945	540.0945	-0.16	1	9793.26	C27H18ClF3N4OS	(M+H)+
541.0895	541.0895	-0.09	1	12503.29	C27H18ClF3N4OS	(M+H)+
542.0922	542.0918	-0.74	1	3917.52	C27H18ClF3N4OS	(M+H)+
543.0892	543.0901	1.66	1	997.55	C27H18ClF3N4OS	(M+H)+
561.0737	561.0734	-0.48	1	5293.78	C27H18ClF3N4OS	(M+Na)+
562.0777	562.0764	-1.14	1	1791.7	C27H18ClF3N4OS	(M+Na)+
563.0708	563.0714	1.05	1	2218.61	C27H18ClF3N4OS	(M+Na)+
1099.1553	1099.1576	2.07	1	60.47	C27H18ClF3N4OS	(2M+Na)+

4.28 Compound 29c



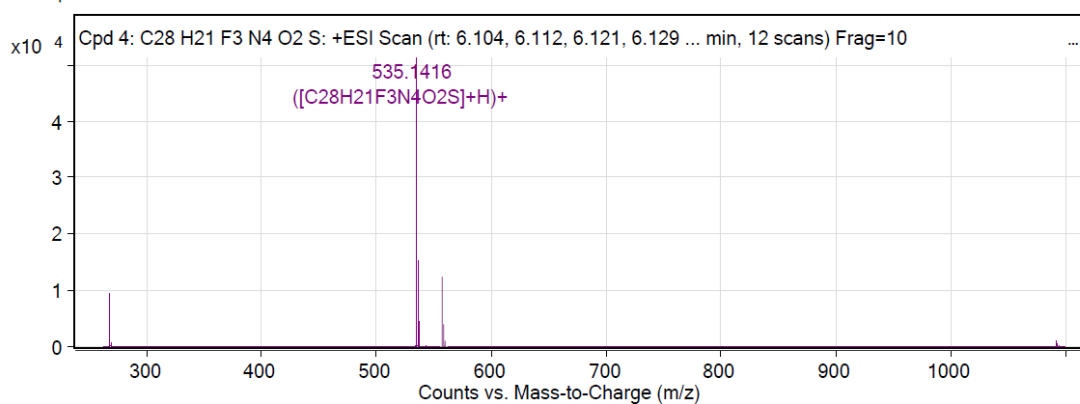


EI MS (70eV)



ESI-QTOF (positive ionization)

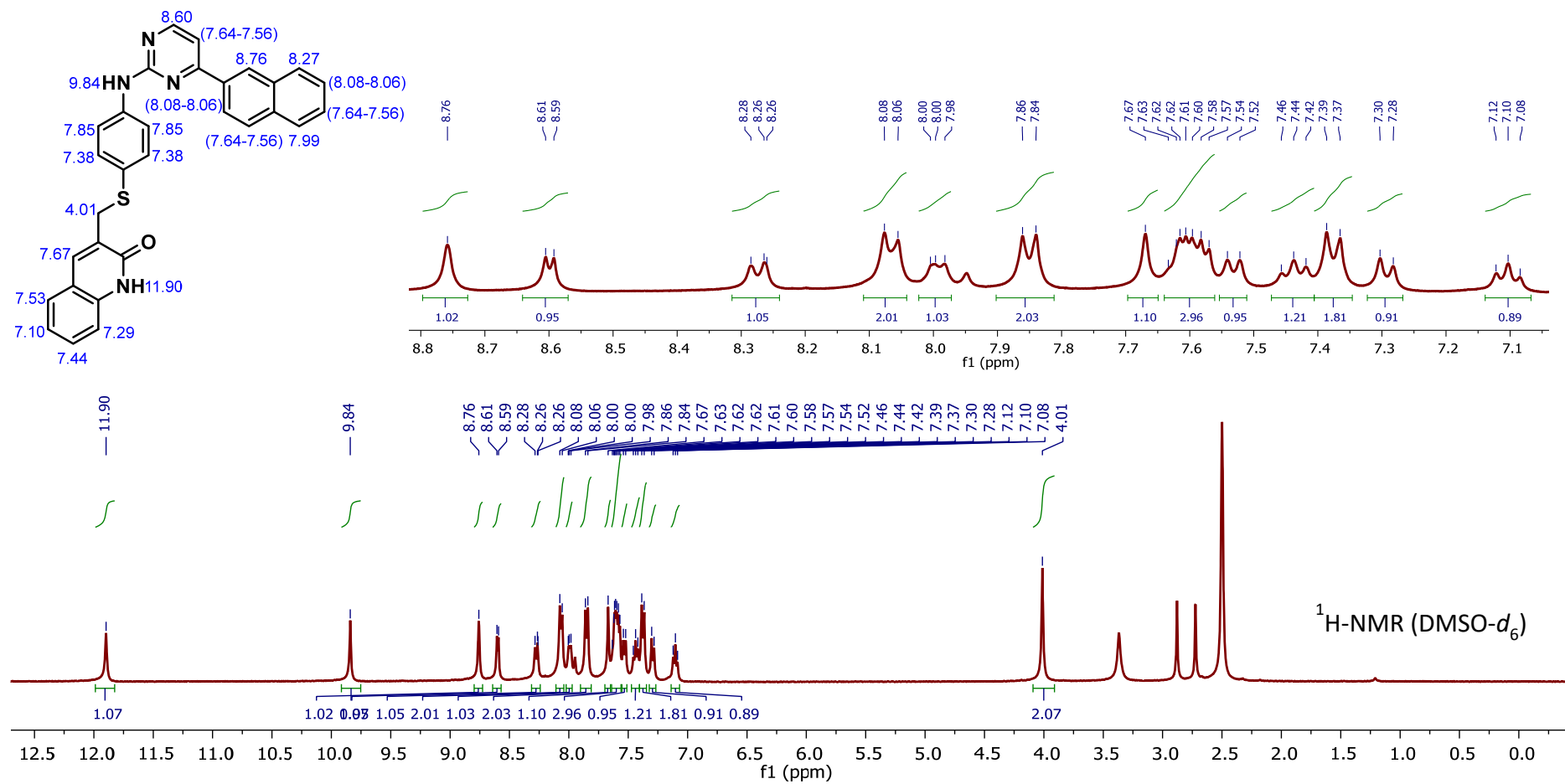
MS Zoomed Spectrum

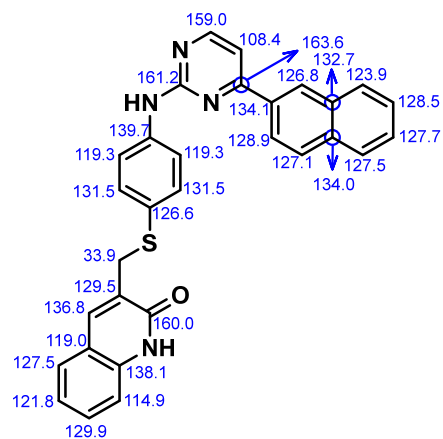


MS Spectrum Peak List

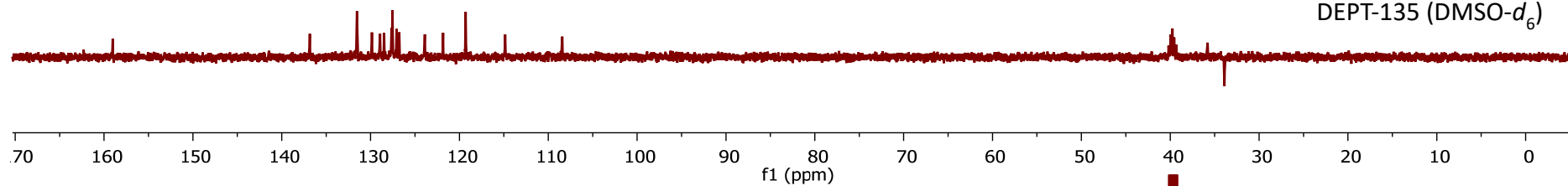
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
268.0741	268.0741	0.27	2	9462.26	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+2H) ⁺ 2
268.5756	268.5756	0.15	2	3198.57	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+2H) ⁺ 2
269.0752	269.0748	-1.14	2	934.05	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+2H) ⁺ 2
535.1416	535.141	-1.04	1	51348.98	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+H) ⁺
536.1445	536.144	-0.92	1	16004.3	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+H) ⁺
537.1433	537.1424	-1.55	1	4650.11	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+H) ⁺
557.1231	557.123	-0.22	1	12574.94	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+Na) ⁺
558.1263	558.126	-0.7	1	4061.59	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+Na) ⁺
559.1251	559.1244	-1.35	1	1216.16	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(M+Na) ⁺
1091.2563	1091.2567	0.31	1	1051.75	C ₂₈ H ₂₁ F ₃ N ₄ O ₂ S	(2M+Na) ⁺

4.29 Compound 30a

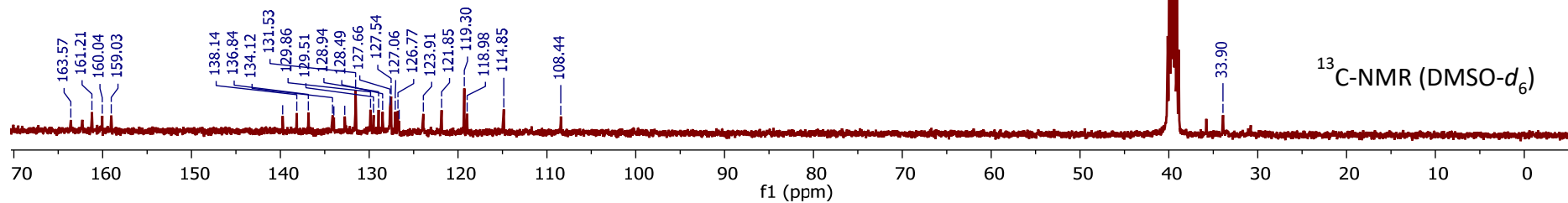




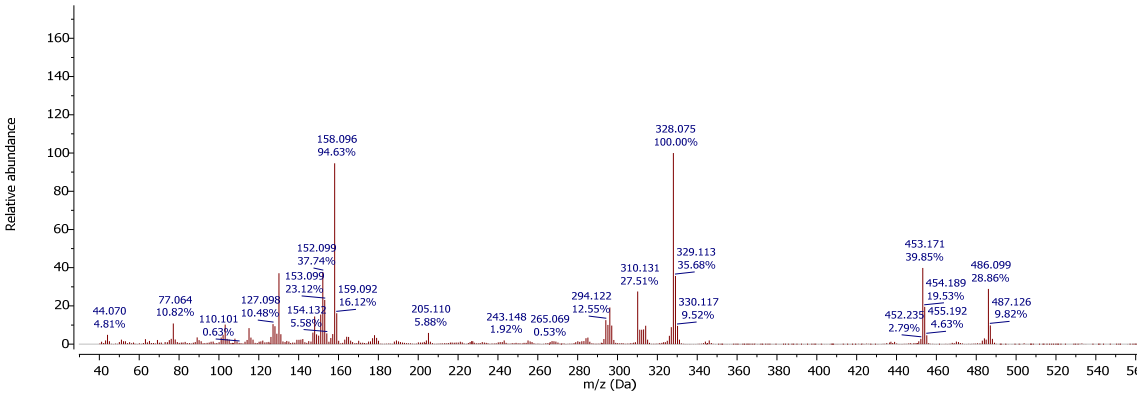
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

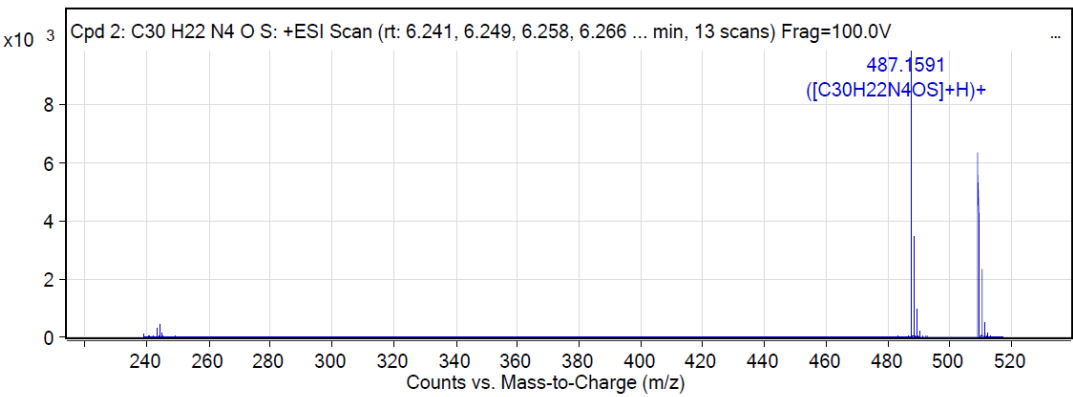


EI MS (70eV)



ESI-QTOF (positive ionization)

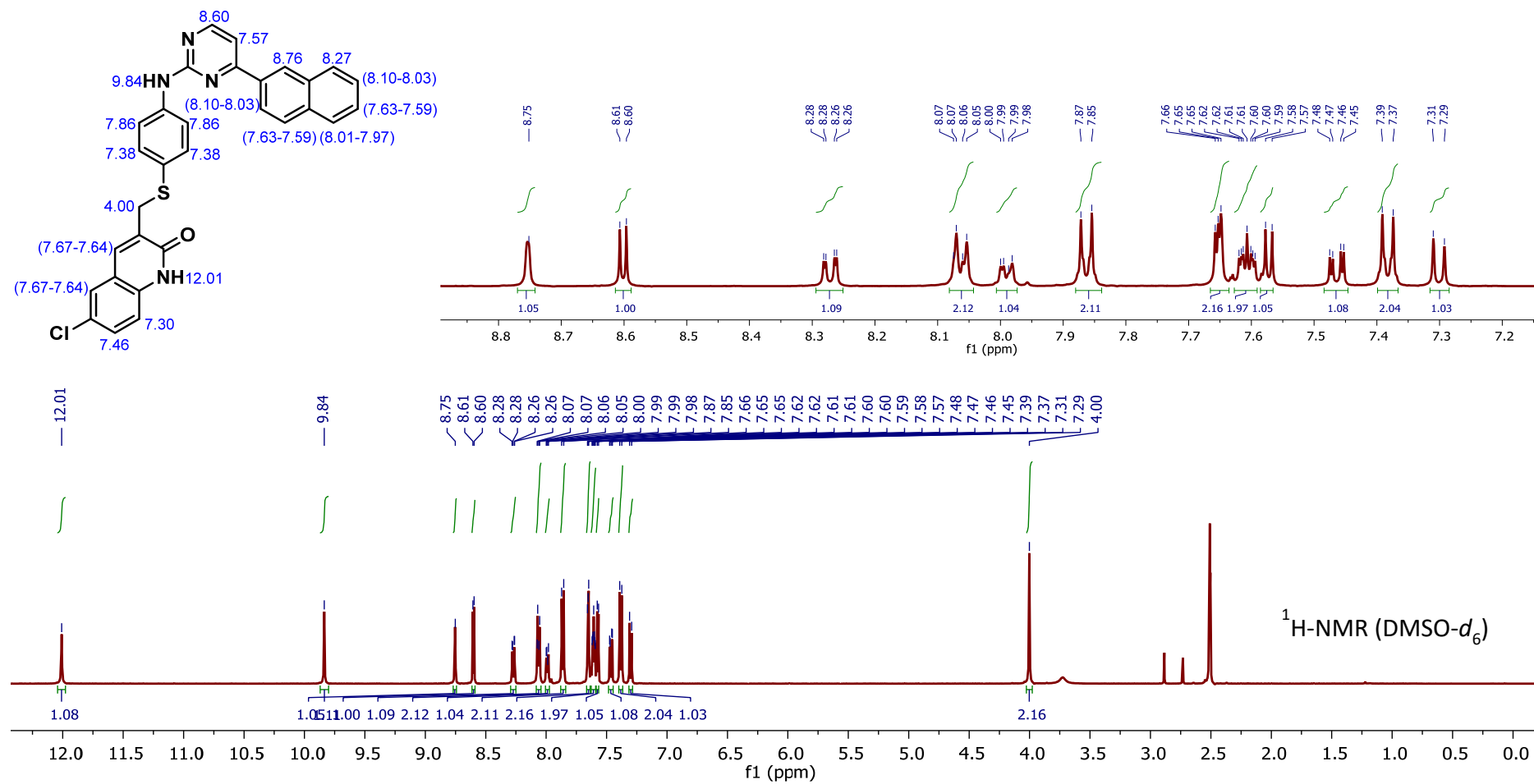
MS Zoomed Spectrum

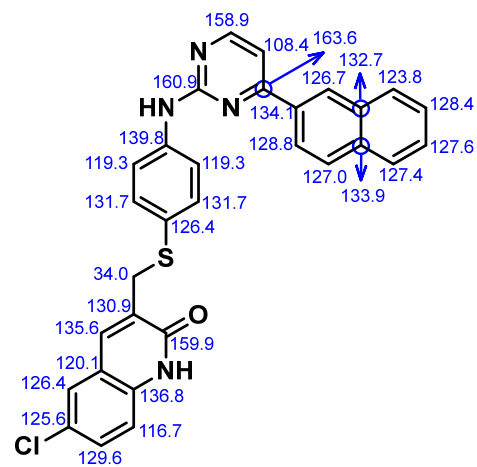


MS Spectrum Peak List

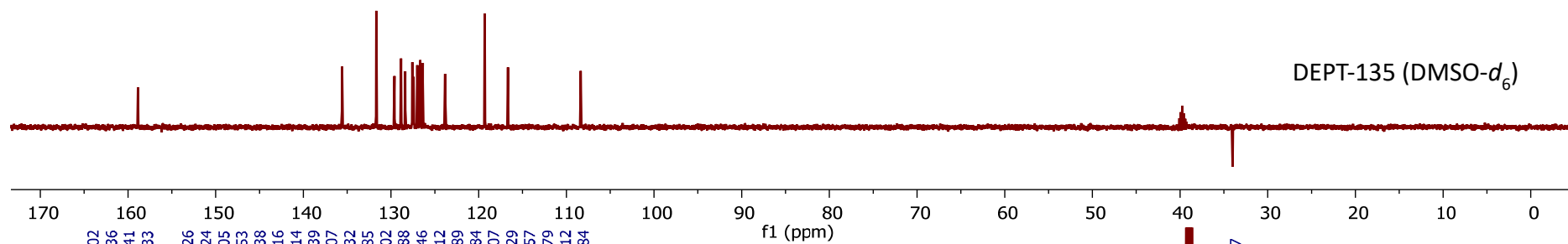
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
244.0825	244.083		2		497.6 C ₃₀ H ₂₂ N ₄ OS	(M+2H)+2
244.5853	244.5845	-3.32	2		121.62 C ₃₀ H ₂₂ N ₄ OS	(M+2H)+2
245.0794	245.0838	18.26	2		54.57 C ₃₀ H ₂₂ N ₄ OS	(M+2H)+2
487.1591	487.1587	-0.73	1		9911.09 C ₃₀ H ₂₂ N ₄ OS	(M+H)+
488.1618	488.1617	-0.18	1		3507.15 C ₃₀ H ₂₂ N ₄ OS	(M+H)+
489.161	489.1604	-1.3	1		998.93 C ₃₀ H ₂₂ N ₄ OS	(M+H)+
509.1411	509.1407	-0.95	1		6441.07 C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
510.1432	510.1437		1		2417.24 C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
511.1432	511.1423	-1.77	1		575.29 C ₃₀ H ₂₂ N ₄ OS	(M+Na)+
512.1463	512.1428	-6.91	1		102.76 C ₃₀ H ₂₂ N ₄ OS	(M+Na)+

4.30 Compound 30b

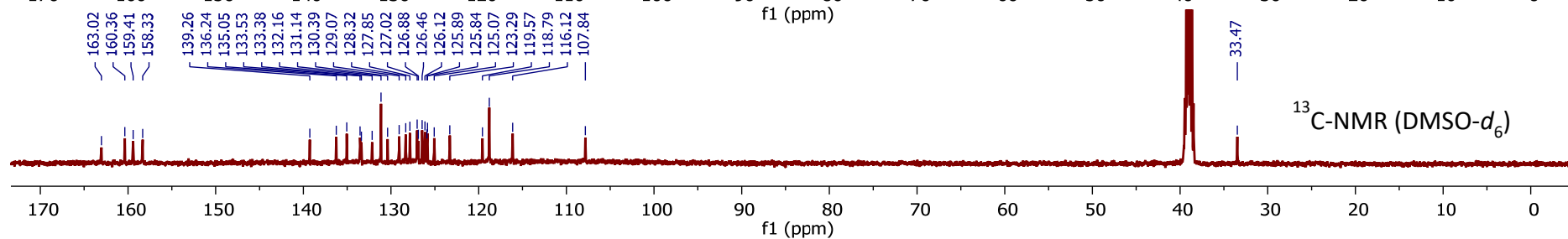




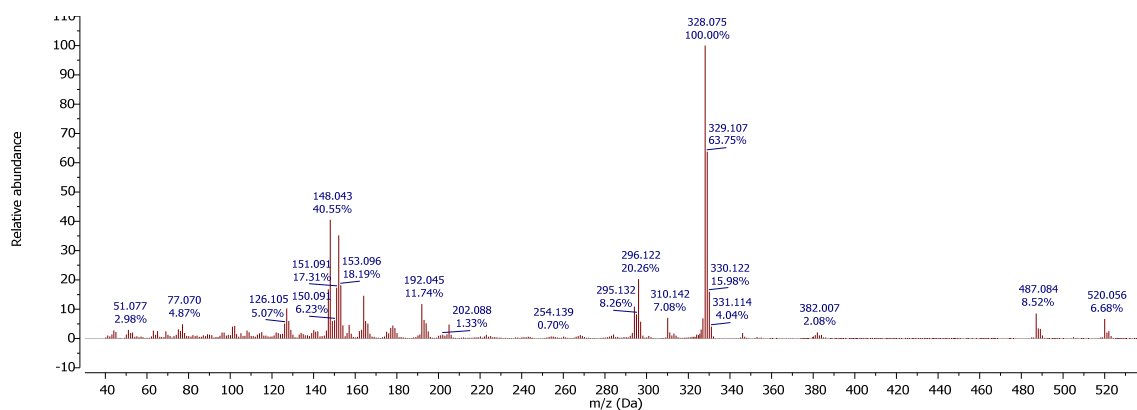
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

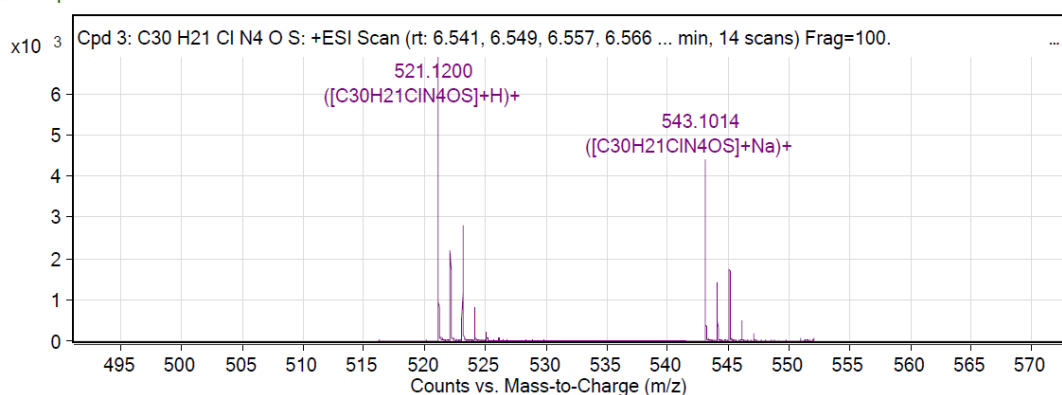


EI MS (70eV)



ESI-QTOF (positive ionization)

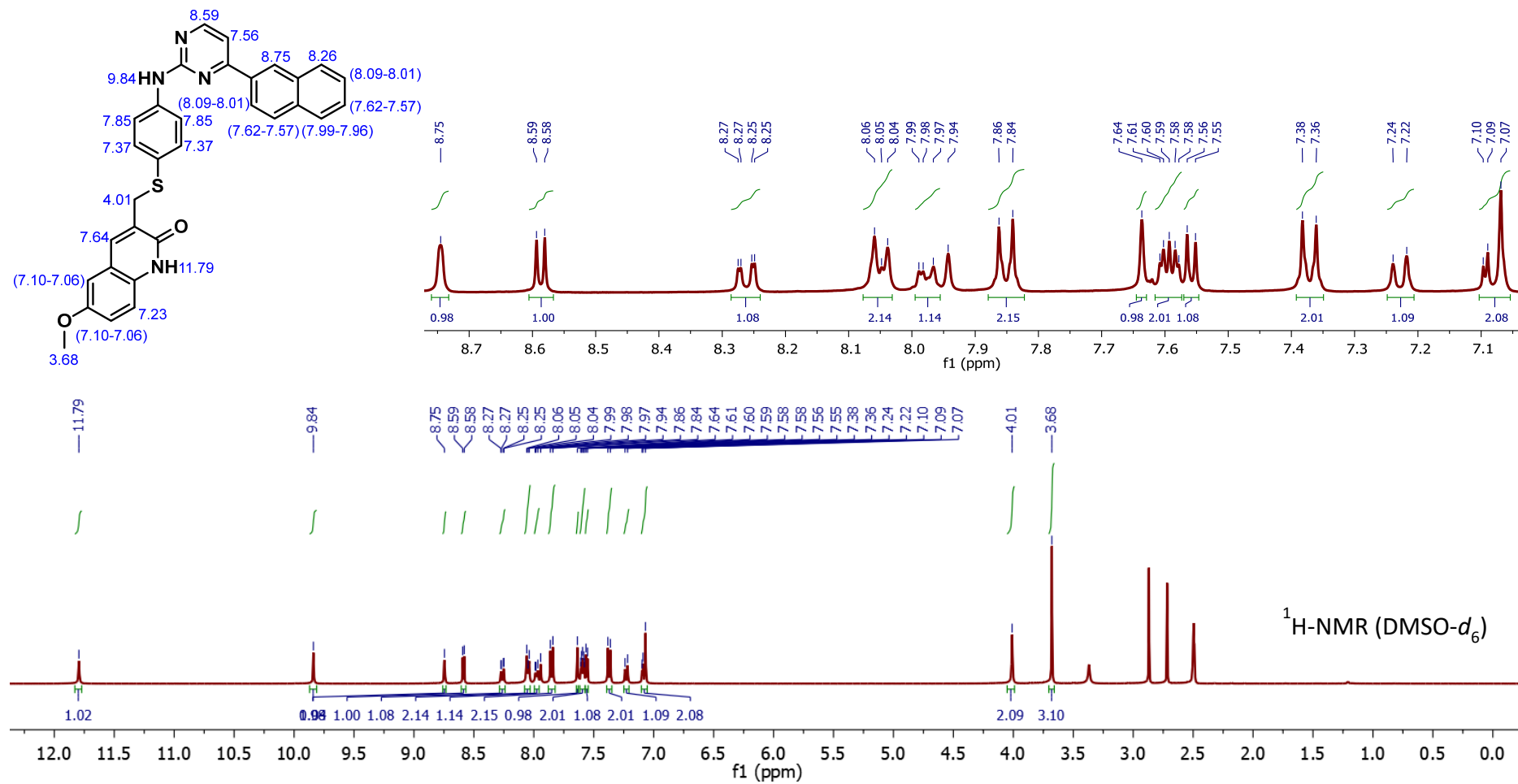
MS Zoomed Spectrum

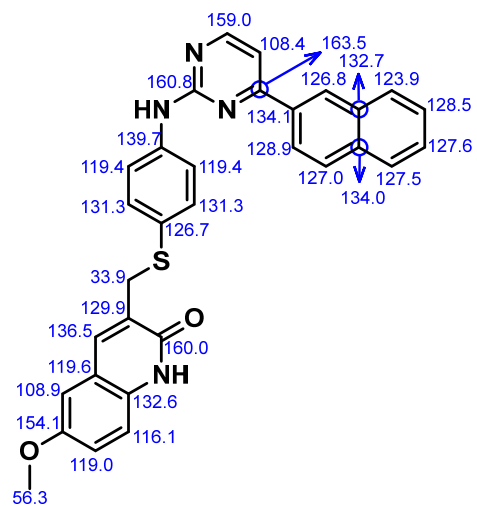


MS Spectrum Peak List

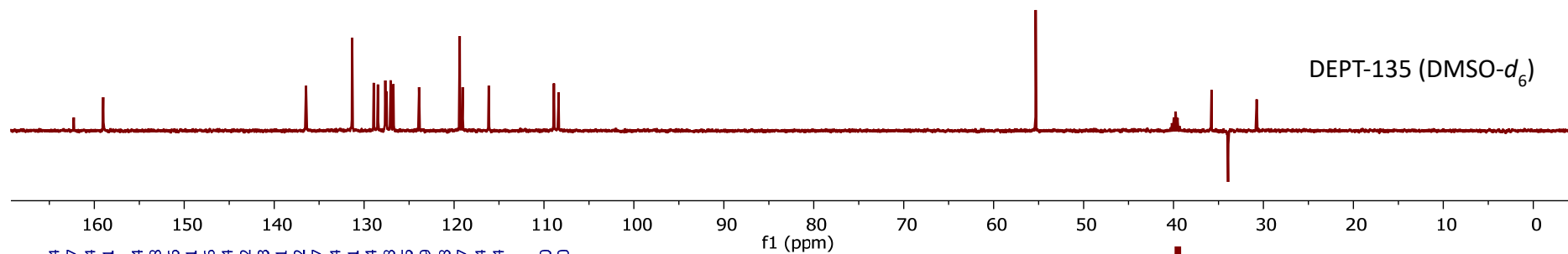
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
521.12	521.1197	-0.43	1	6953.13	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+H) ⁺
522.1225	522.1228	0.41	1	2321.15	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+H) ⁺
523.1184	523.1179	-0.9	1	2869.15	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+H) ⁺
524.1206	524.1201	-0.91	1	840.5	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+H) ⁺
525.1218	525.1189	-5.56	1	235.49	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+H) ⁺
543.1014	543.1017	0.59	1	4442.43	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+Na) ⁺
544.1049	544.1047	-0.44	1	1485.43	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+Na) ⁺
545.0992	545.0999	1.25	1	1813.92	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+Na) ⁺
546.1036	546.1021	-2.75	1	545.87	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+Na) ⁺
547.101	547.1009	-0.21	1	175.92	C ₃₀ H ₂₁ ClN ₄ O ₅ S	(M+Na) ⁺

4.31 Compound 30c

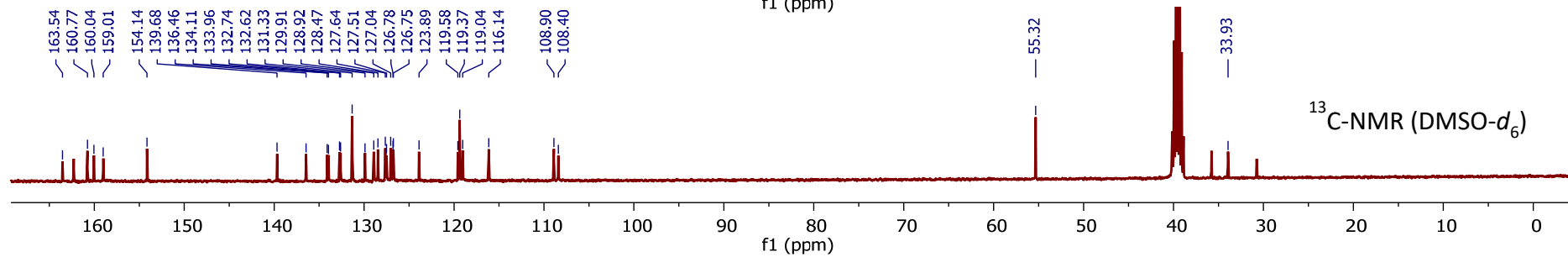




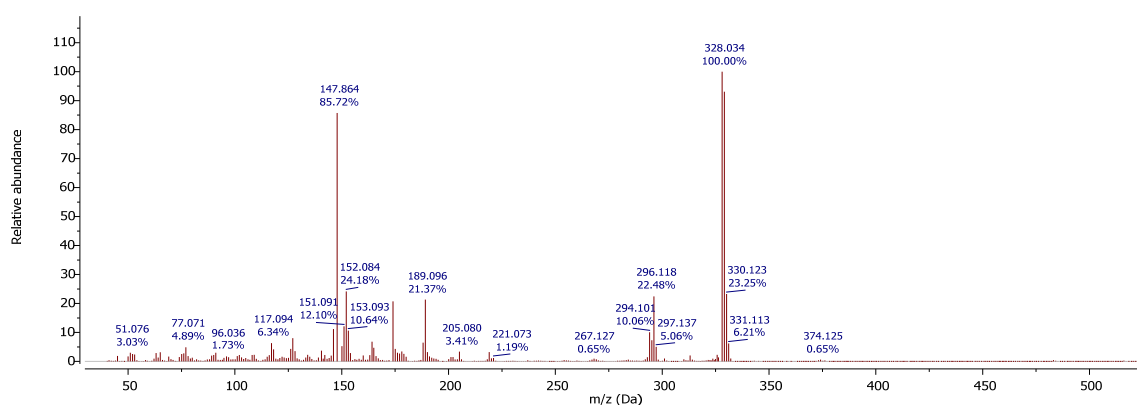
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

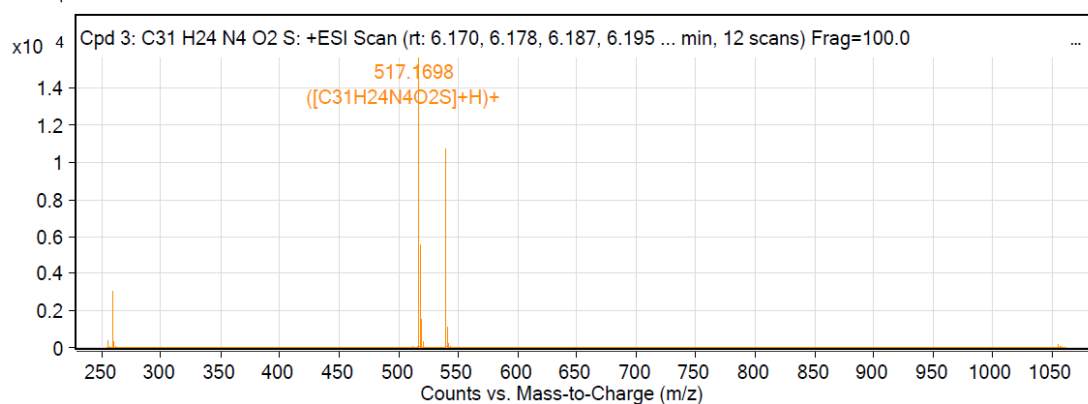


EI MS (70eV)



ESI-QTOF (positive ionization)

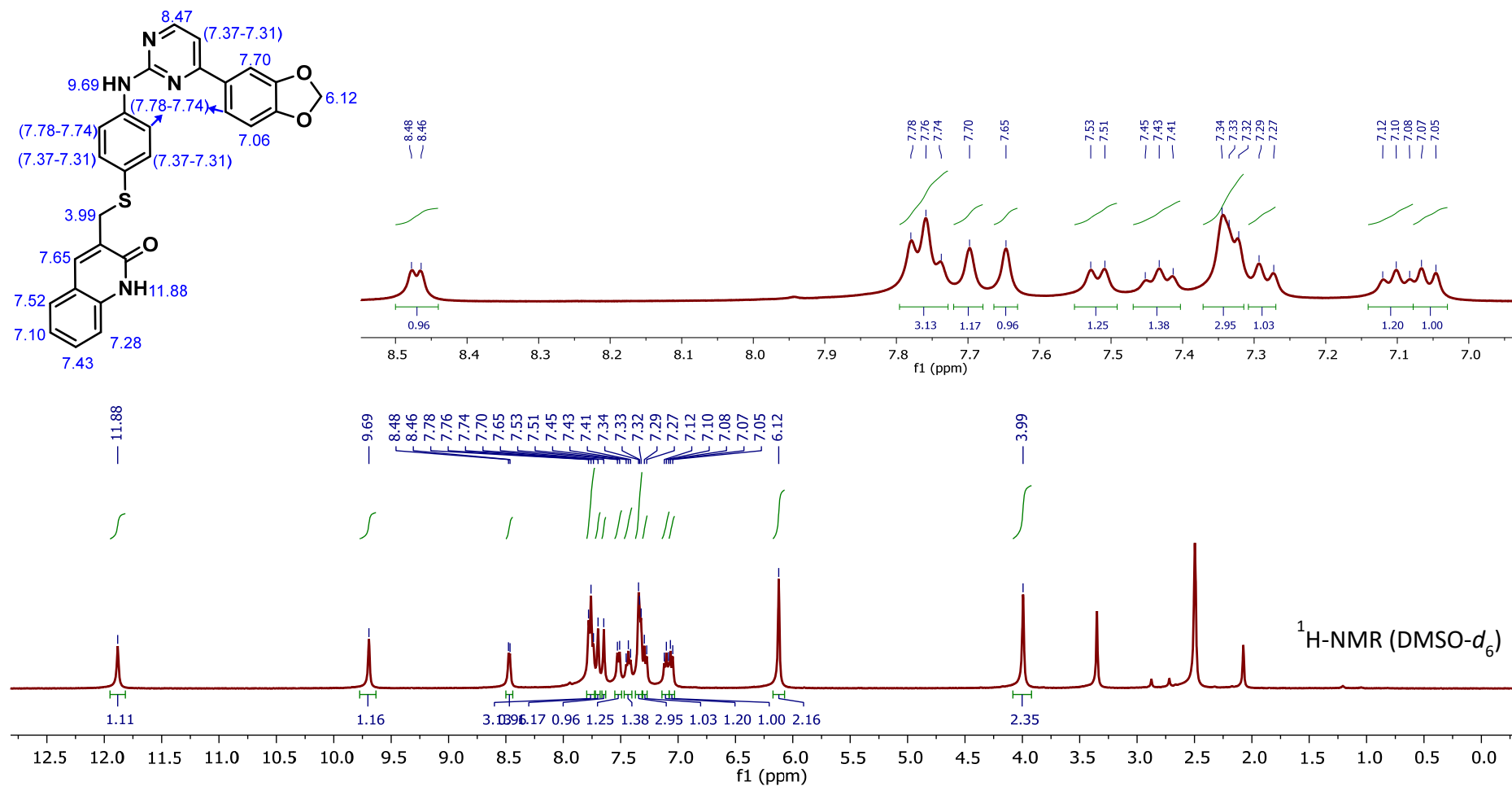
MS Zoomed Spectrum

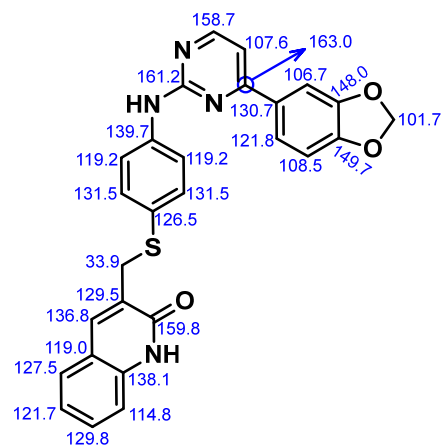


MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
259.0884	259.0883	-0.48	2	3151.79	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+2H)+2
259.5893	259.5898	1.98	2	1104.27	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+2H)+2
260.0897	260.0892	-1.67	2	368.27	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+2H)+2
517.1698	517.1693	-1.06	1	15760.97	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+H)+
518.1728	518.1723	-0.94	1	5645.06	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+H)+
519.1722	519.1712	-1.98	1	1609.85	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+H)+
539.1517	539.1512	-0.93	1	11045.04	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+Na)+
540.1551	540.1543	-1.52	1	3947.27	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+Na)+
541.155	541.1531	-3.5	1	1184.69	C ₃₁ H ₂₄ N ₄ O ₂ S	(M+Na)+
1055.3142	1055.3132	-0.95	1	210.75	C ₃₁ H ₂₄ N ₄ O ₂ S	(2M+Na)+

4.32 Compound 31a

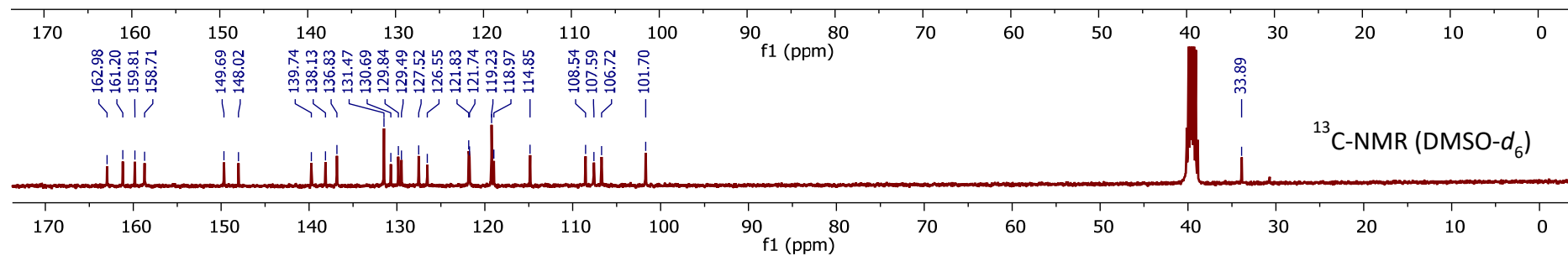




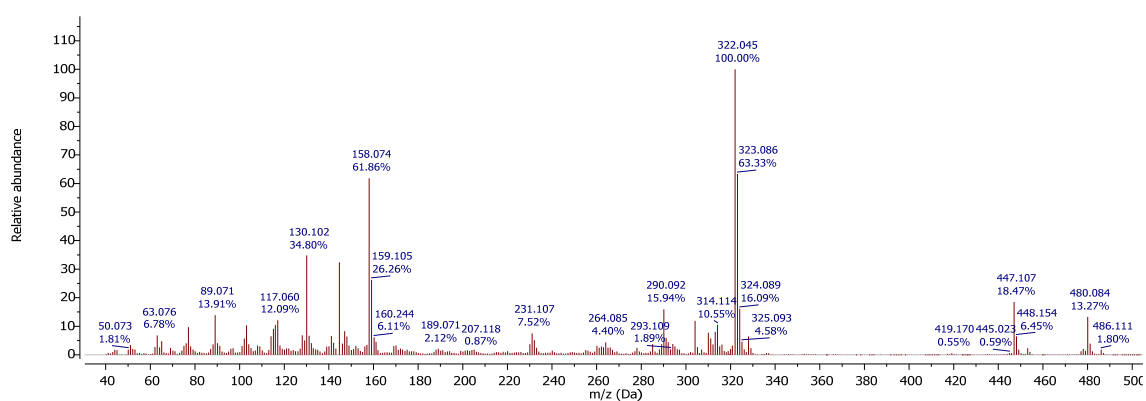
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

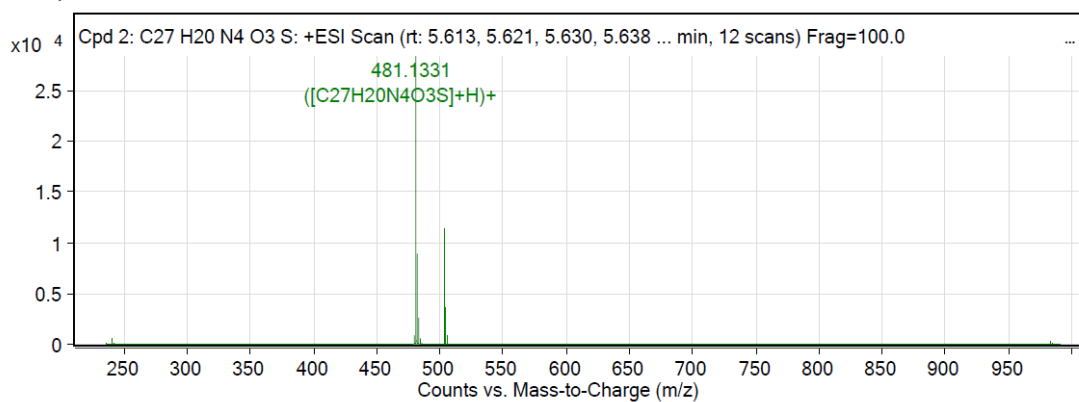


EI MS (70eV)



ESI-QTOF (positive ionization)

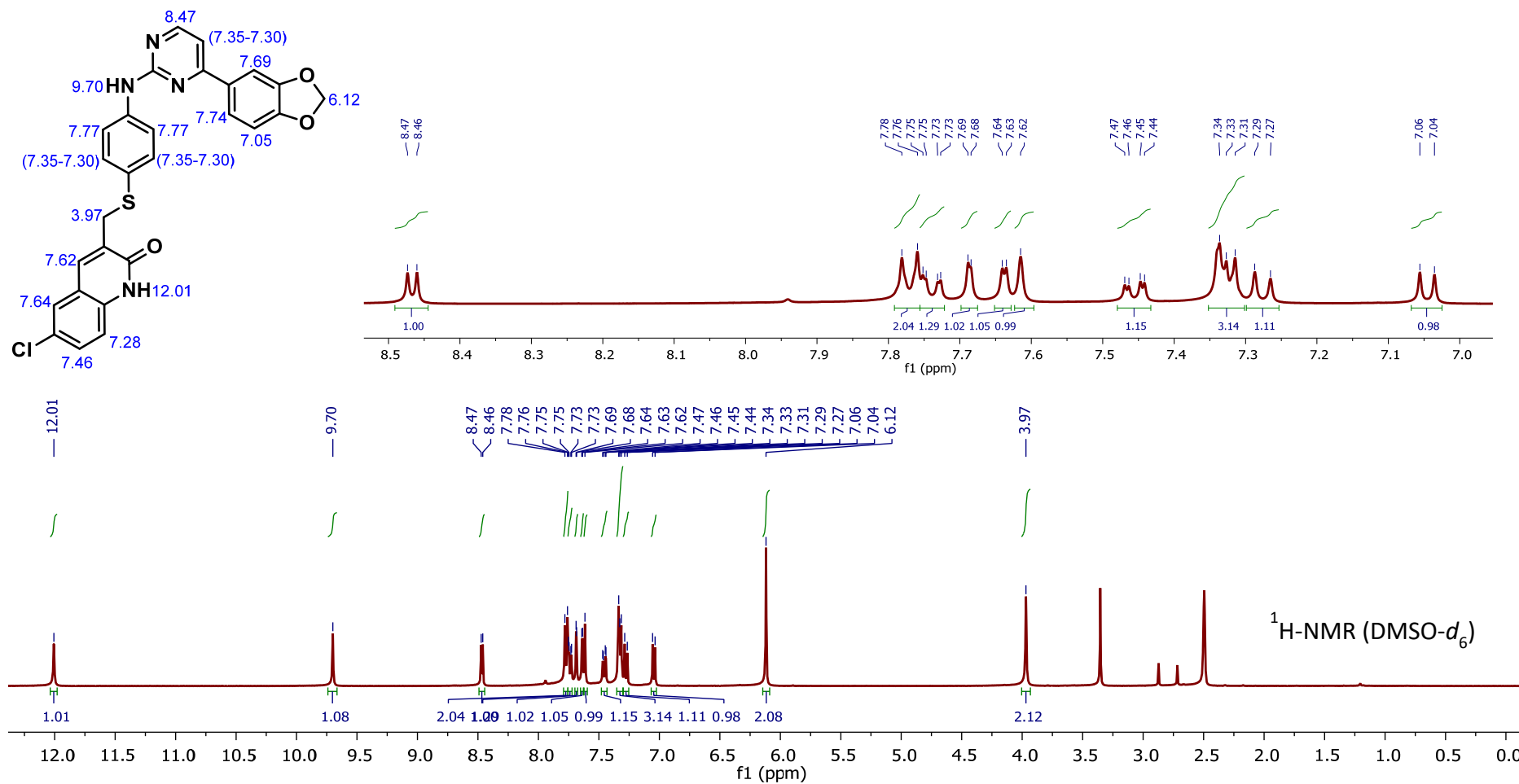
MS Zoomed Spectrum

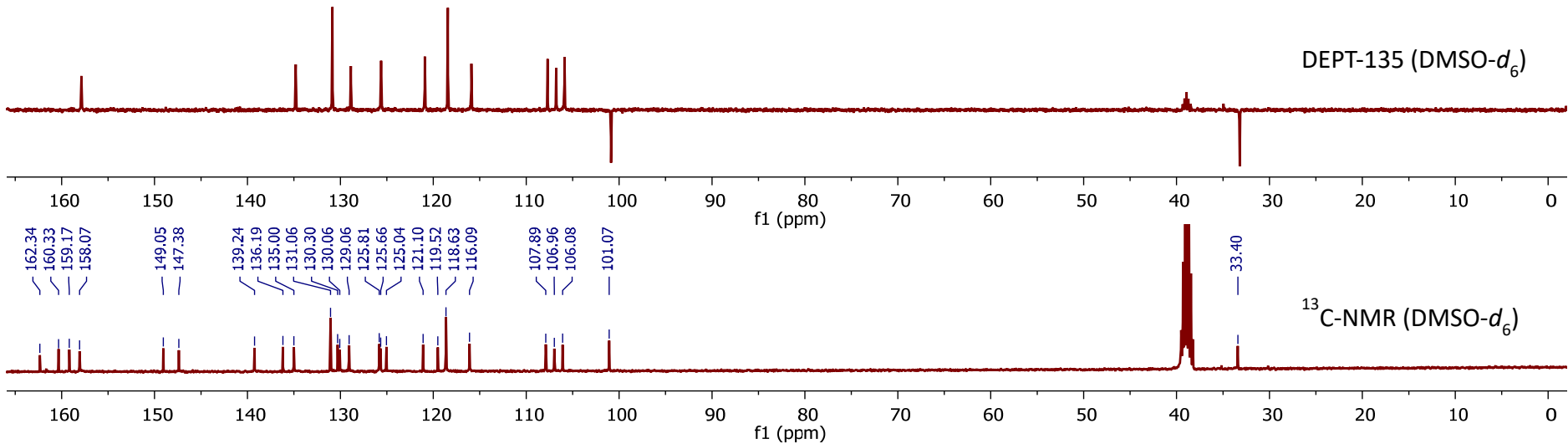


MS Spectrum Peak List

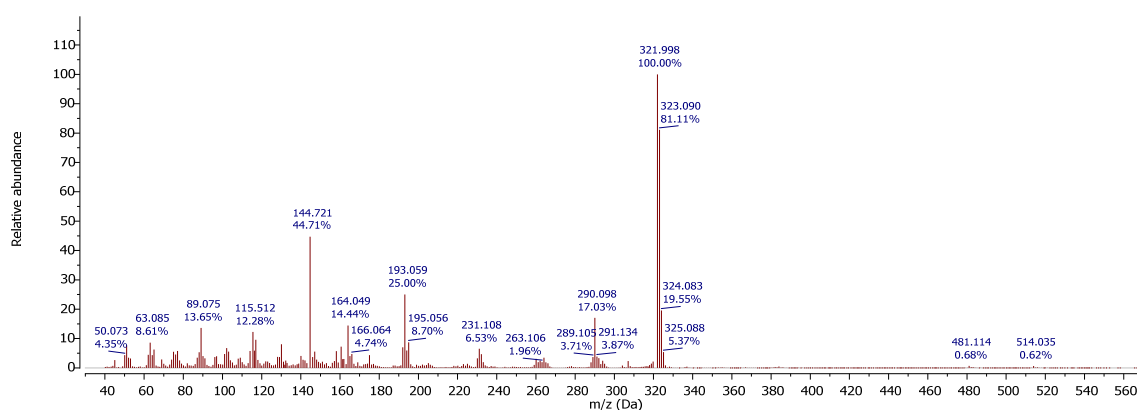
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
241.0696	241.0701	1.93	2	654.72	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+2H)+2
481.1331	481.1329	-0.47	1	29280.21	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H)+
482.1361	482.1359	-0.51	1	8975.86	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H)+
483.1347	483.1342	-1.13	1	2638.49	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+H)+
503.115	503.1148	-0.28	1	11622.33	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na)+
504.1176	504.1178	0.4	1	3718.28	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na)+
505.1169	505.1161	-1.49	1	1042.77	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na)+
506.1125	506.1169	8.6	1	186.36	C ₂₇ H ₂₀ N ₄ O ₃ S	(M+Na)+
983.2422	983.2404	-1.77	1	352.25	C ₂₇ H ₂₀ N ₄ O ₃ S	(2M+Na)+
984.2449	984.2434	-1.44	1	200.29	C ₂₇ H ₂₀ N ₄ O ₃ S	(2M+Na)+

4.33 Compound 31b



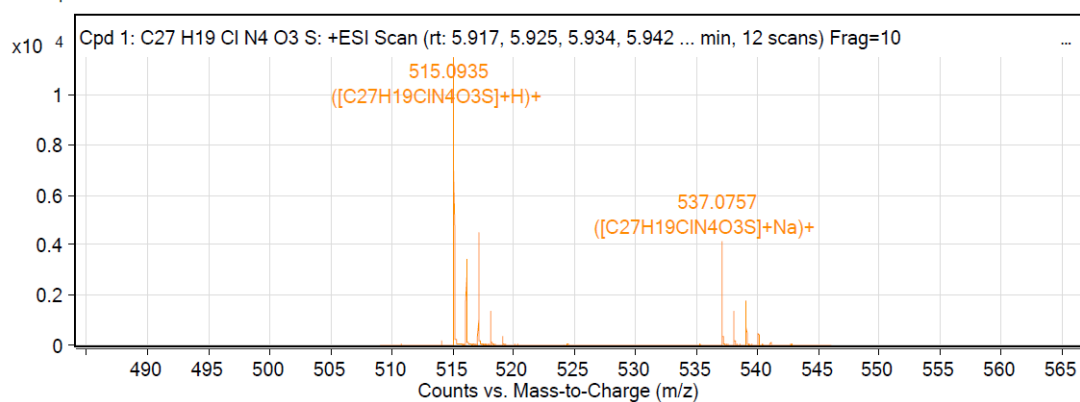


EI MS (70eV)



ESI-QTOF (positive ionization)

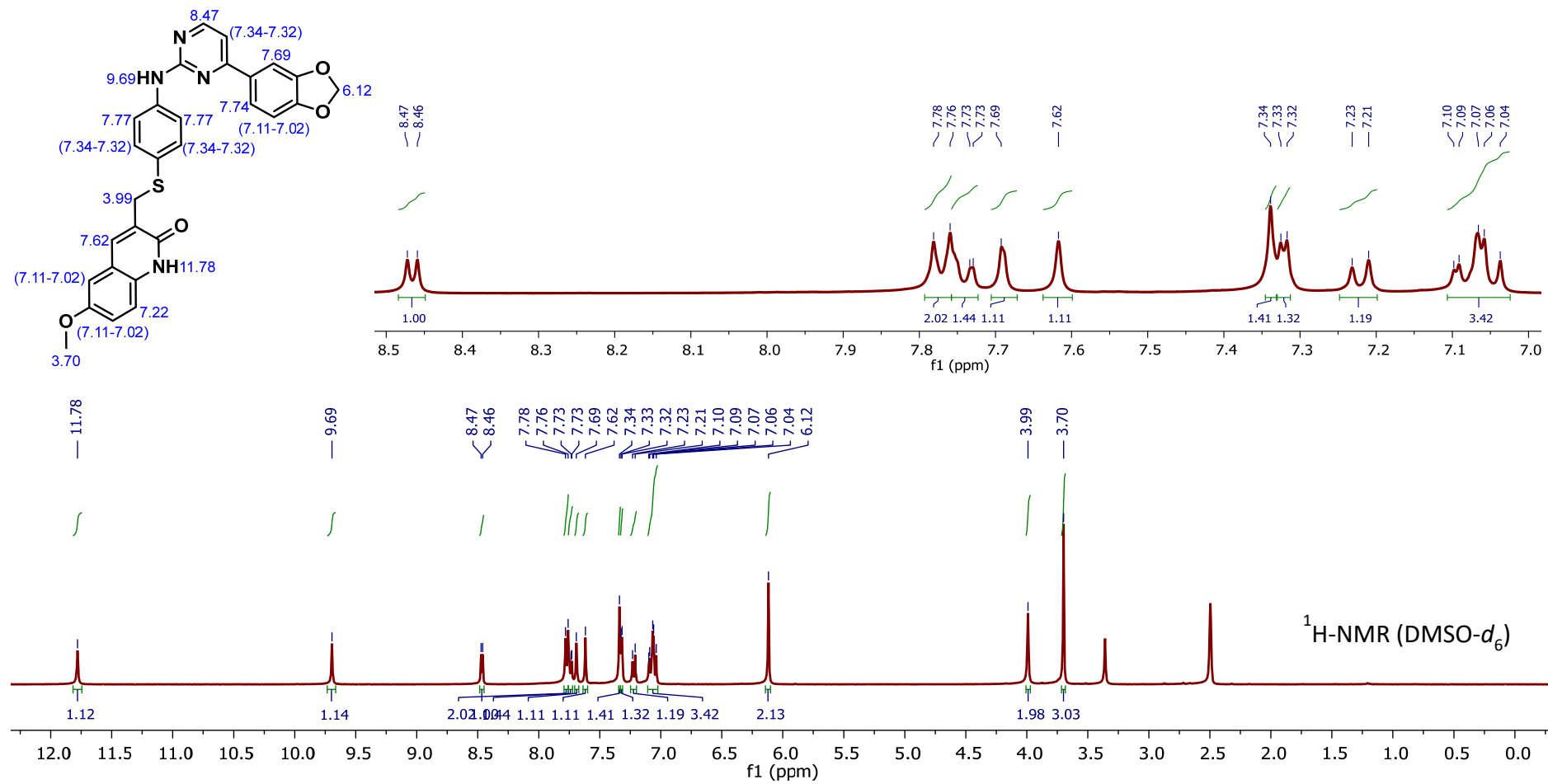
MS Zoomed Spectrum

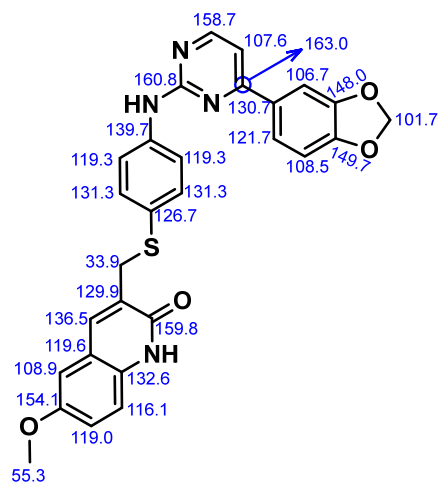


MS Spectrum Peak List

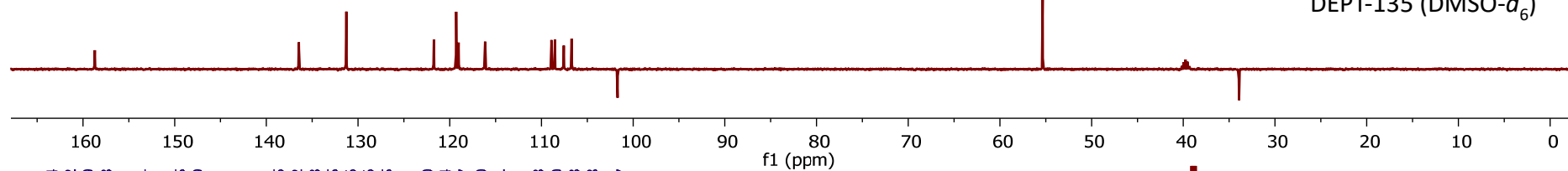
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
514.085	514.0861	2.22	1	145.65	C ₂₇ H ₁₉ ClN ₄ O ₃ S	M+
515.0935	515.0939	0.84	1	11522.77	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H)+
516.0969	516.0969	0.05	1	3560.53	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H)+
517.0919	517.092	0.16	1	4642.79	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H)+
518.0935	518.0943	1.54	1	1356.07	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H)+
519.0937	519.0927	-1.93	1	351.39	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+H)+
537.0757	537.0759	0.23	1	4185.63	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+Na)+
538.0784	538.0788	0.85	1	1410.28	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+Na)+
539.0735	539.0739	0.8	1	1793.18	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+Na)+
540.0759	540.0762	0.64	1	533.48	C ₂₇ H ₁₉ ClN ₄ O ₃ S	(M+Na)+

4.34 Compound 31c

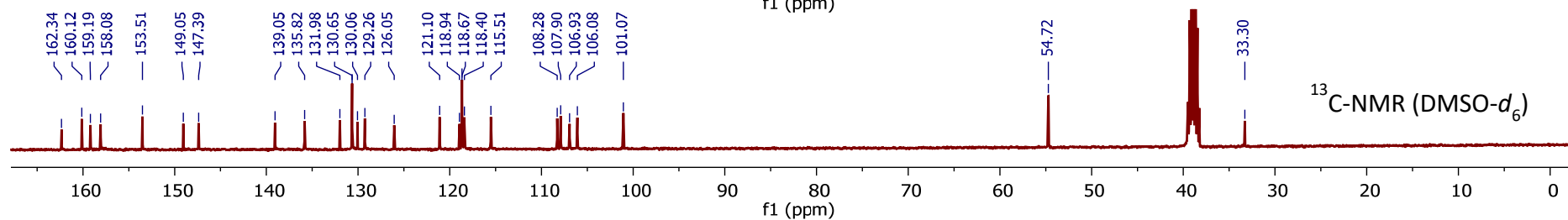




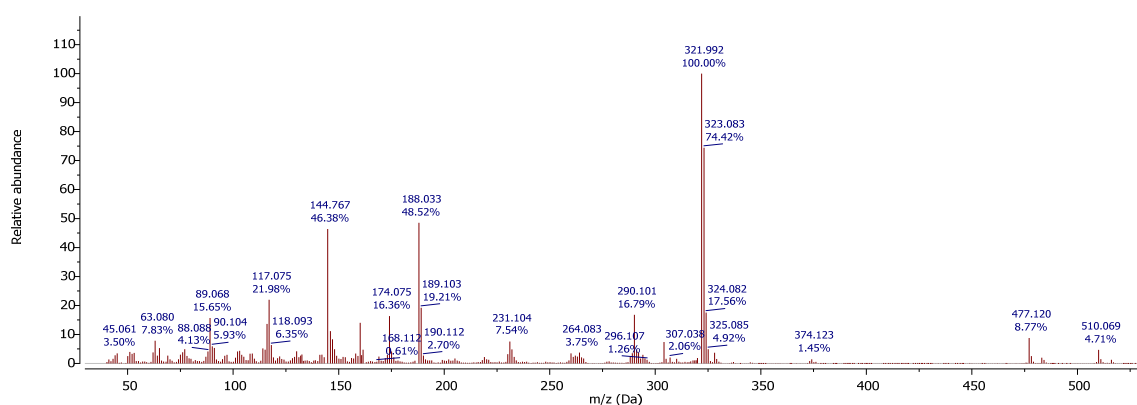
DEPT-135 ($\text{DMSO}-d_6$)



^{13}C -NMR ($\text{DMSO}-d_6$)

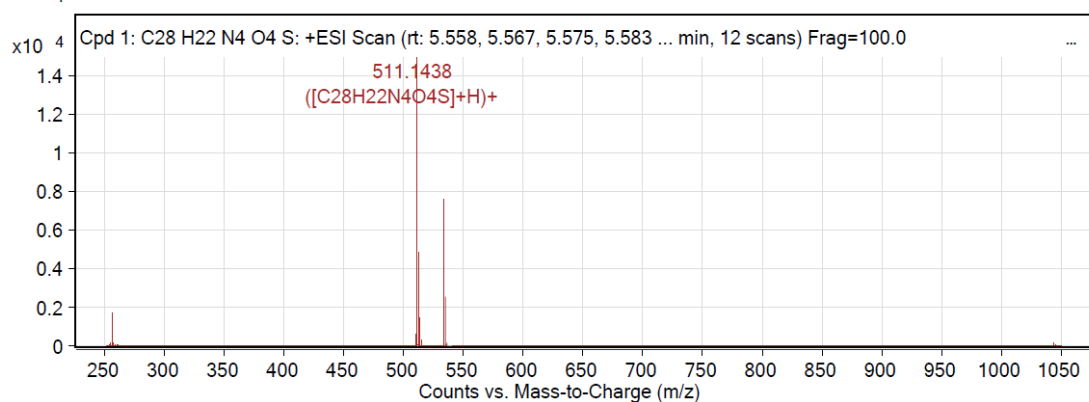


EI MS (70eV)



ESI-QTOF (positive ionization)

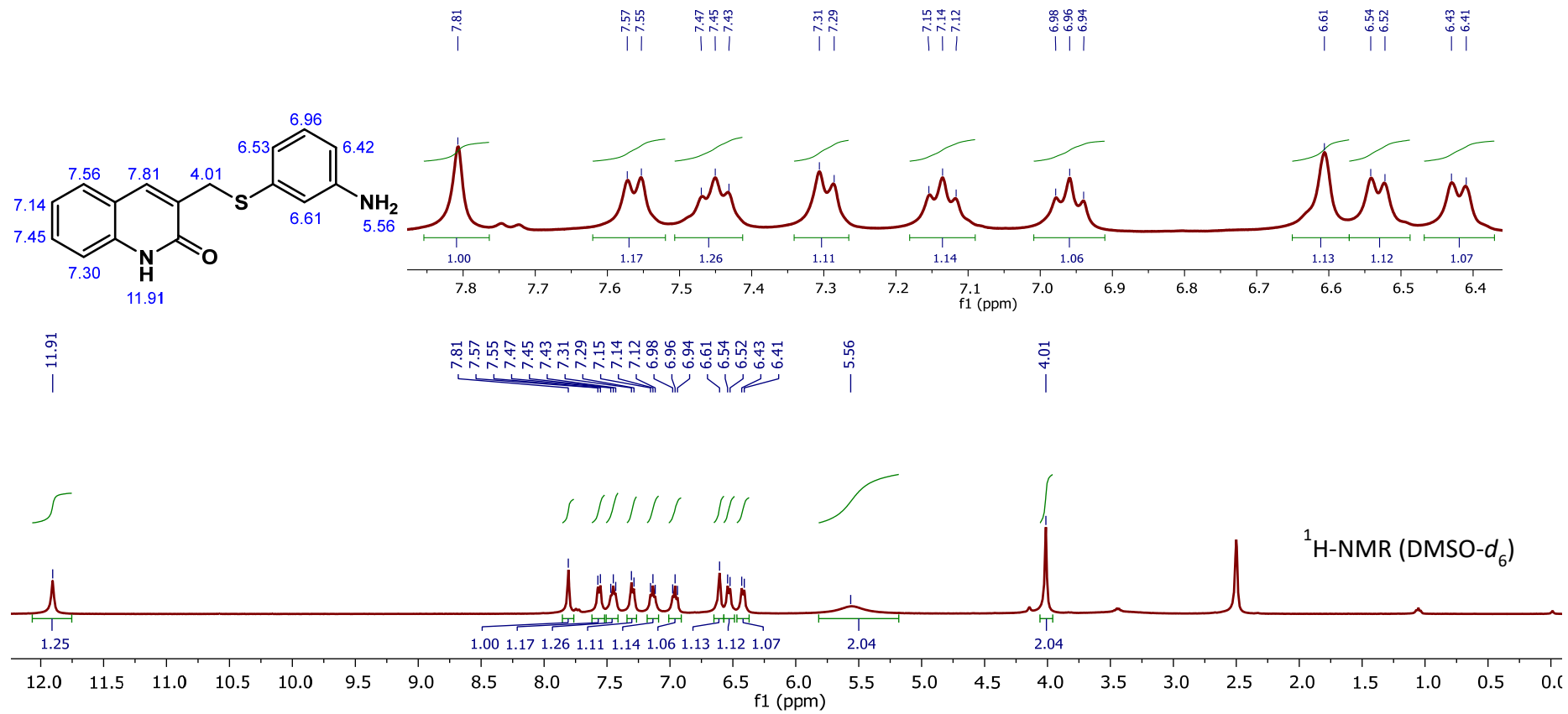
MS Zoomed Spectrum

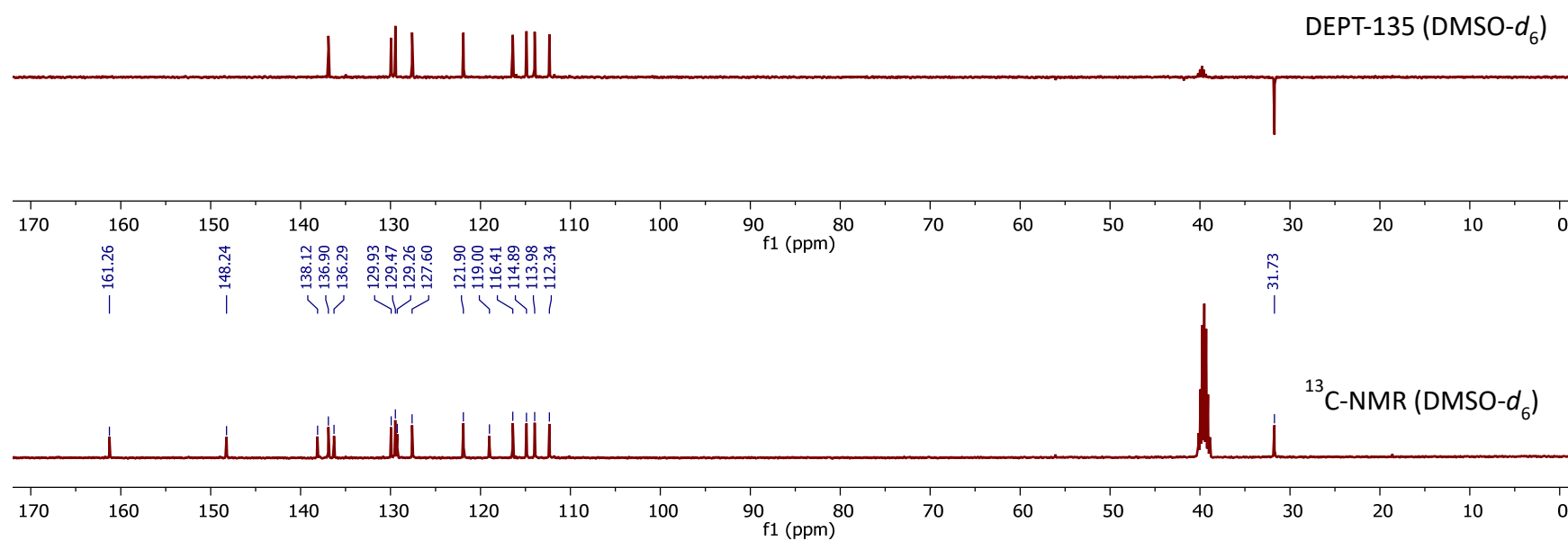
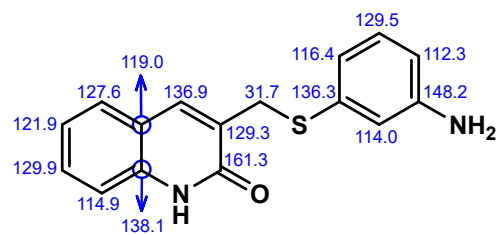


MS Spectrum Peak List

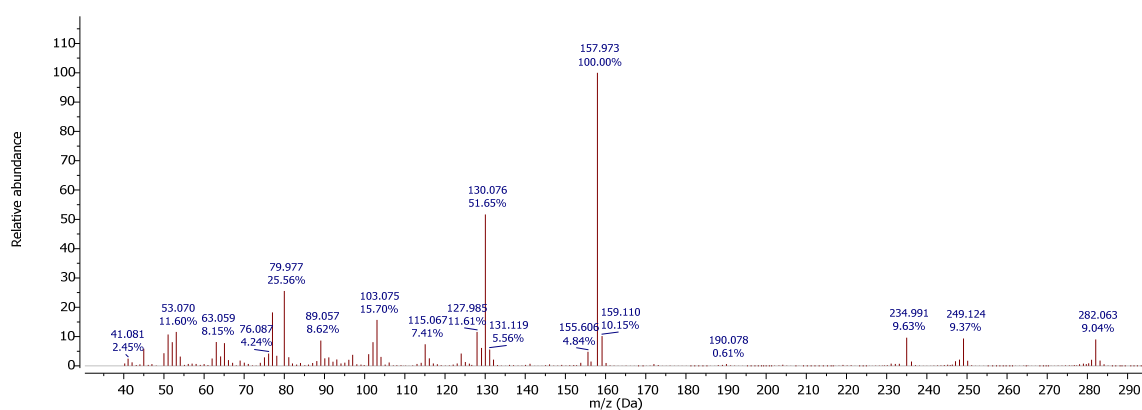
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
256.0746	256.0754	2.93	2	1763.84	C28H22N4O4S	(M+2H)+2
256.5772	256.5769	-1.17	2	685.52	C28H22N4O4S	(M+2H)+2
257.0777	257.0761	-6.04	2	183.36	C28H22N4O4S	(M+2H)+2
511.1438	511.1435	-0.71	1	14971.63	C28H22N4O4S	(M+H)+
512.1462	512.1465	0.55	1	4953.16	C28H22N4O4S	(M+H)+
513.1455	513.145	-0.93	1	1537.28	C28H22N4O4S	(M+H)+
533.1252	533.1254	0.42	1	7665.06	C28H22N4O4S	(M+Na)+
534.1284	534.1284	0.01	1	2610.76	C28H22N4O4S	(M+Na)+
535.1272	535.1269	-0.46	1	736.35	C28H22N4O4S	(M+Na)+
1043.2579	1043.2616	3.53	1	83.51	C28H22N4O4S	(2M+Na)+

4.35 Compound 32a



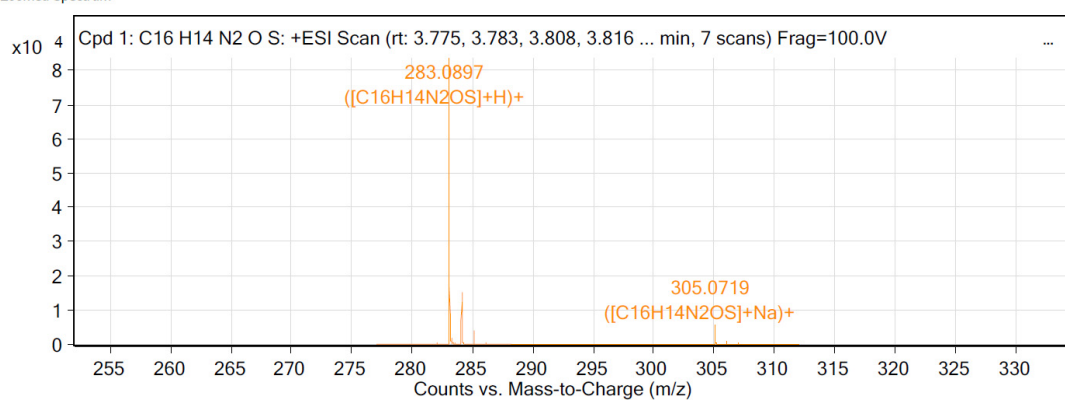


EI MS (70eV)



ESI-QTOF (positive ionization)

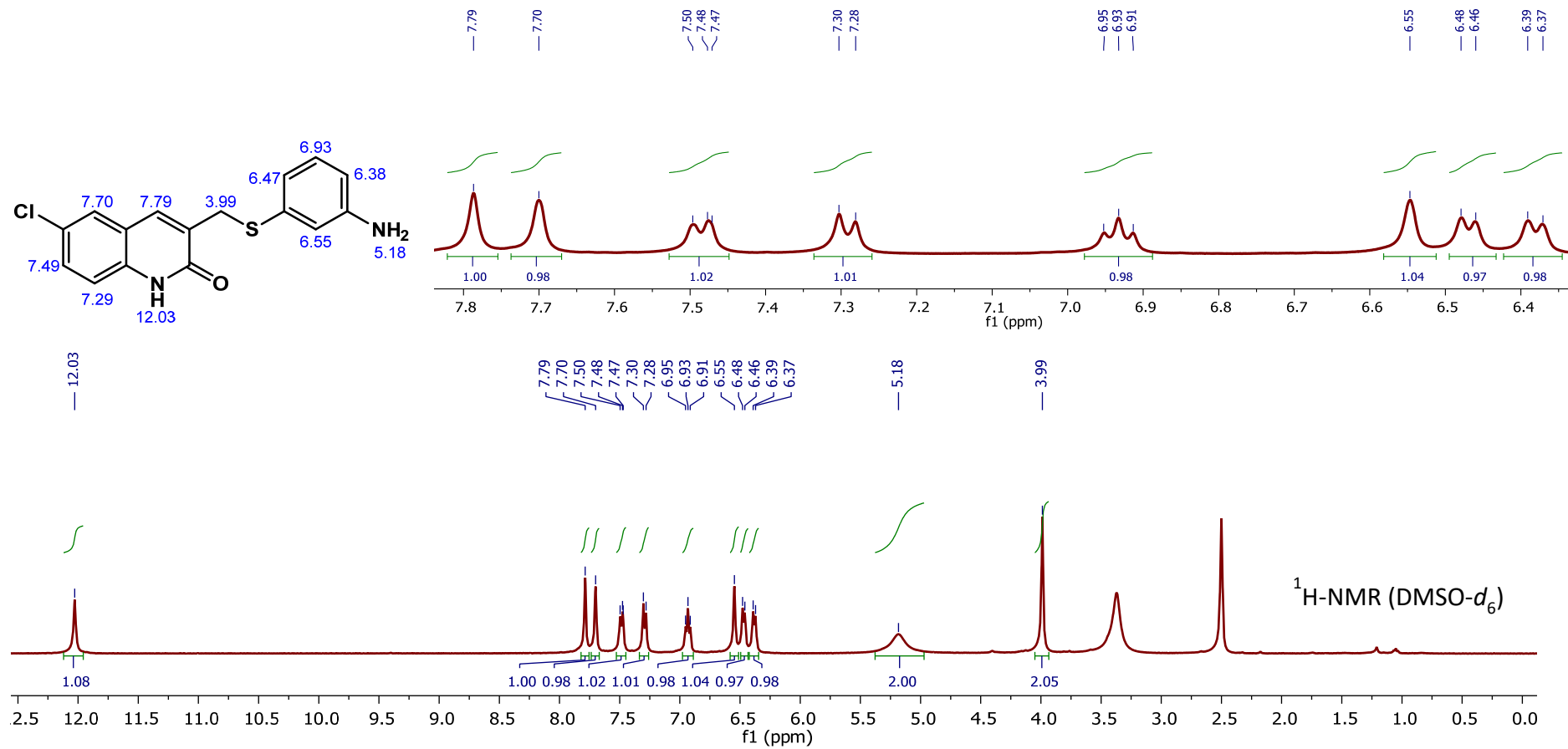
MS Zoomed Spectrum

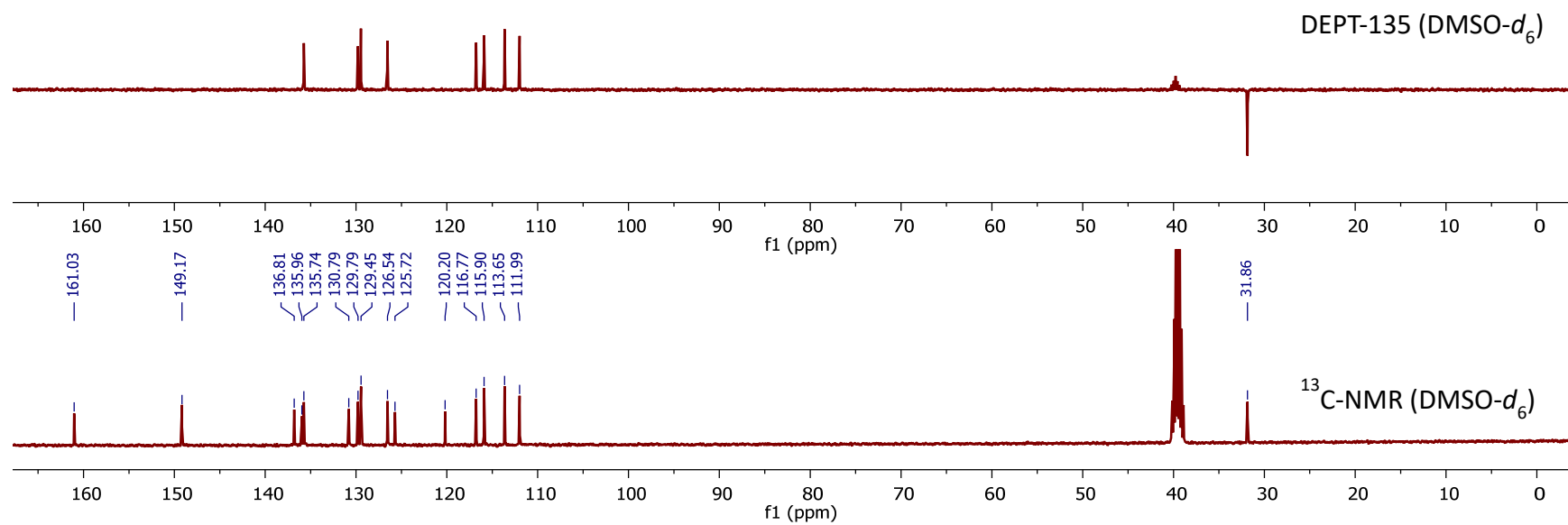
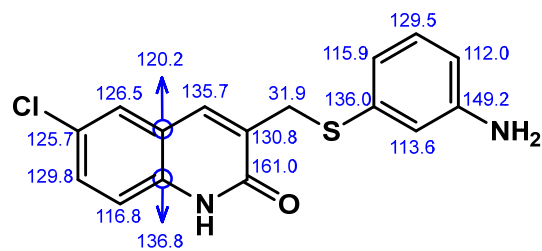


MS Spectrum Peak List

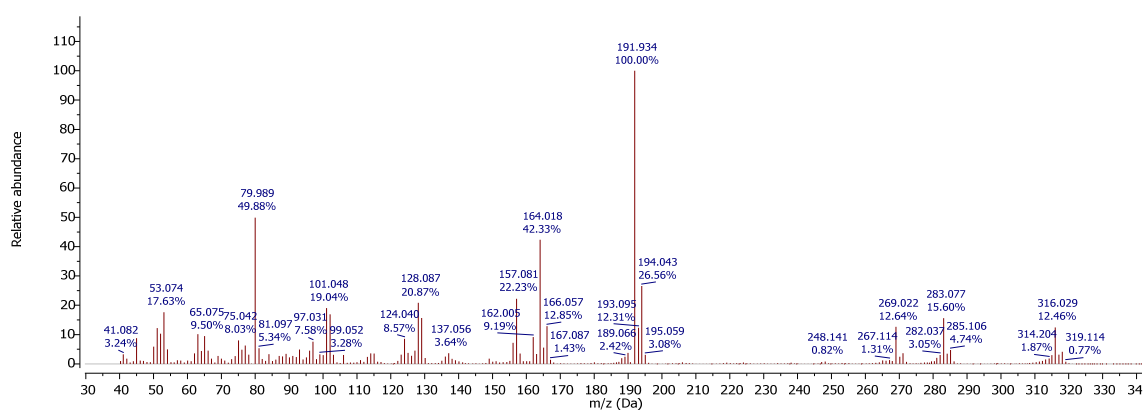
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
282.0827	282.0821	-1.93	1	538.14	C16H14N2OS	M+
283.0897	283.09	0.8	1	84261.67	C16H14N2OS	(M+H)+
284.0929	284.0929	0.02	1	15045.32	C16H14N2OS	(M+H)+
285.0885	285.0887	0.89	1	4221.72	C16H14N2OS	(M+H)+
305.0719	305.0719	0.16	1	5652.01	C16H14N2OS	(M+Na)+
306.0753	306.0749	-1.28	1	1184.37	C16H14N2OS	(M+Na)+
307.0701	307.0707	1.83	1	367.66	C16H14N2OS	(M+Na)+

4.36 Compound 32b



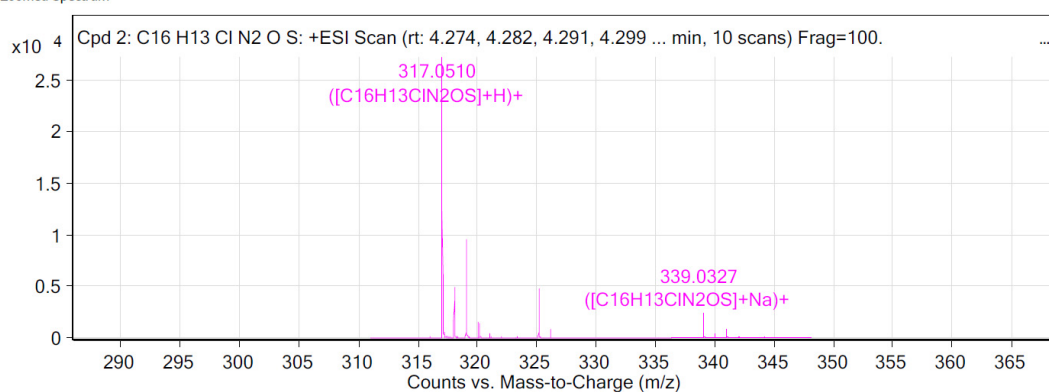


EI MS (70eV)



ESI-QTOF (positive ionization)

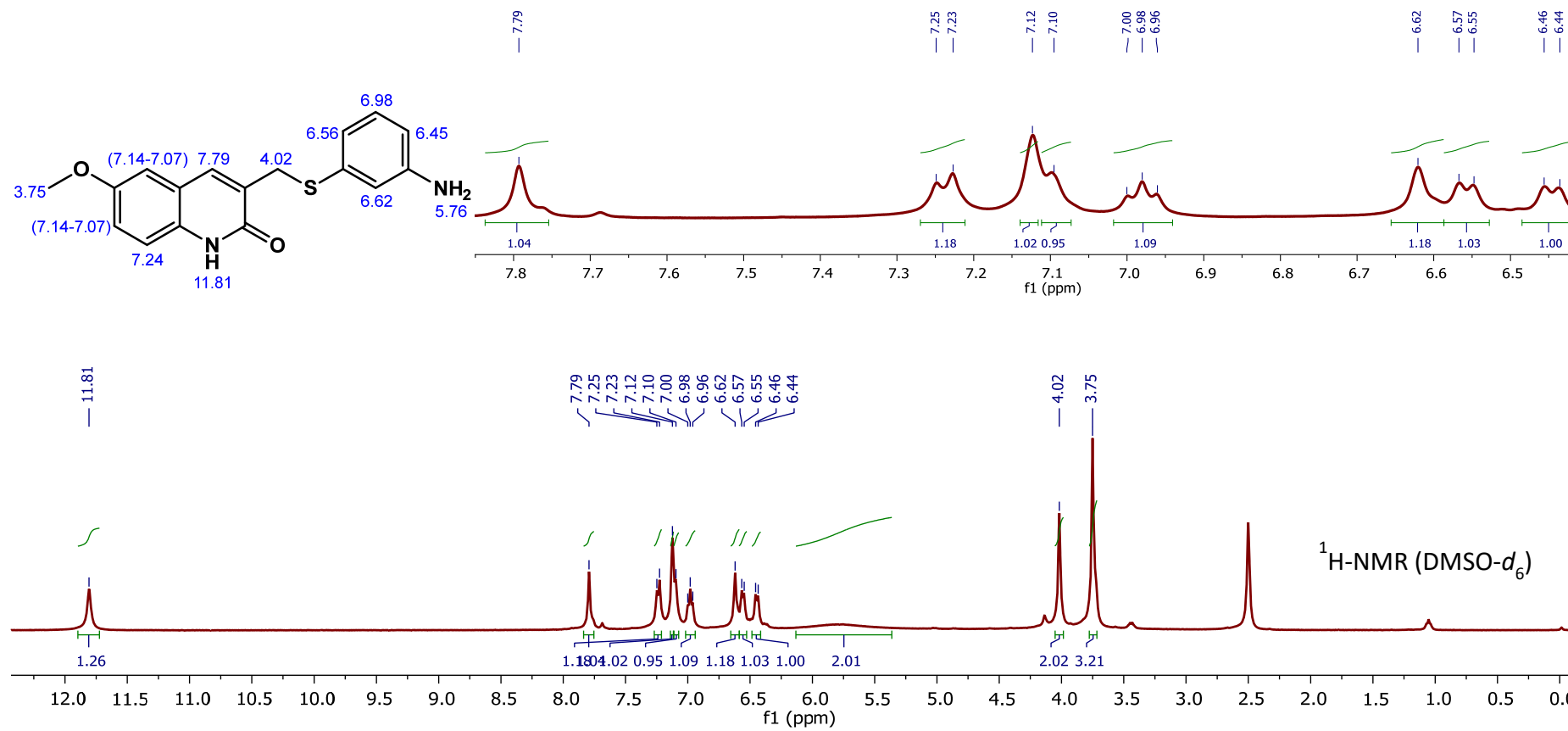
MS Zoomed Spectrum

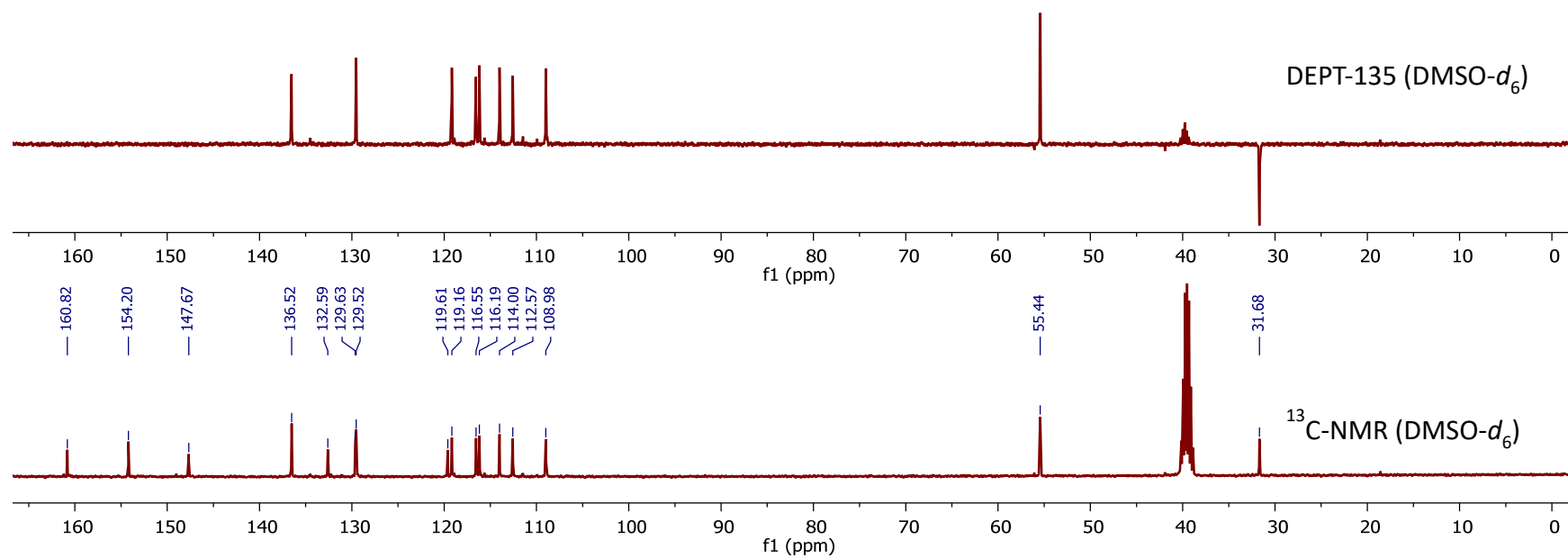
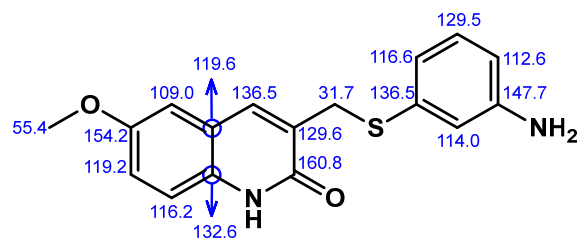


MS Spectrum Peak List

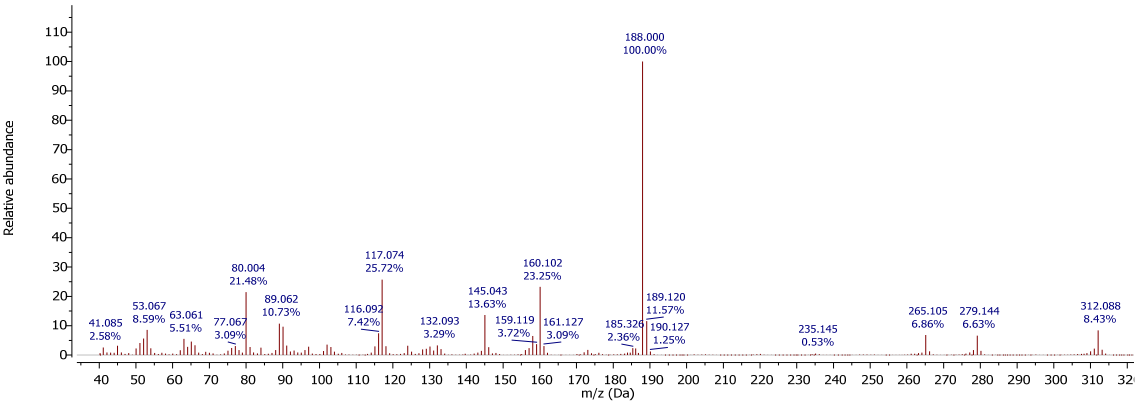
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
316.045	316.0432	-5.68	1	103.78	C ₁₆ H ₁₃ ClN ₂ OS	M+
317.051	317.051	0	1	27328.75	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
318.0537	318.054	0.83	1	5062.02	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
319.0482	319.0483	0.49	1	9851.85	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
320.0515	320.051	-1.44	1	1715.77	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
321.0484	321.0471	-4.17	1	507.61	C ₁₆ H ₁₃ ClN ₂ OS	(M+H) ⁺
339.0327	339.0329	0.79	1	2483.84	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
340.0363	340.0368	1.46	1	401.33	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
341.03	341.0303	0.81	1	915.04	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺
342.0322	342.033	2.33	1	175.25	C ₁₆ H ₁₃ ClN ₂ OS	(M+Na) ⁺

4.37 Compound 32c



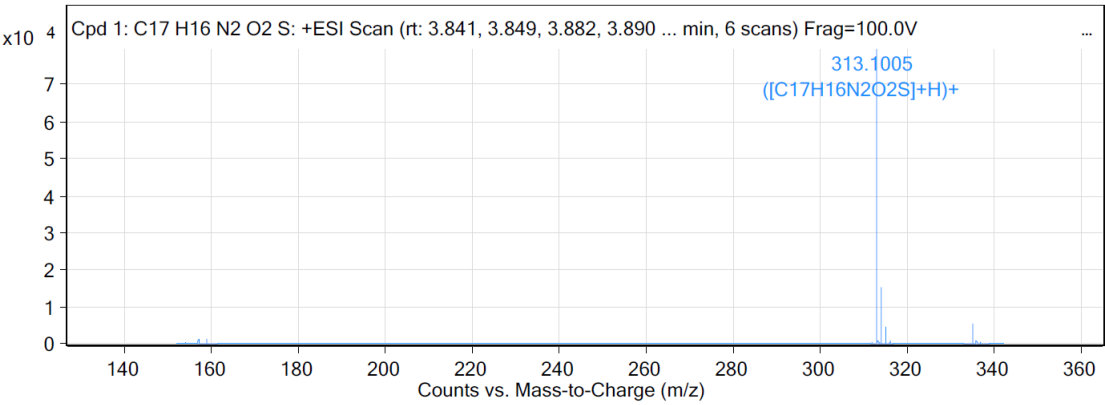


EI MS (70eV)



ESI-QTOF (positive ionization)

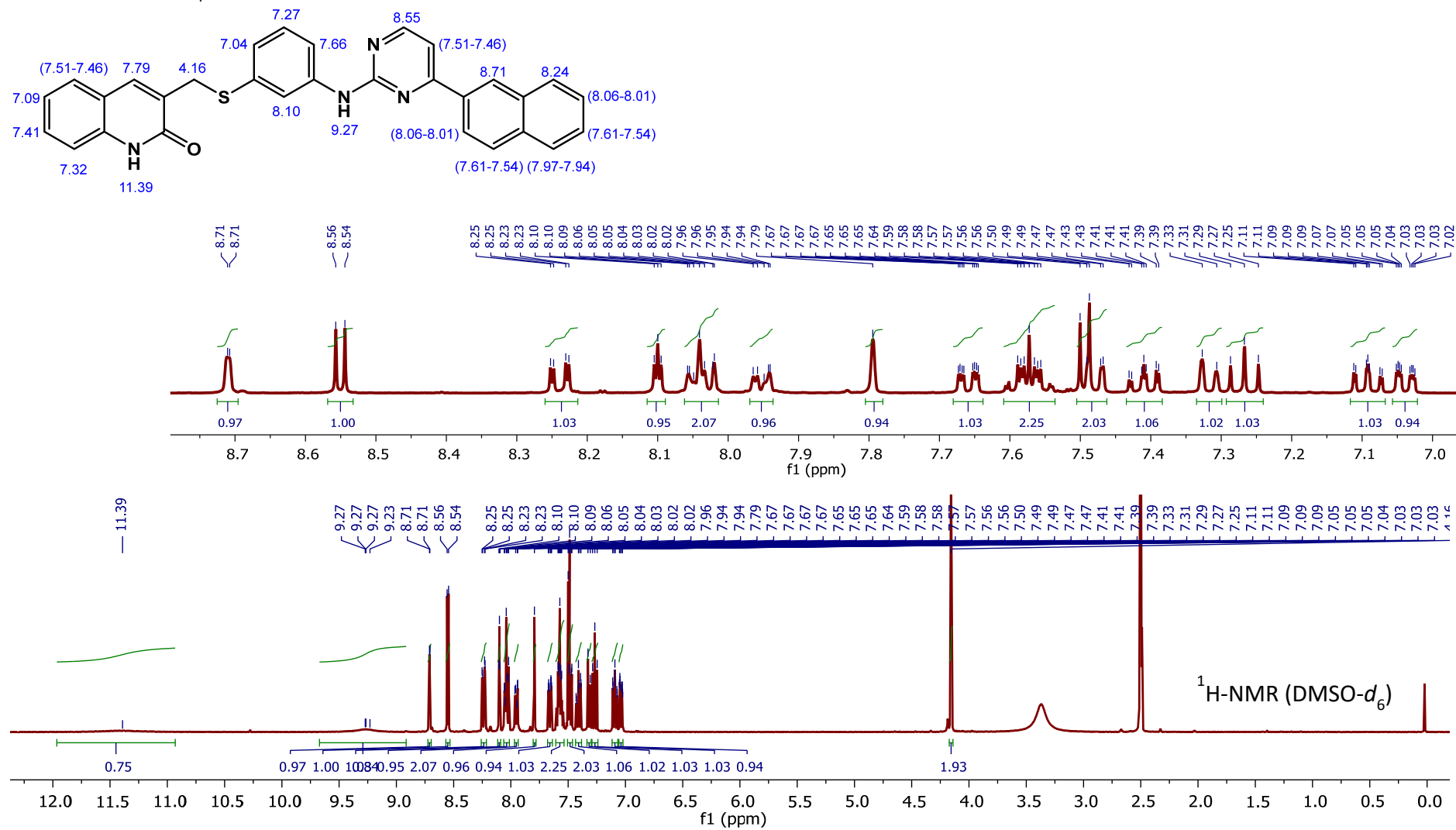
MS Zoomed Spectrum

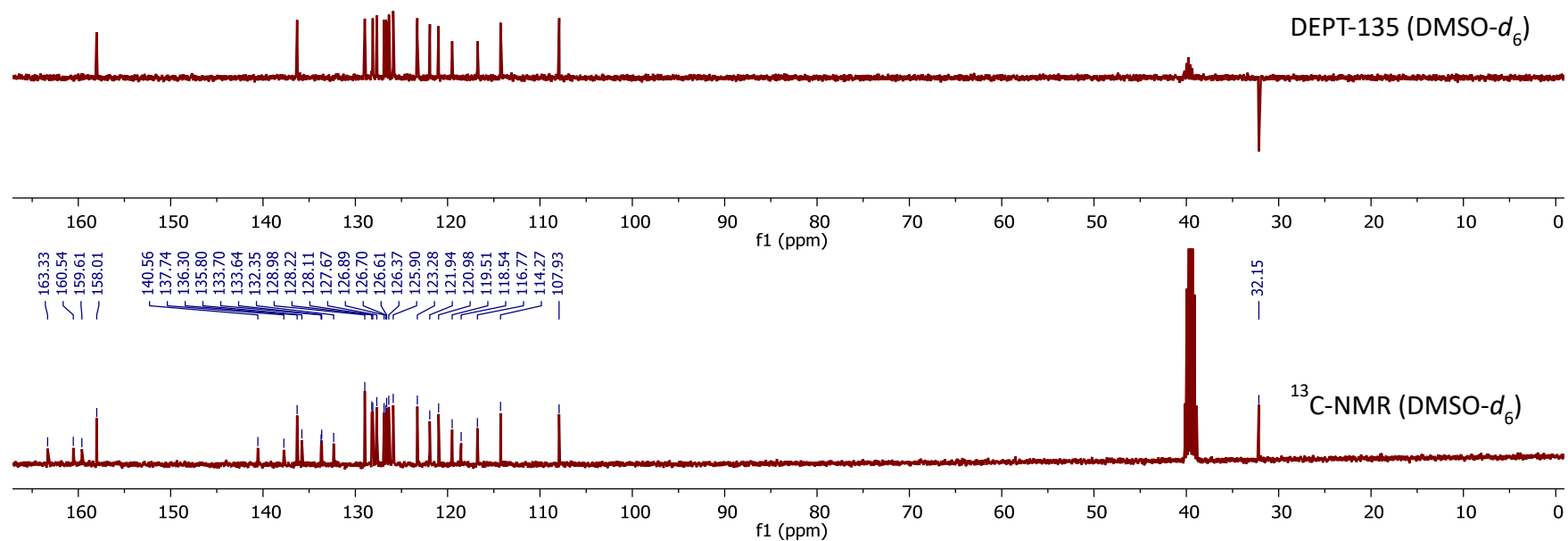
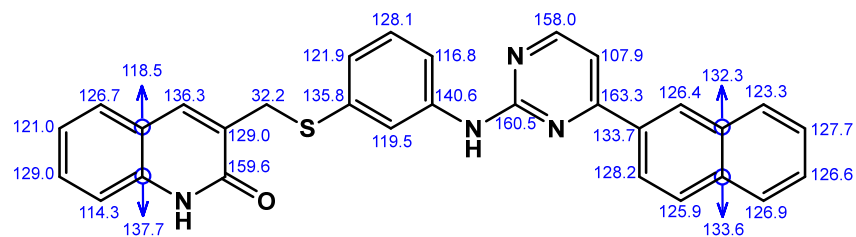


MS Spectrum Peak List

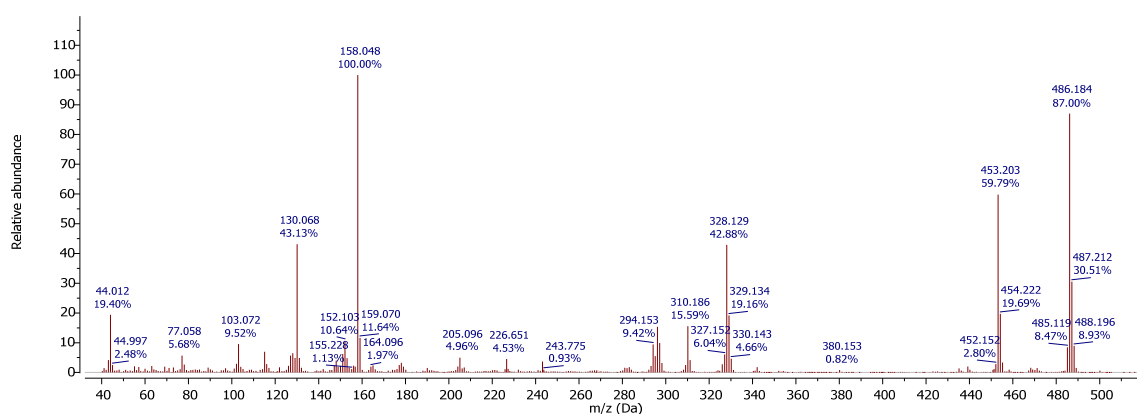
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
157.0534	157.0539	3.1	2	1327.52	C17H16N2O2S	(M+2H)+2
157.5539	157.5554	9.41	2	217.53	C17H16N2O2S	(M+2H)+2
158.057	158.0535	-22.44	2	103.37	C17H16N2O2S	(M+2H)+2
312.0924	312.0927	0.81	1	601.84	C17H16N2O2S	M+
313.1005	313.1005	-0.04	1	81732.62	C17H16N2O2S	(M+H)+
314.1036	314.1035	-0.32	1	15167.51	C17H16N2O2S	(M+H)+
315.0996	315.0997	0.27	1	4440.54	C17H16N2O2S	(M+H)+
335.0826	335.0825	-0.42	1	5570.1	C17H16N2O2S	(M+Na)+
337.081	337.0817	2.09	1	358.39	C17H16N2O2S	(M+Na)+

4.38 Compound 35a



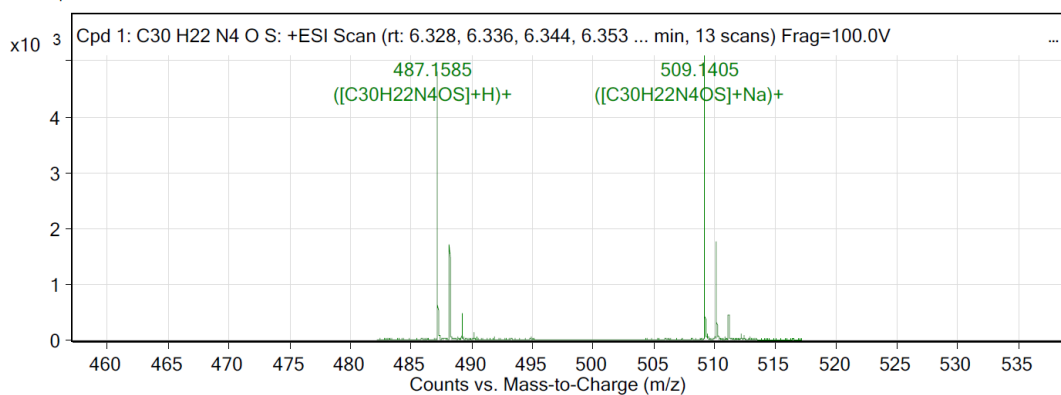


EI MS (70eV)



ESI-QTOF (positive ionization)

MS Zoomed Spectrum

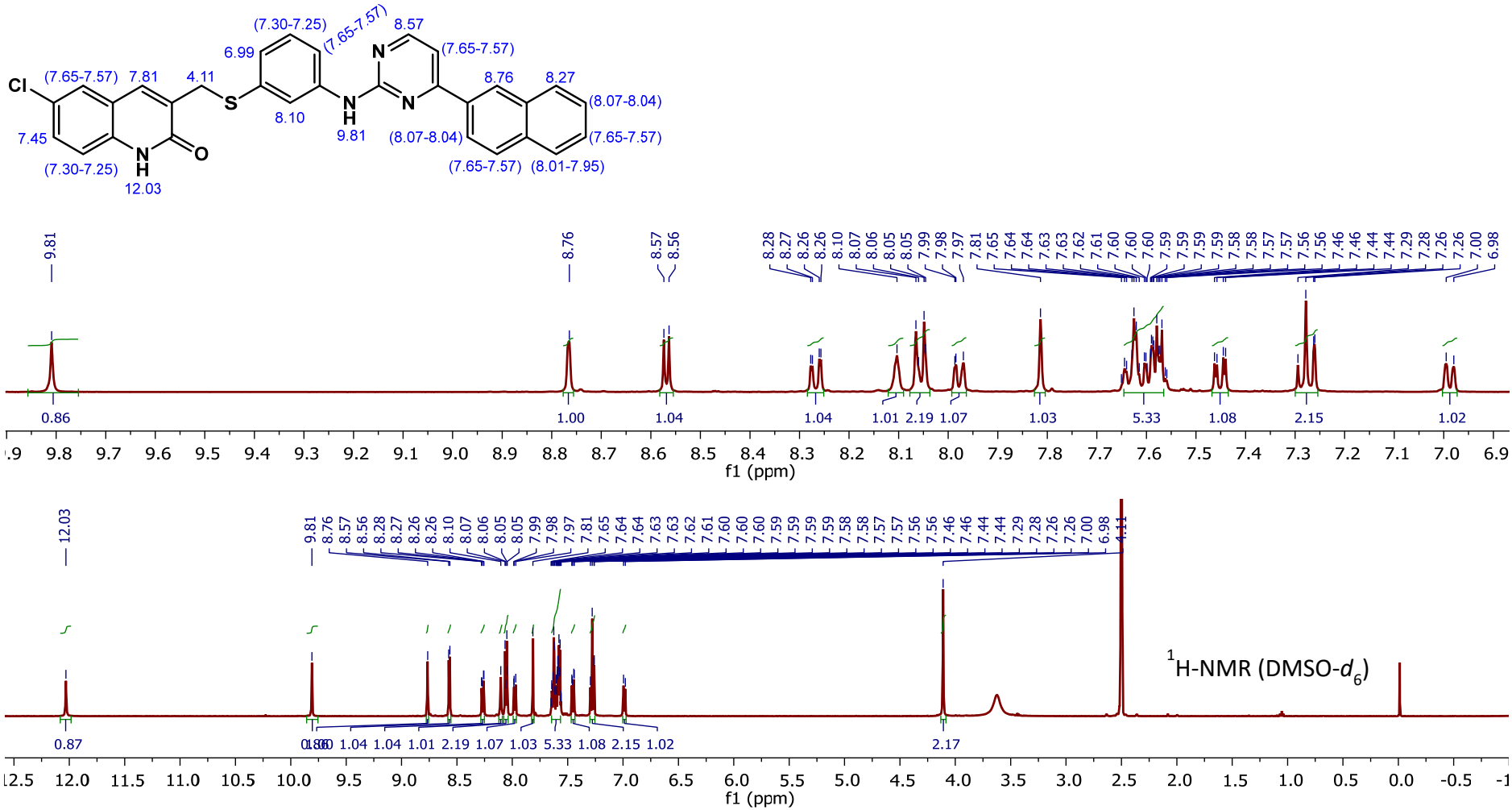


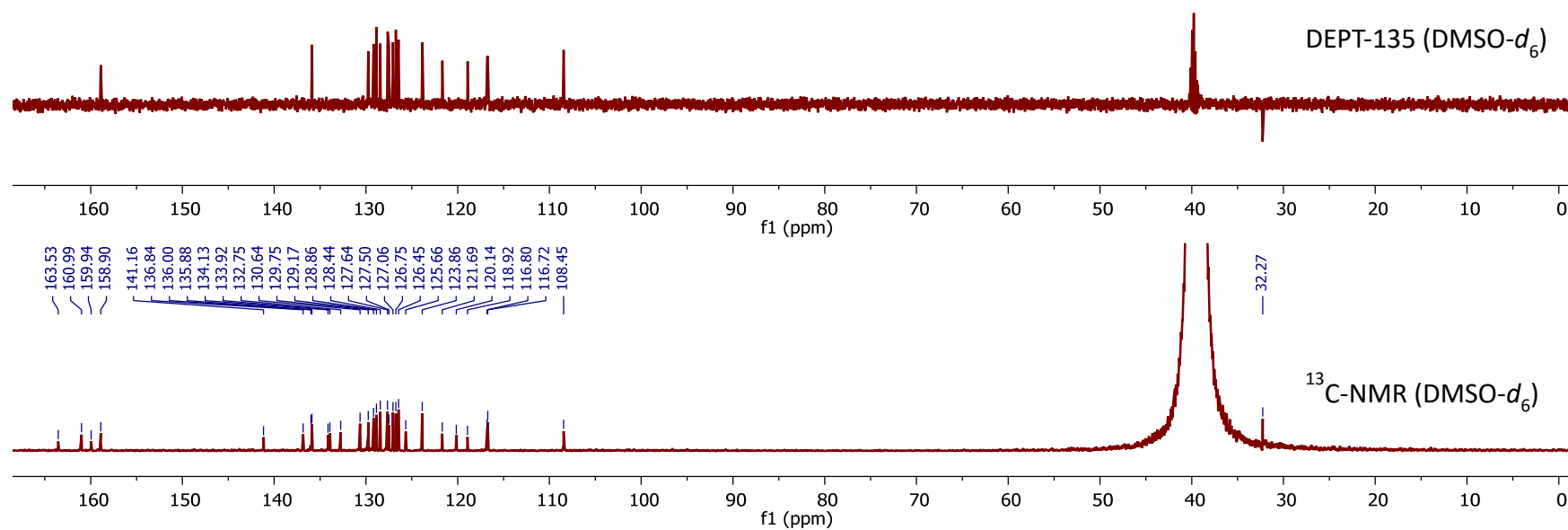
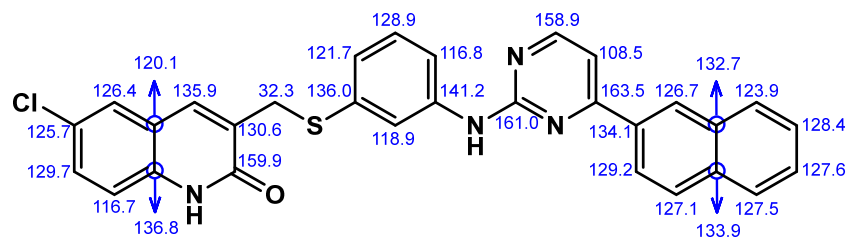
MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
487.1585	487.1587	0.48	1	4914.18	C ₃₀ H ₂₂ N ₄ O ₅	(M+H) ⁺
488.1618	488.1617	-0.13	1	1750.32	C ₃₀ H ₂₂ N ₄ O ₅	(M+H) ⁺
489.1595	489.1604	1.83	1	516.34	C ₃₀ H ₂₂ N ₄ O ₅	(M+H) ⁺
490.1622	490.1608	-2.83	1	78.4	C ₃₀ H ₂₂ N ₄ O ₅	(M+H) ⁺
509.1405	509.1407	0.35	1	5170.75	C ₃₀ H ₂₂ N ₄ O ₅	(M+Na) ⁺
510.1434	510.1437	0.59	1	1867.81	C ₃₀ H ₂₂ N ₄ O ₅	(M+Na) ⁺
511.1418	511.1423	1.13	1	513.31	C ₃₀ H ₂₂ N ₄ O ₅	(M+Na) ⁺
512.1422	512.1428	1	1	82.34	C ₃₀ H ₂₂ N ₄ O ₅	(M+Na) ⁺

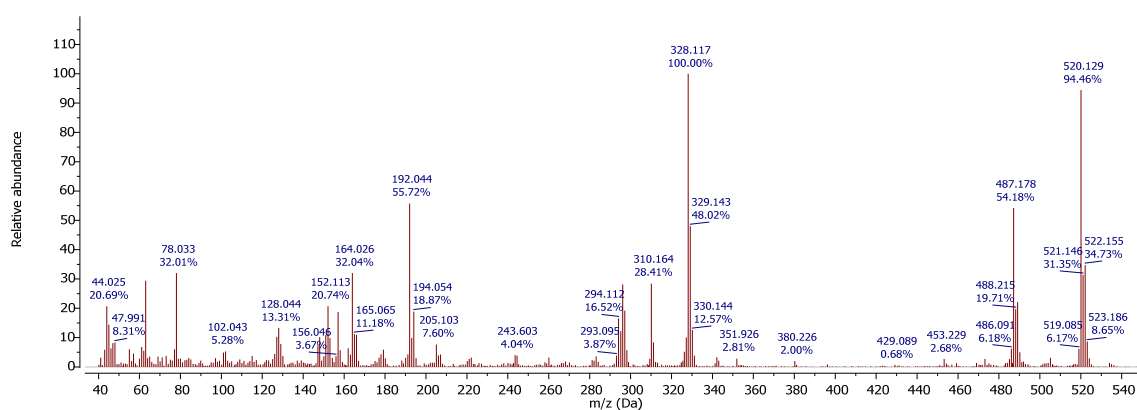
4.39

Compound 35b



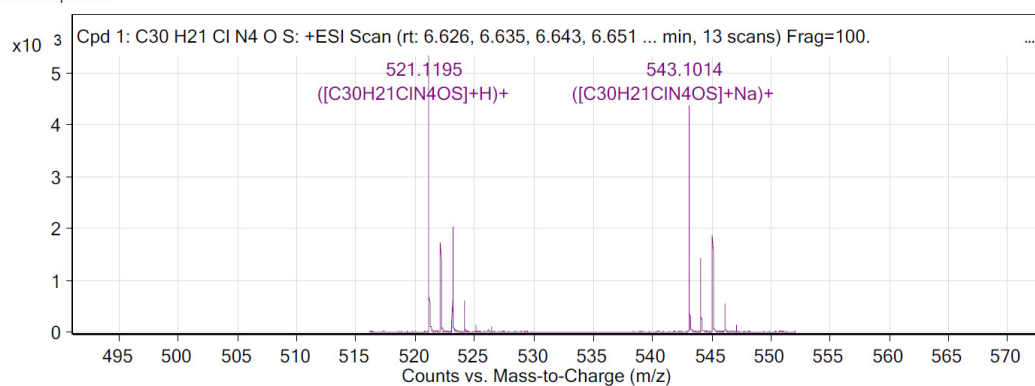


EI MS (70eV)



ESI-QTOF (positive ionization)

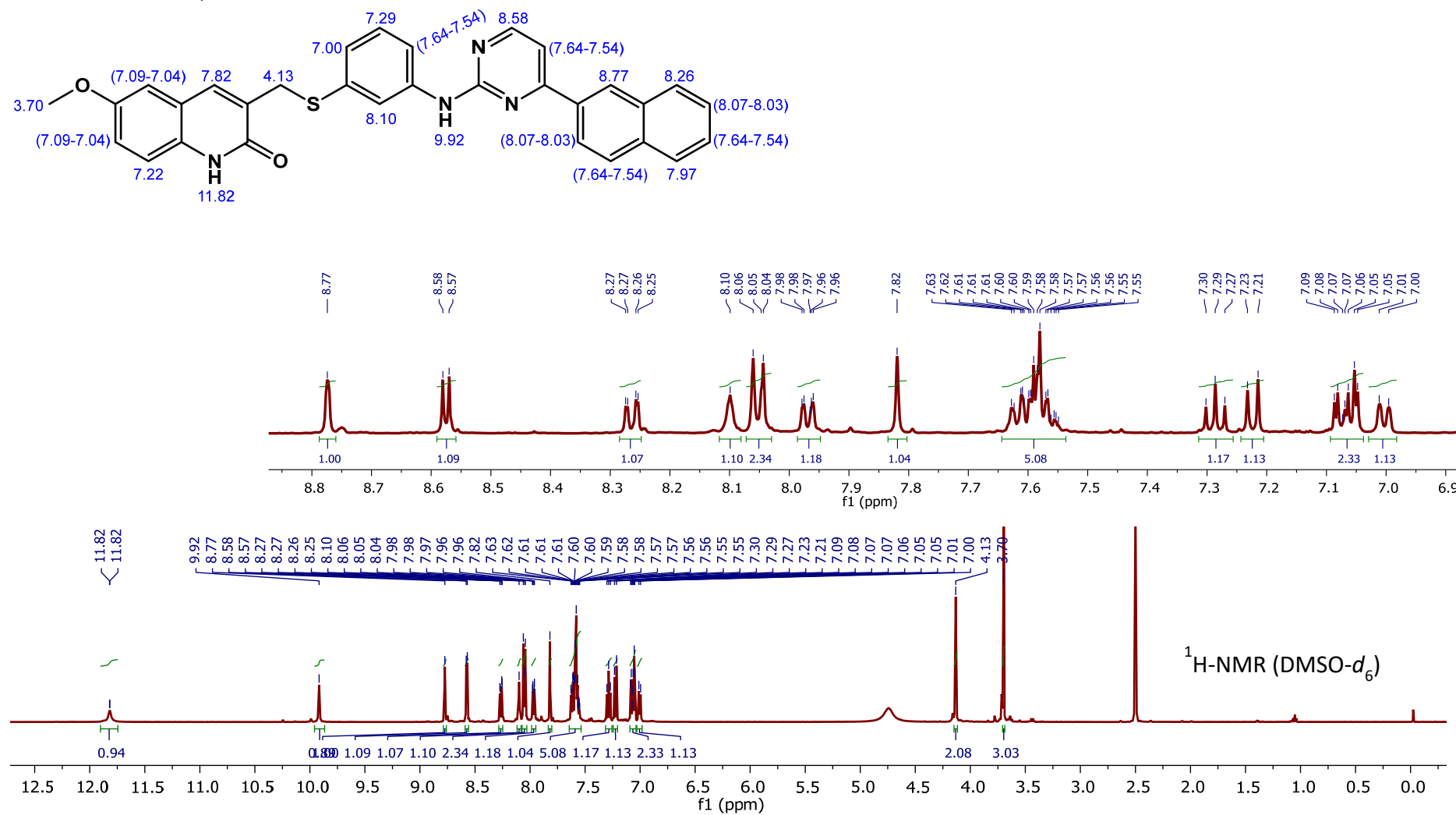
MS Zoomed Spectrum

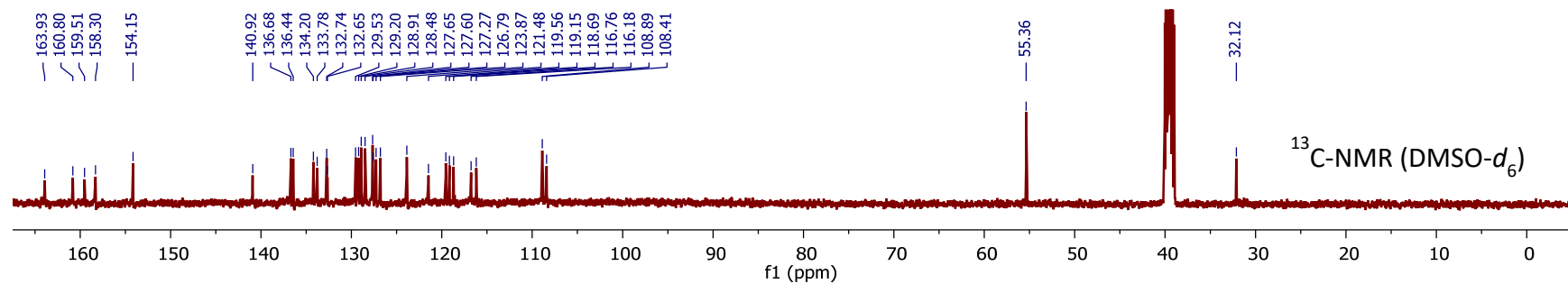
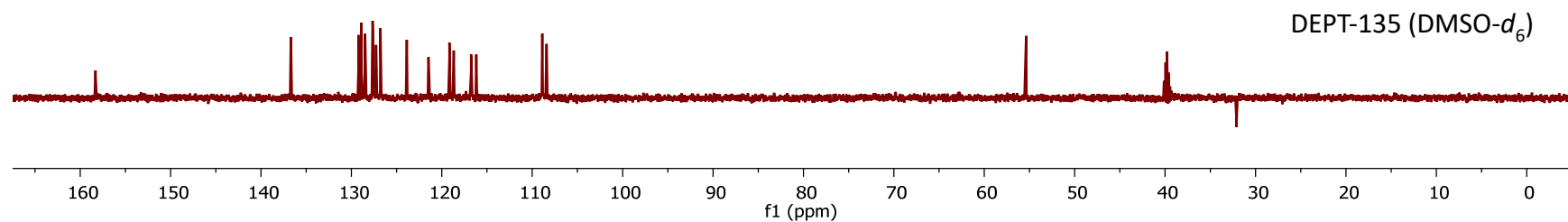
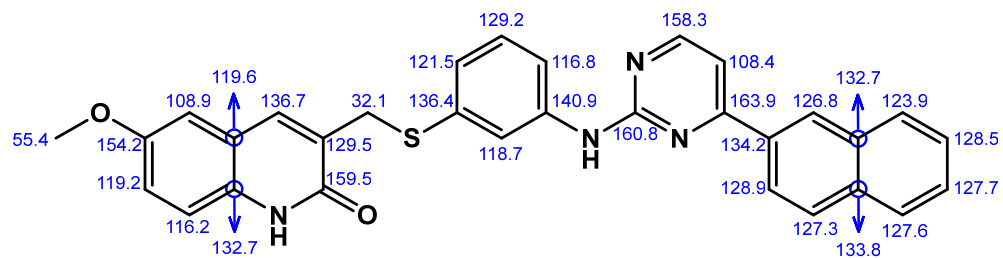


MS Spectrum Peak List

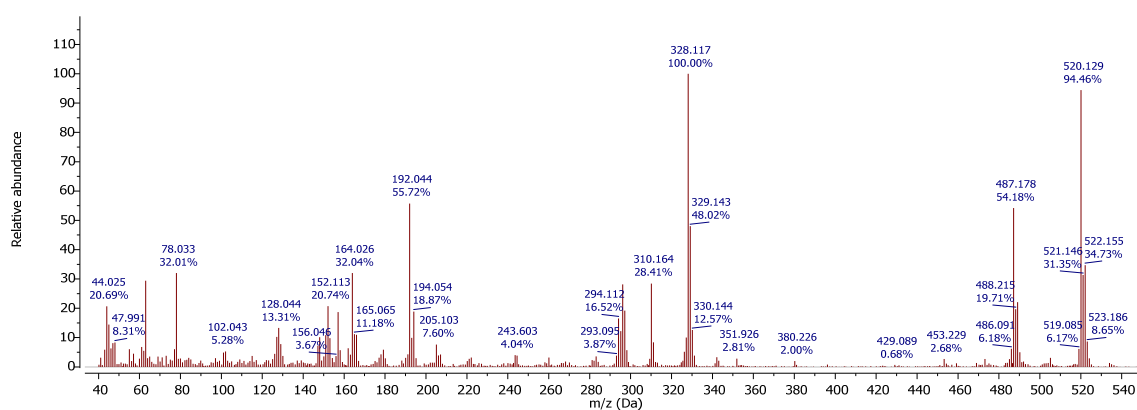
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
521.1195	521.1197	0.48	1	5458.62	C ₃₀ H ₂₁ ClN ₄ OS	(M+H)+
522.1225	522.1228	0.56	1	1815.21	C ₃₀ H ₂₁ ClN ₄ OS	(M+H)+
523.117	523.1179	1.75	1	2090.69	C ₃₀ H ₂₁ ClN ₄ OS	(M+H)+
524.1203	524.1201	-0.34	1	619.73	C ₃₀ H ₂₁ ClN ₄ OS	(M+H)+
525.1183	525.1189	1.13	1	126.98	C ₃₀ H ₂₁ ClN ₄ OS	(M+H)+
543.1014	543.1017	0.45	1	4458.7	C ₃₀ H ₂₁ ClN ₄ OS	(M+Na)+
544.1047	544.1047	0.02	1	1534.79	C ₃₀ H ₂₁ ClN ₄ OS	(M+Na)+
545.1003	545.0999	-0.83	1	1950.36	C ₃₀ H ₂₁ ClN ₄ OS	(M+Na)+
546.1009	546.1021	2.20	1	372.63	C ₃₀ H ₂₁ ClN ₄ OS	(M+Na)+
547.1014	547.1009	-0.92	1	126.62	C ₃₀ H ₂₁ ClN ₄ OS	(M+Na)+

4.40 Compound 35c



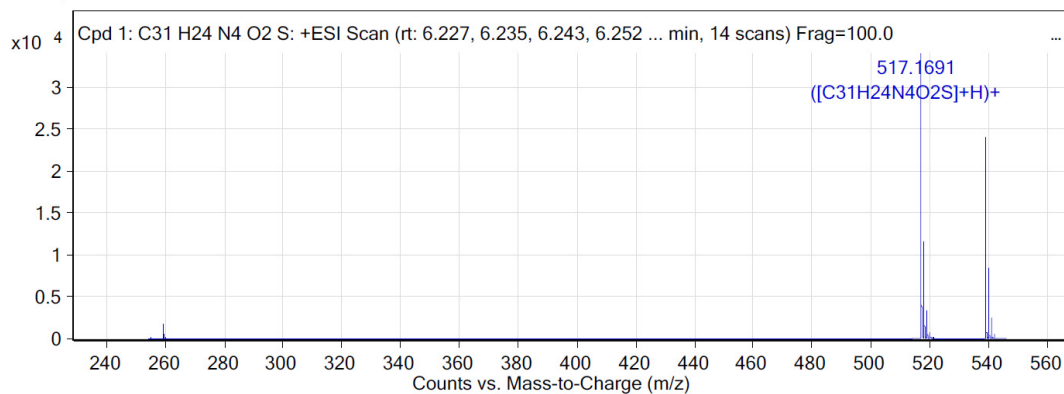


EI MS (70eV)



ESI-QTOF (positive ionization)

MS Zoomed Spectrum



MS Spectrum Peak List

m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
259.0882	259.0883	0.29	2	1807.07	C31H24N4O2S	(M+2H)+2
259.5901	259.5898	-1.32	2	601.35	C31H24N4O2S	(M+2H)+2
260.0892	260.0892	-0.06	2	184.95	C31H24N4O2S	(M+2H)+2
517.1691	517.1693	0.43	1	35187.08	C31H24N4O2S	(M+H)+
518.1726	518.1723	-0.53	1	12105.11	C31H24N4O2S	(M+H)+
519.1719	519.1712	-1.29	1	3356.03	C31H24N4O2S	(M+H)+
539.1511	539.1512	0.2	1	24291.18	C31H24N4O2S	(M+Na)+
540.1542	540.1543	0.13	1	8693.75	C31H24N4O2S	(M+Na)+
541.1534	541.1531	-0.5	1	2476.71	C31H24N4O2S	(M+Na)+