

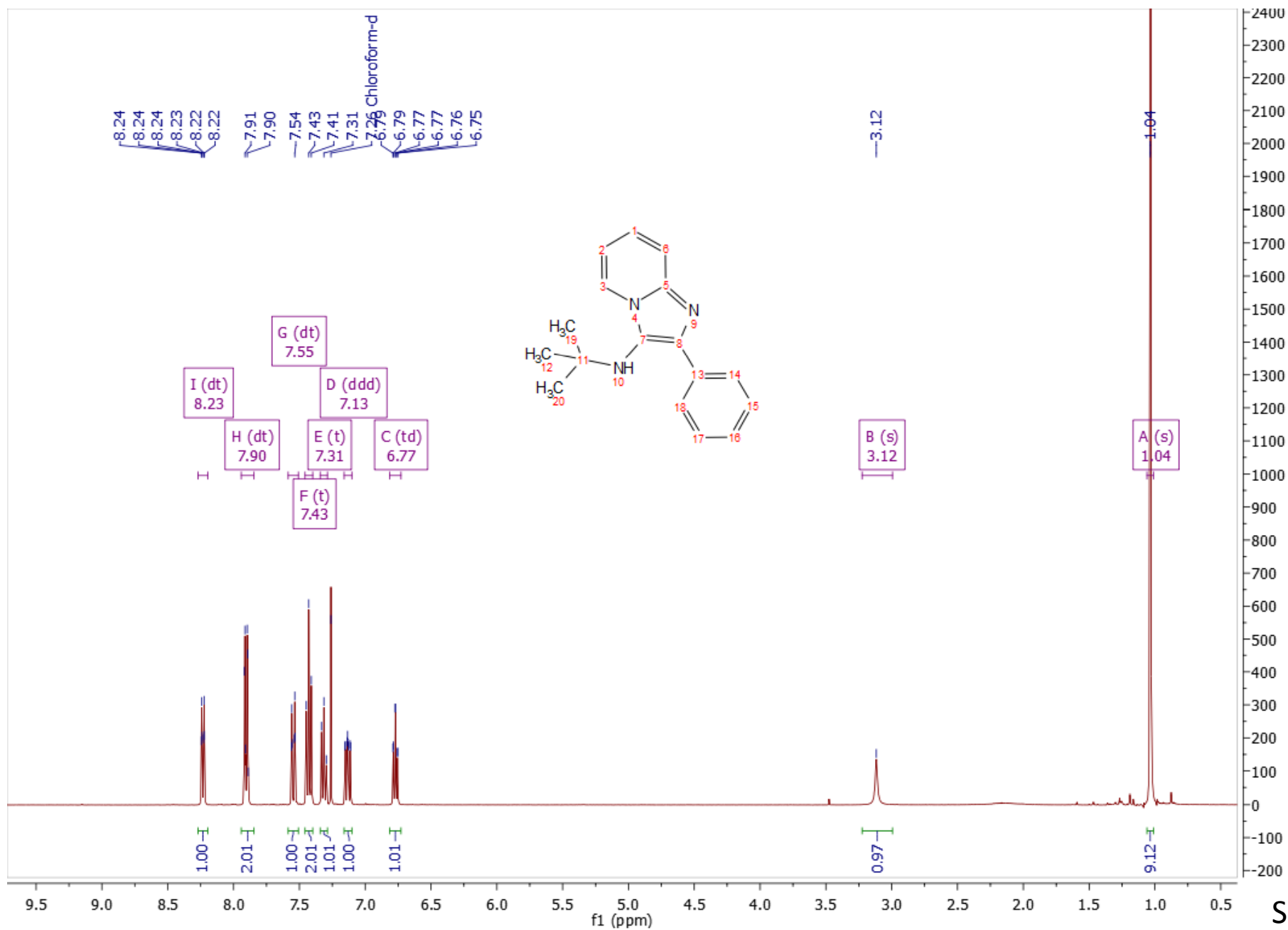
Supporting Information

Antibacterial activities of Groebke-Blackburn-Bienaymé-derived imidazo[1,2-*a*]pyridin-3-amines

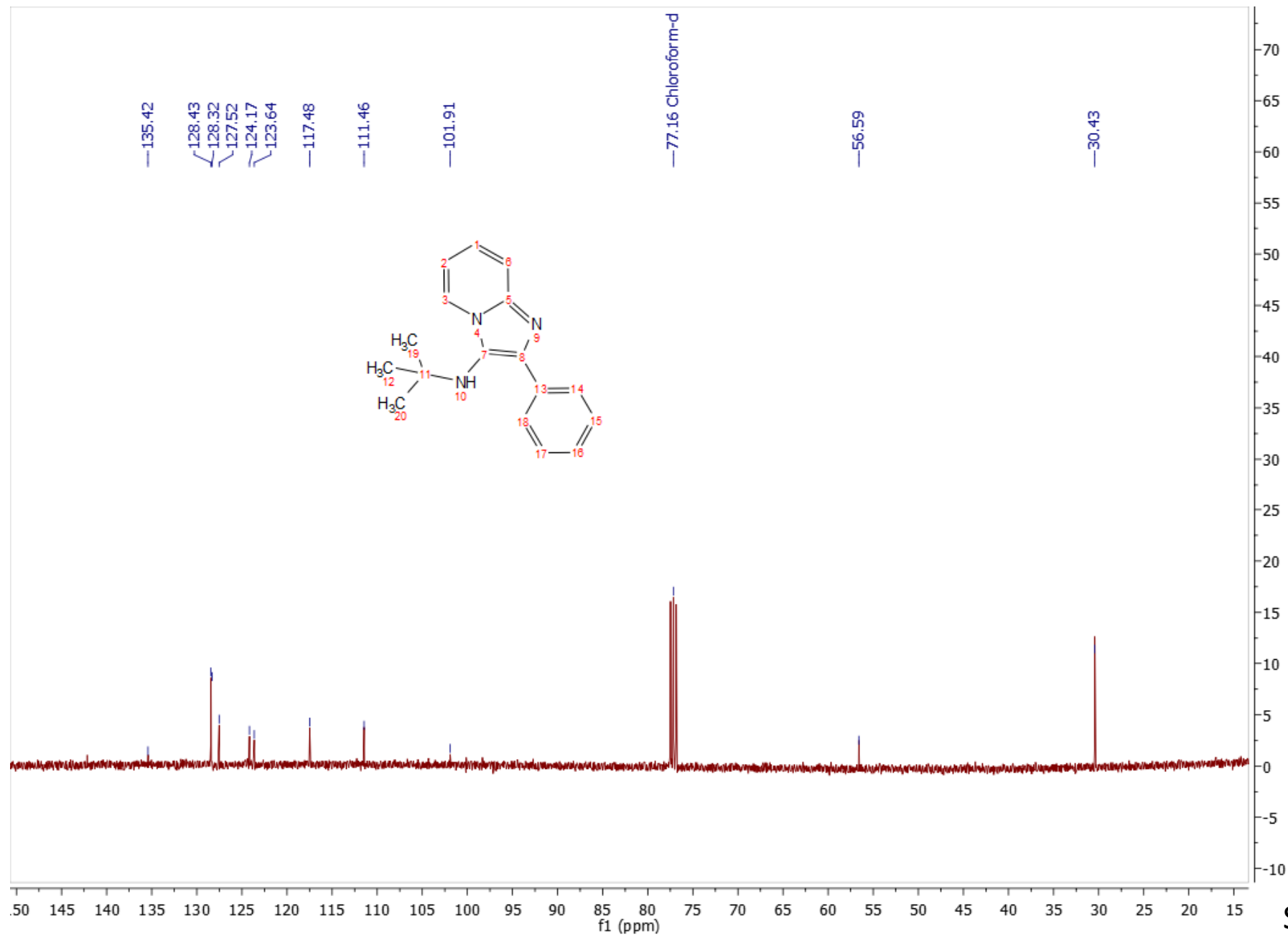
Nikunj M. Shukla, Deepak B. Salunke, Euna Yoo, Cole A. Mutz,
Rajalakshmi Balakrishna, and Sunil A. David*

Department of Medicinal Chemistry,
University of Kansas.

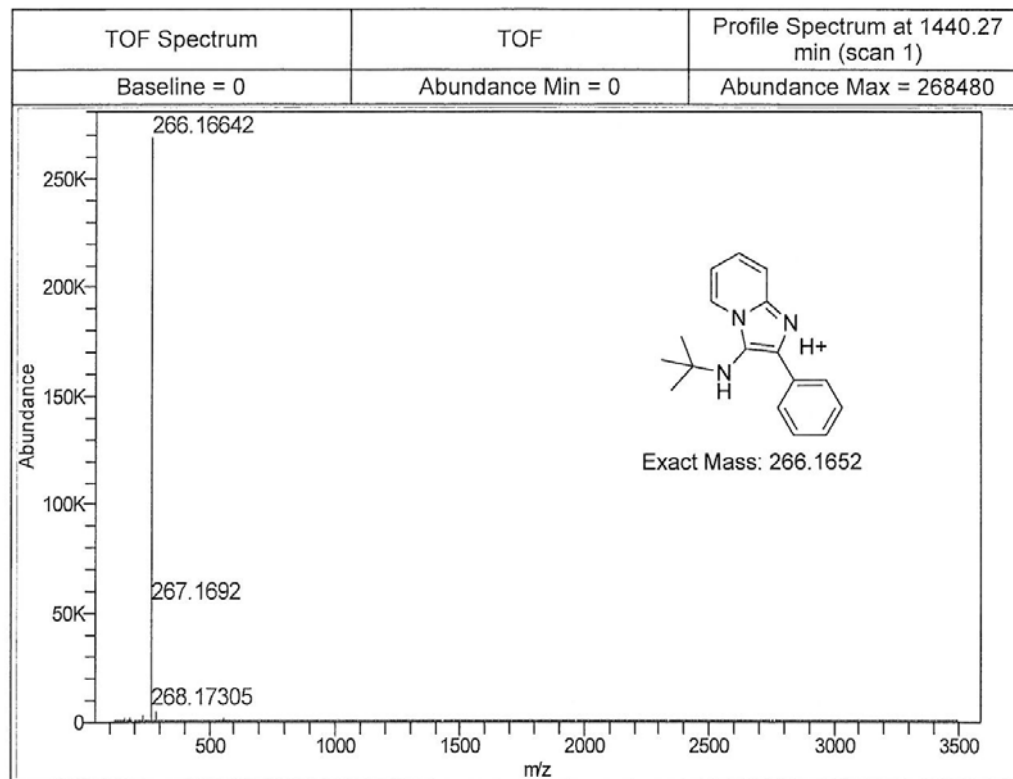
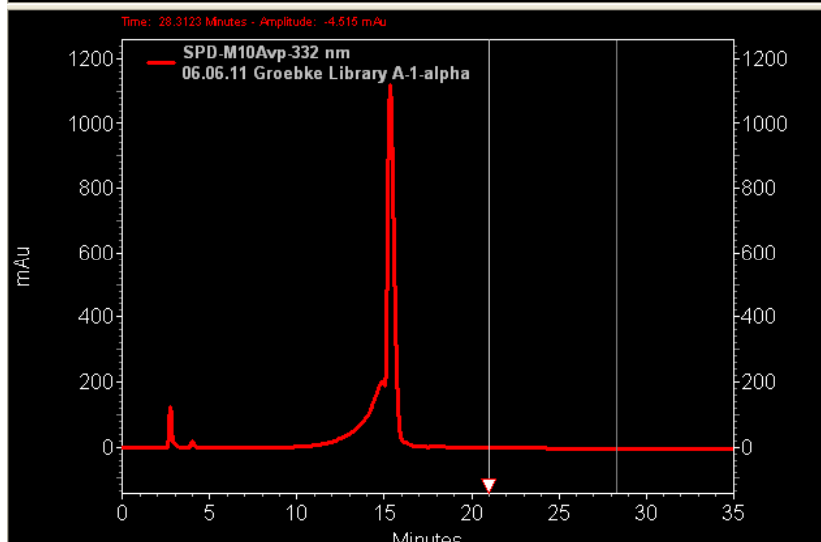
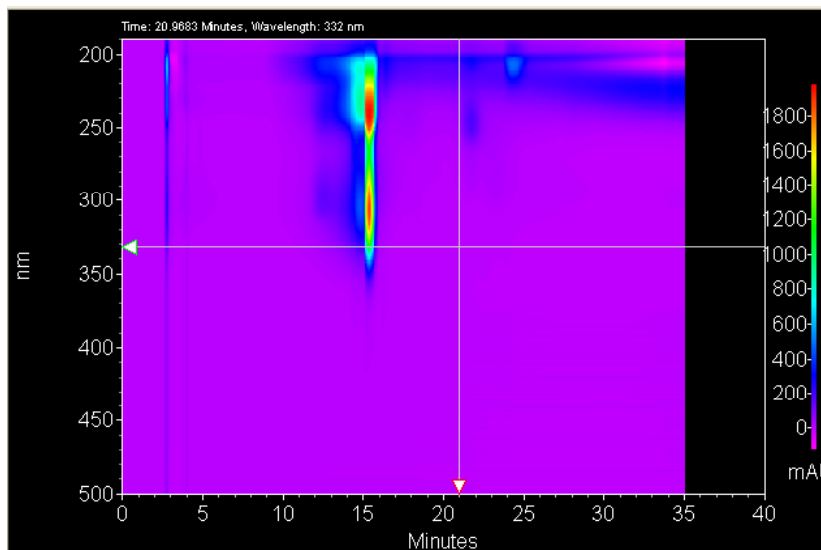
1a ¹H Spectrum



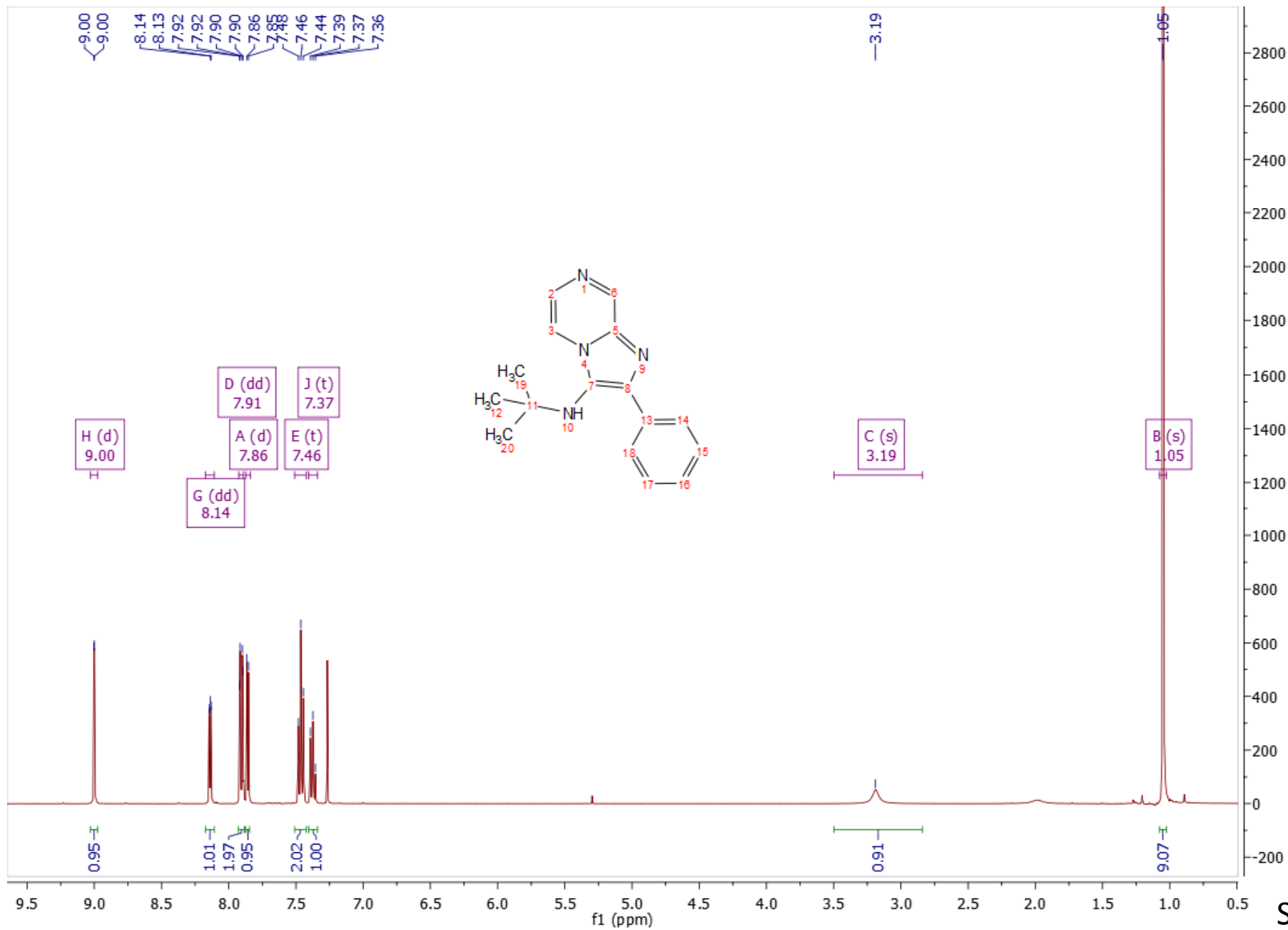
1a ¹³C Spectrum



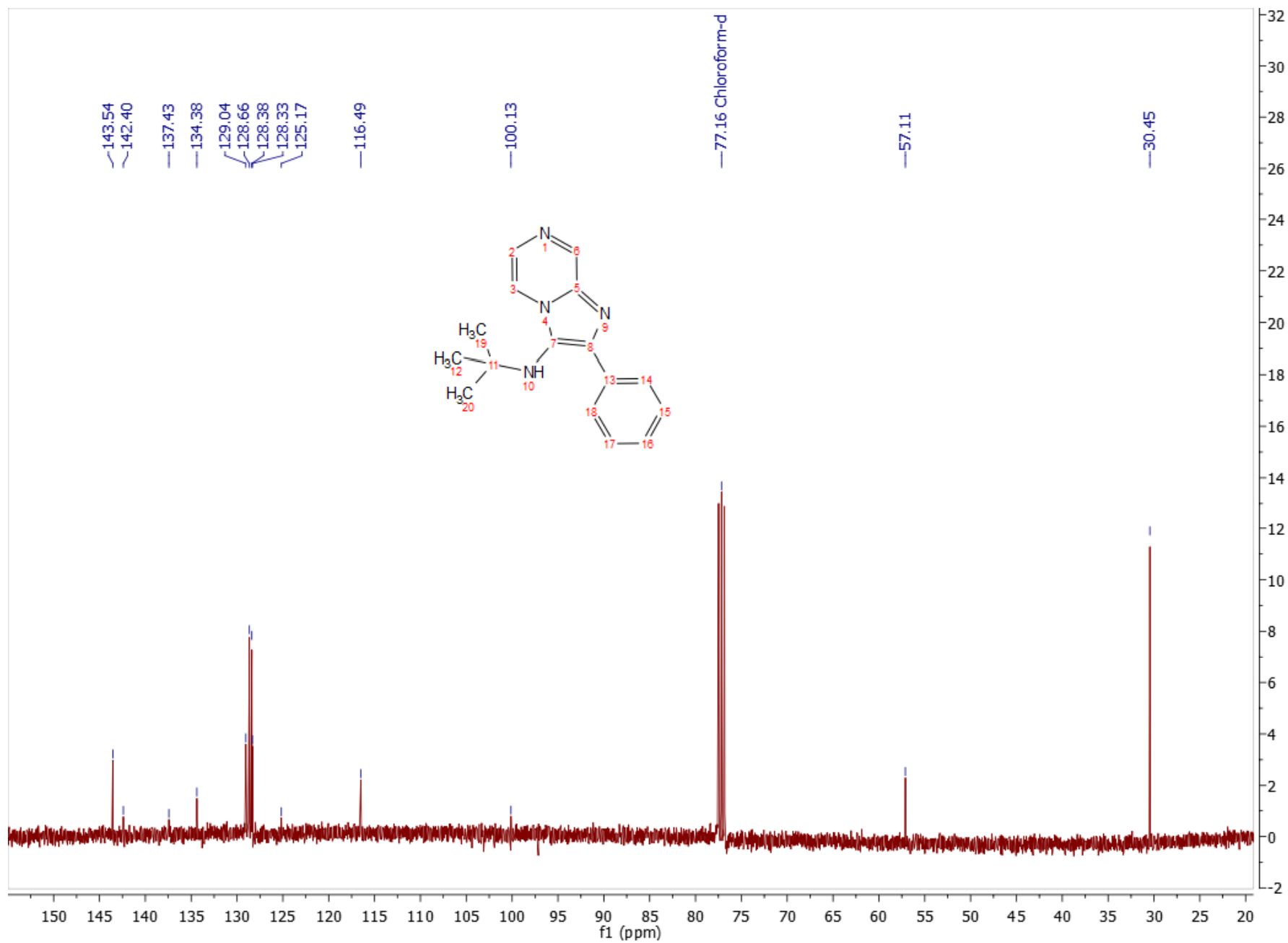
1a LC-MS



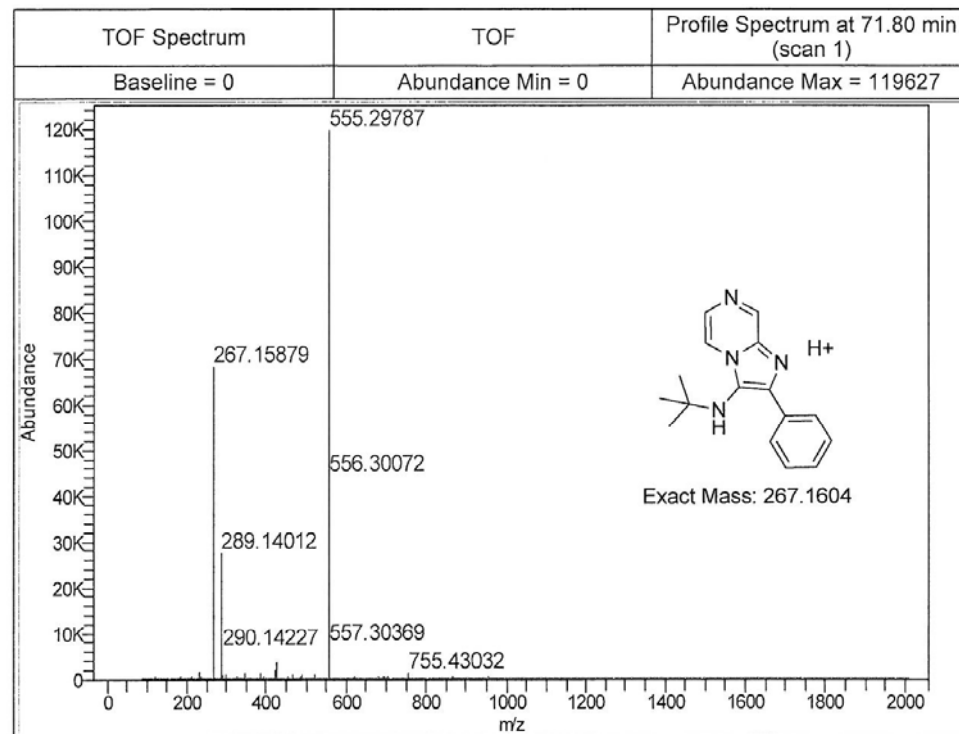
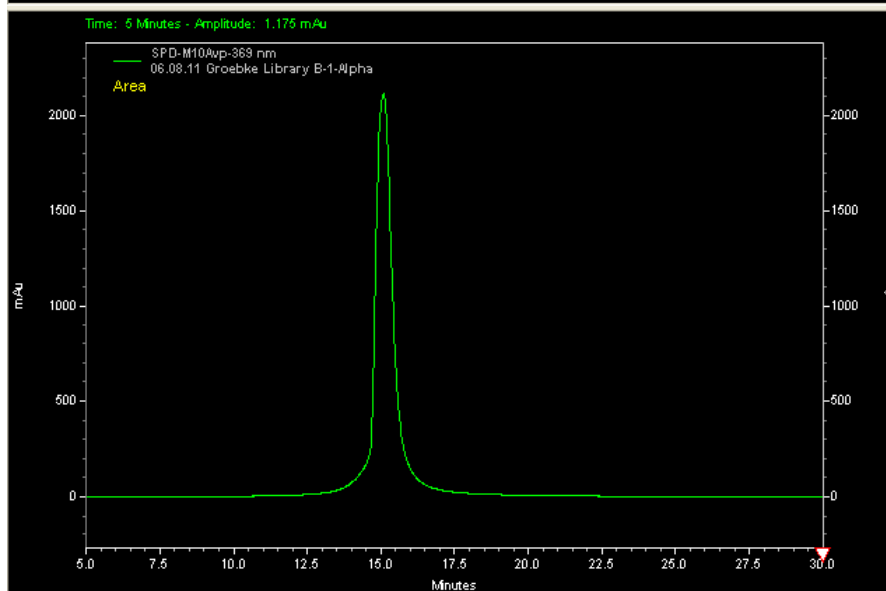
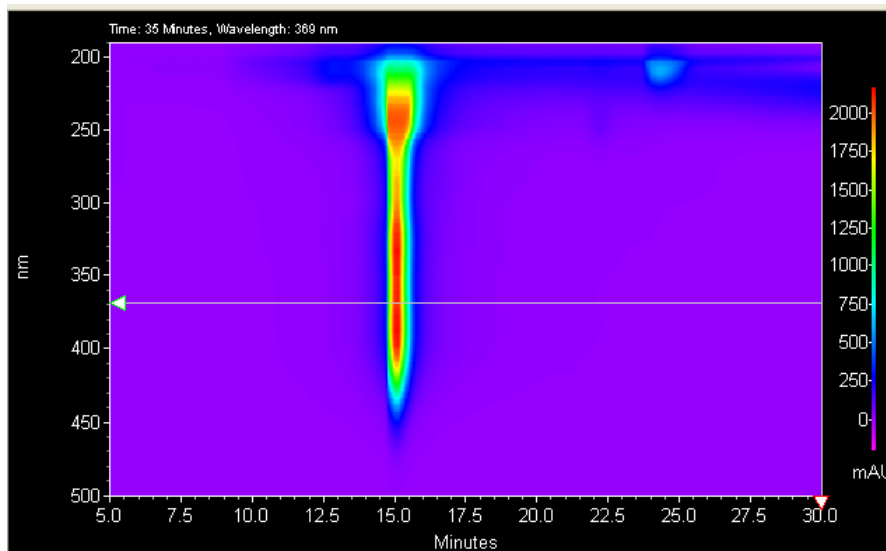
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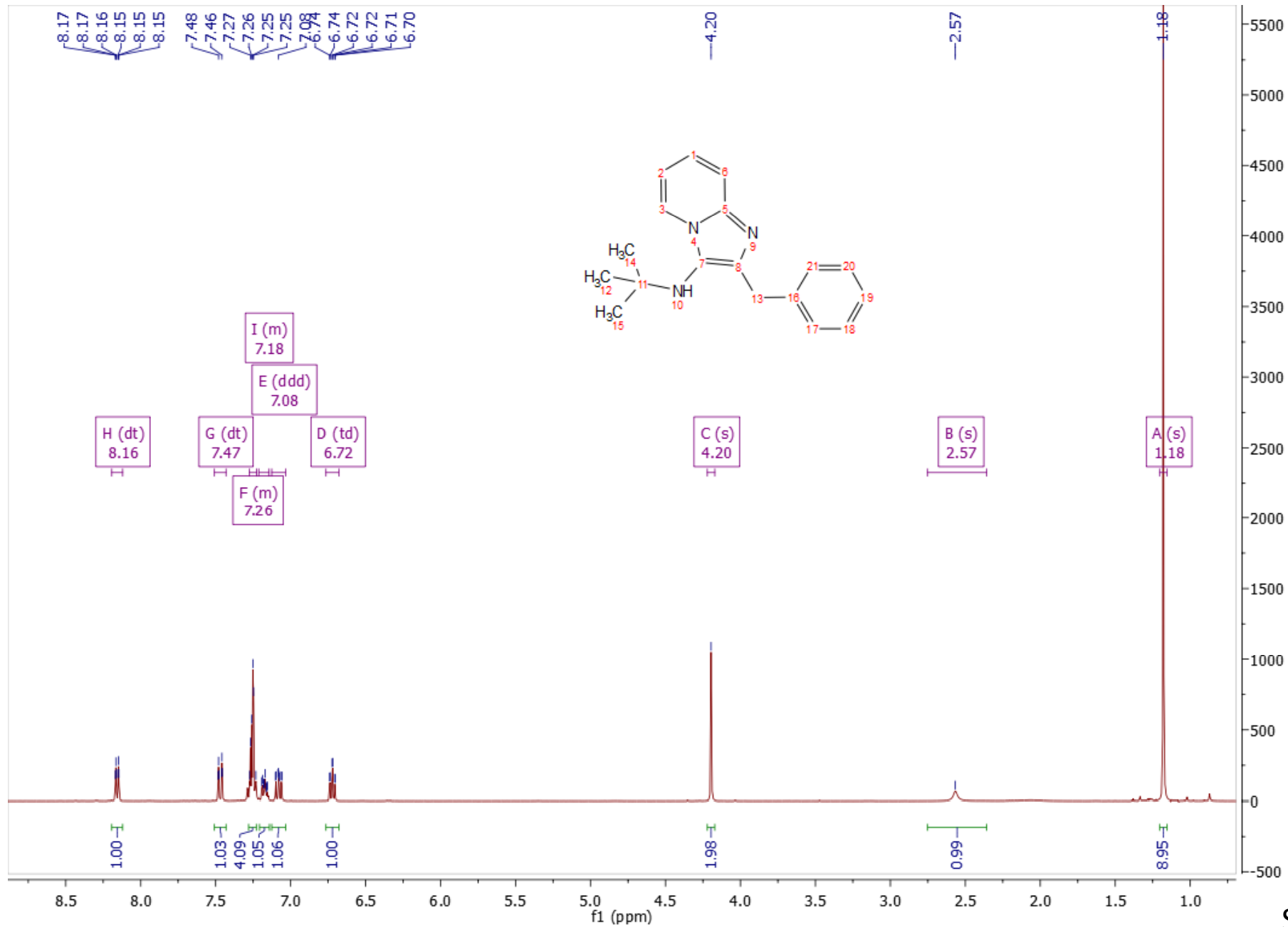
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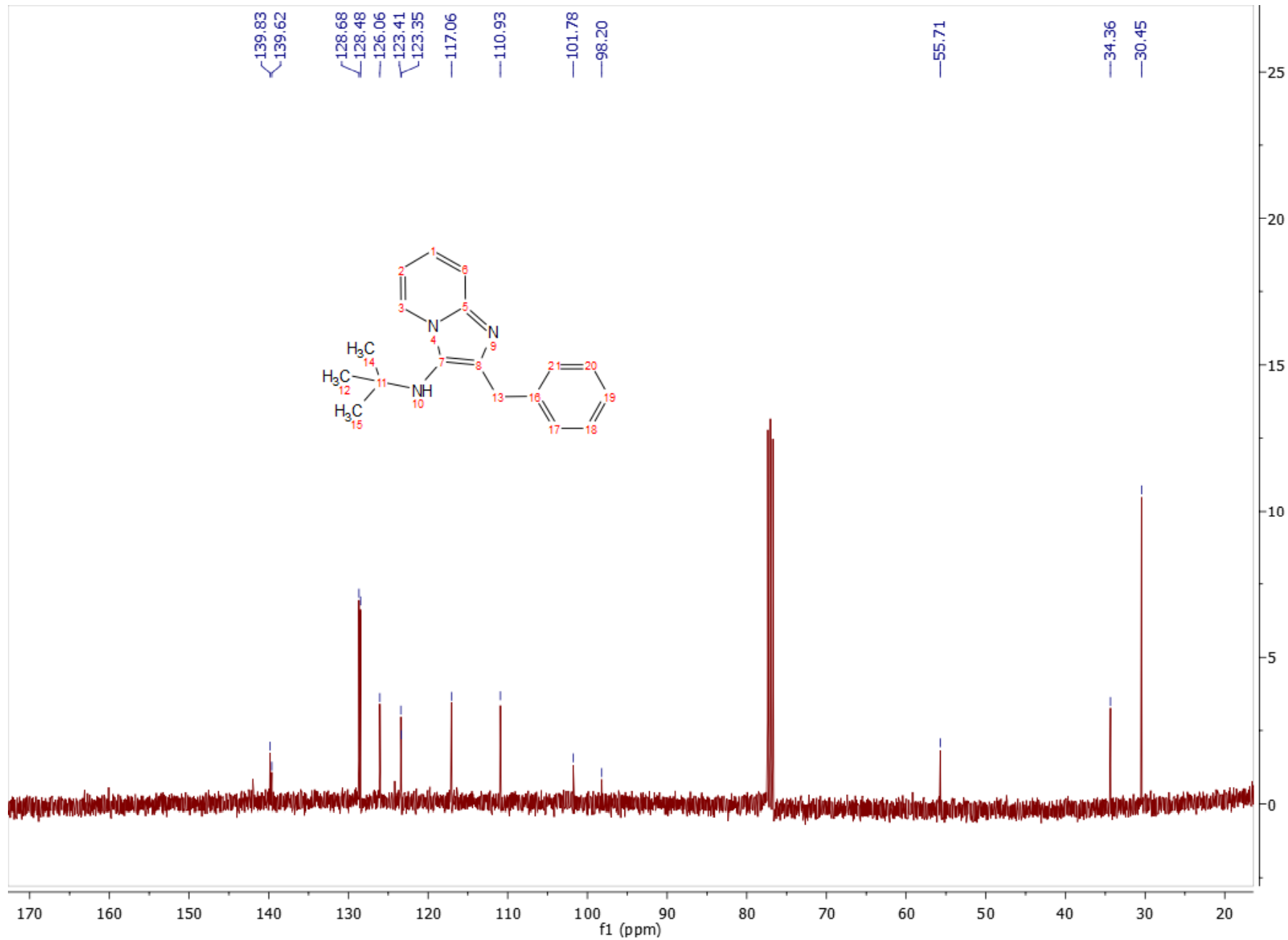
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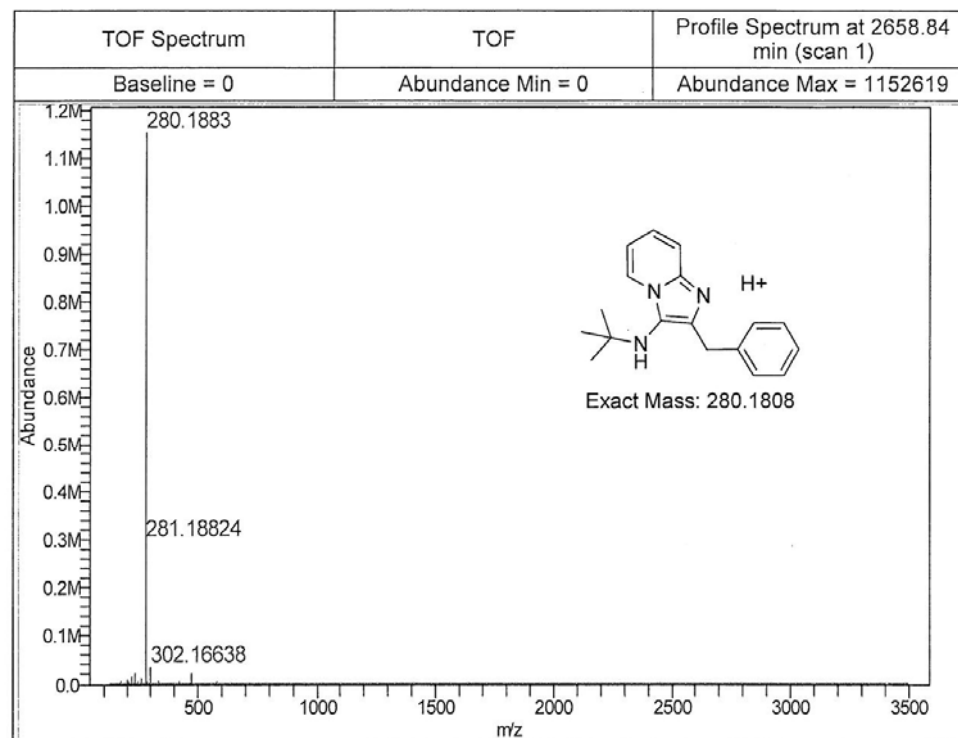
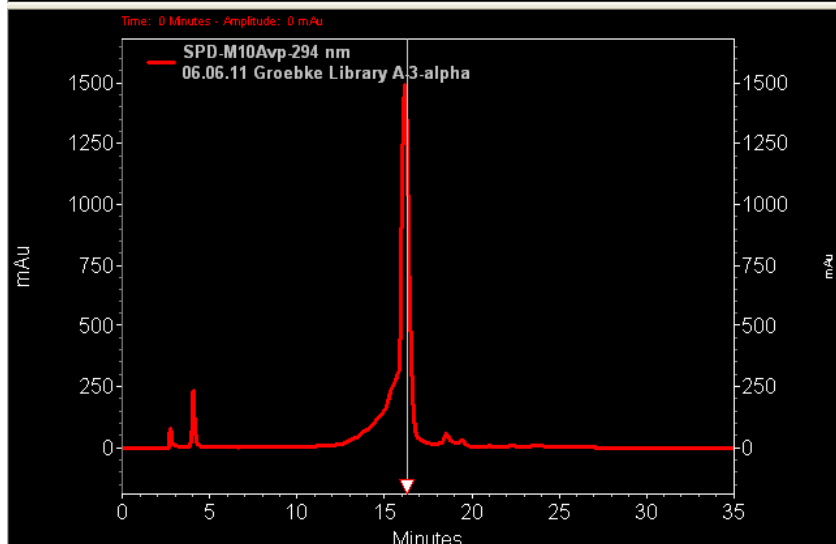
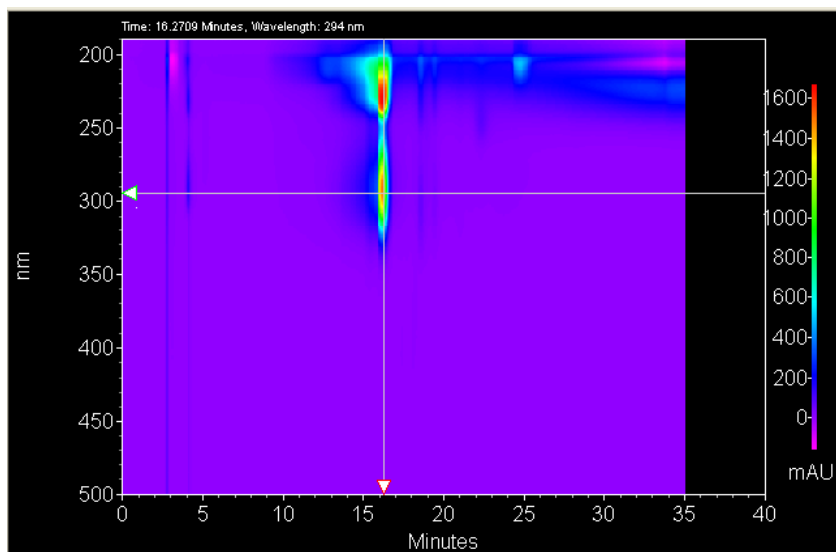
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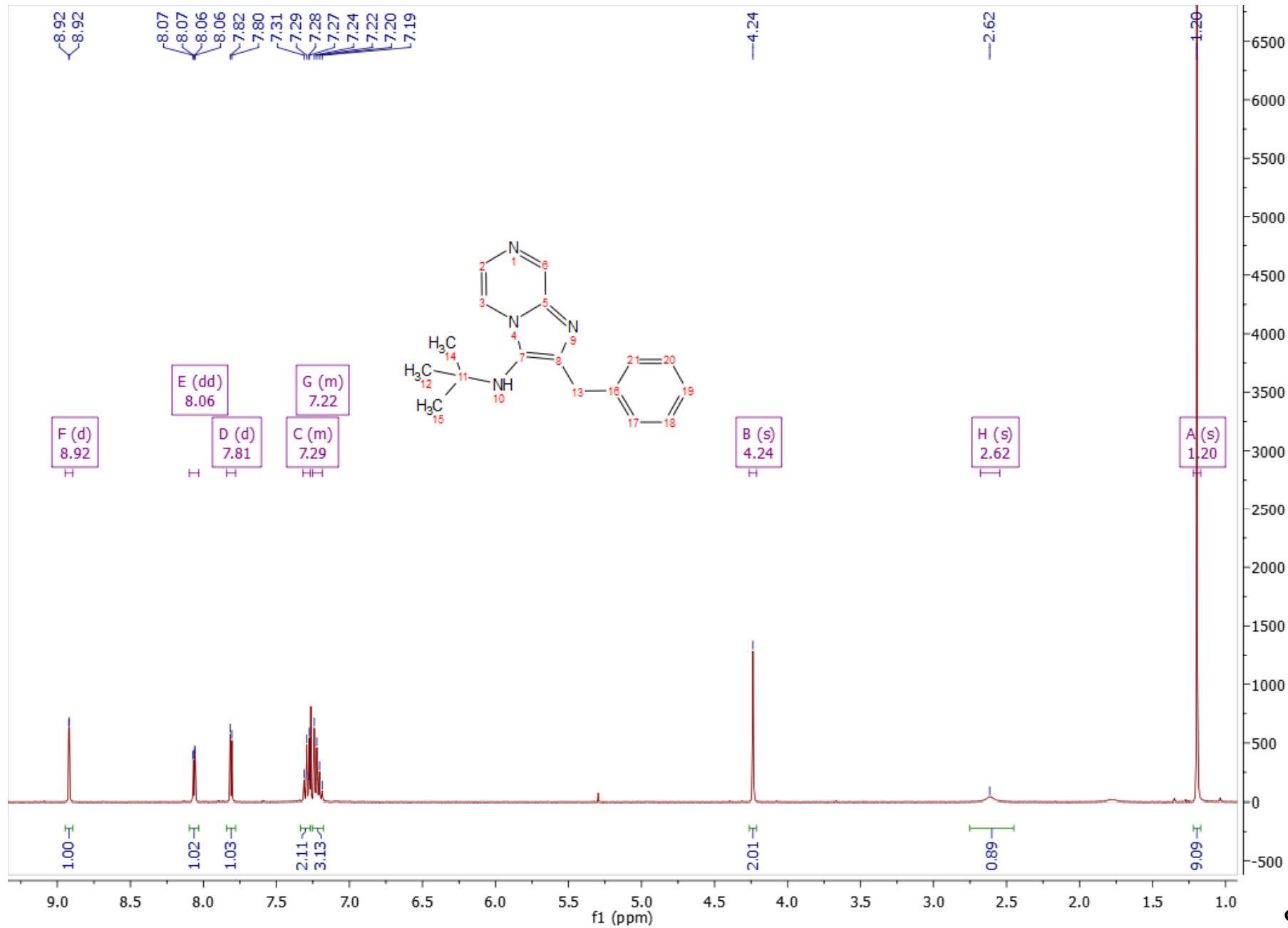
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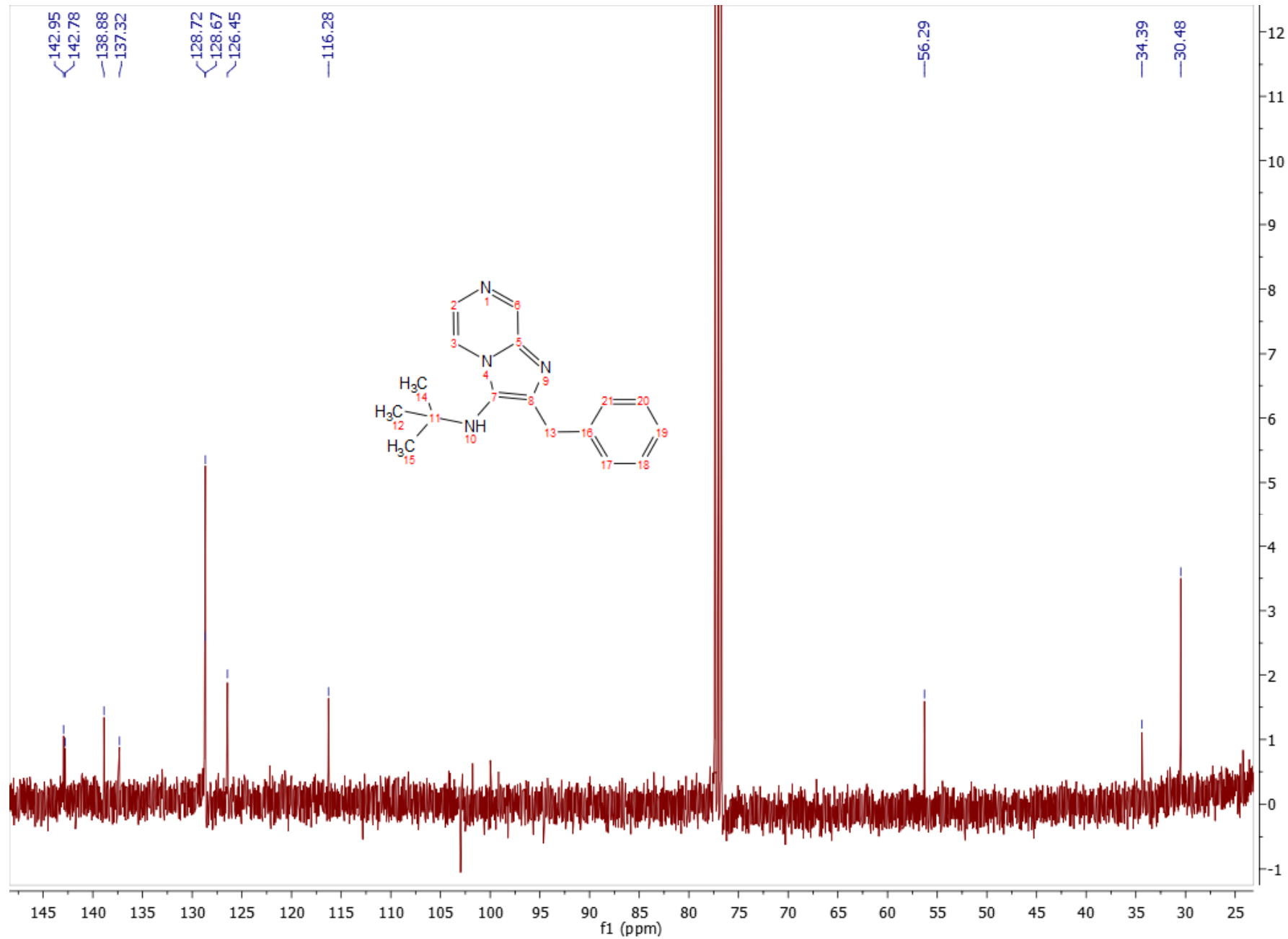
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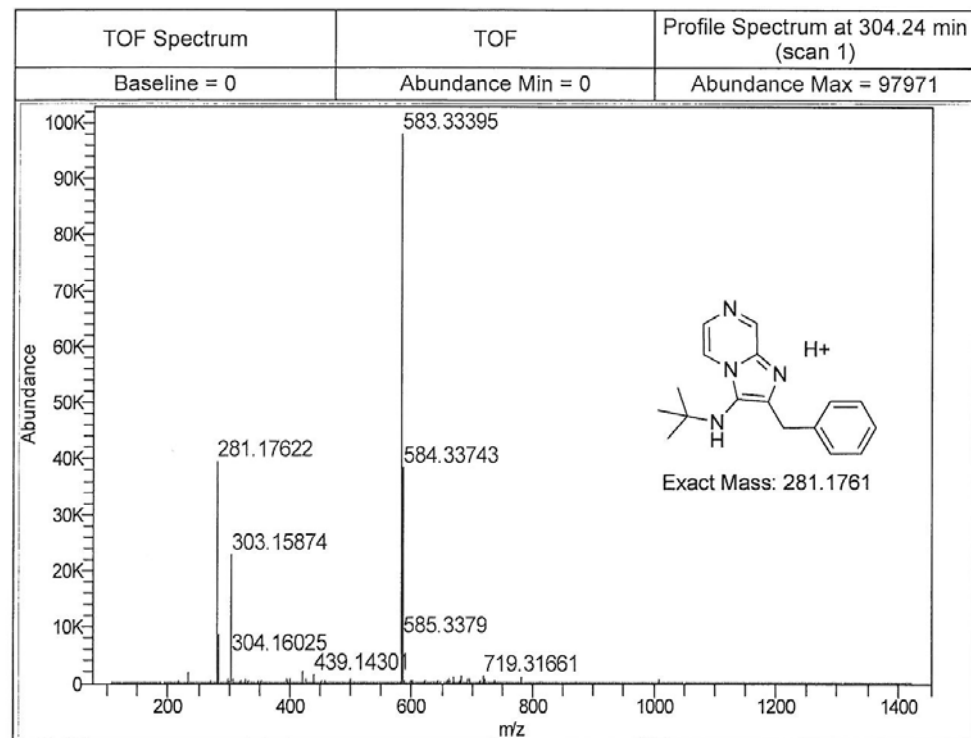
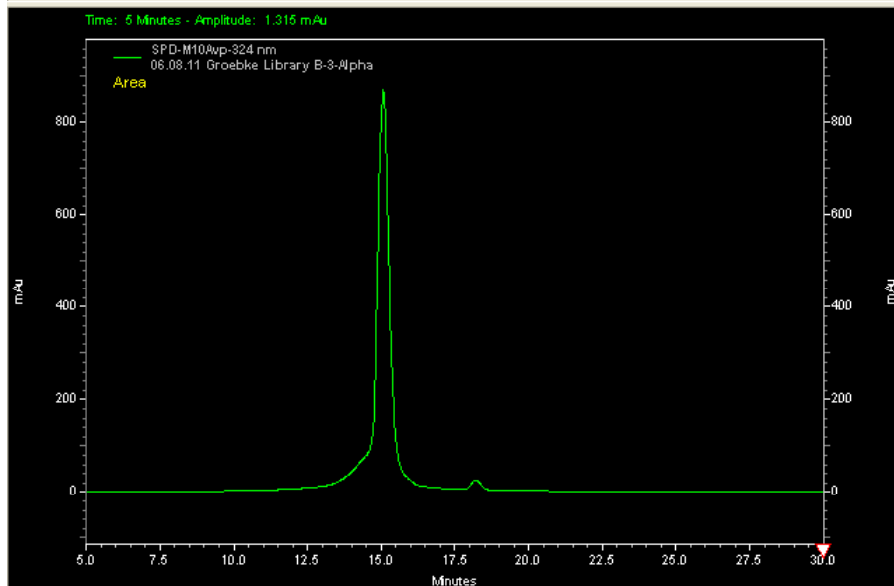
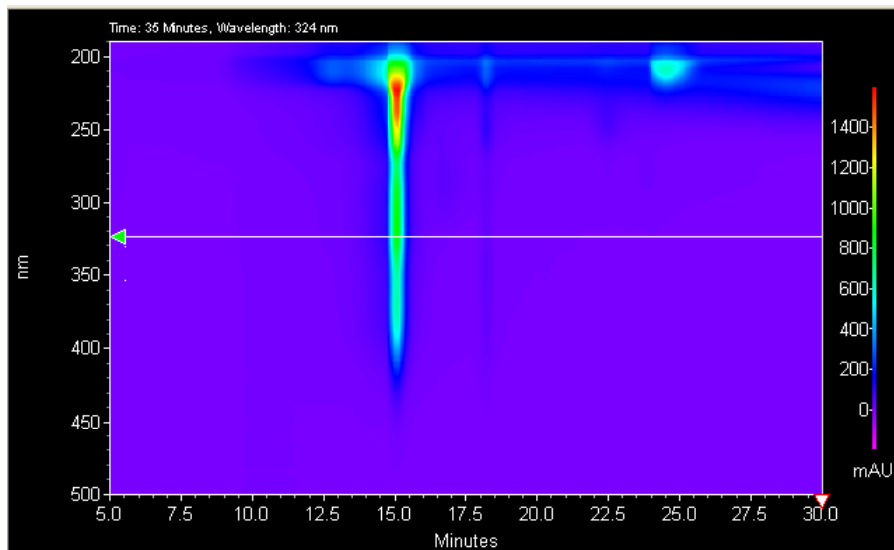
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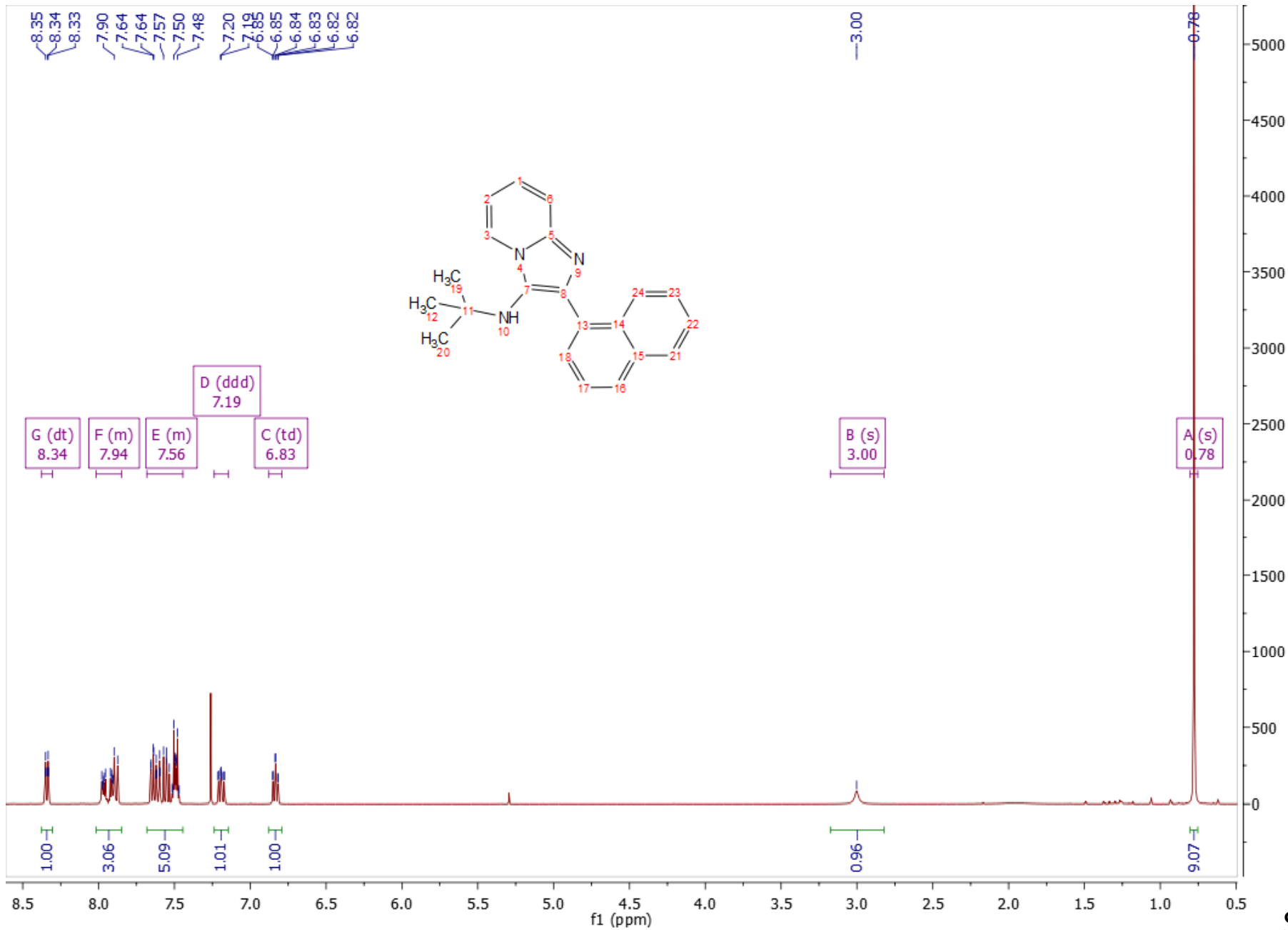
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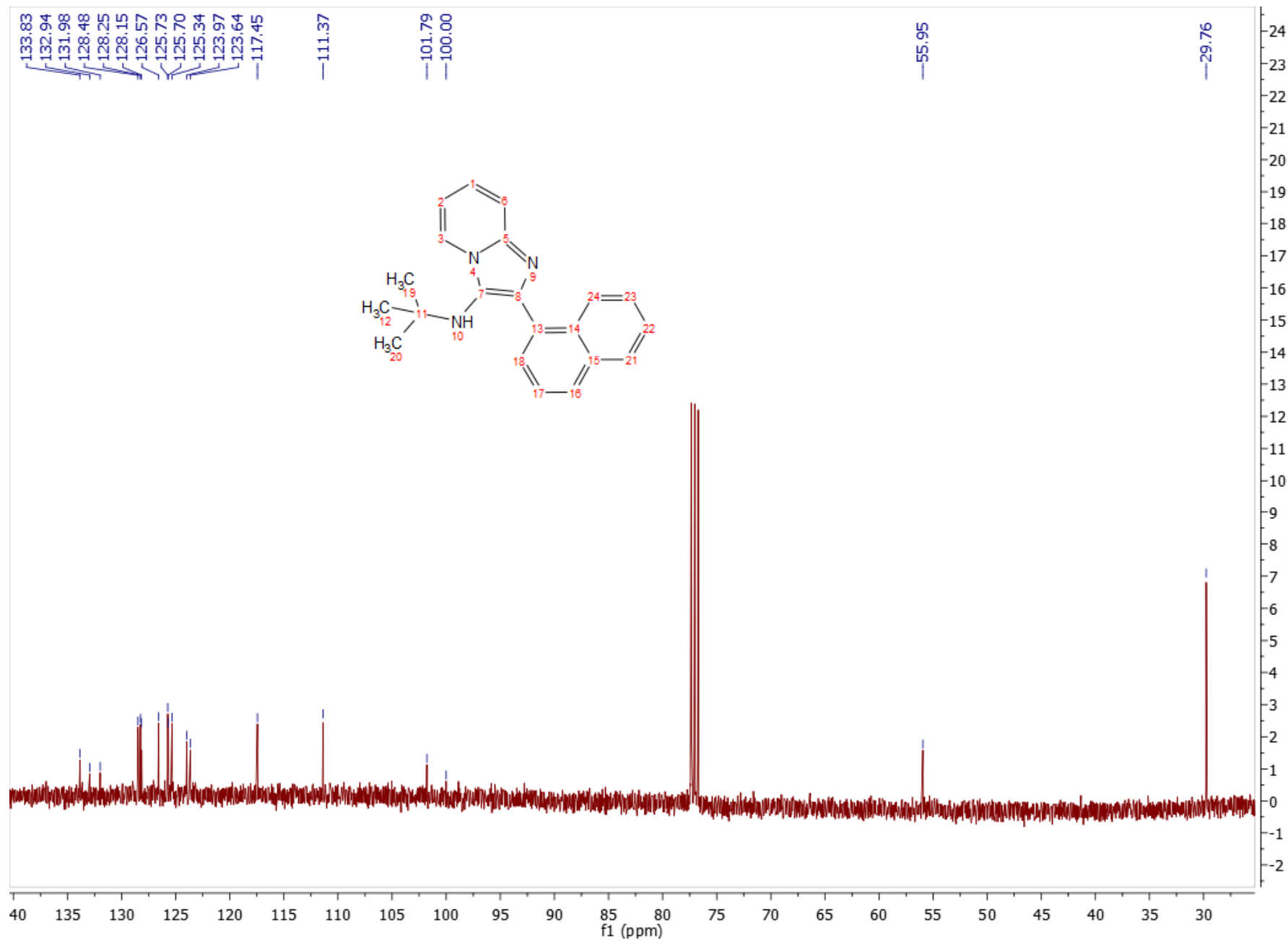
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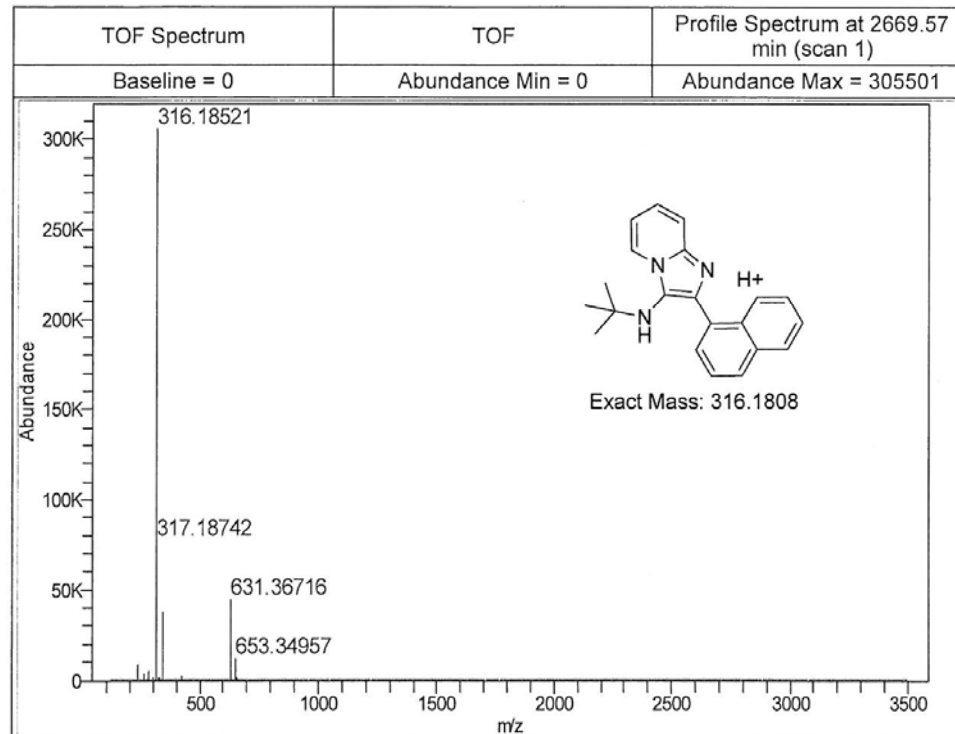
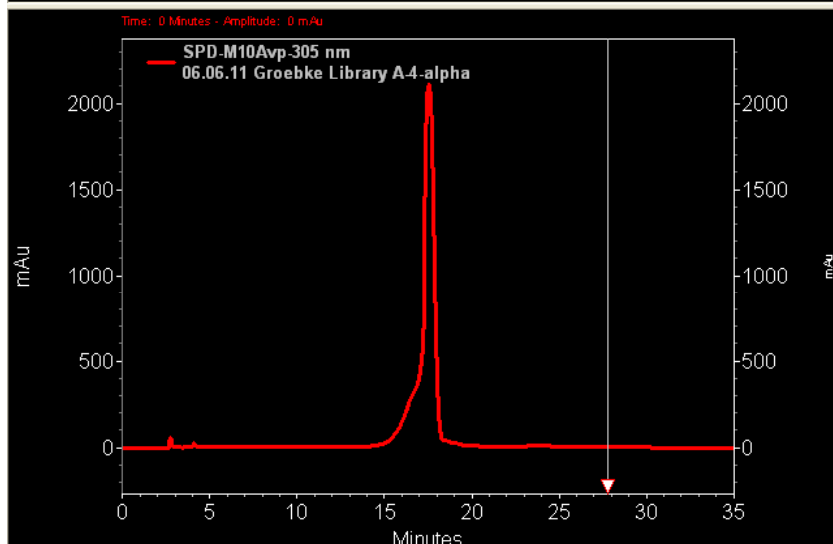
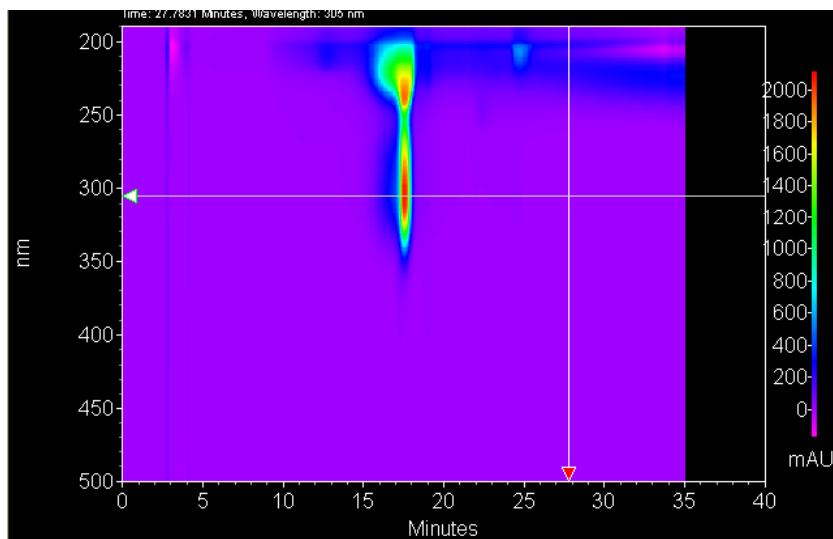
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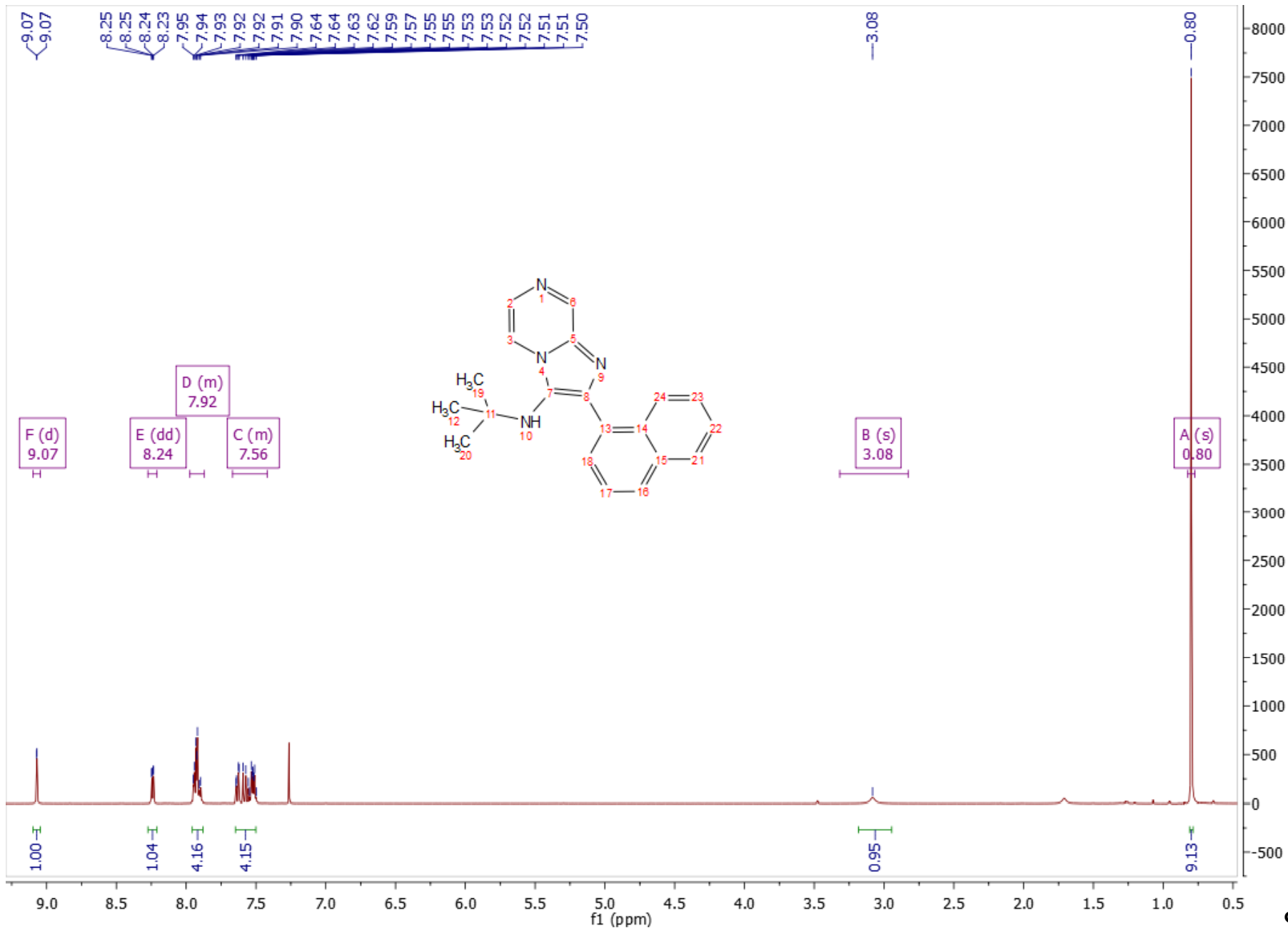
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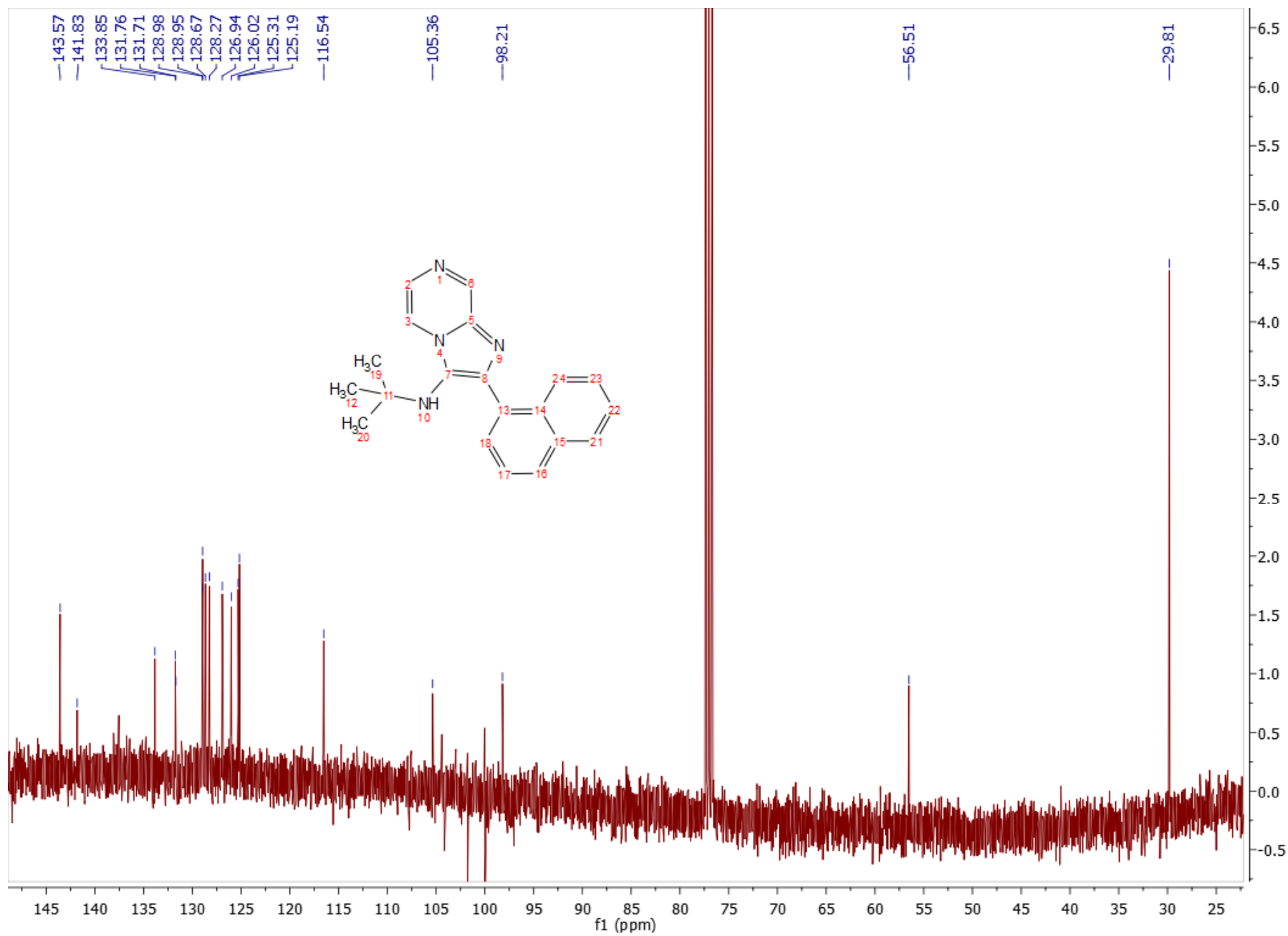
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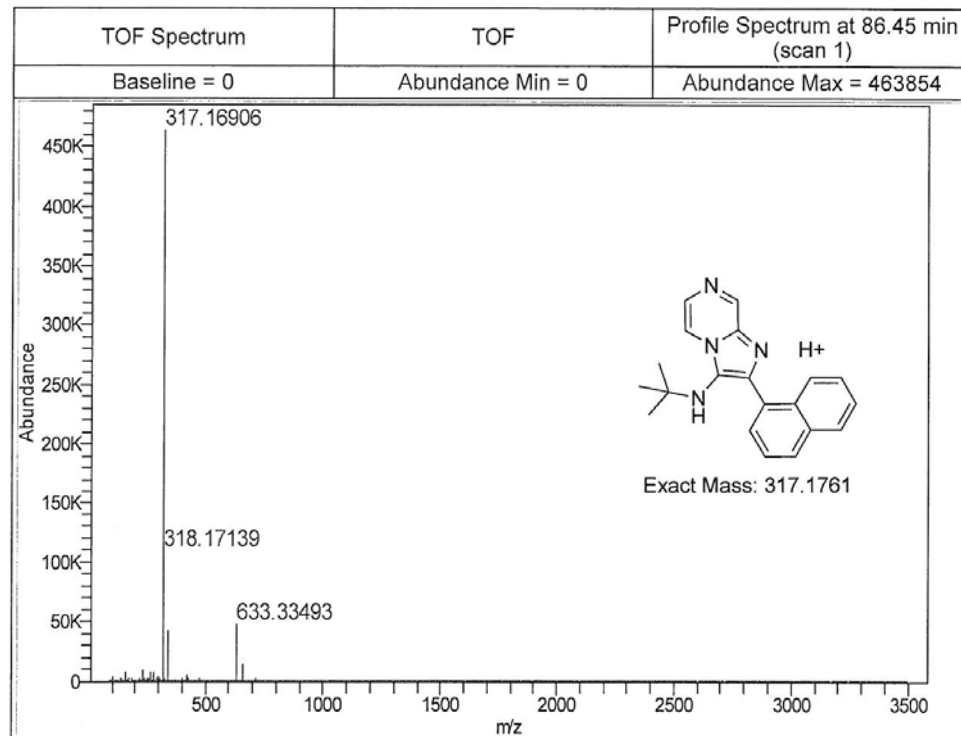
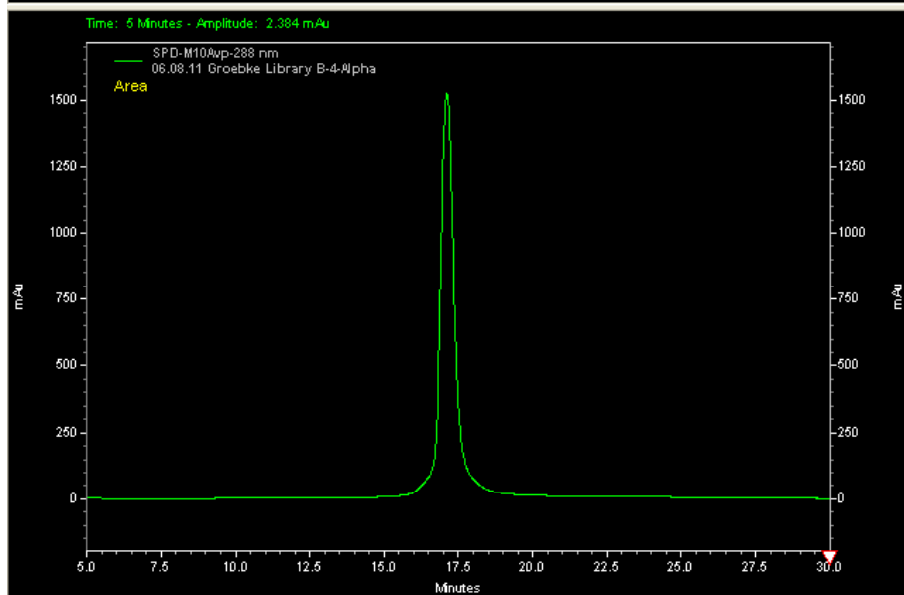
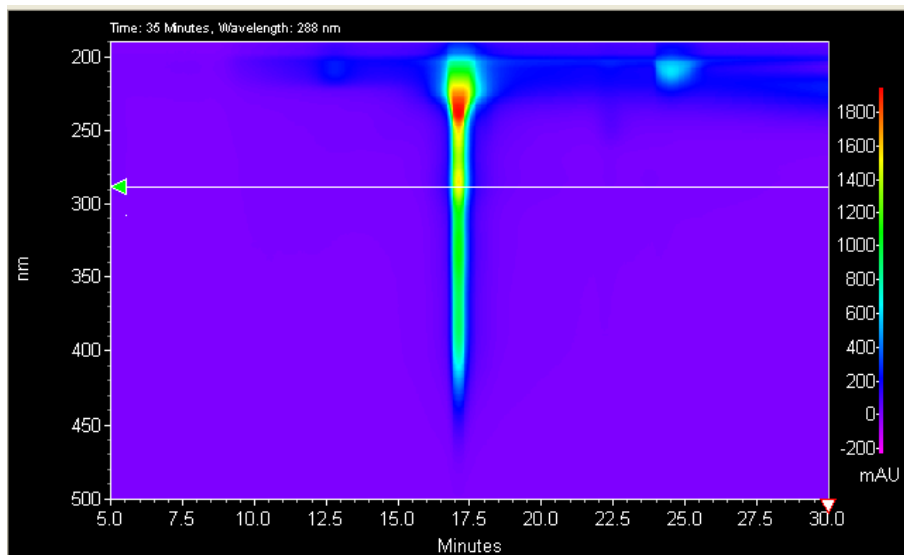
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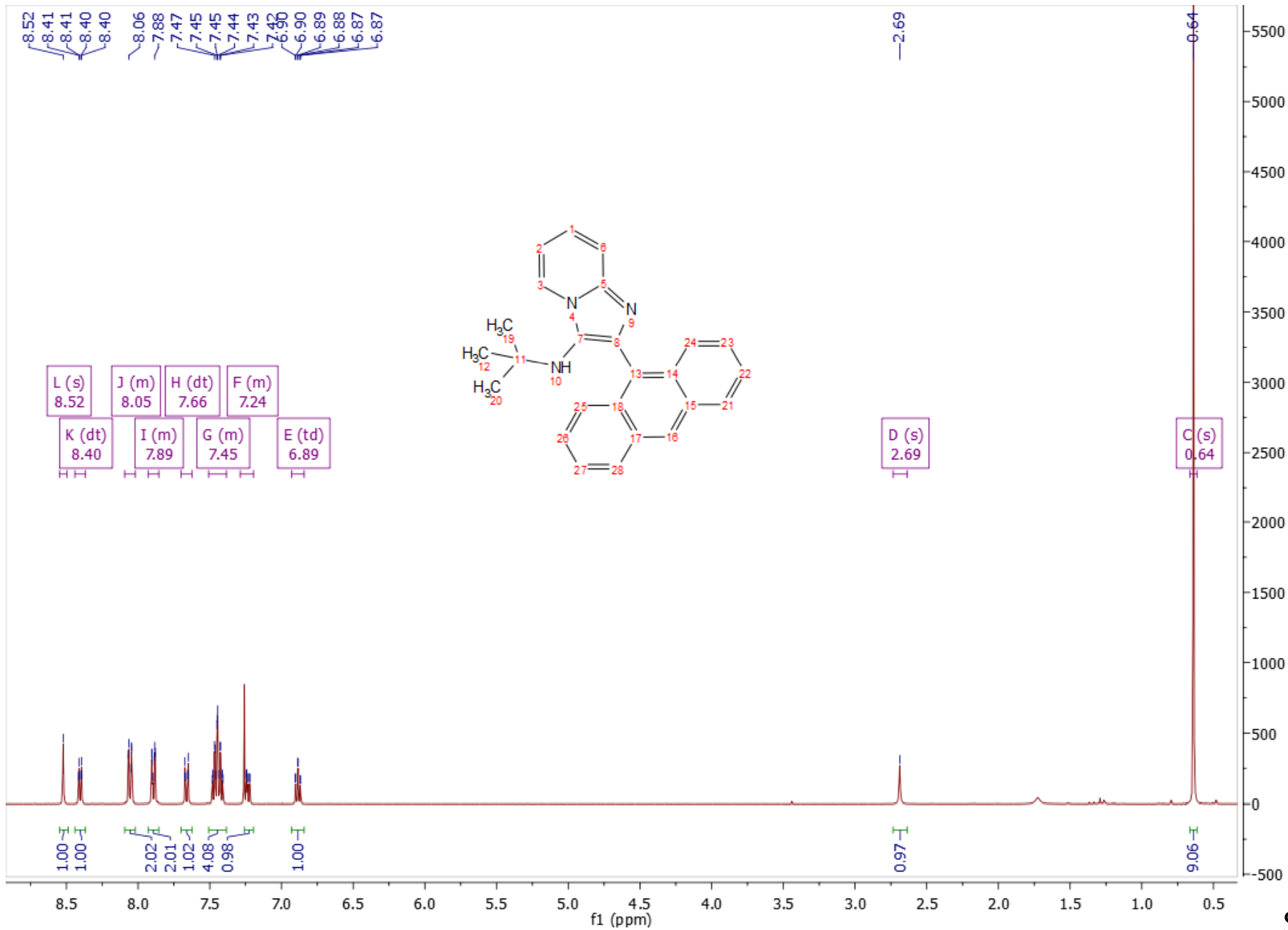
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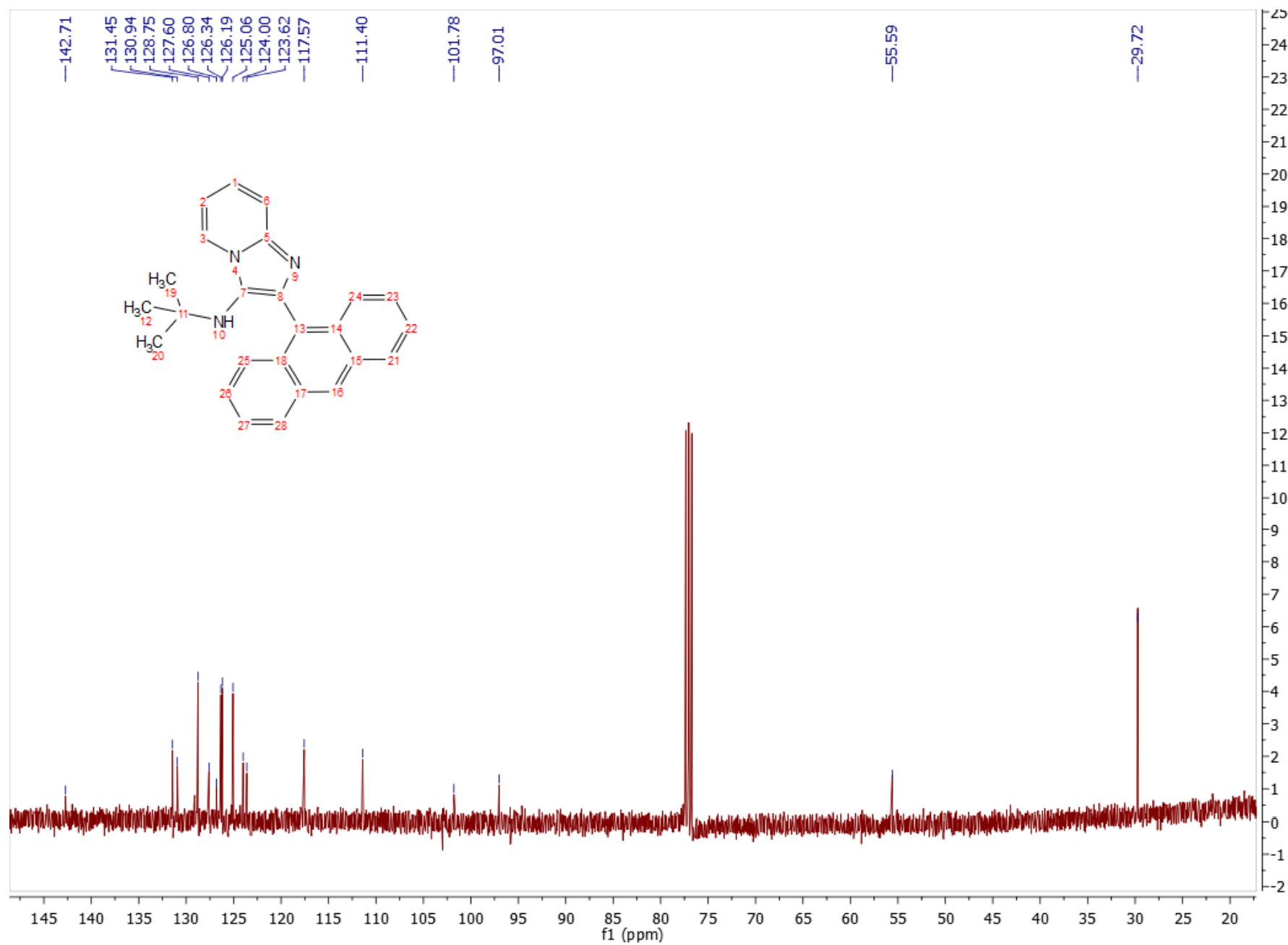
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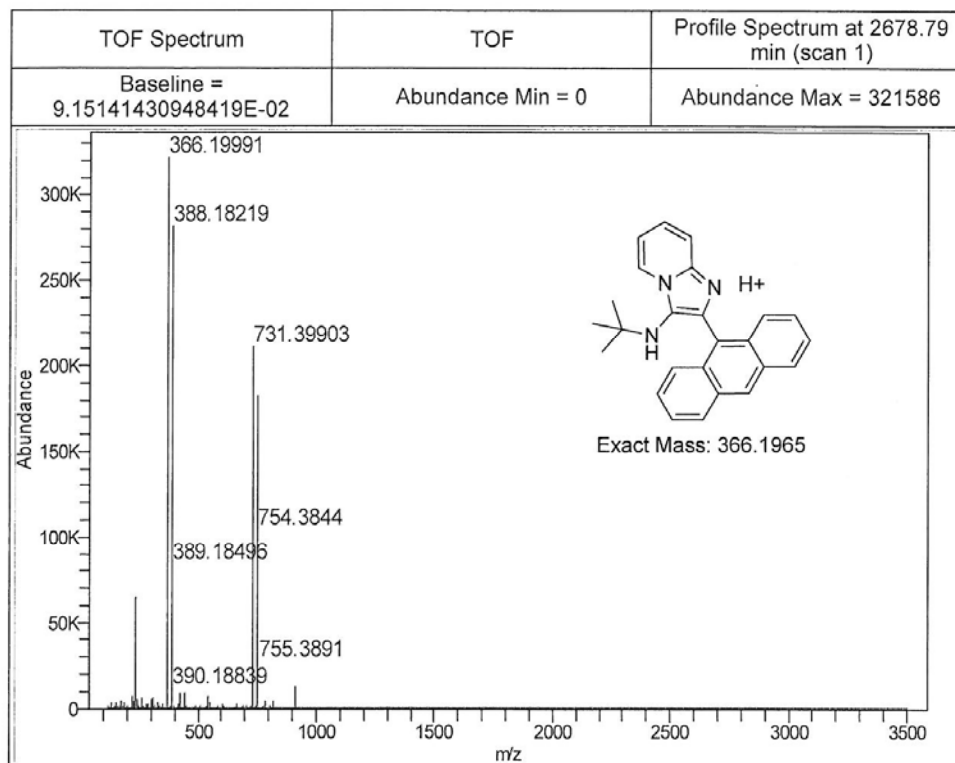
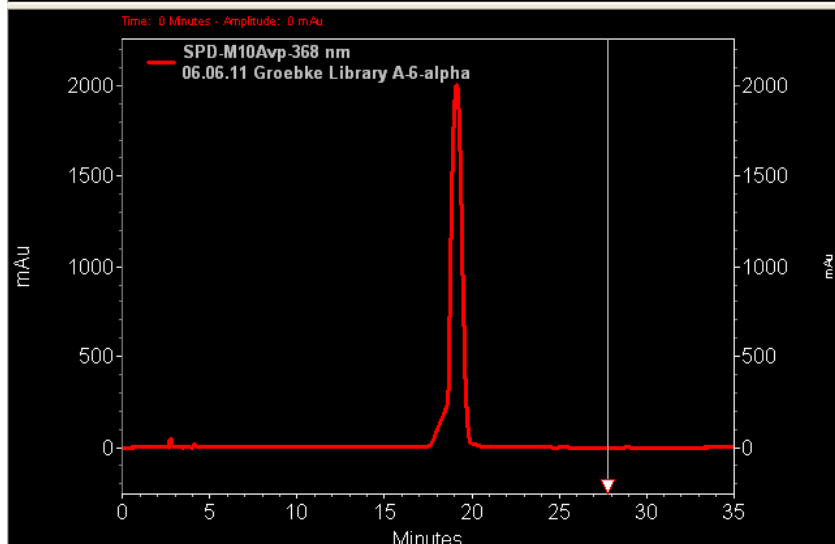
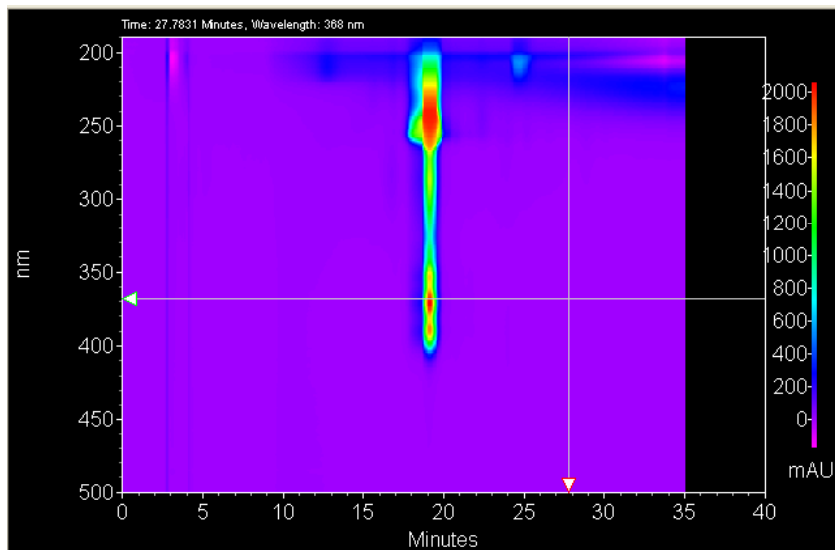
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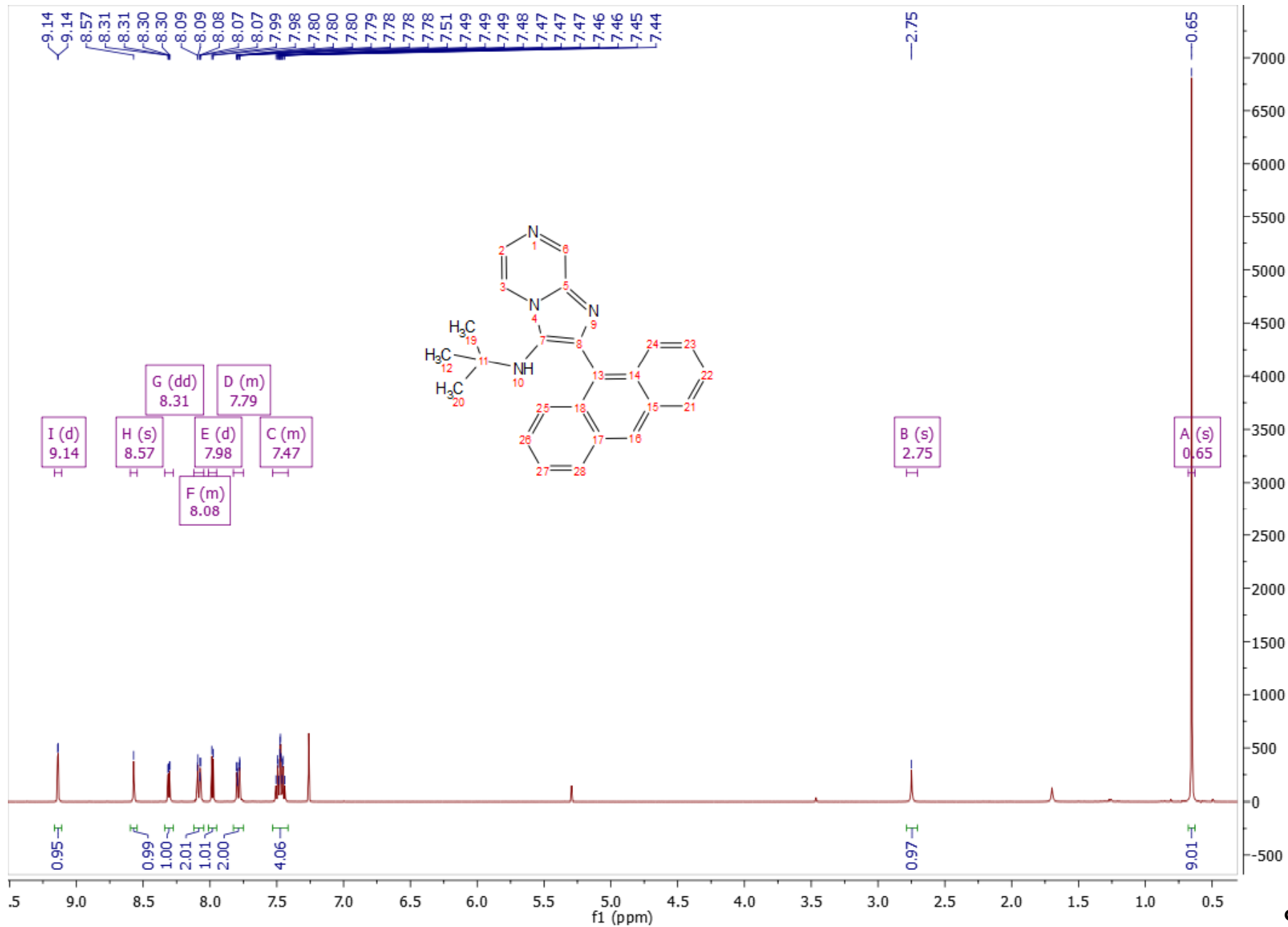
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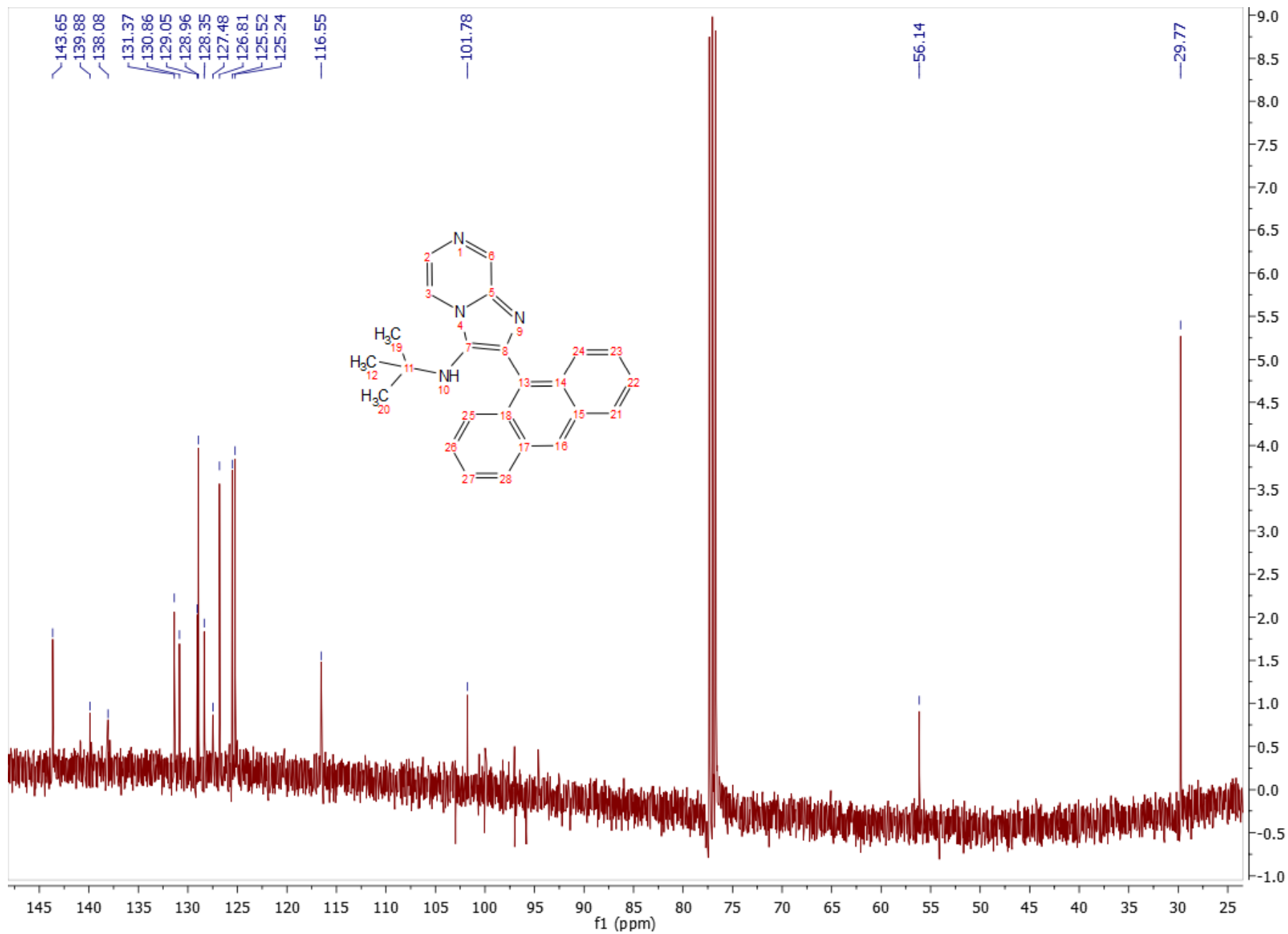
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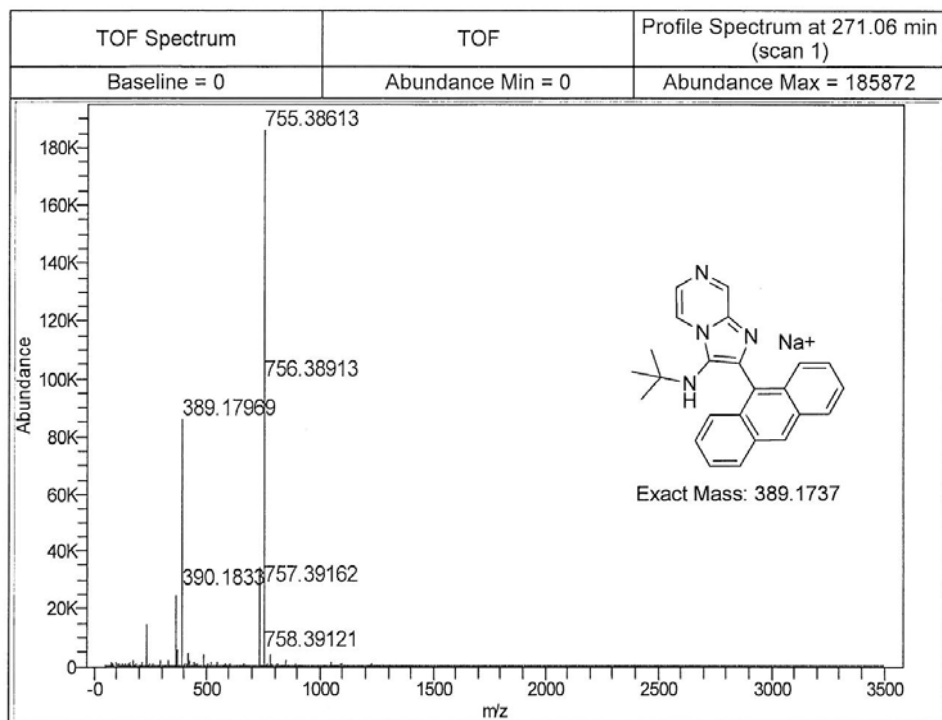
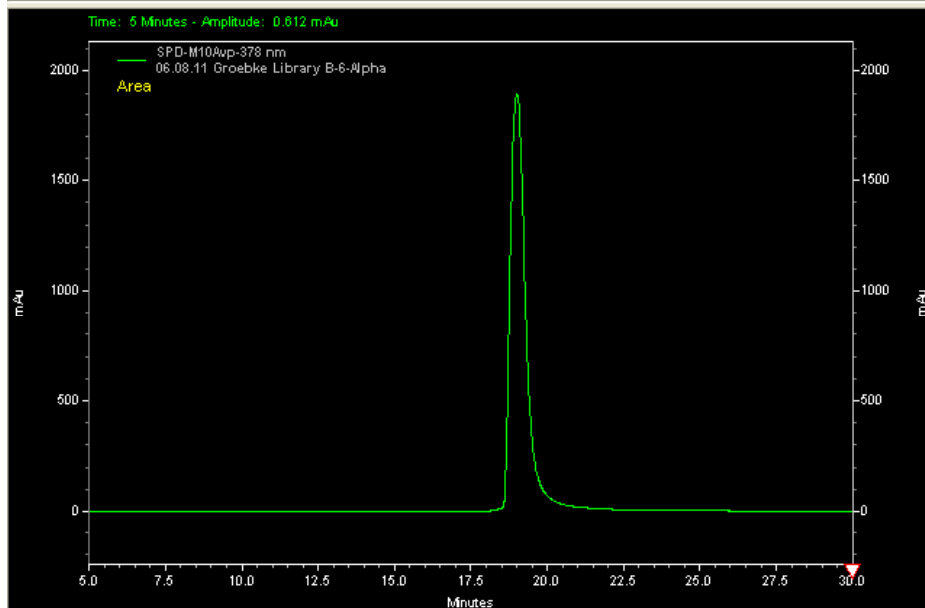
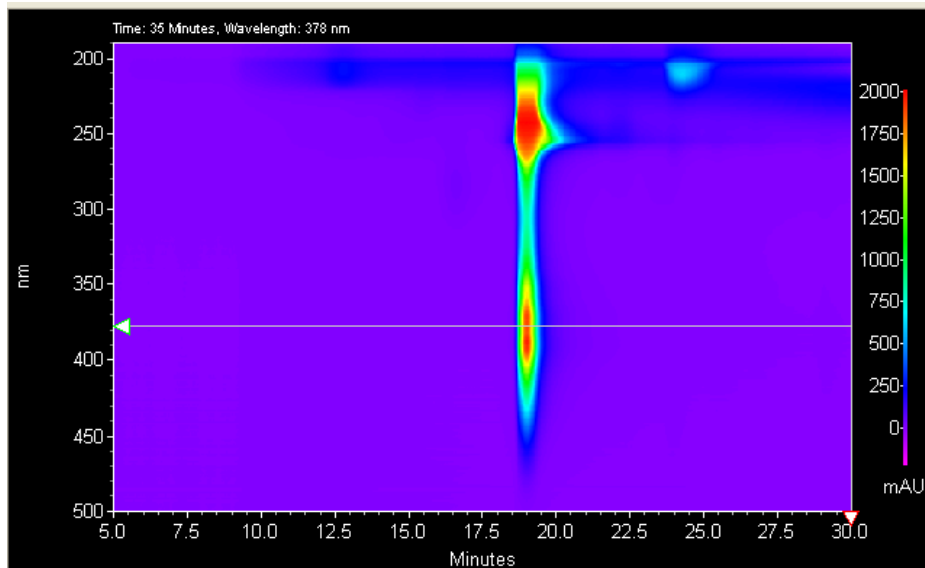
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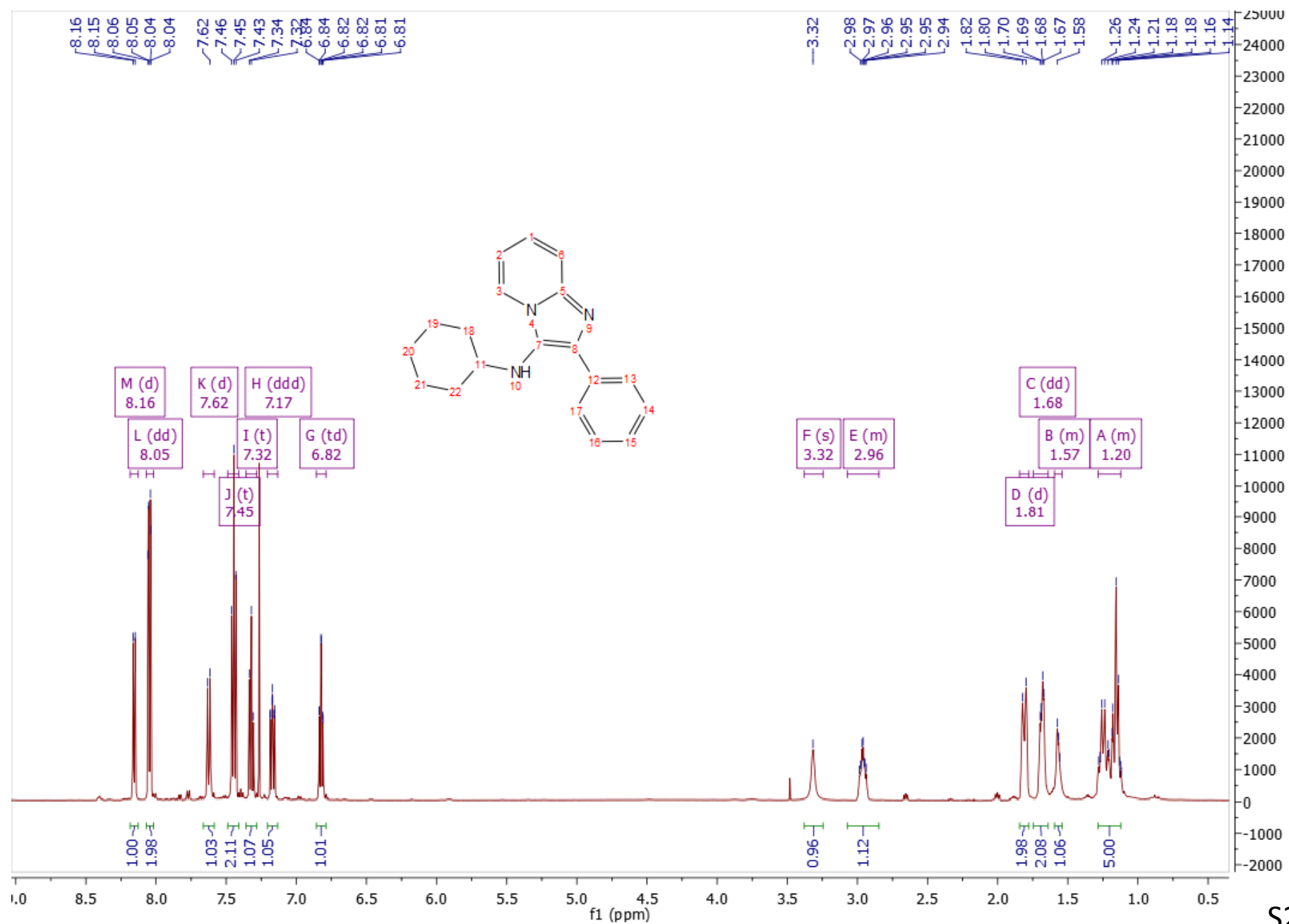
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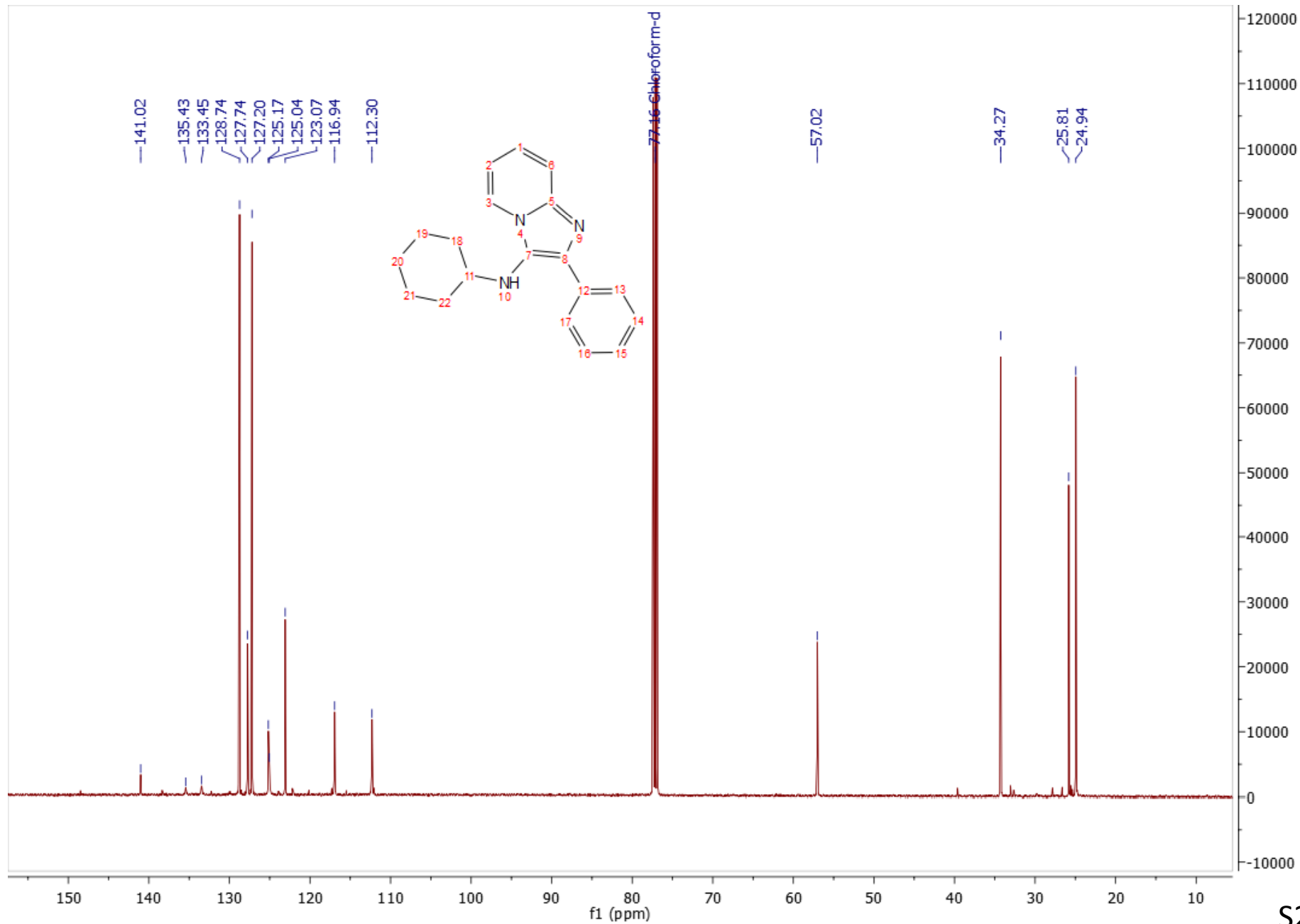
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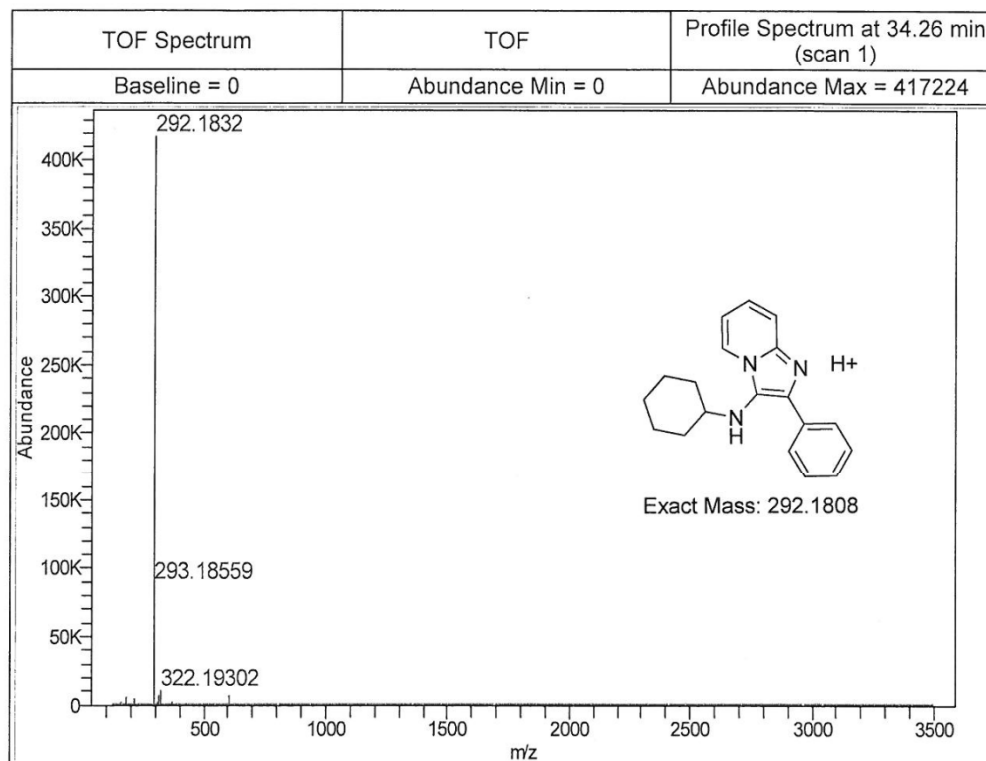
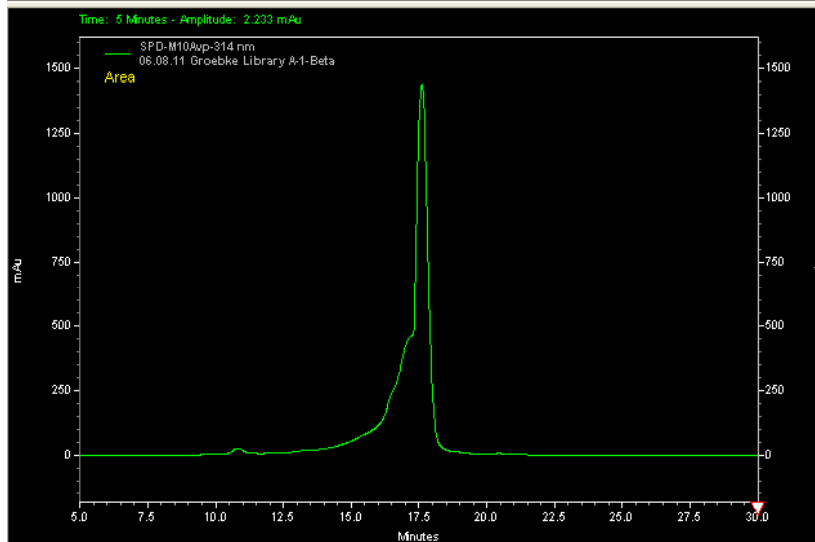
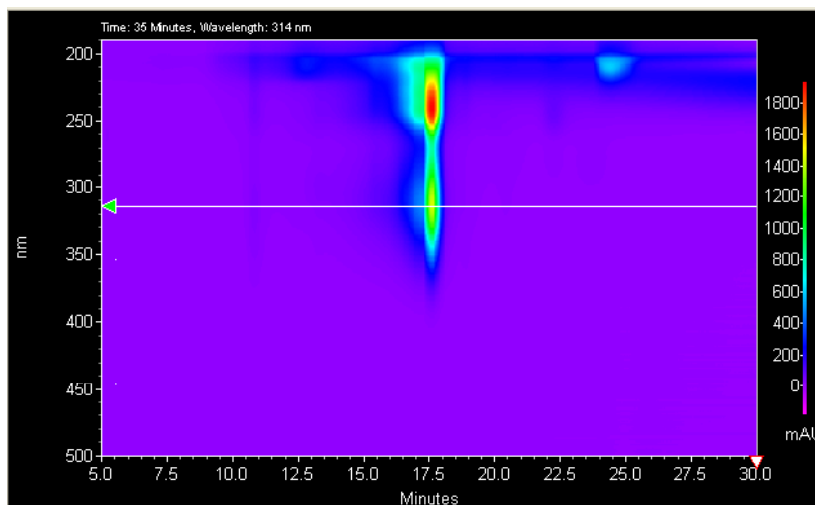
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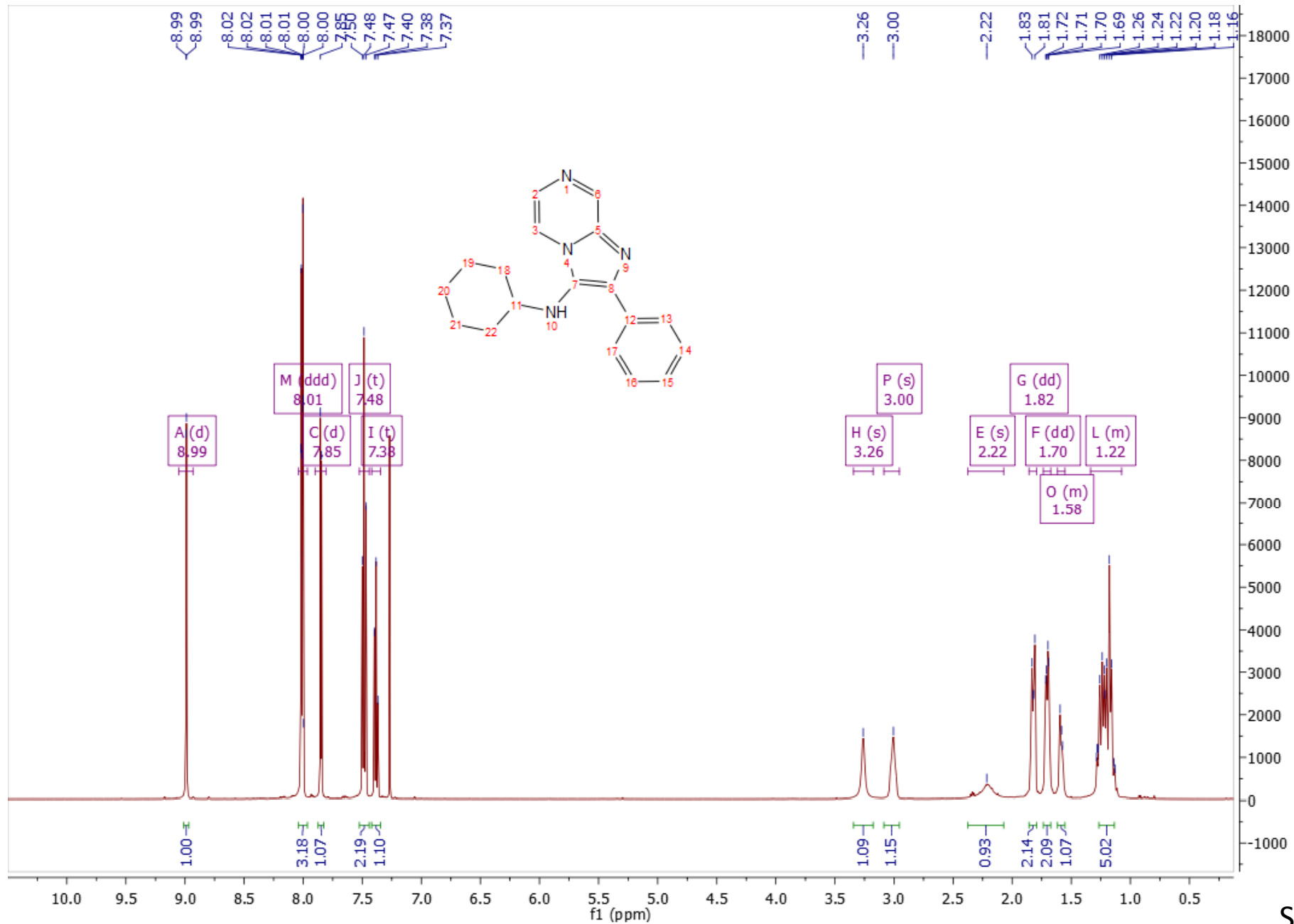
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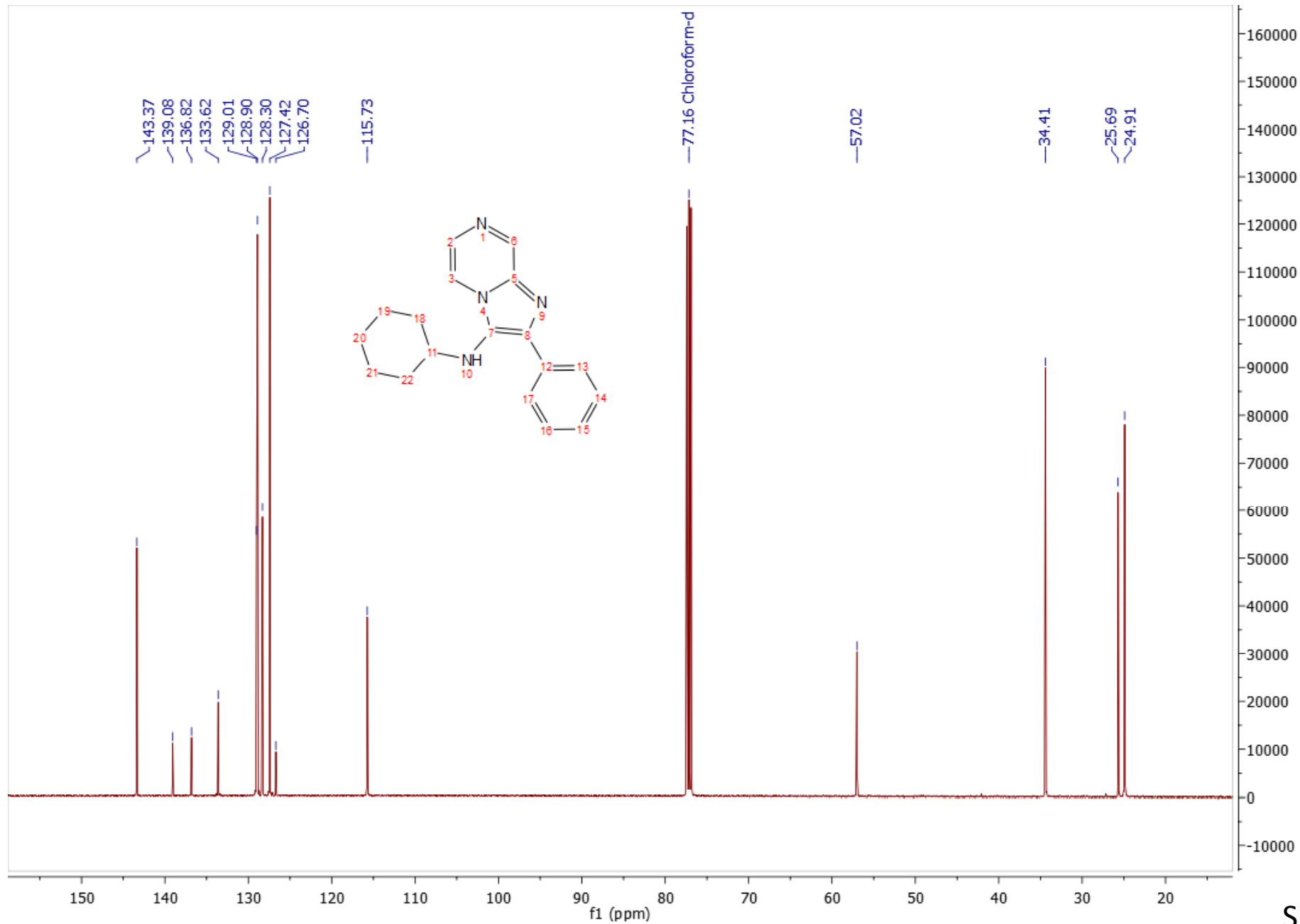
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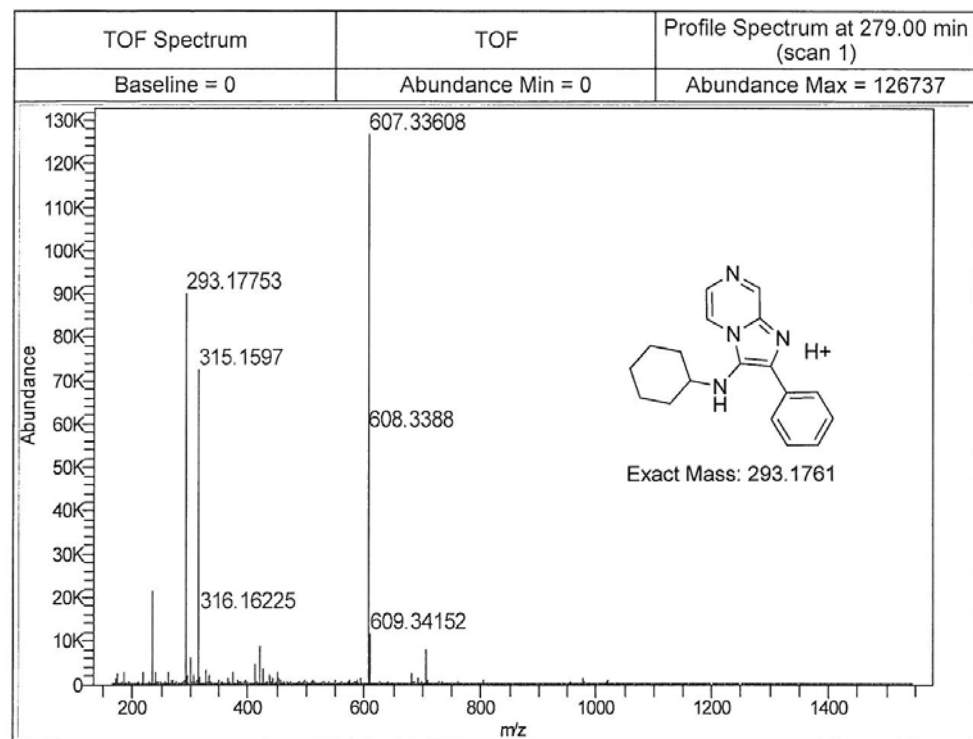
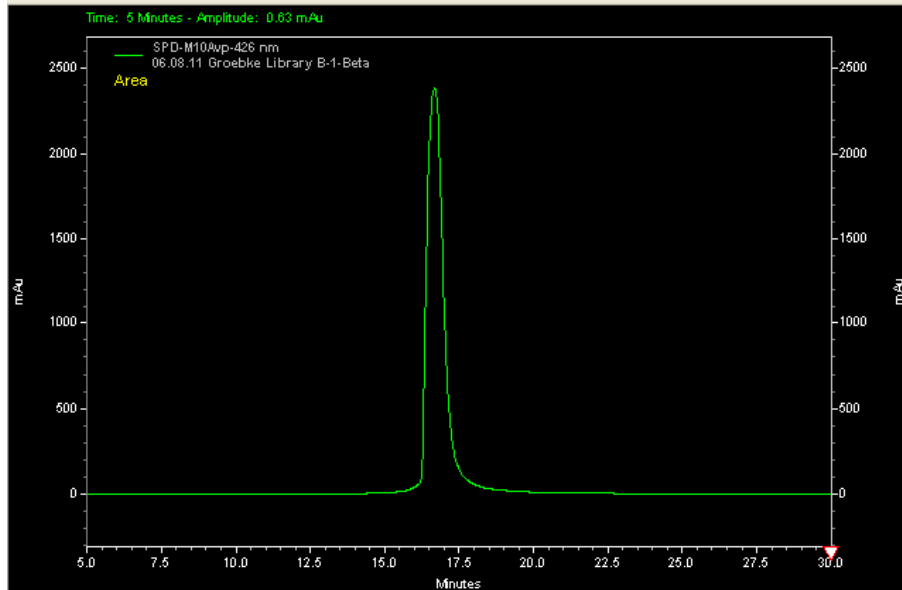
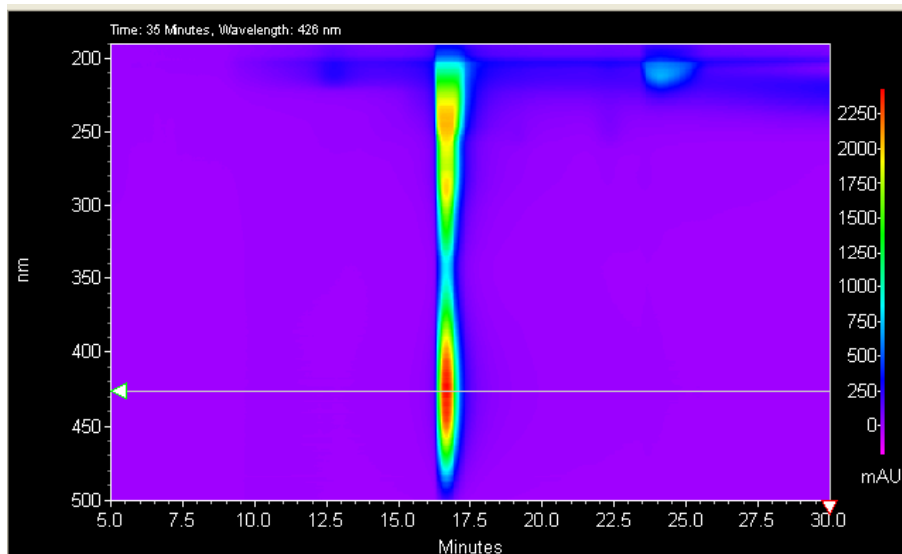
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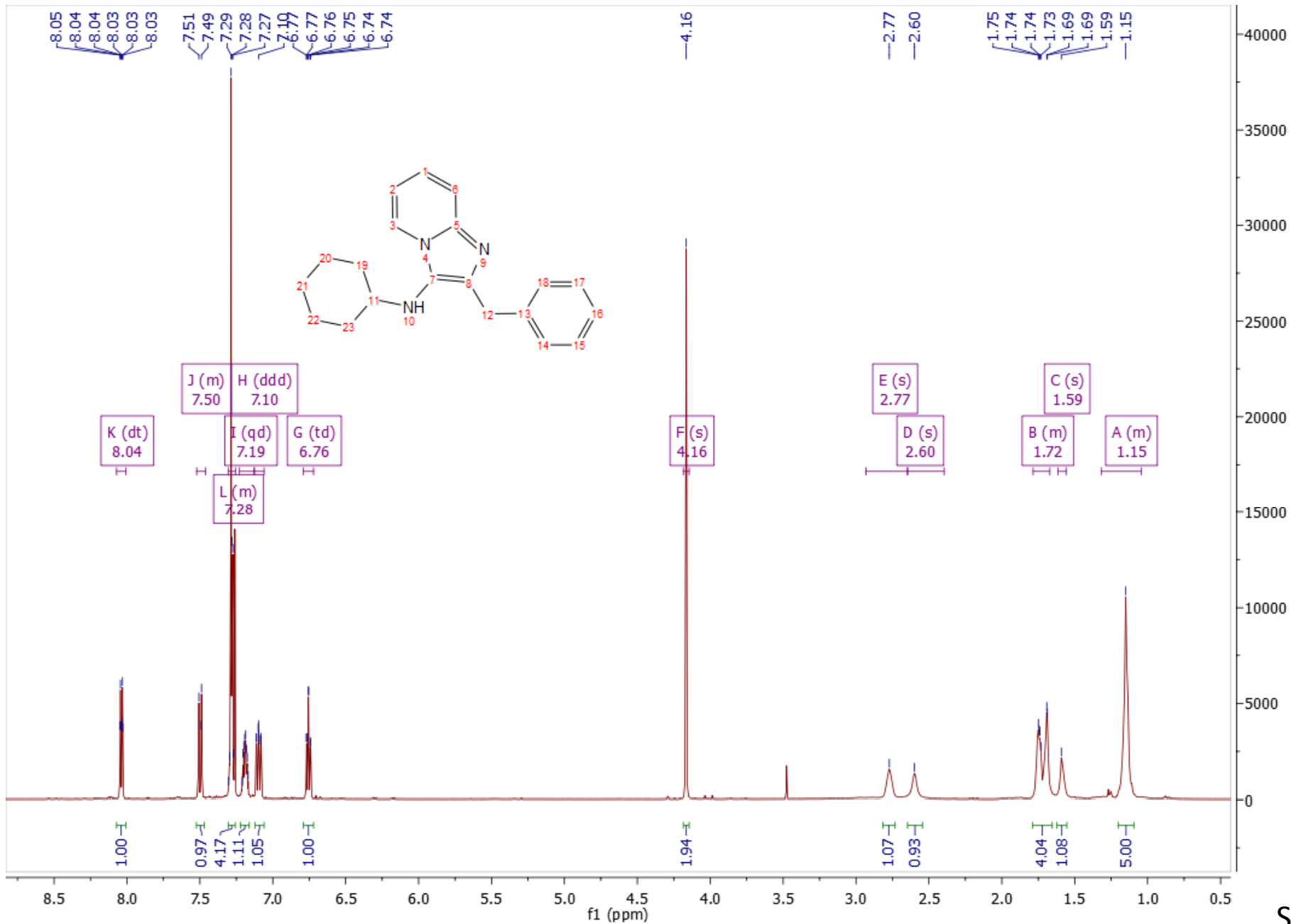
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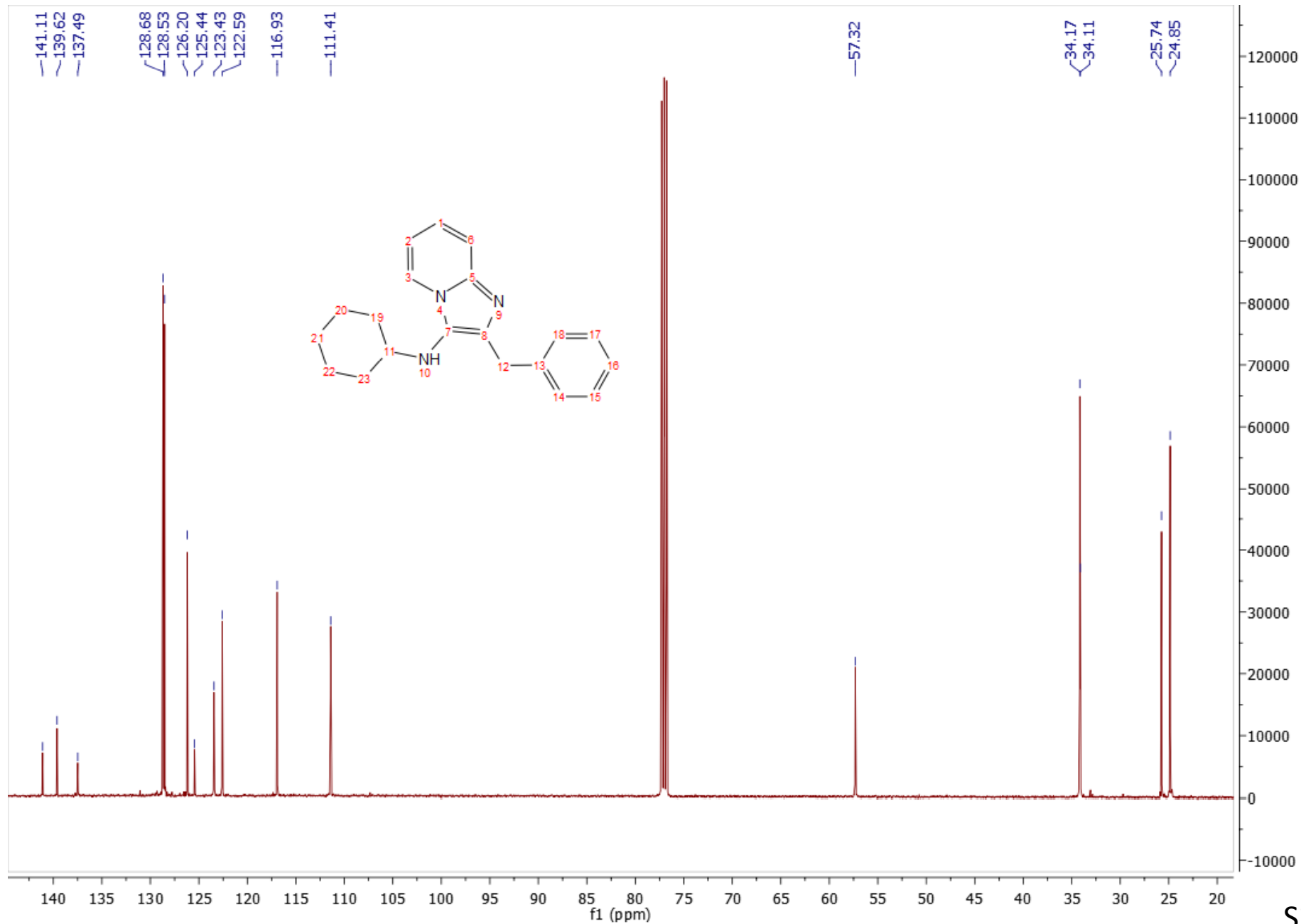
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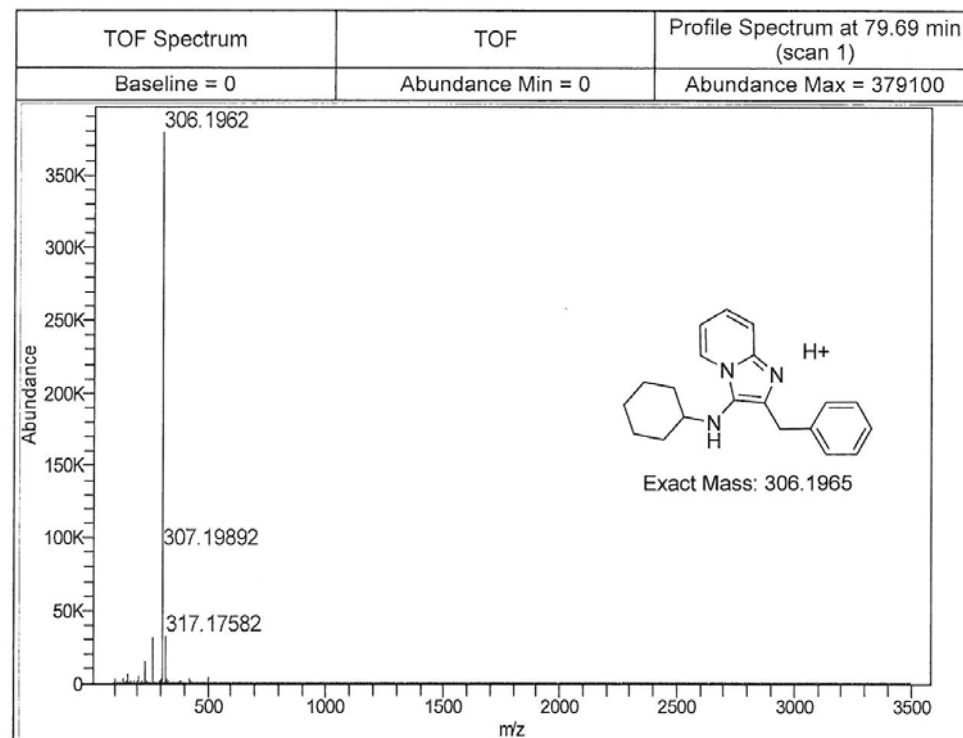
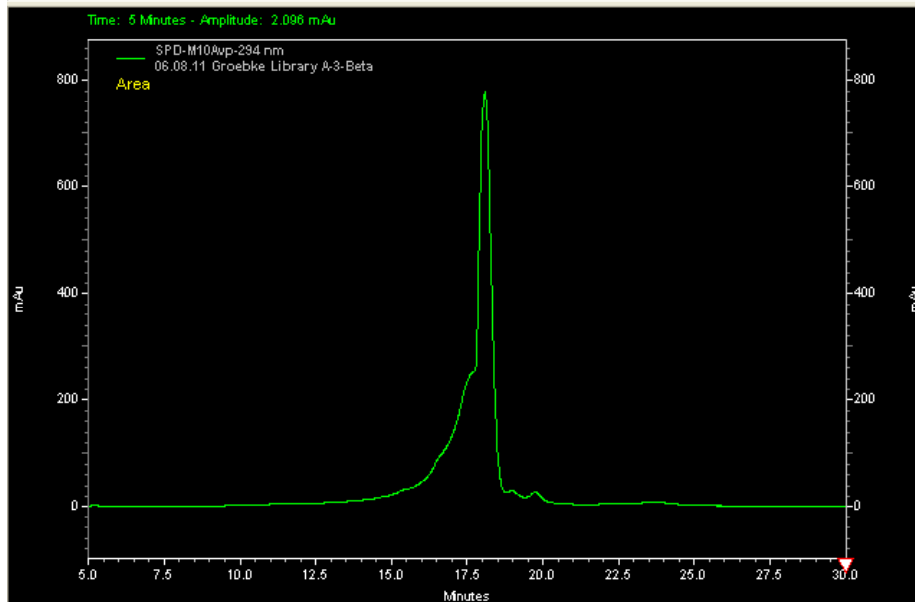
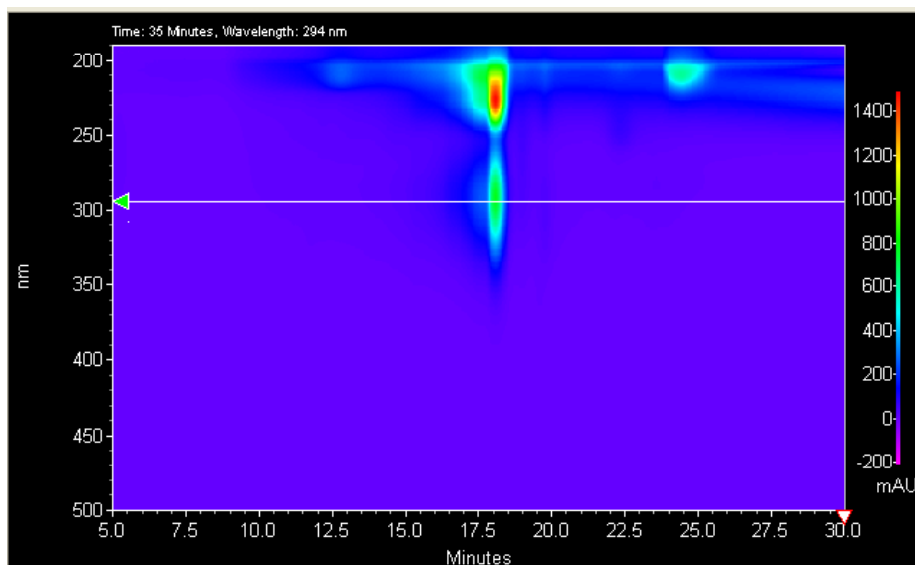
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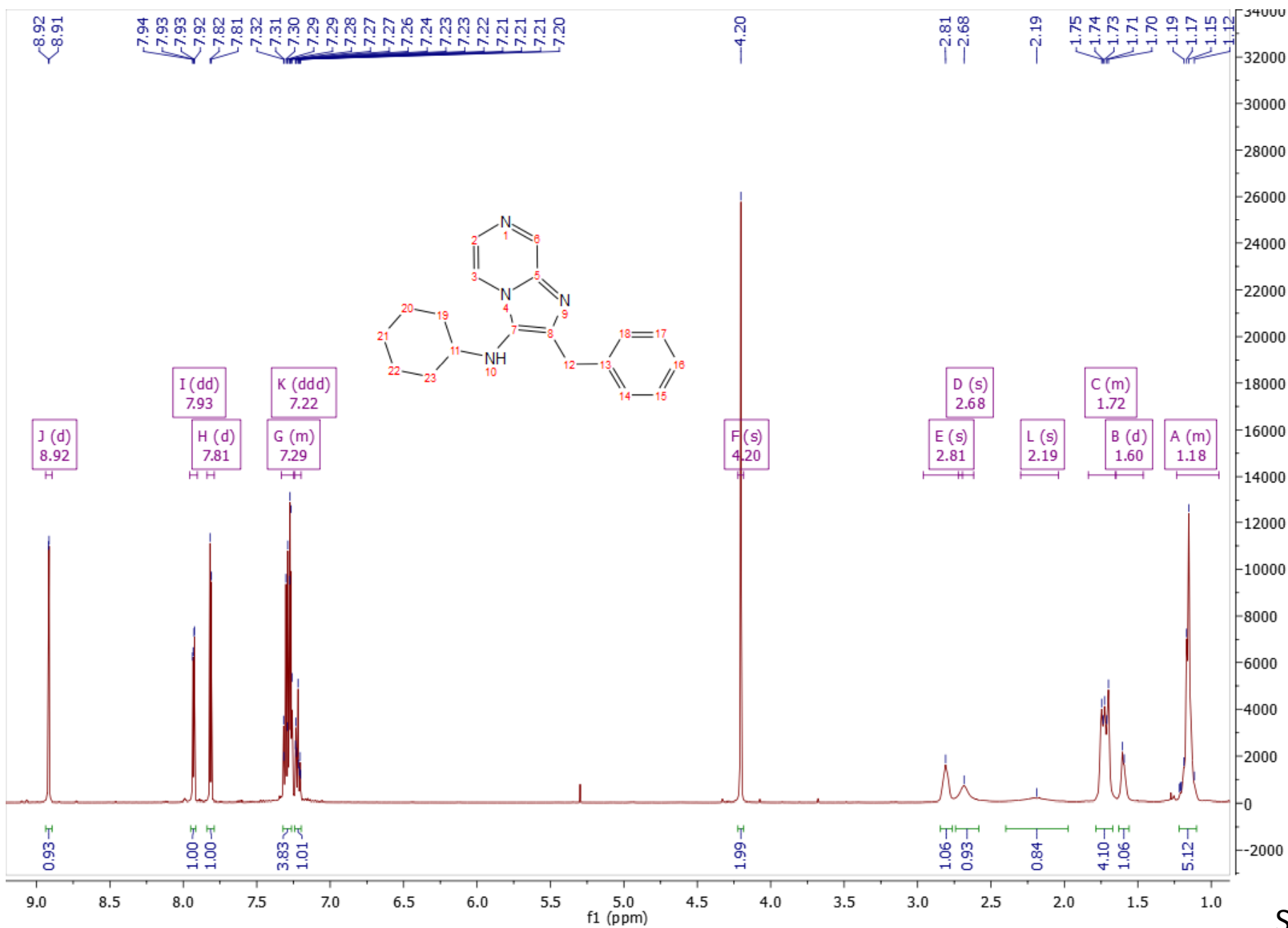
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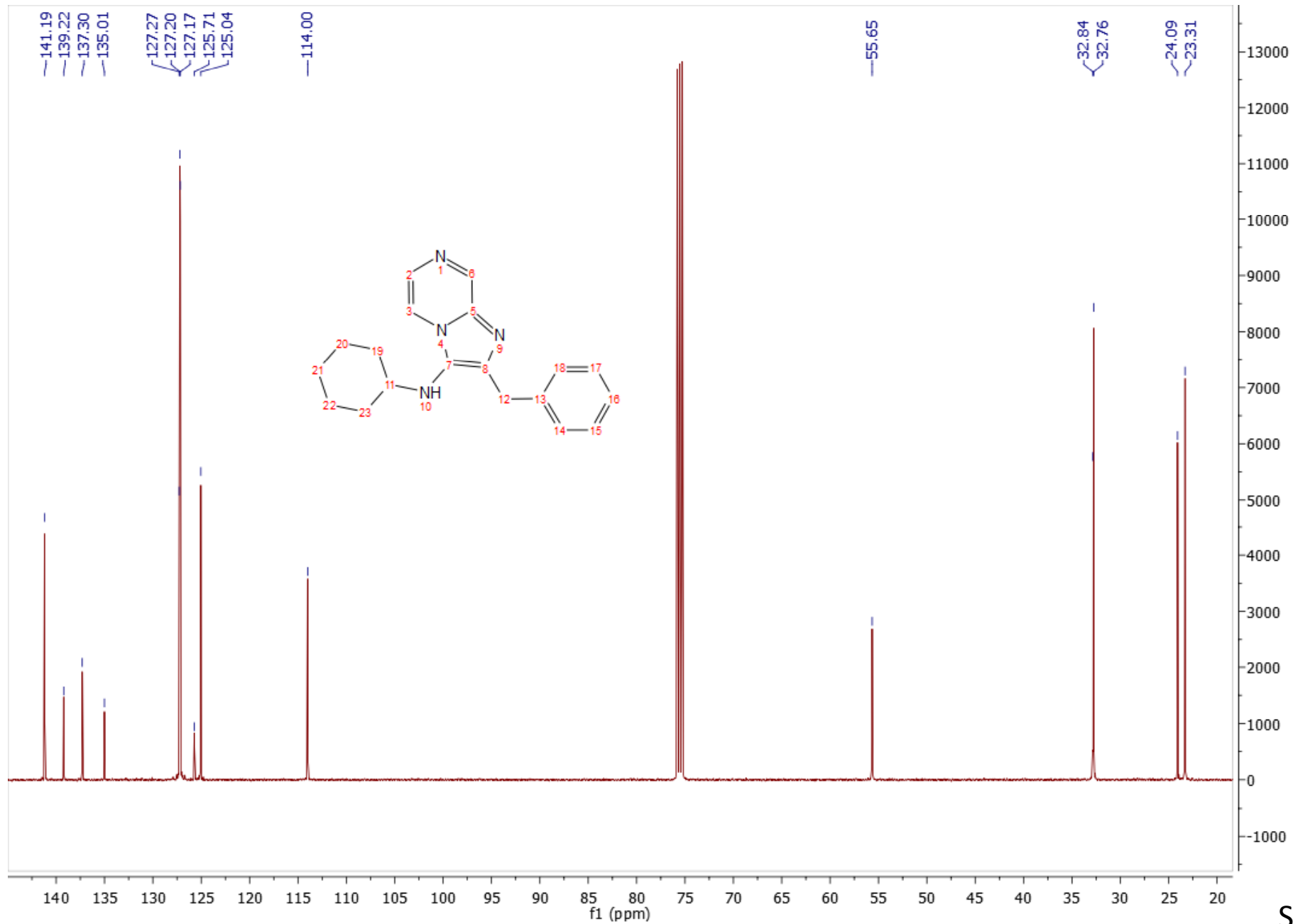
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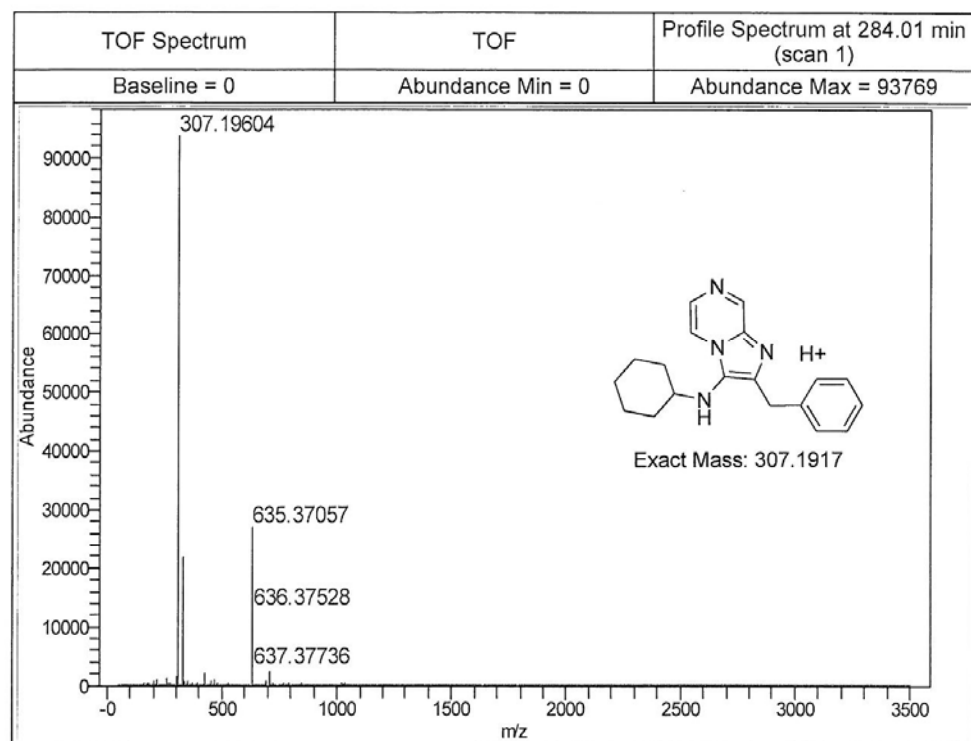
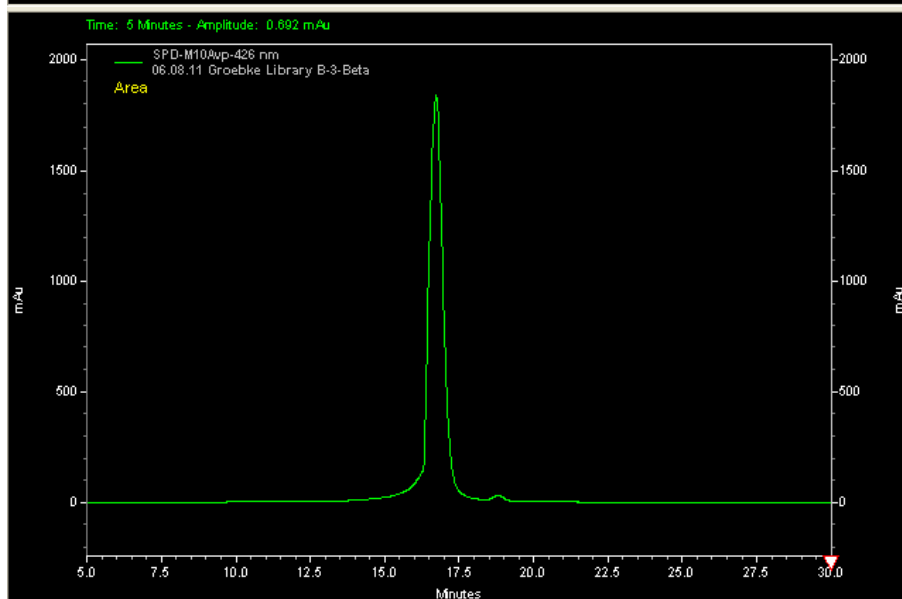
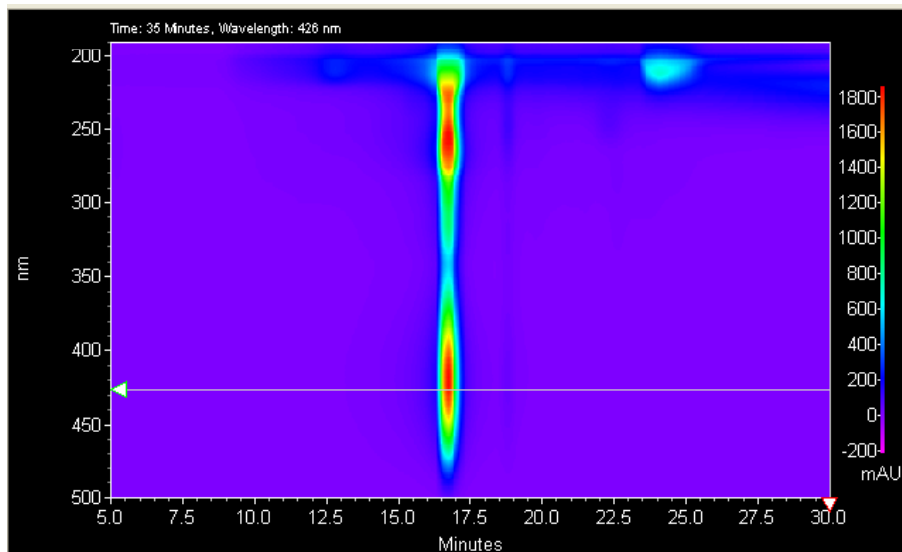
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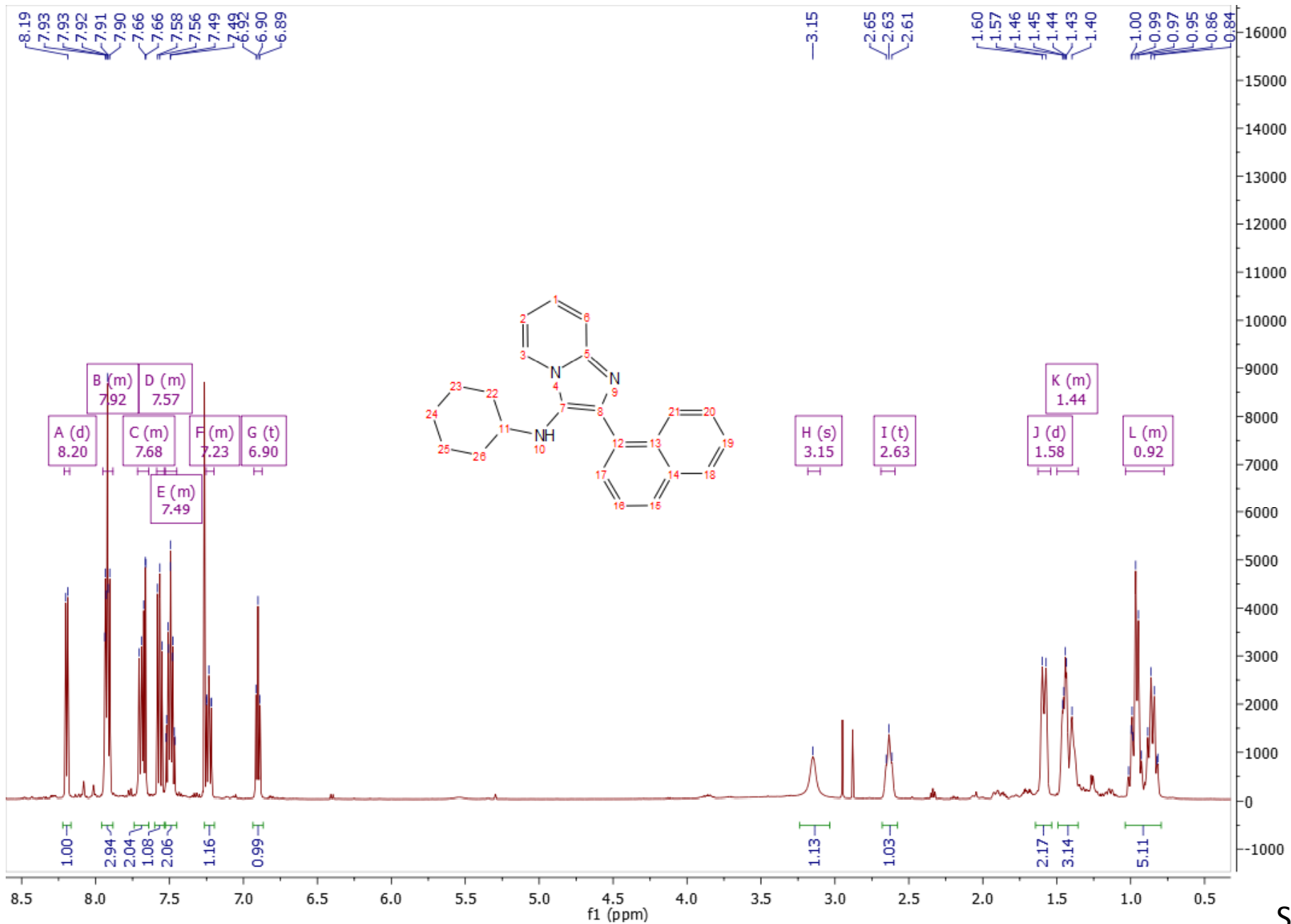
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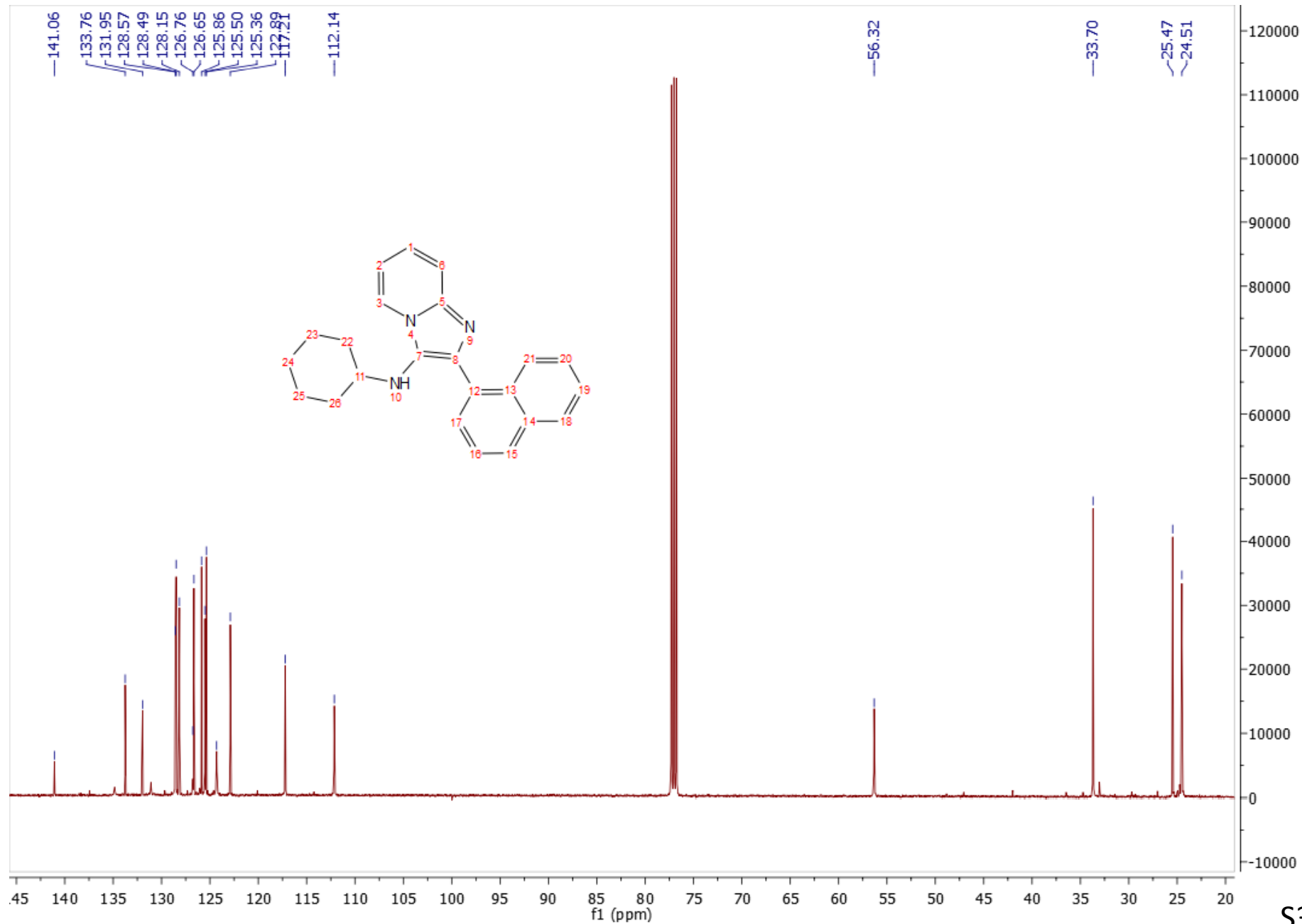
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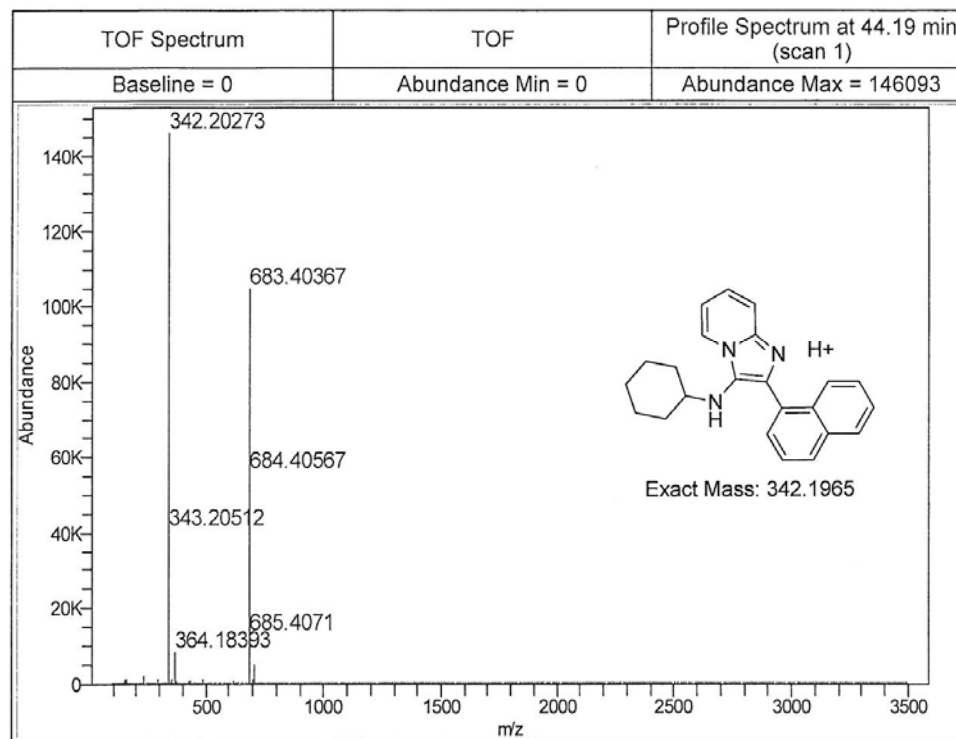
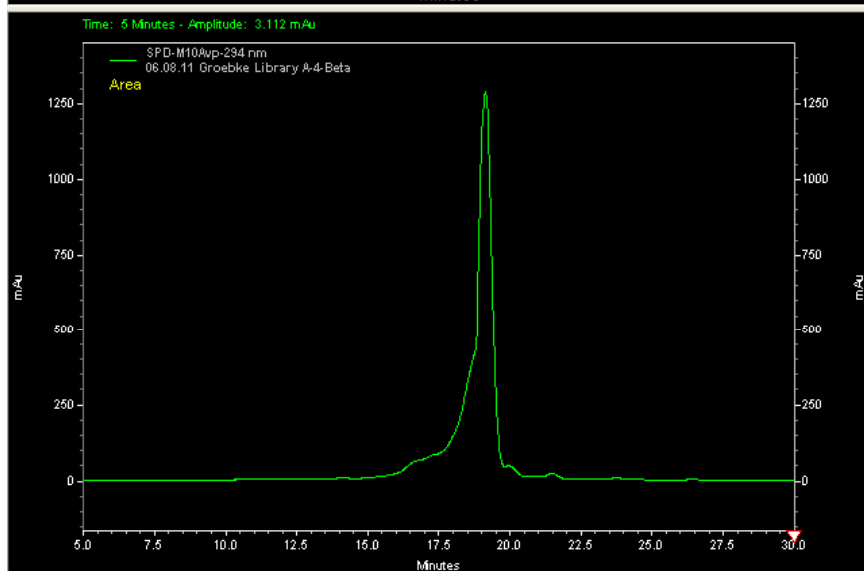
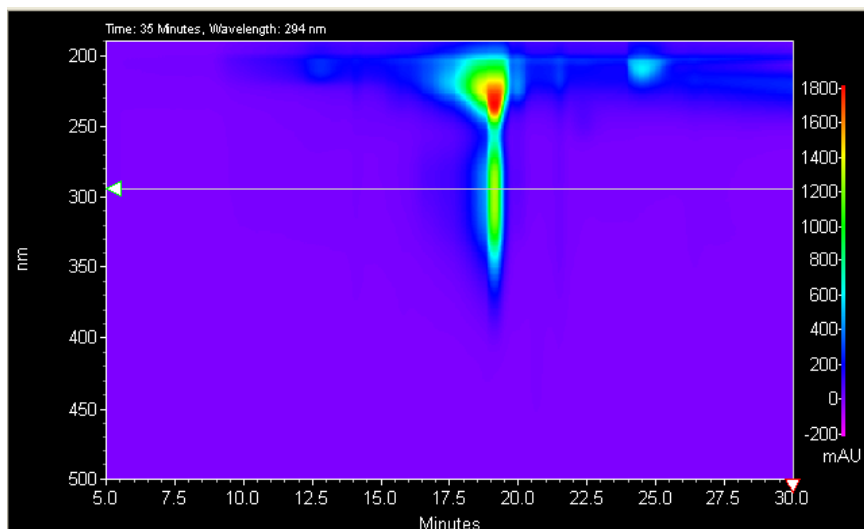
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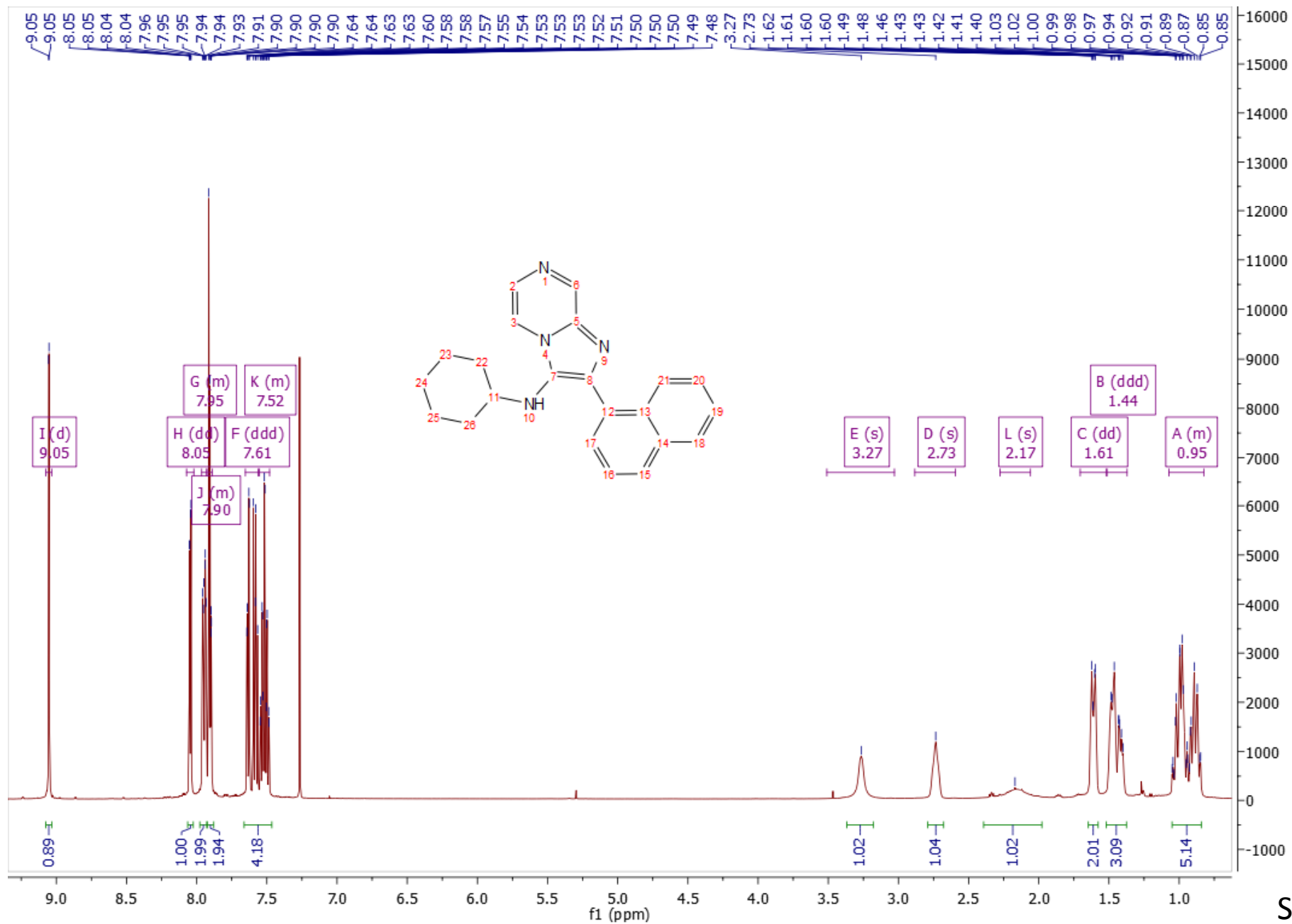
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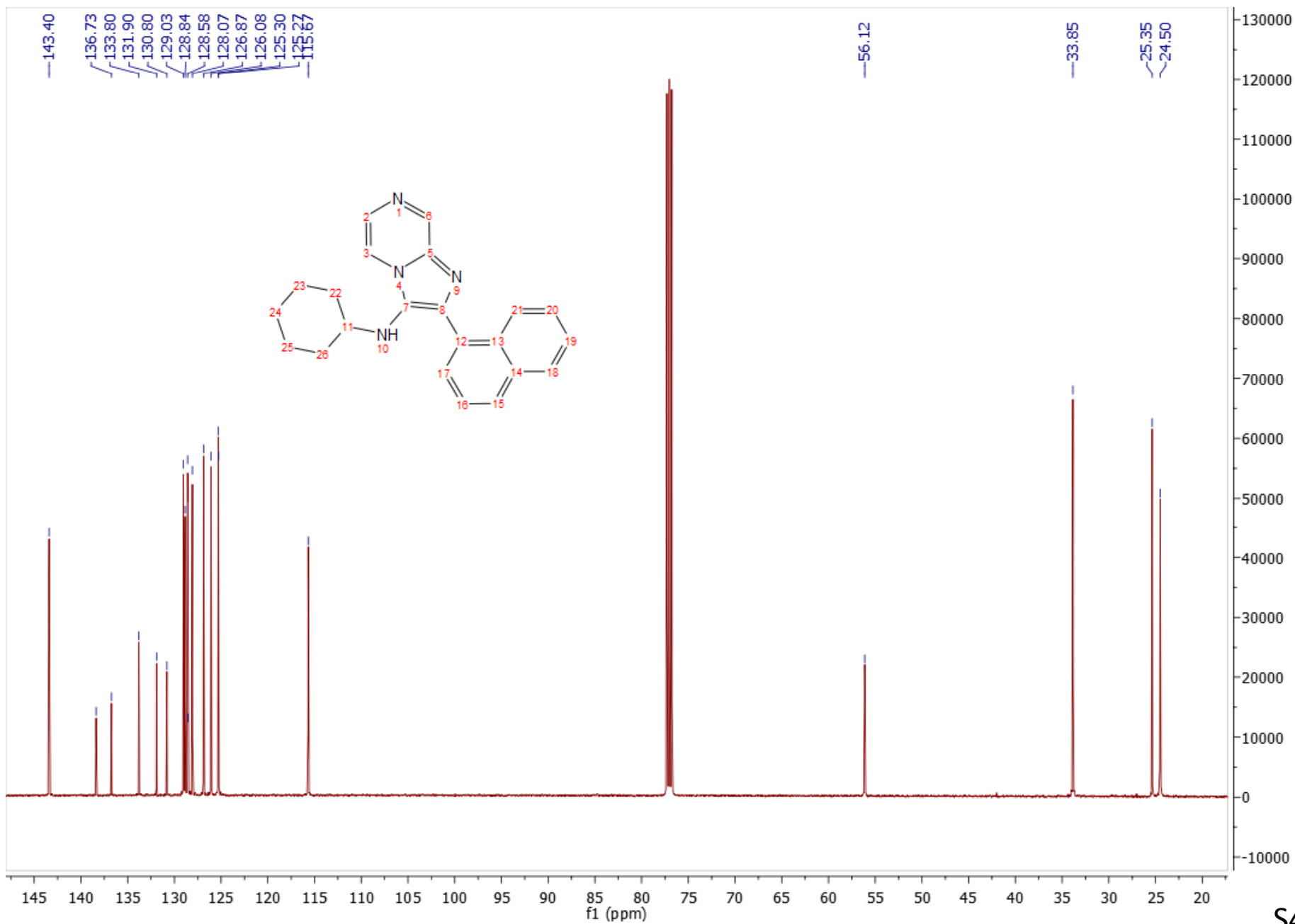
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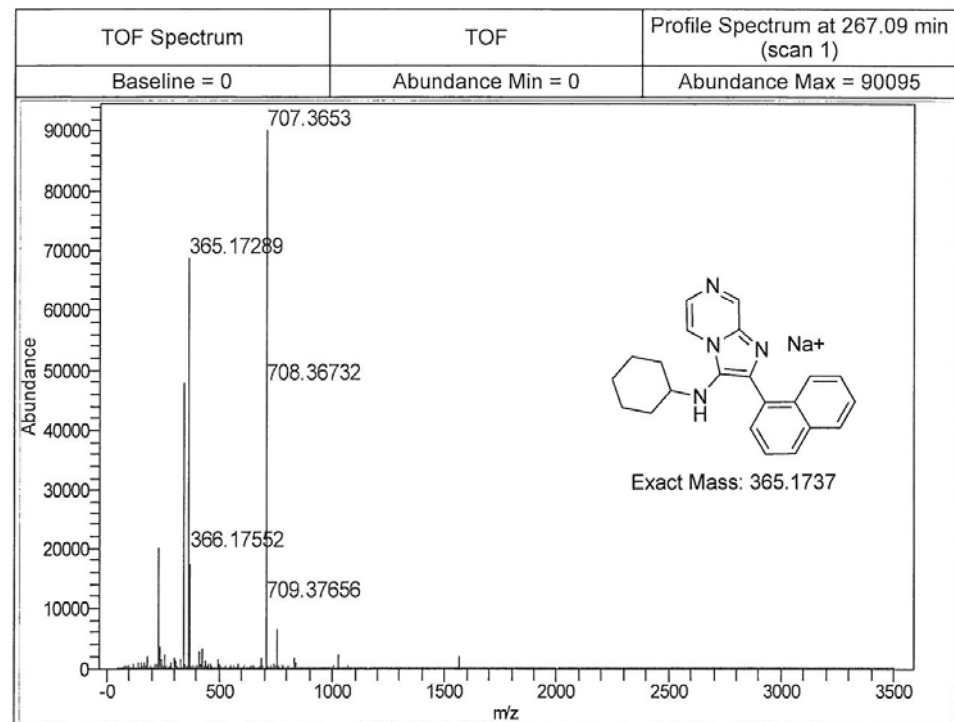
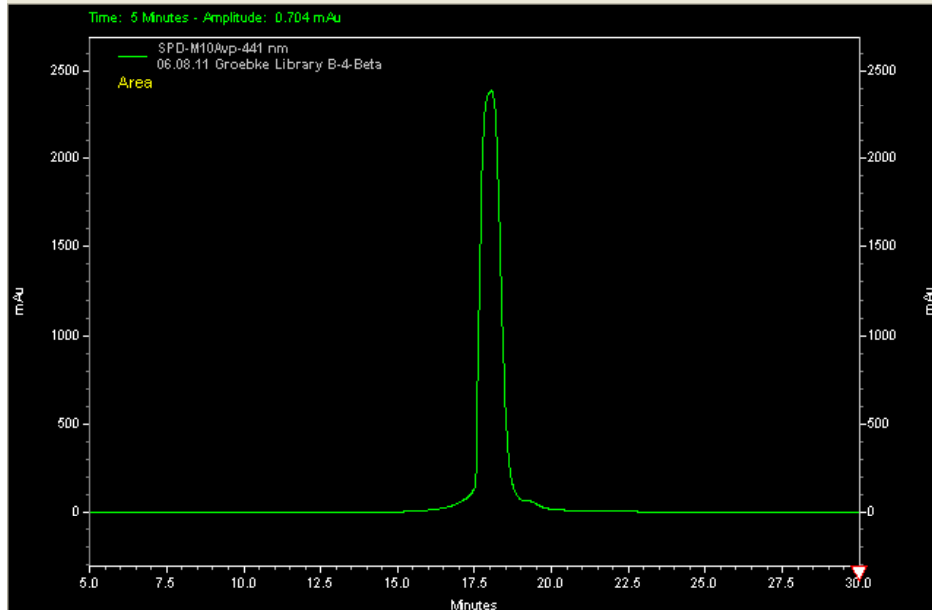
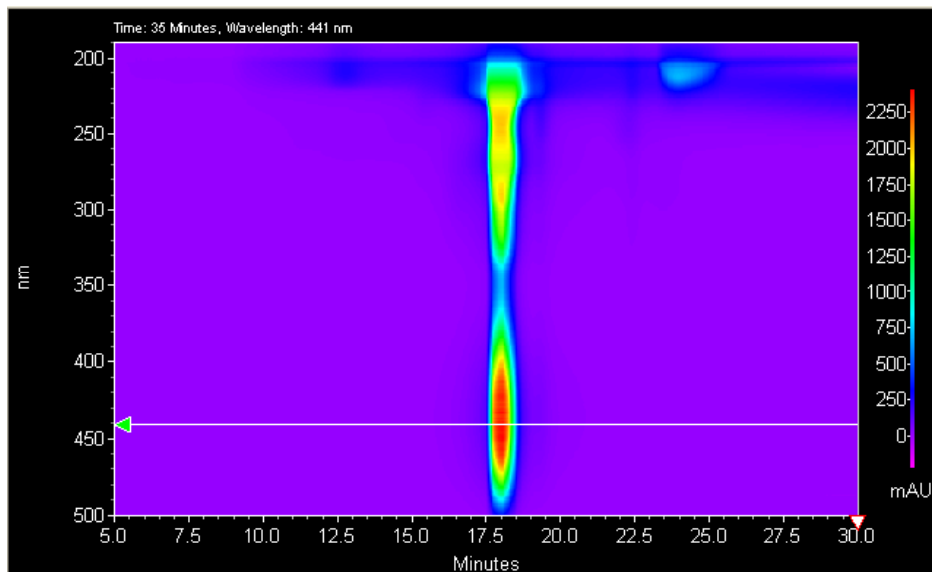
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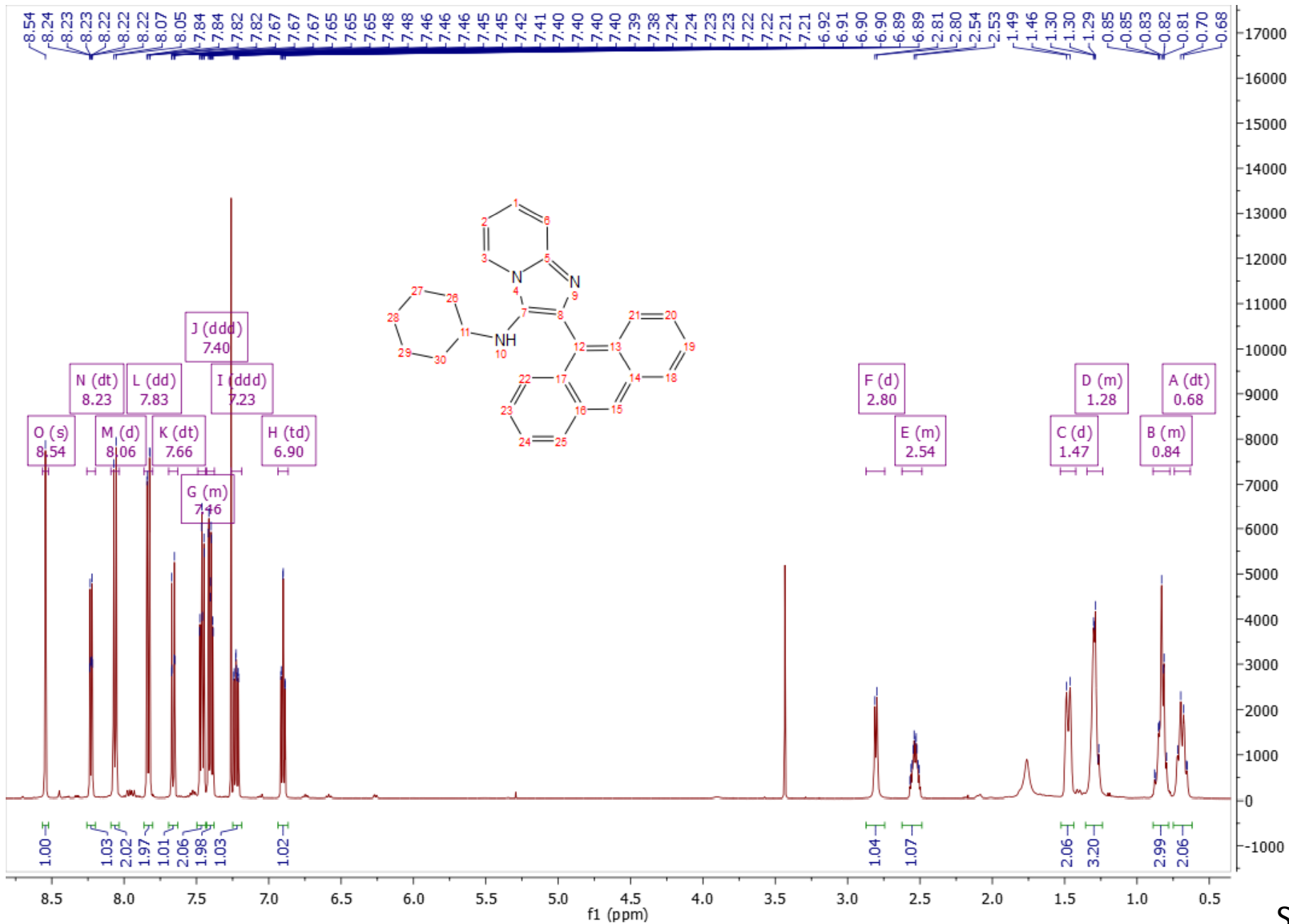
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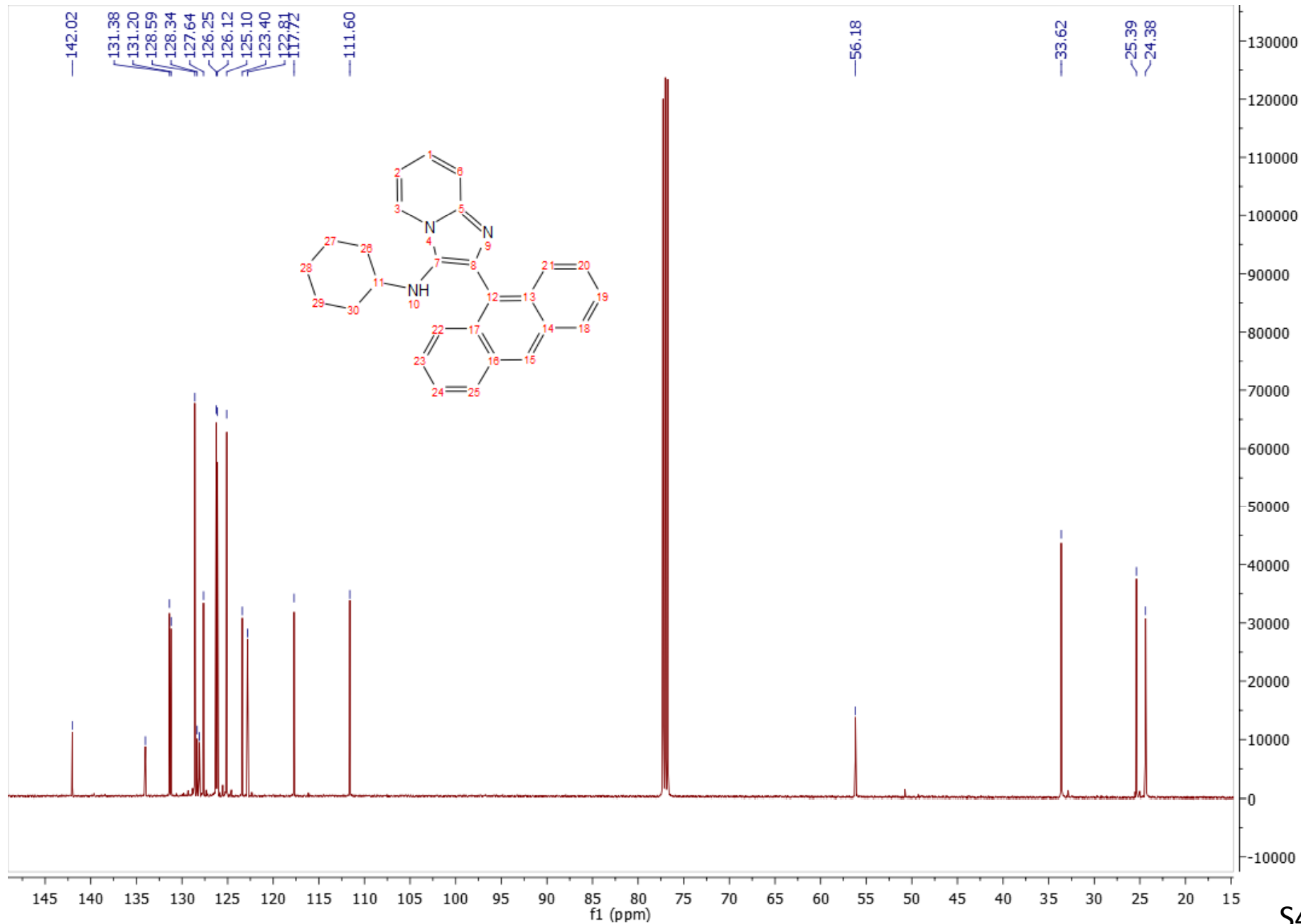
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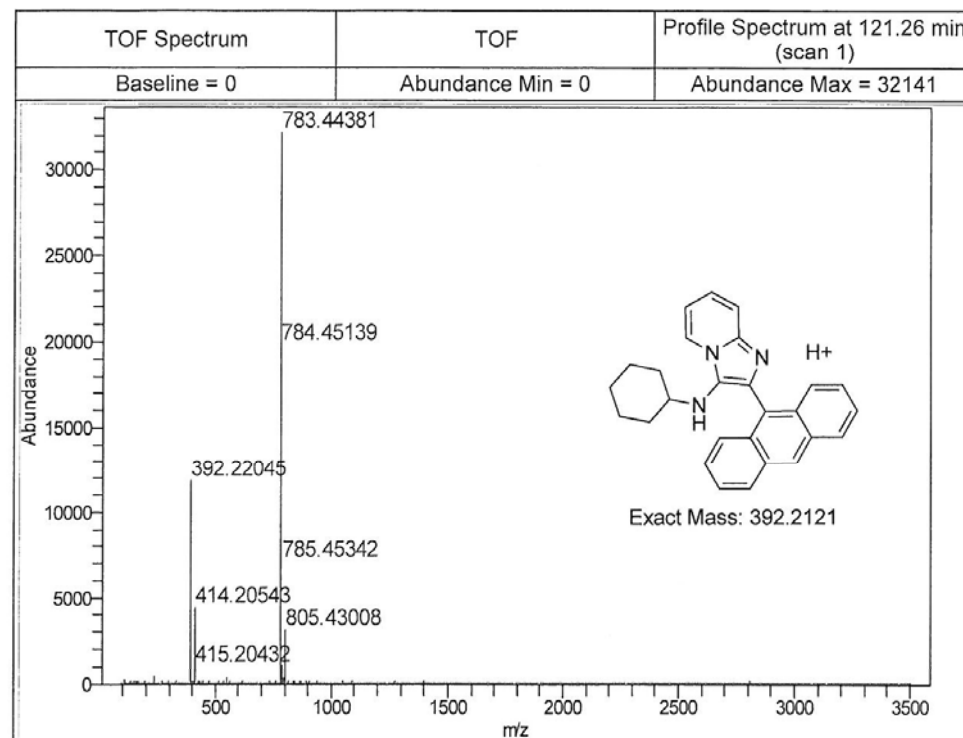
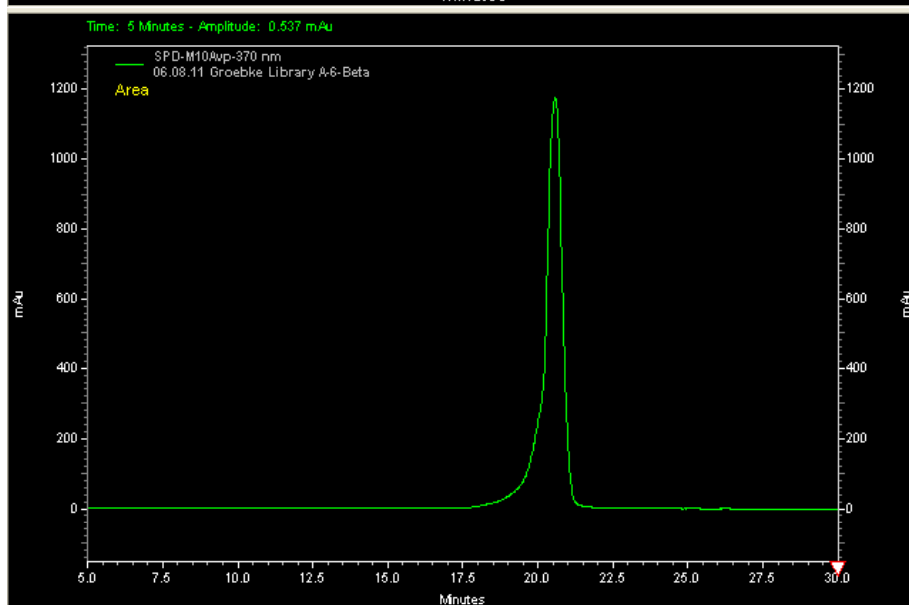
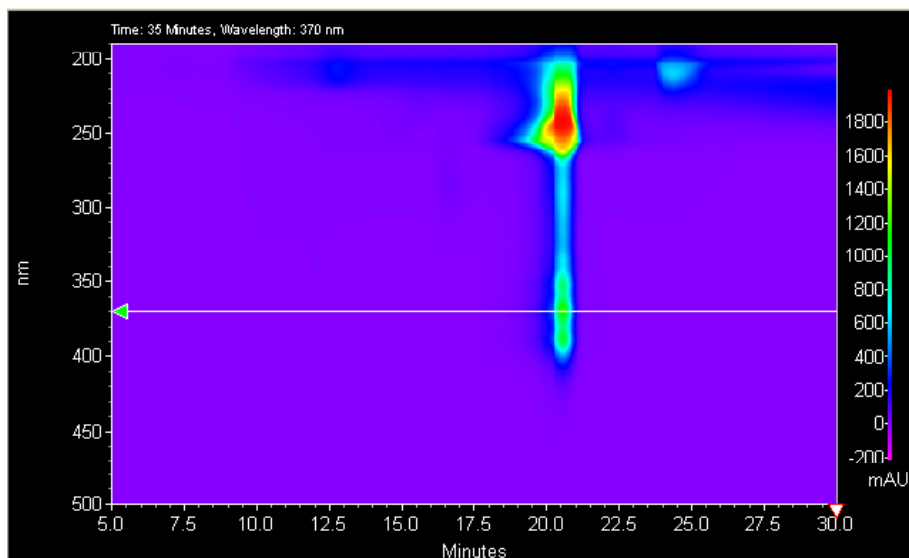
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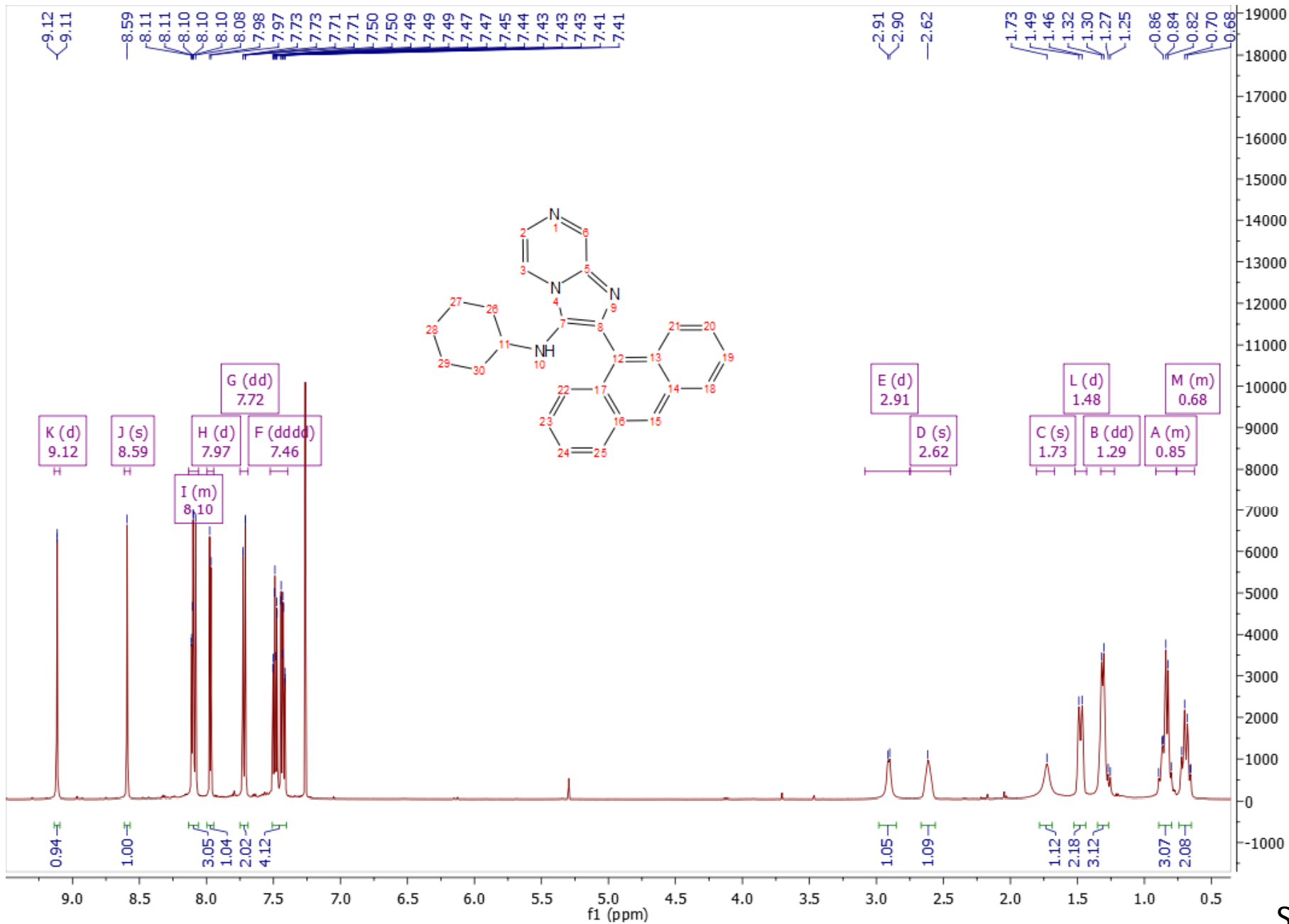
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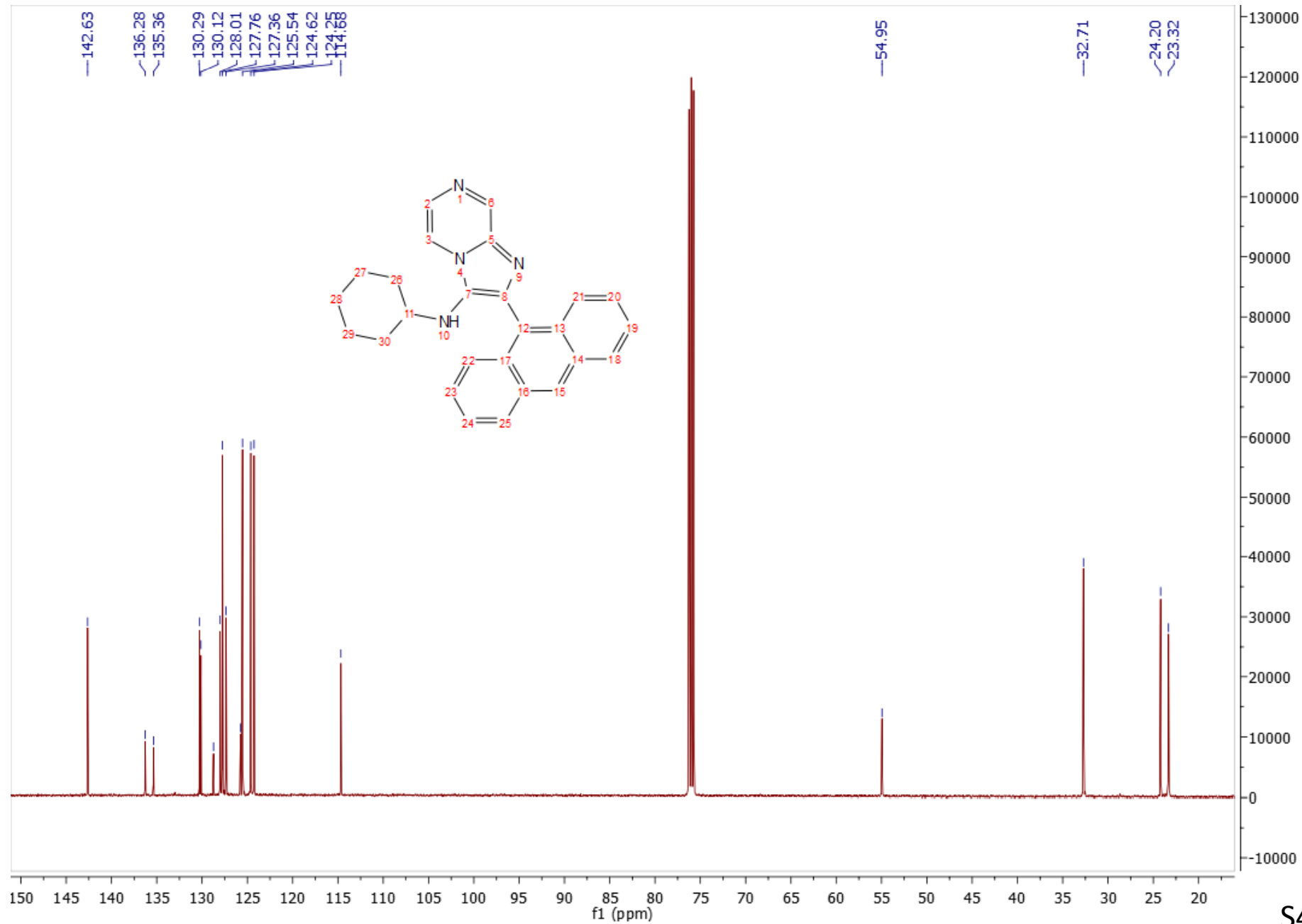
2g MS



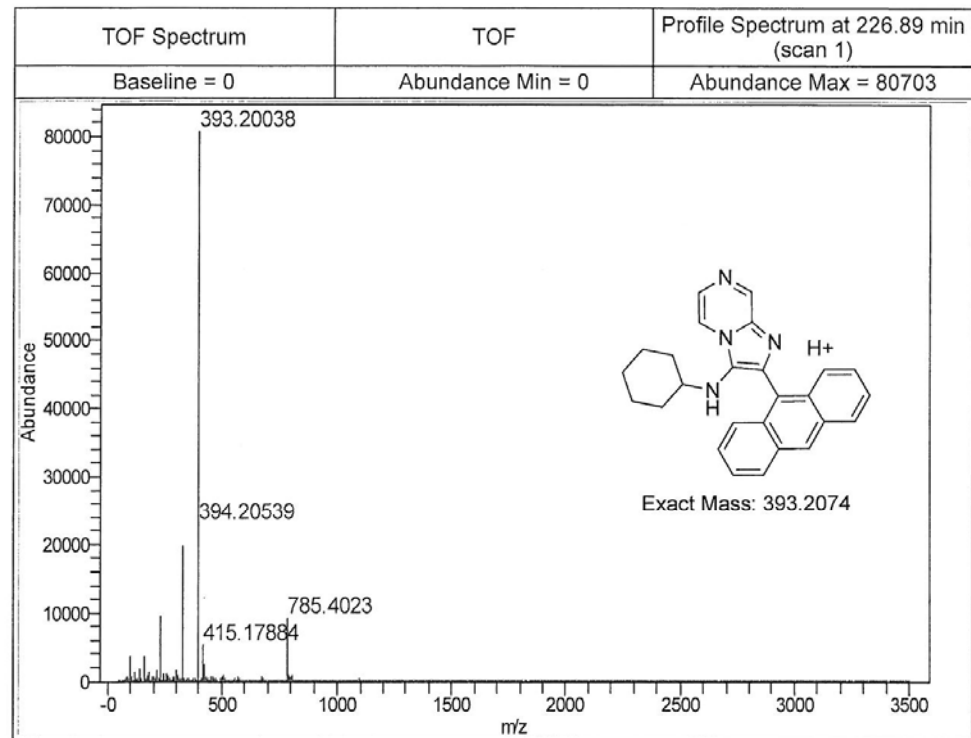
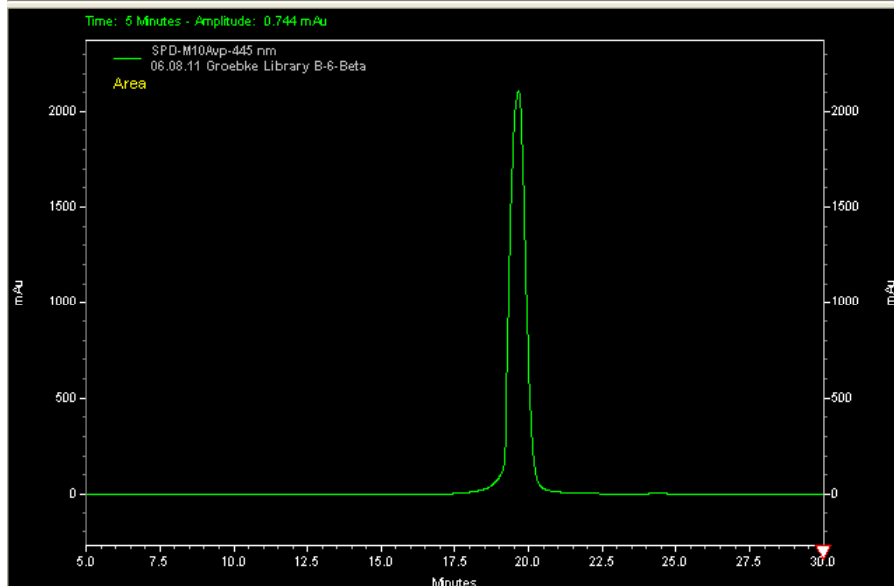
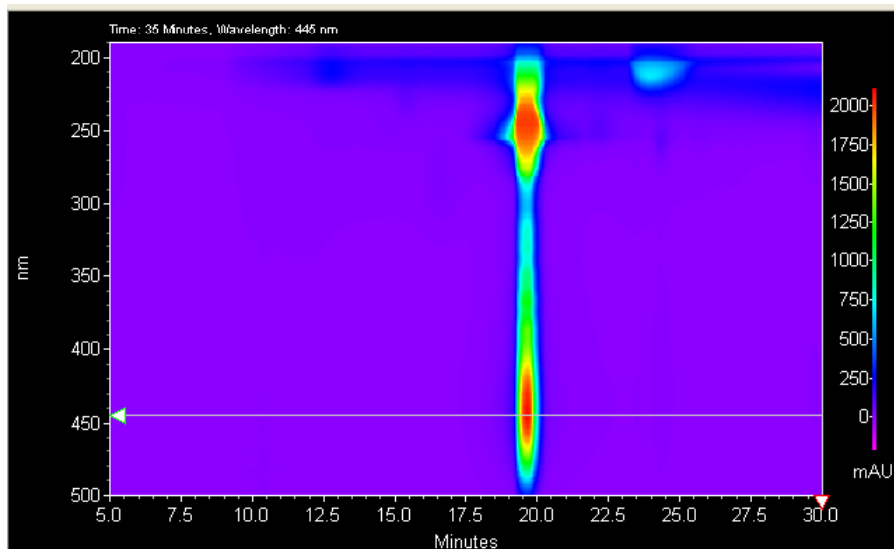
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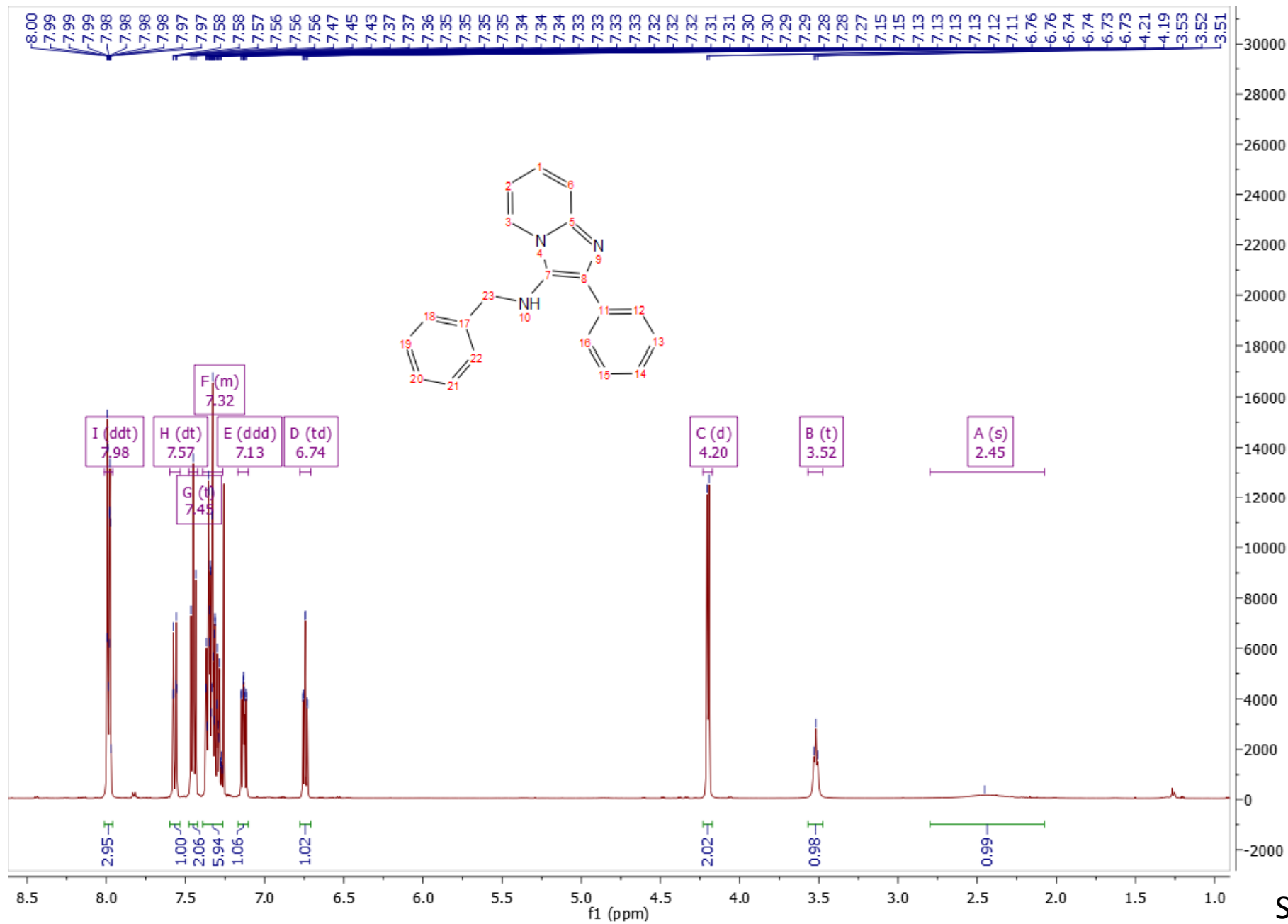
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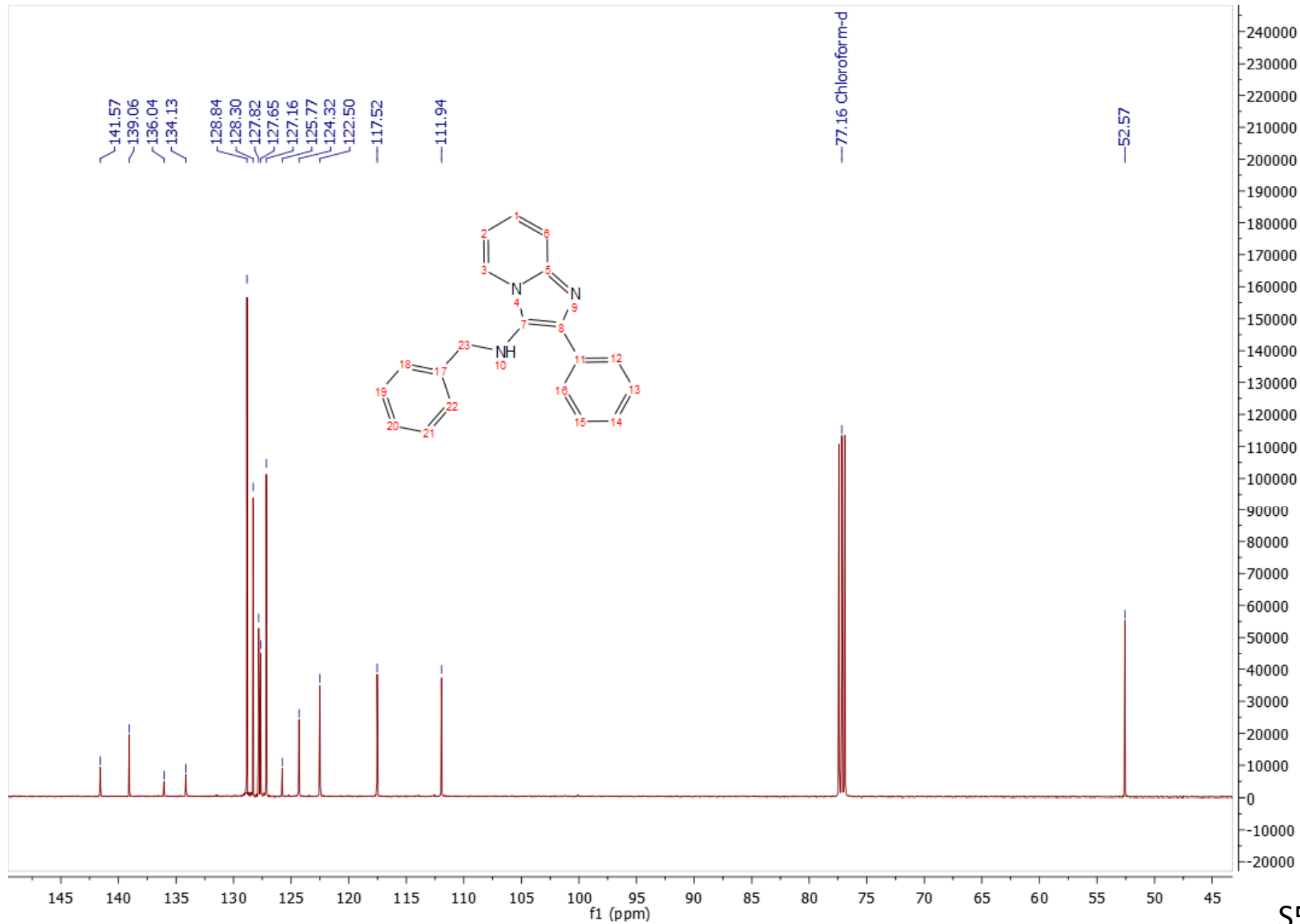
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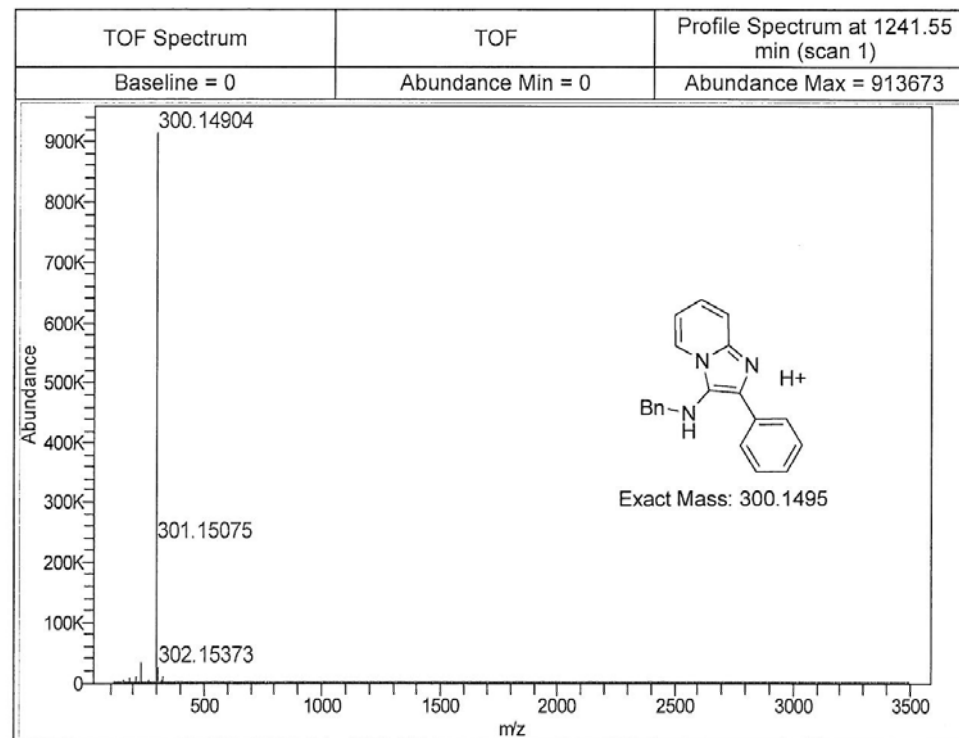
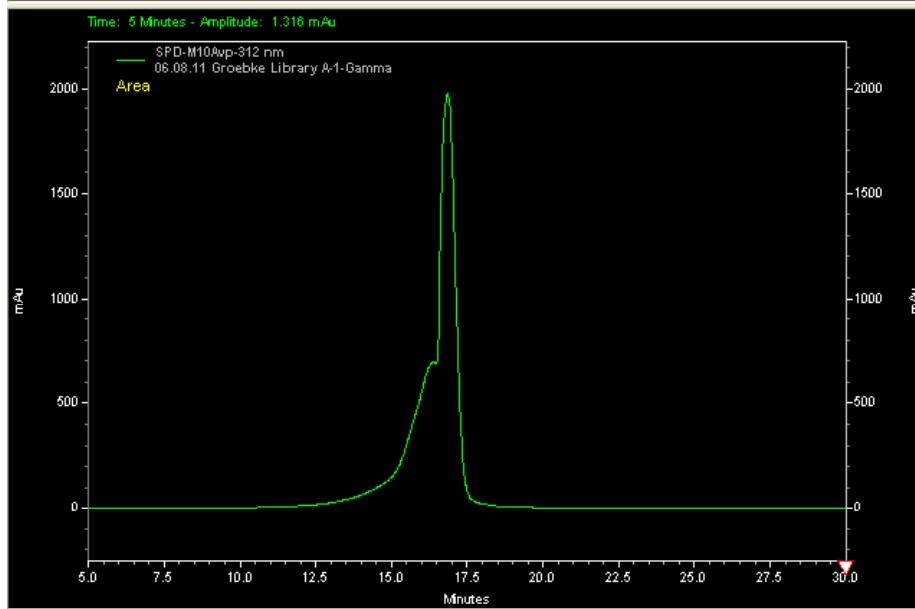
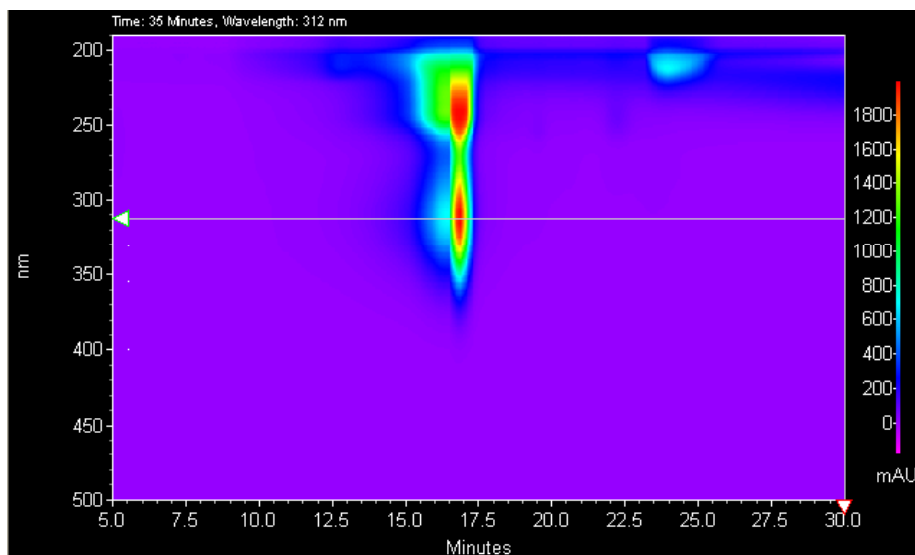
3a ¹H Spectrum



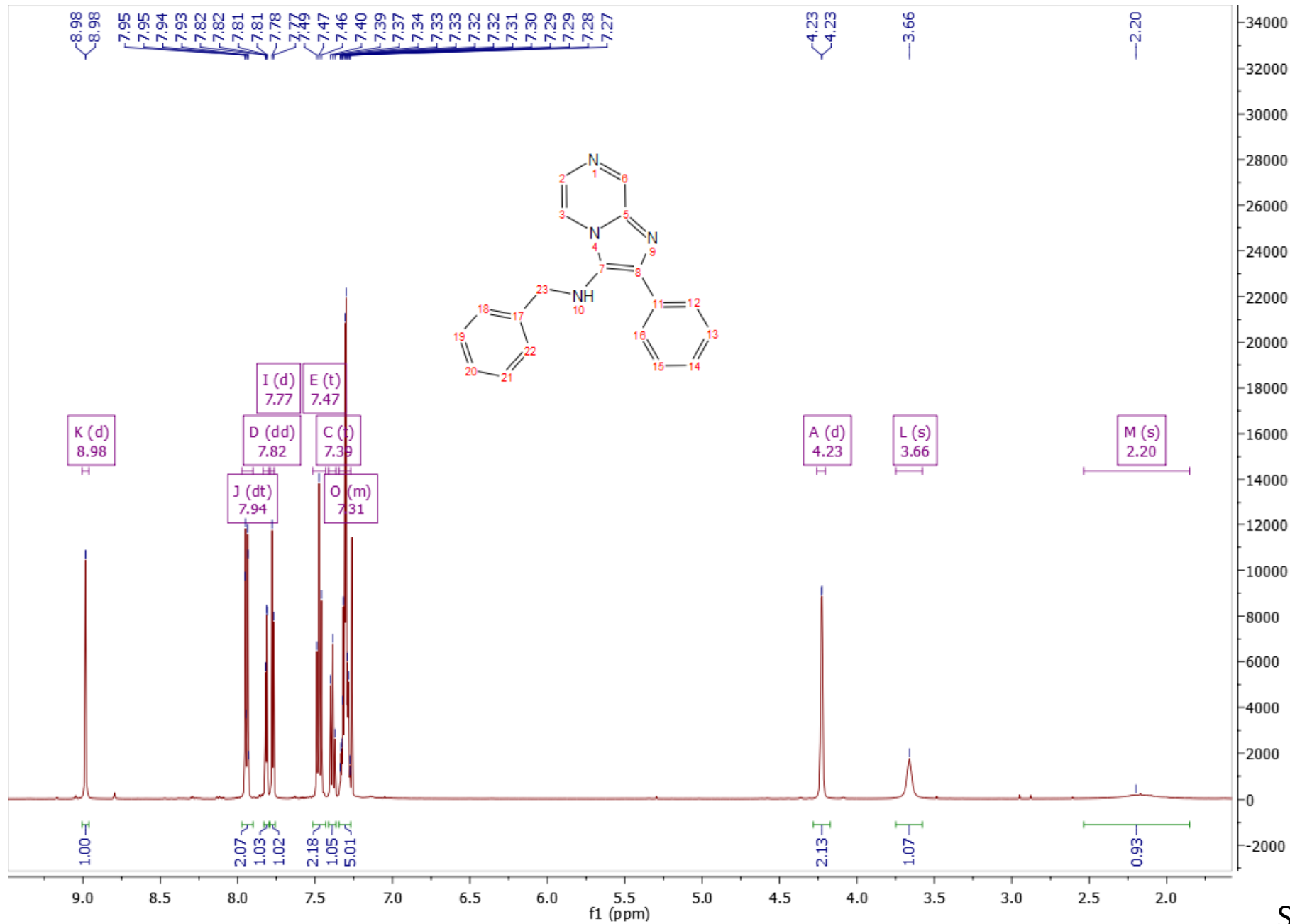
3a ¹³C Spectrum



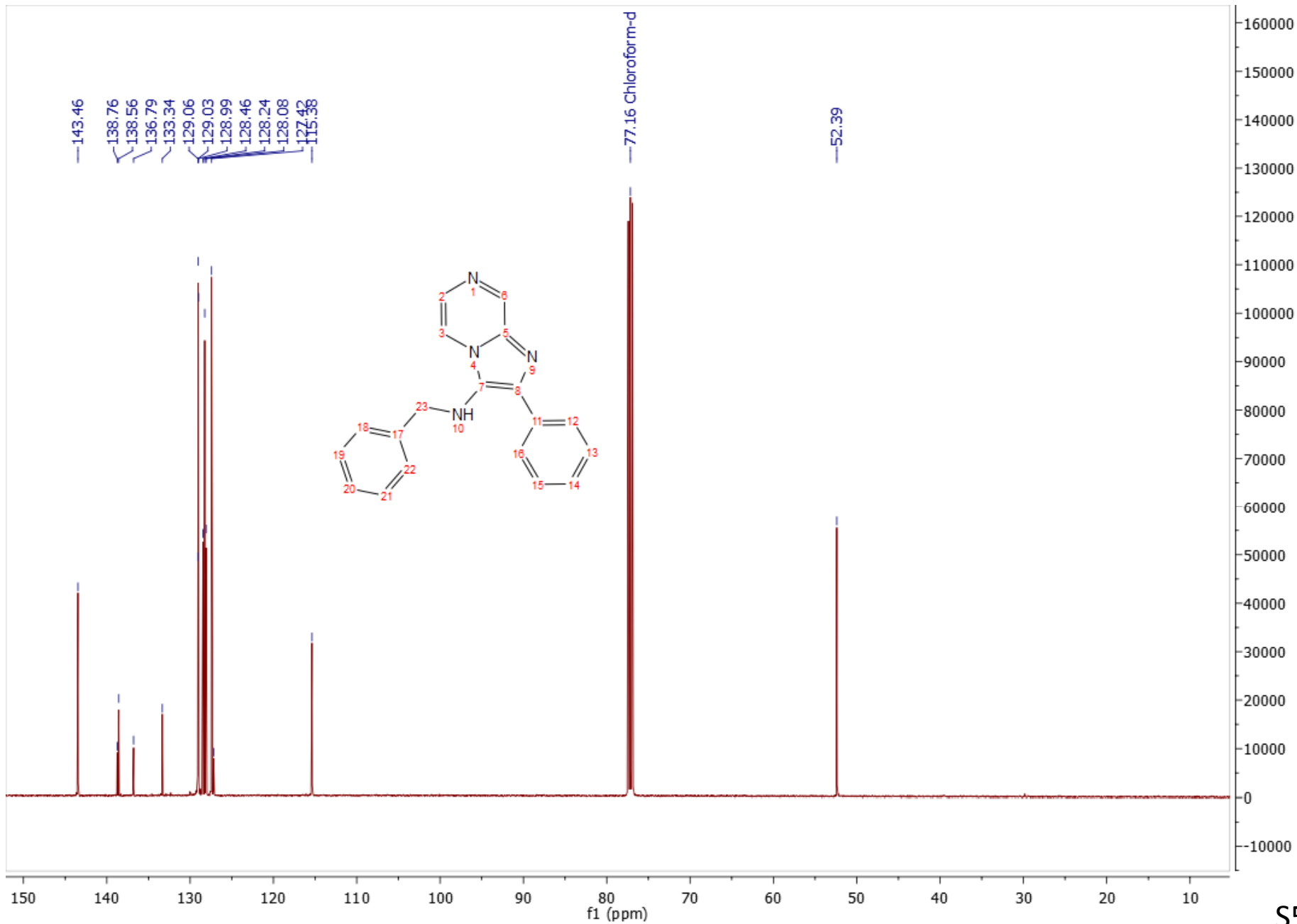
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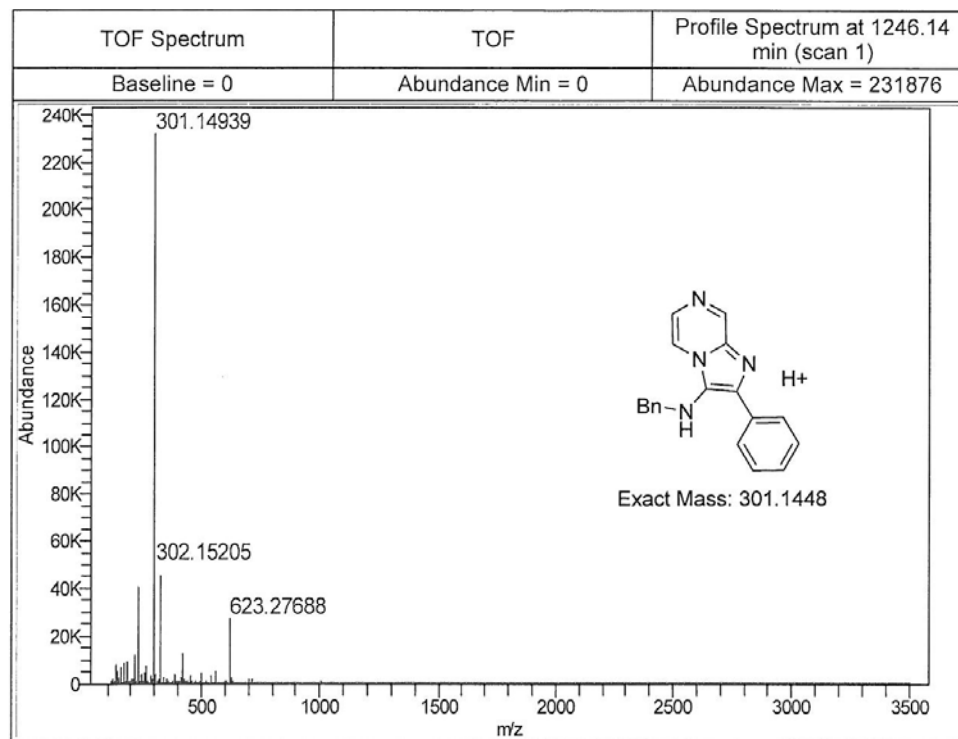
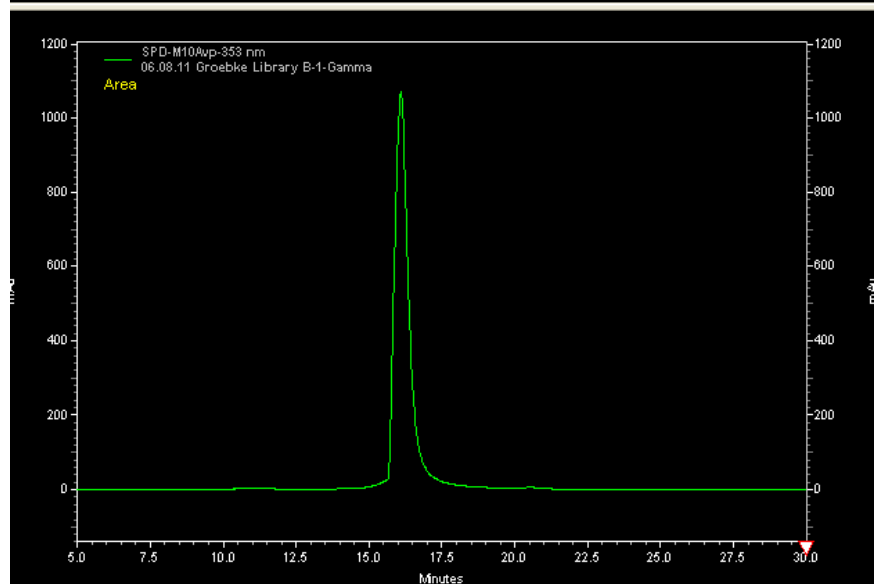
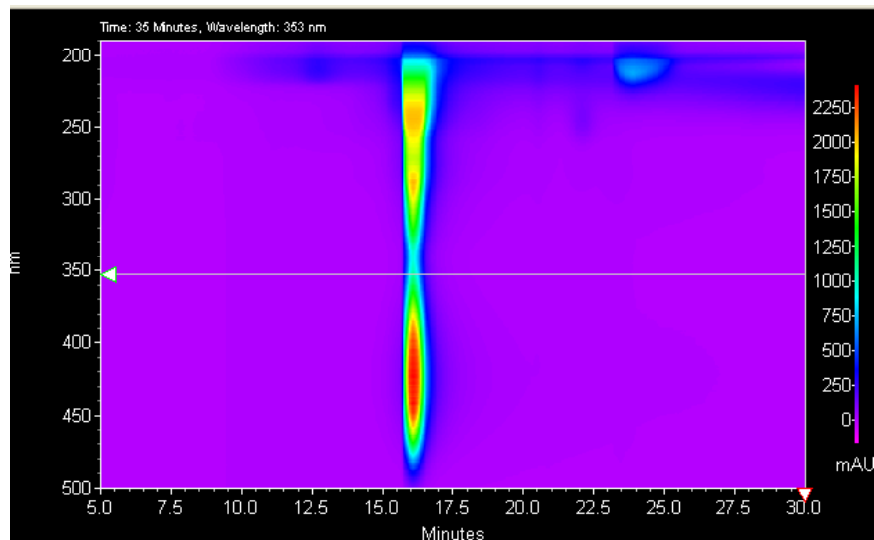
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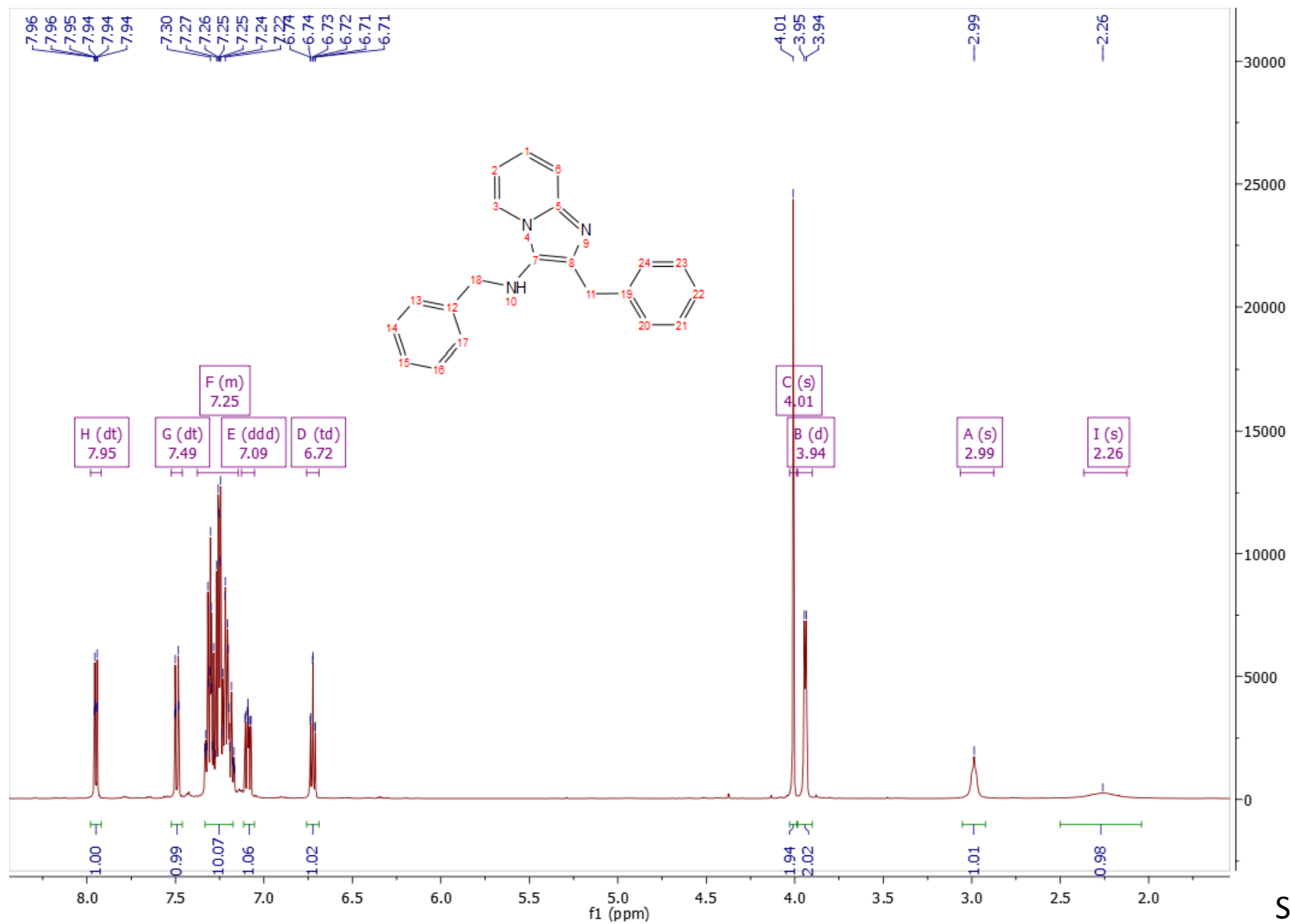
3b ¹³C Spectrum



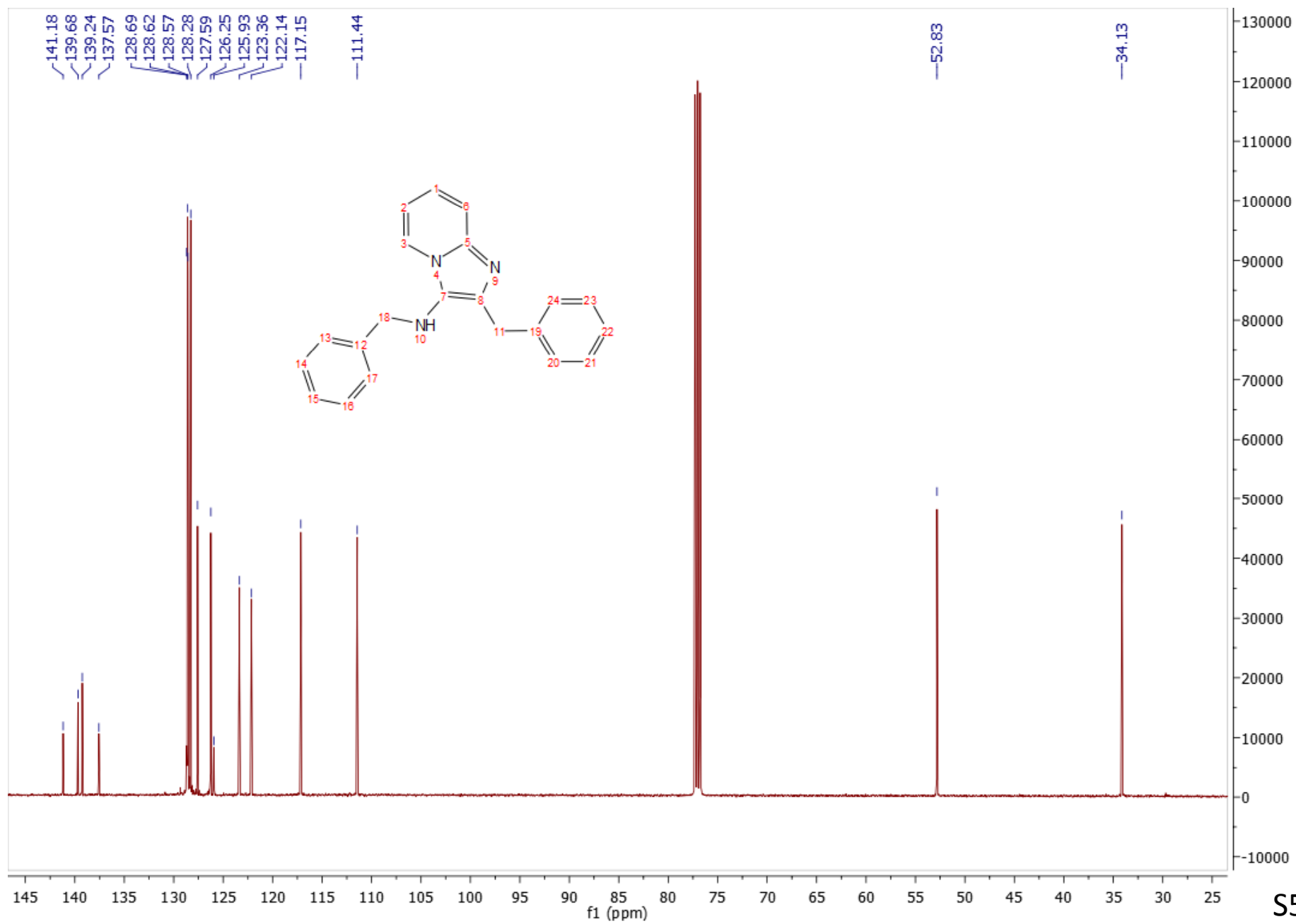
3b LC-MS



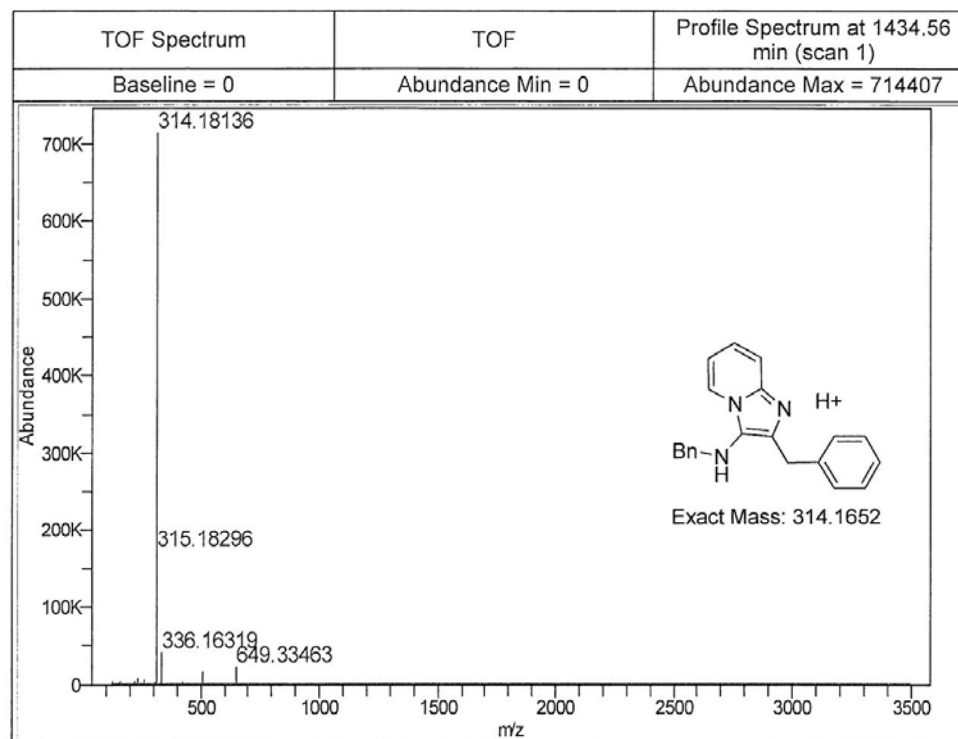
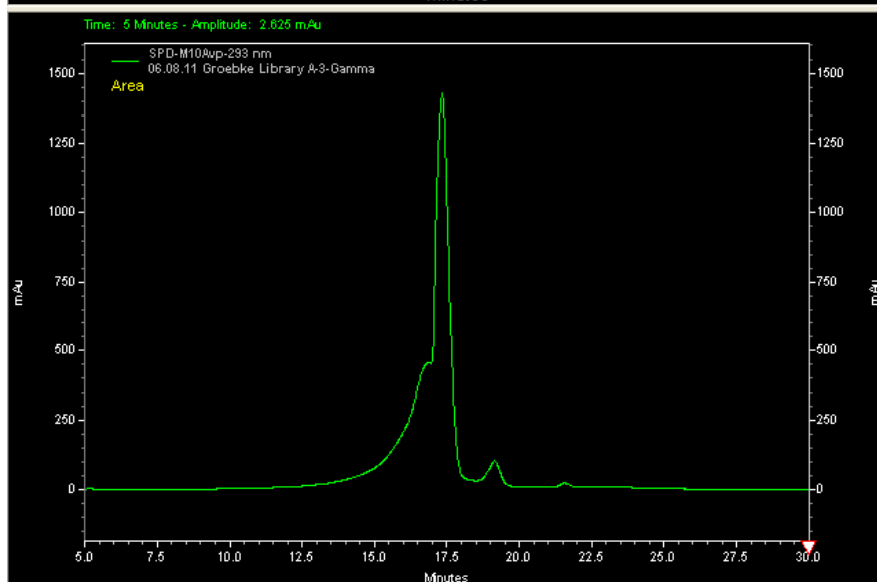
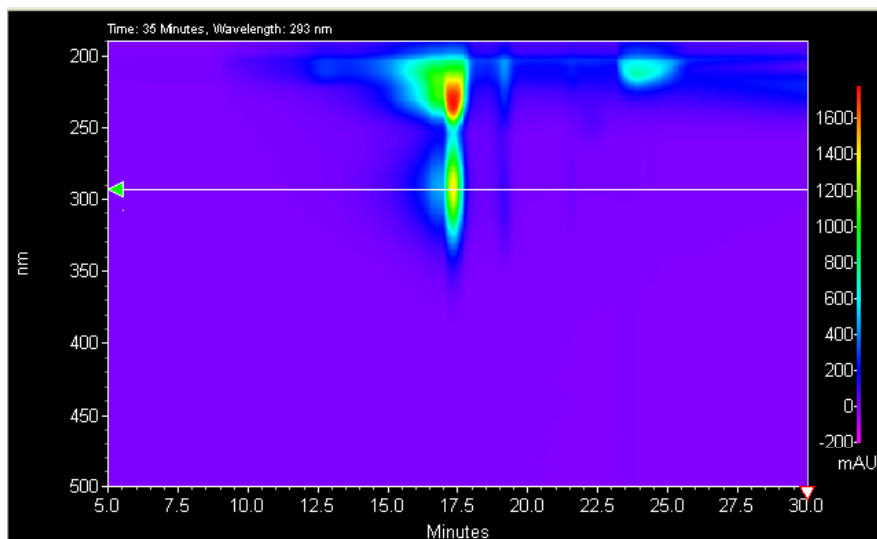
3c ¹H Spectrum



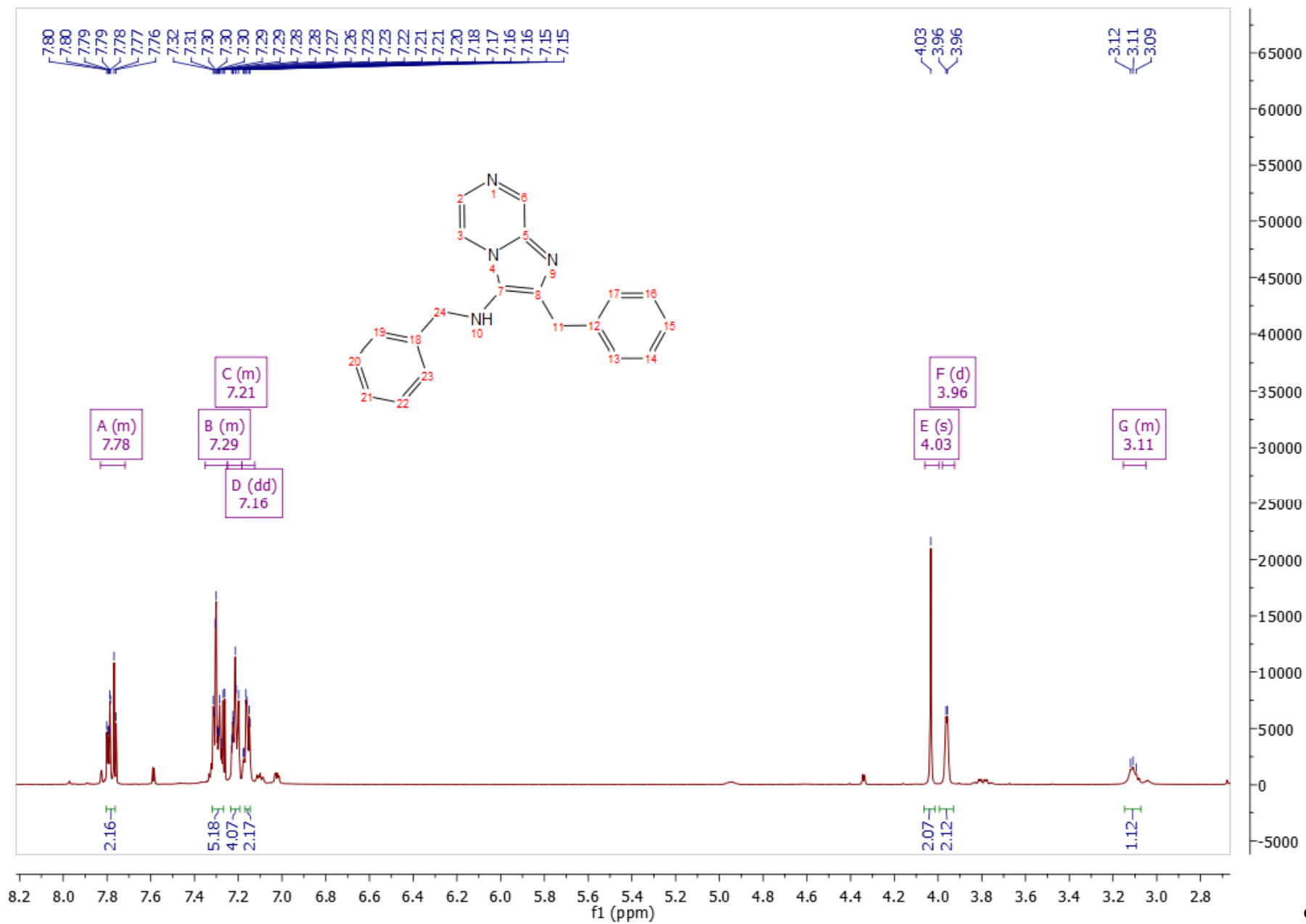
3c ¹³C Spectrum



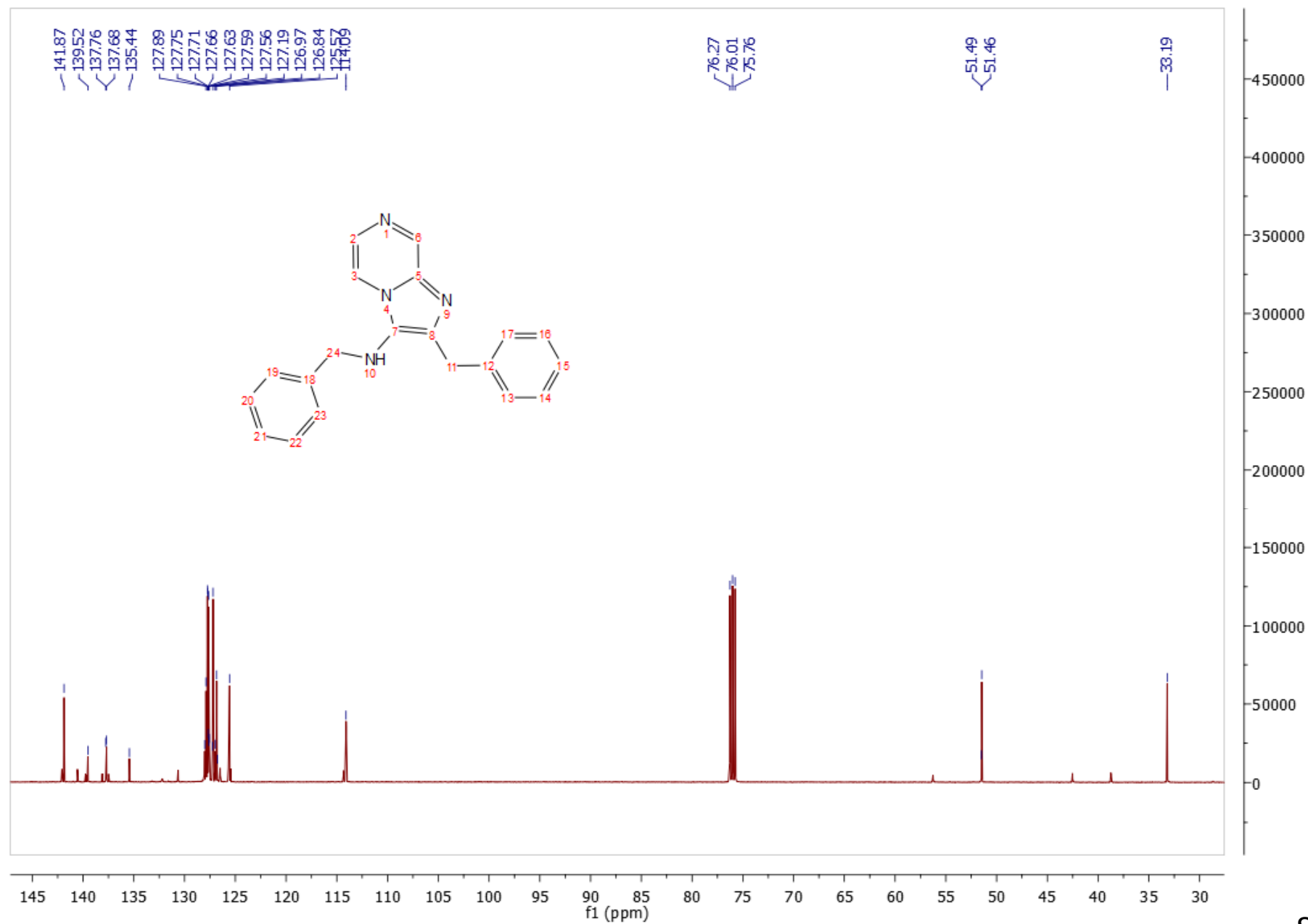
3c LC-MS



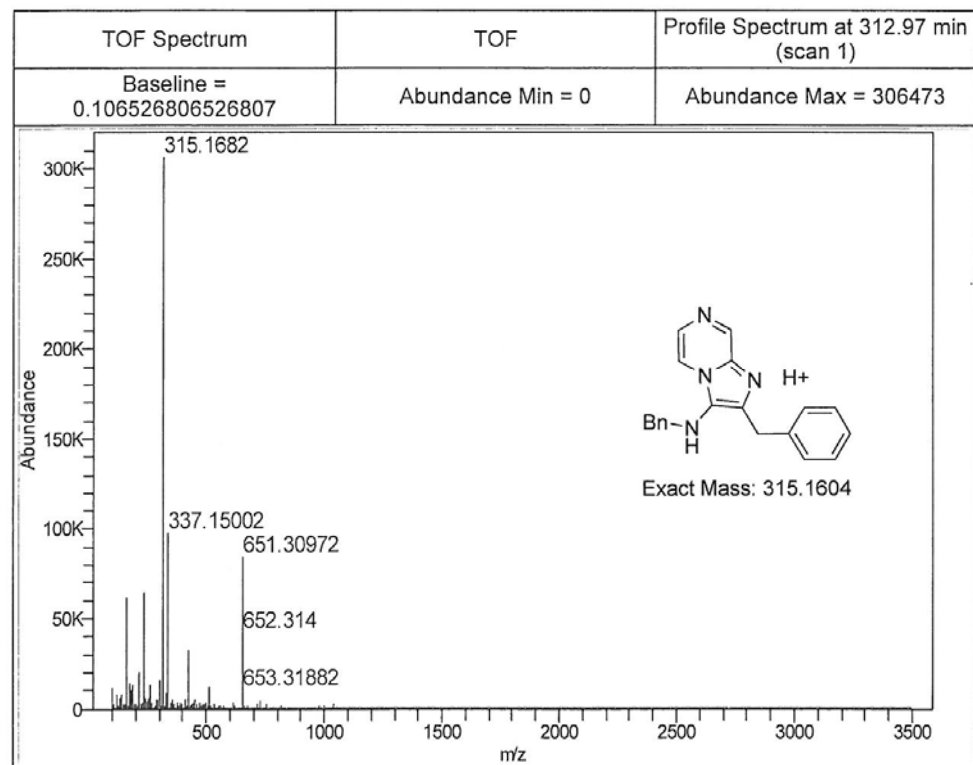
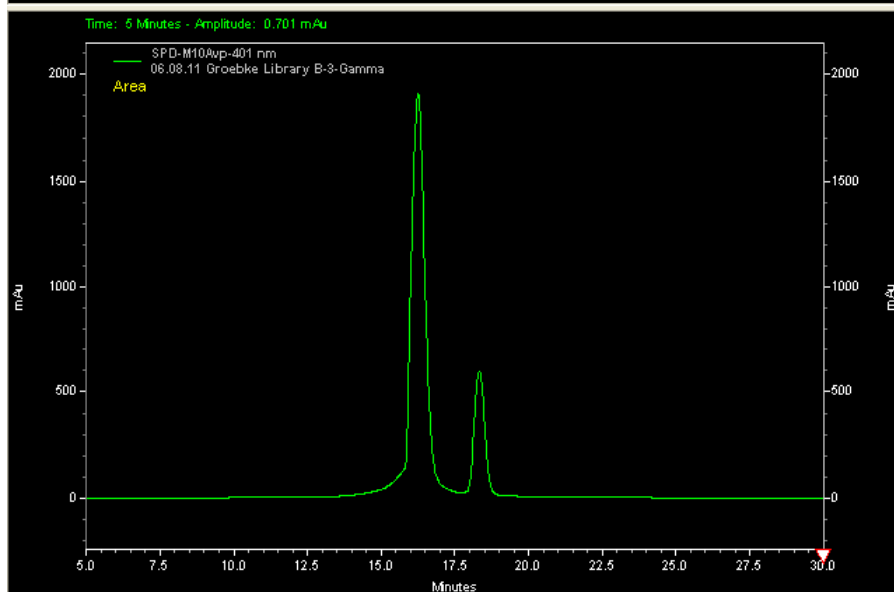
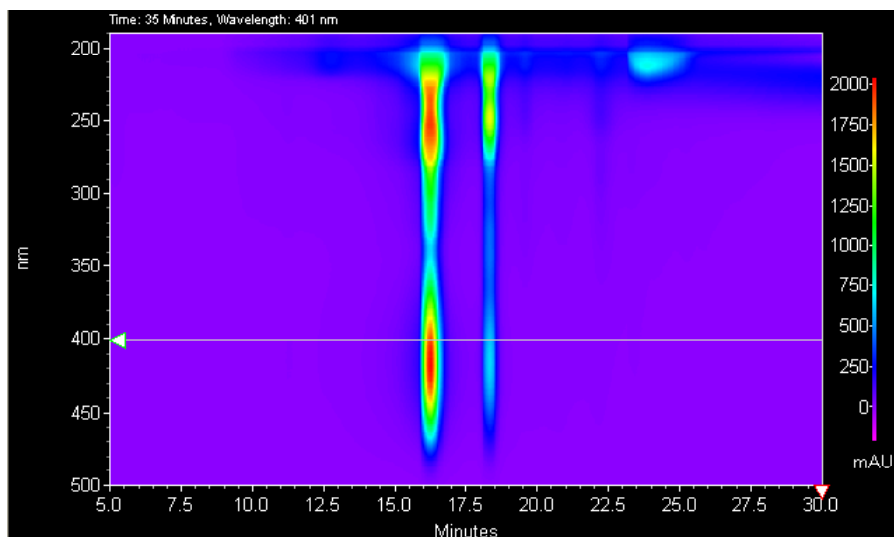
3d ¹H Spectrum



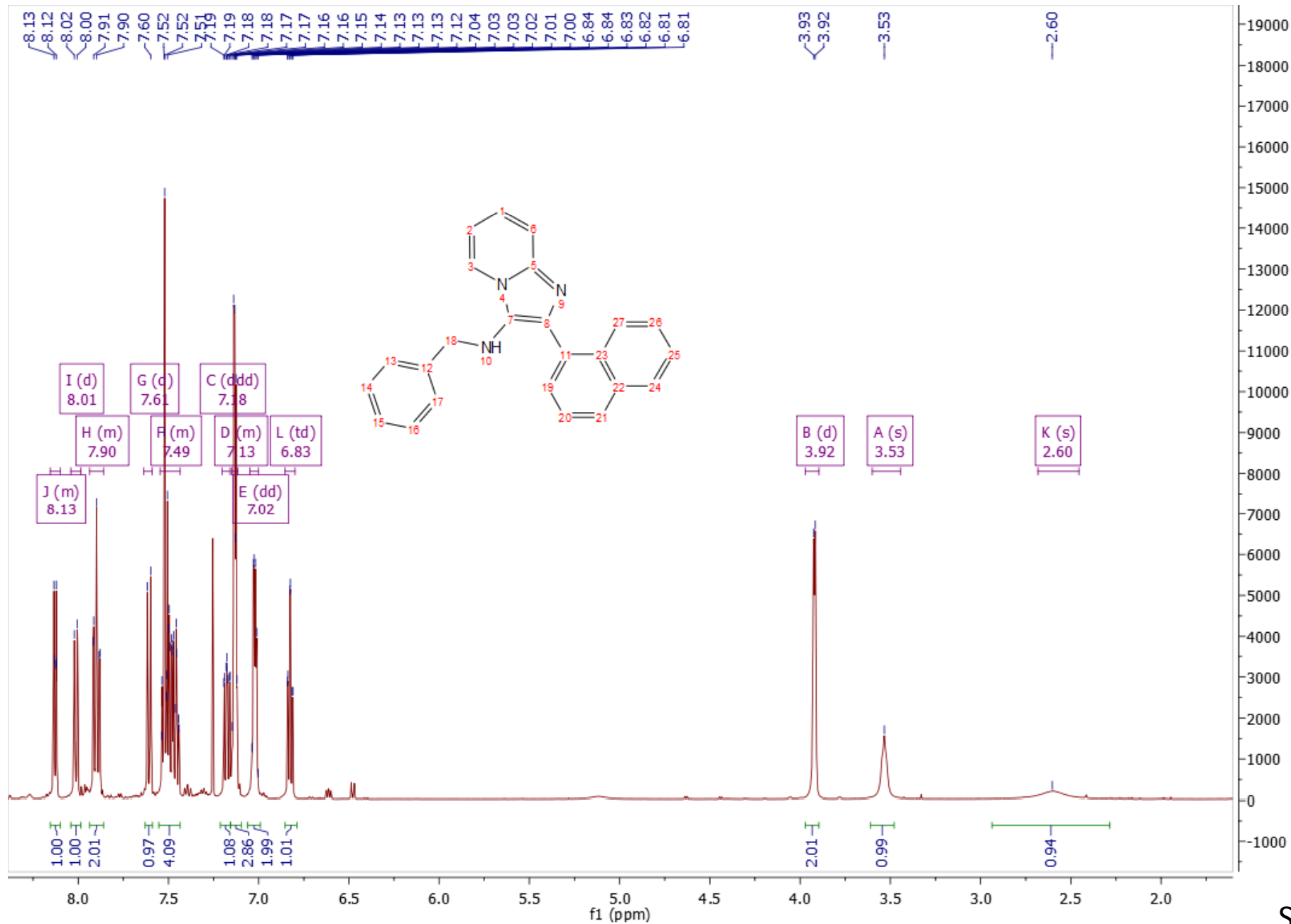
3d ¹³C Spectrum



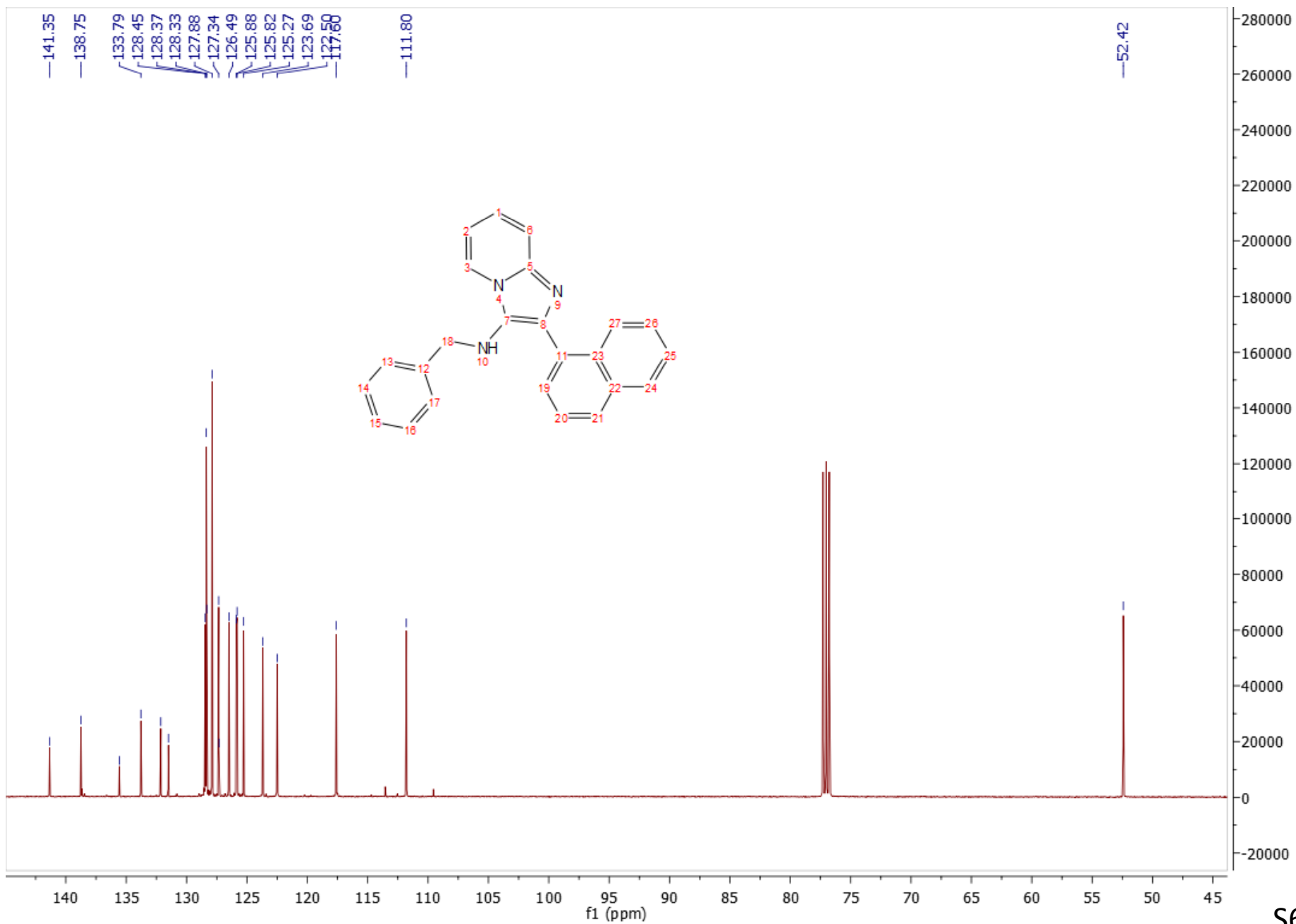
3d LC-MS



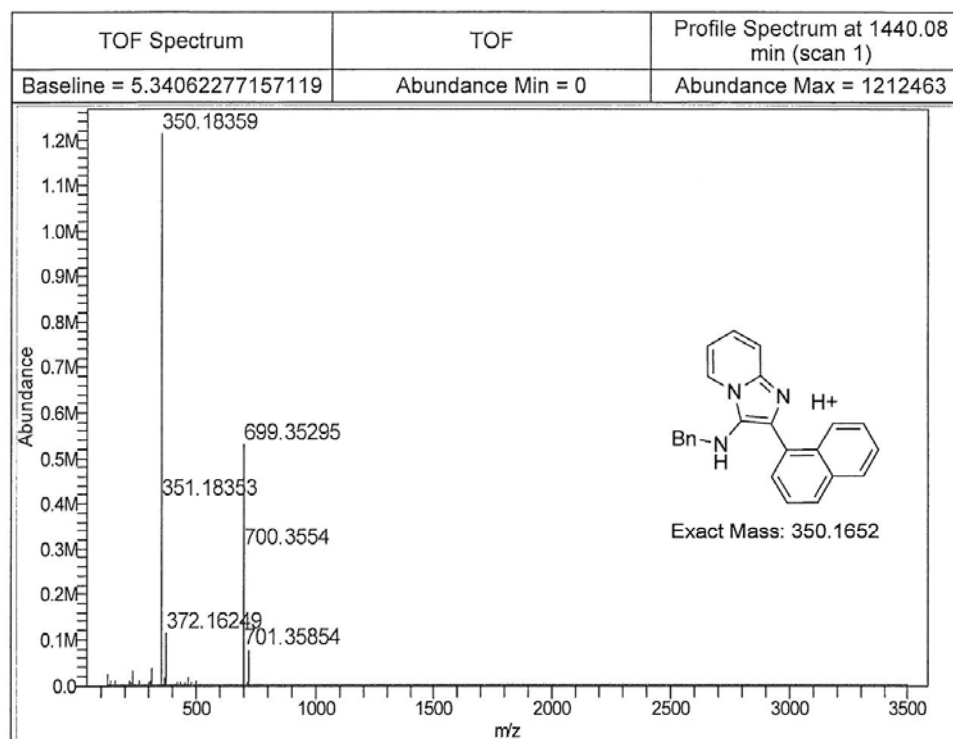
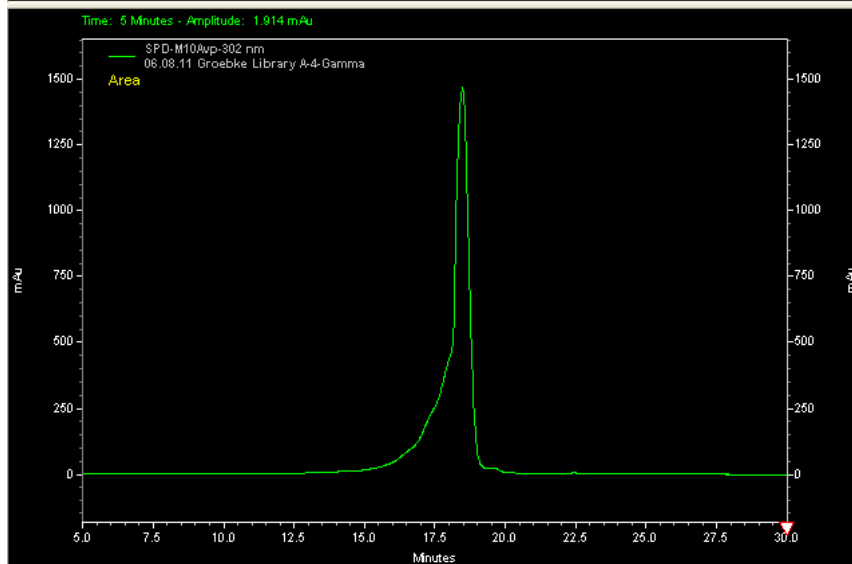
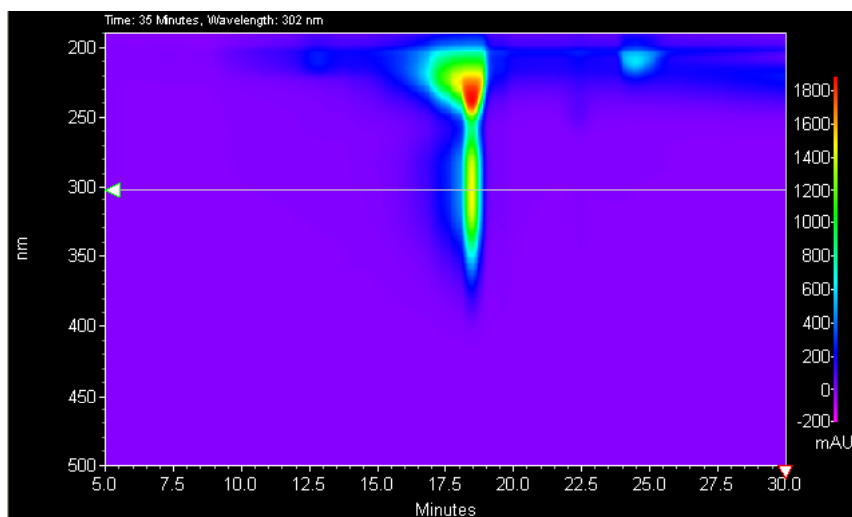
3e ¹H Spectrum



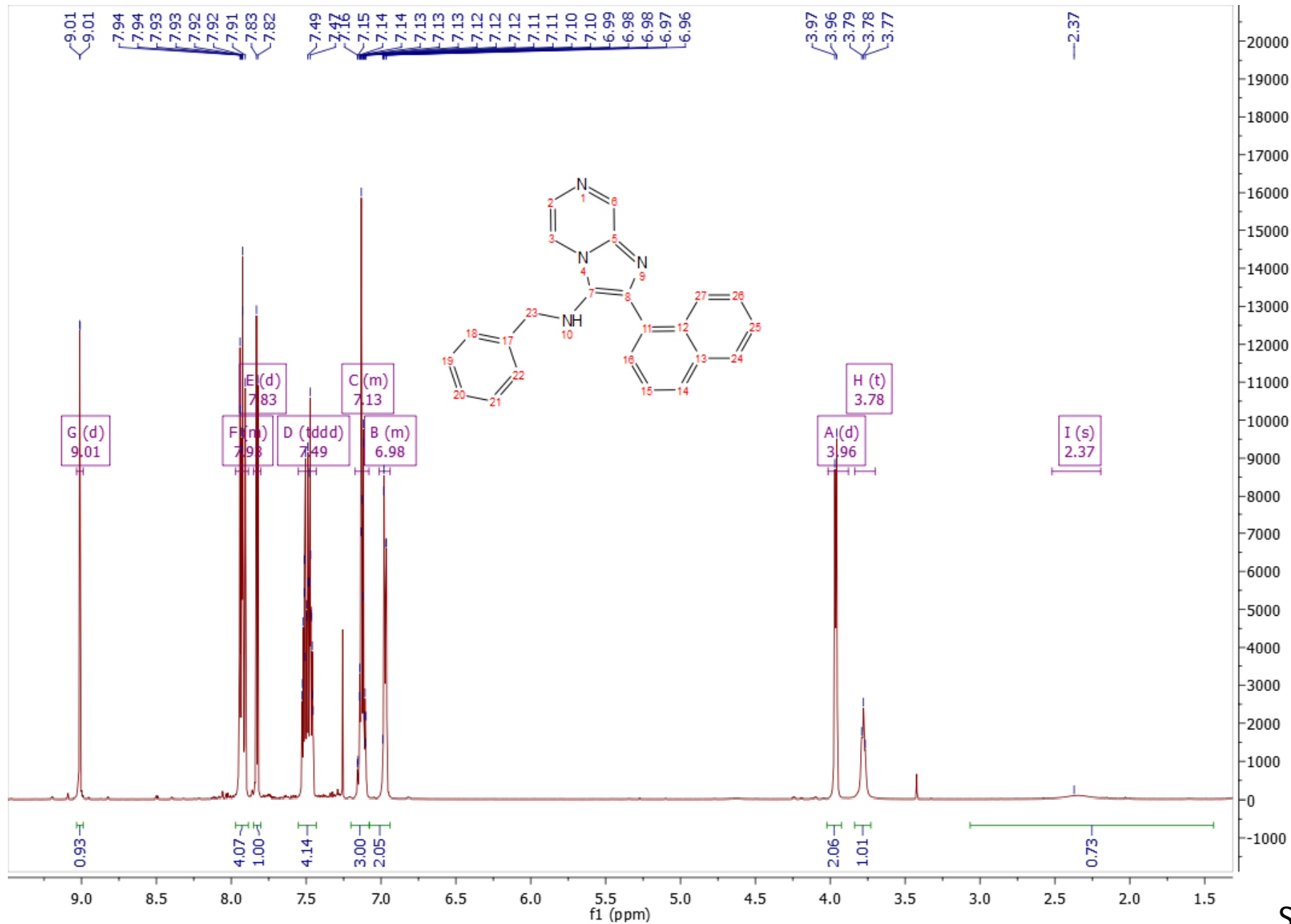
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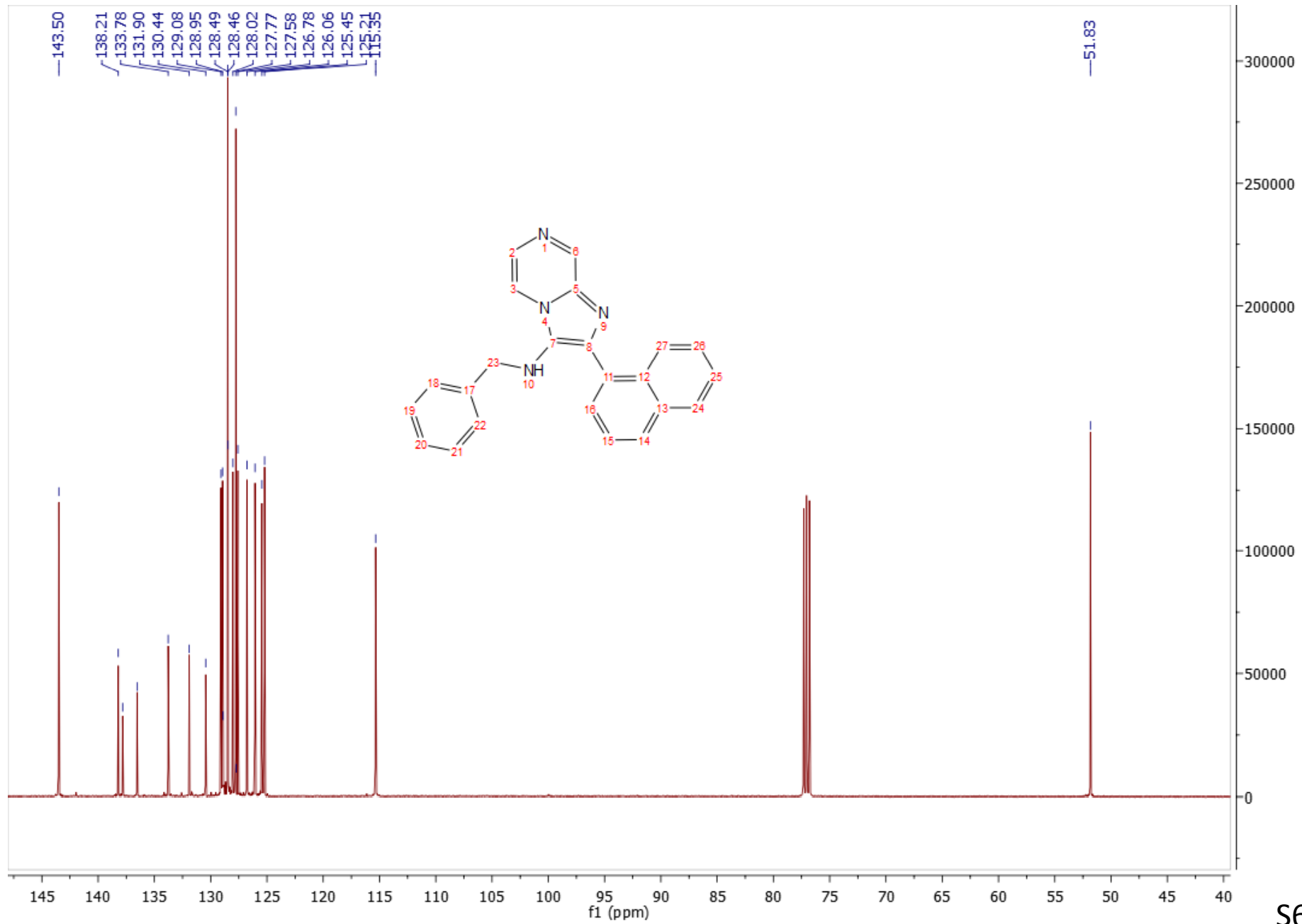
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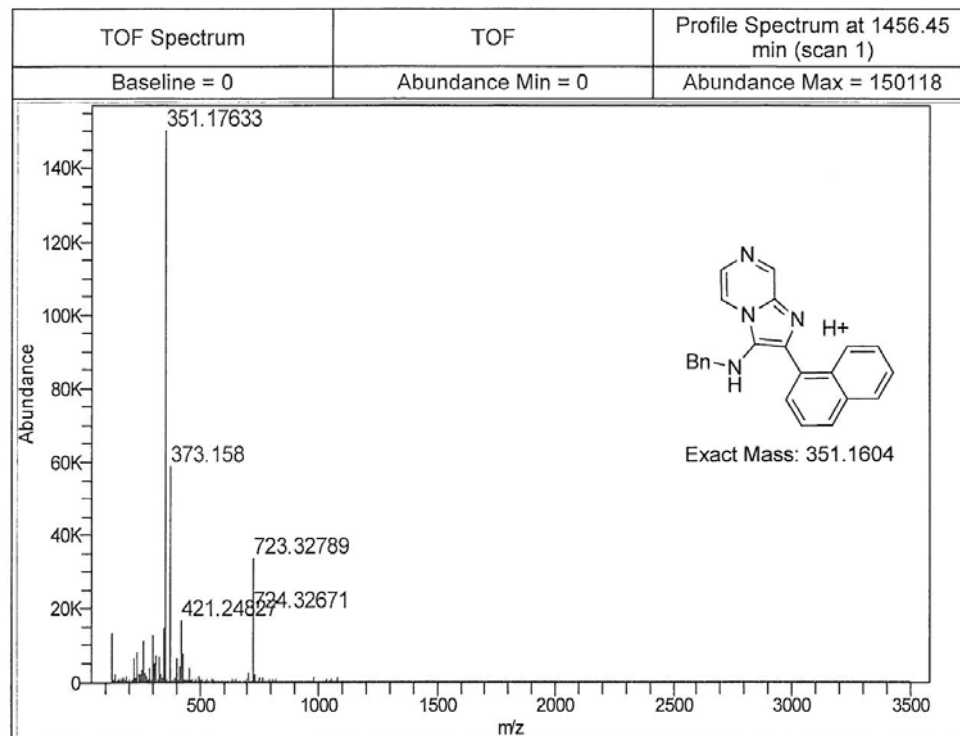
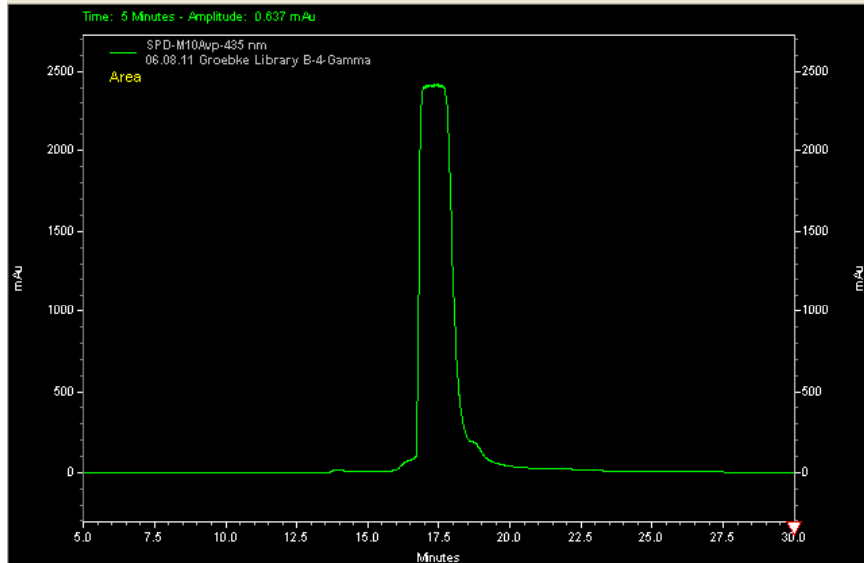
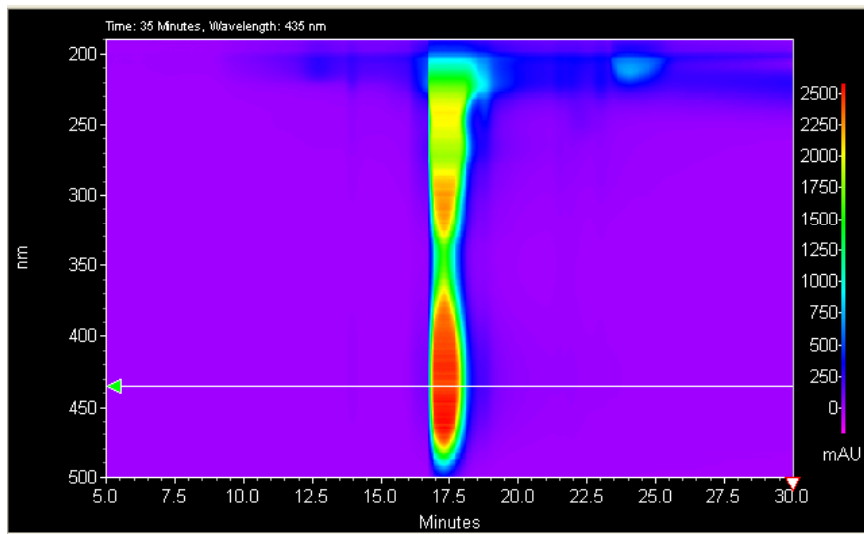
3f ¹H Spectrum



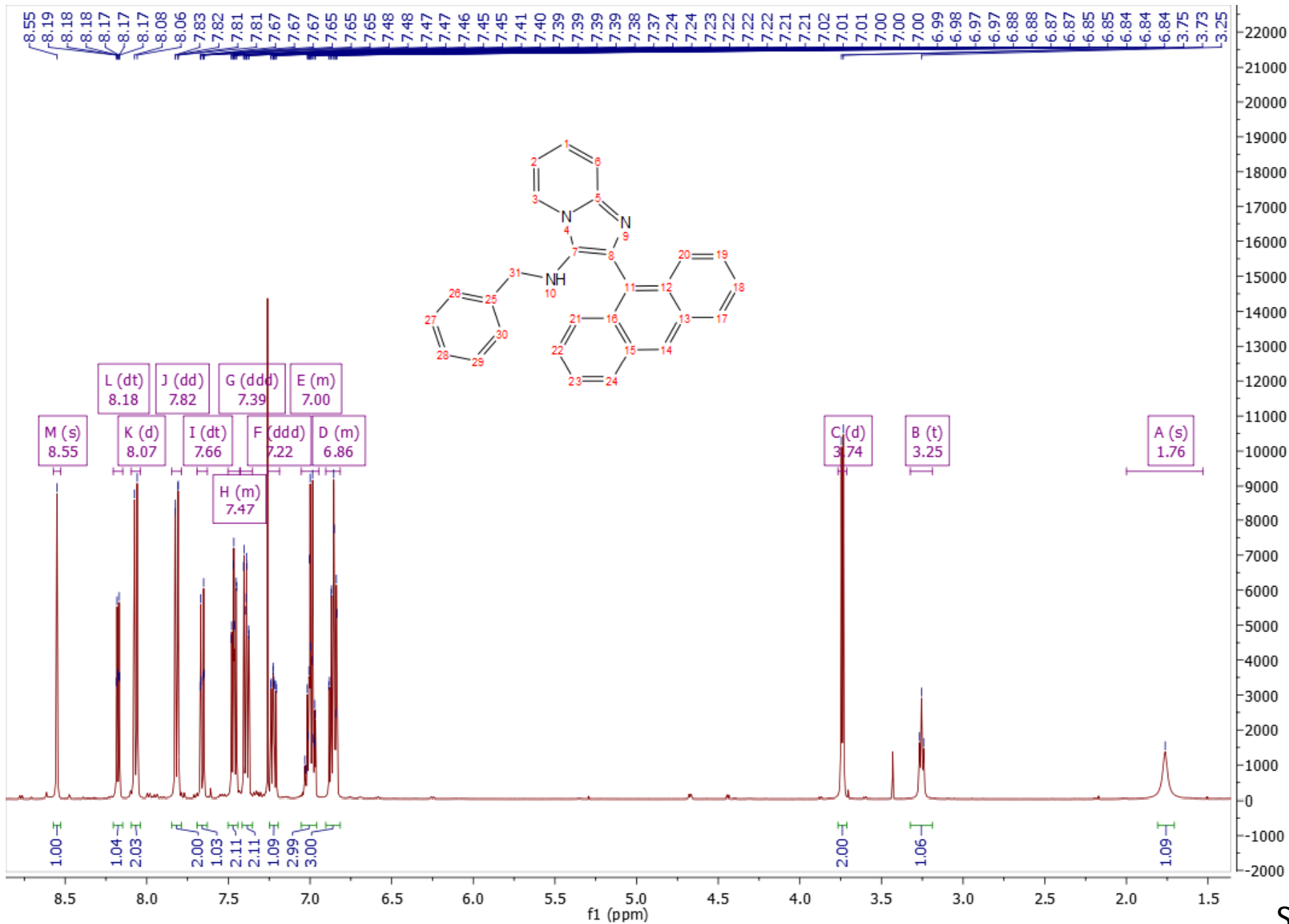
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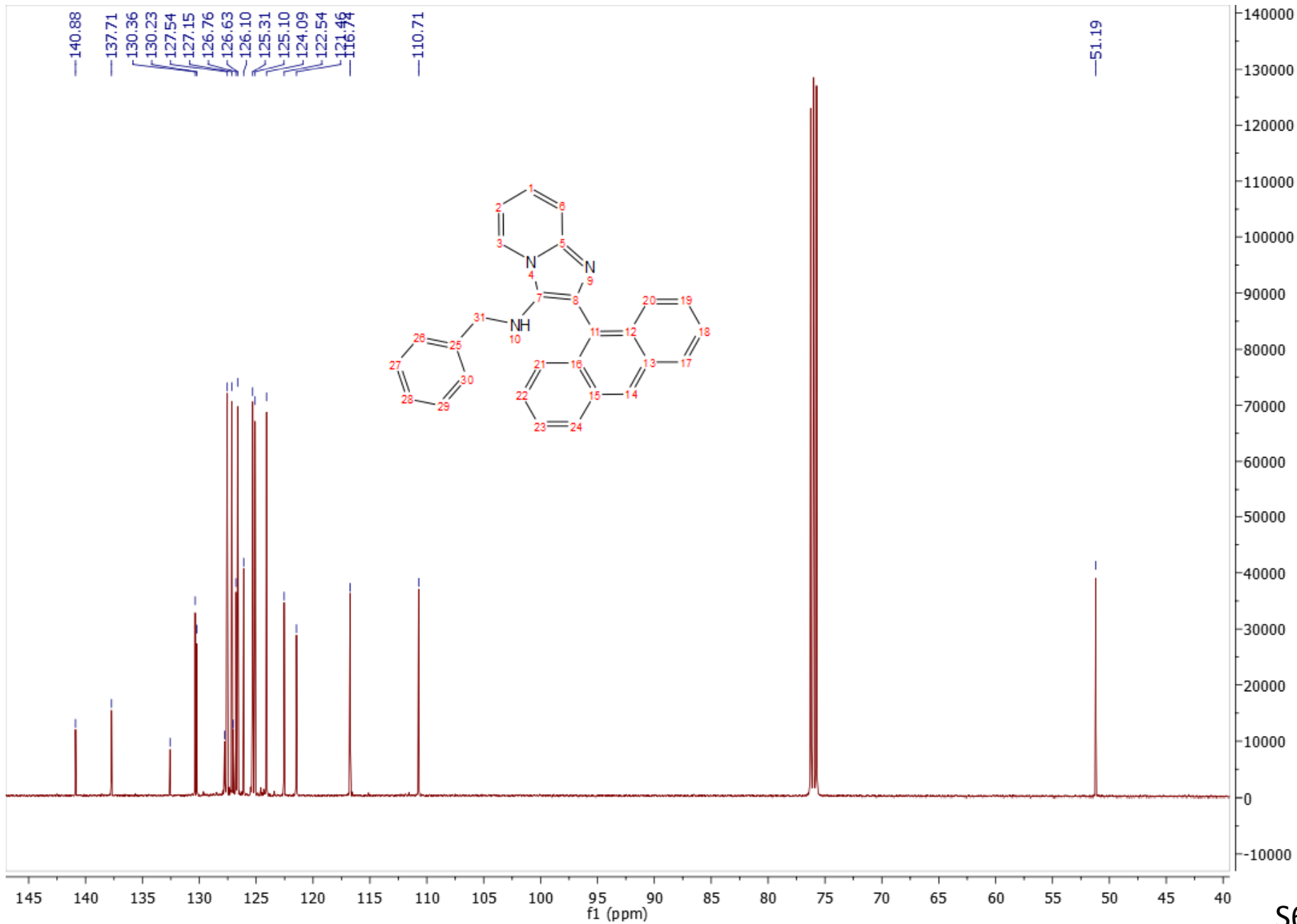
3f LC-MS



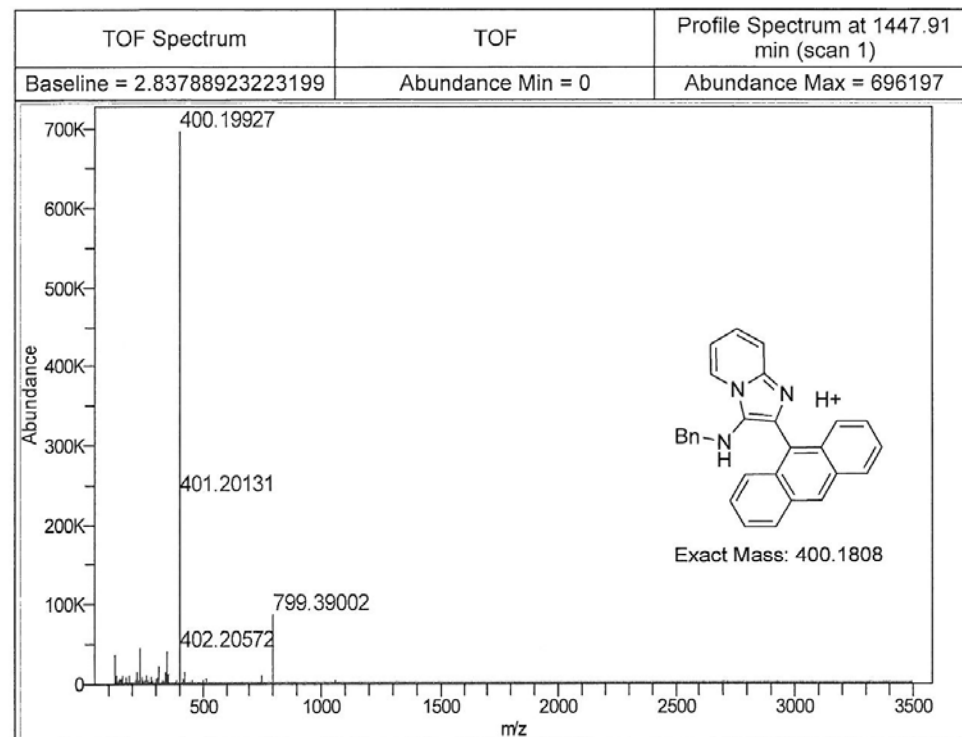
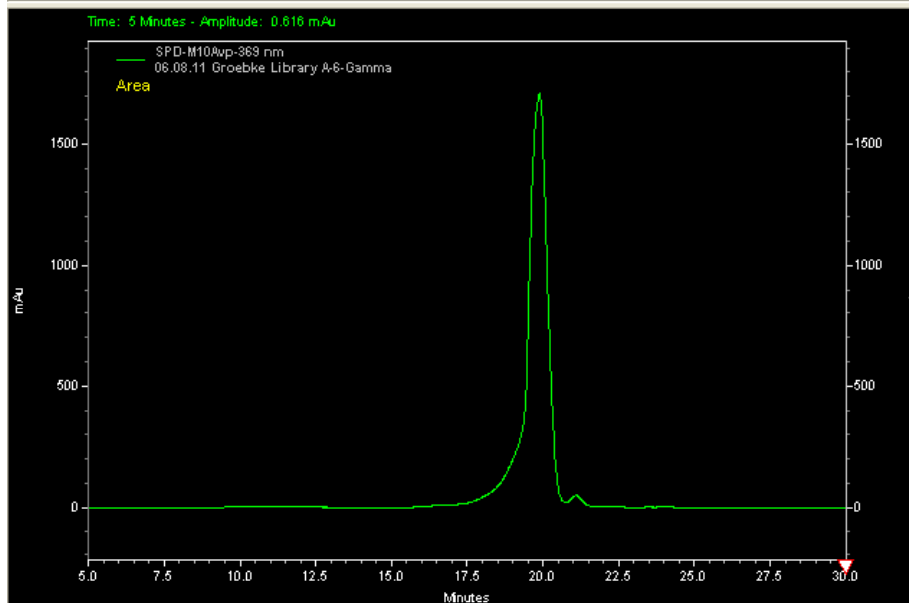
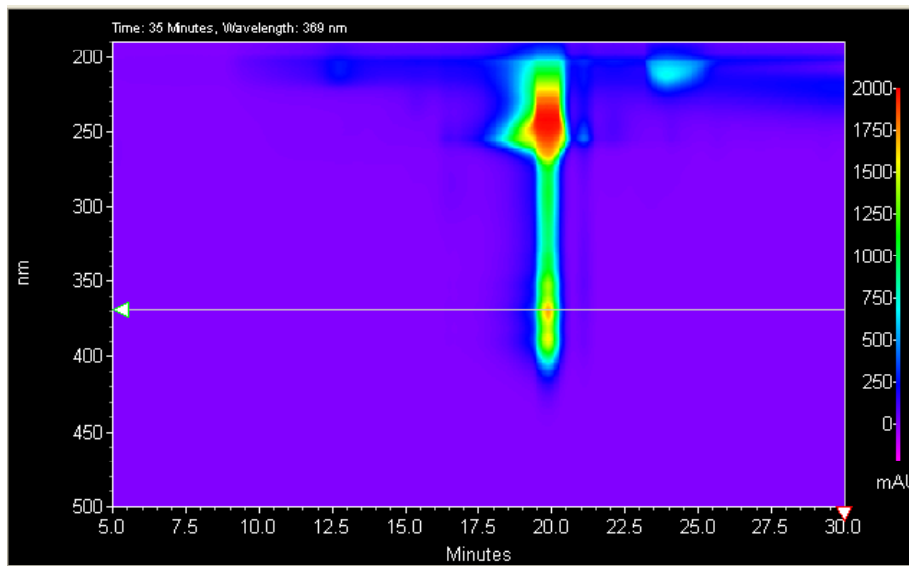
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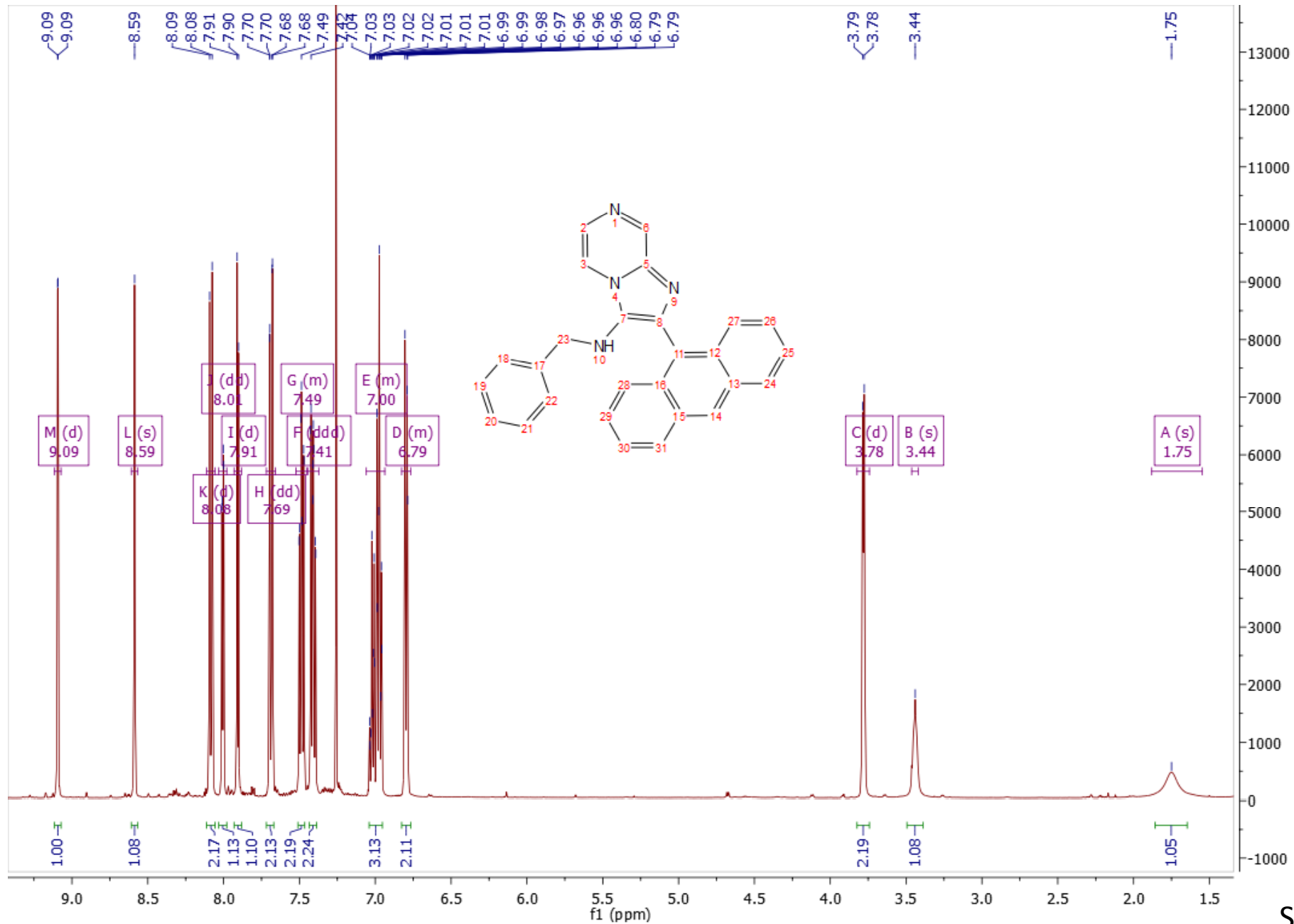
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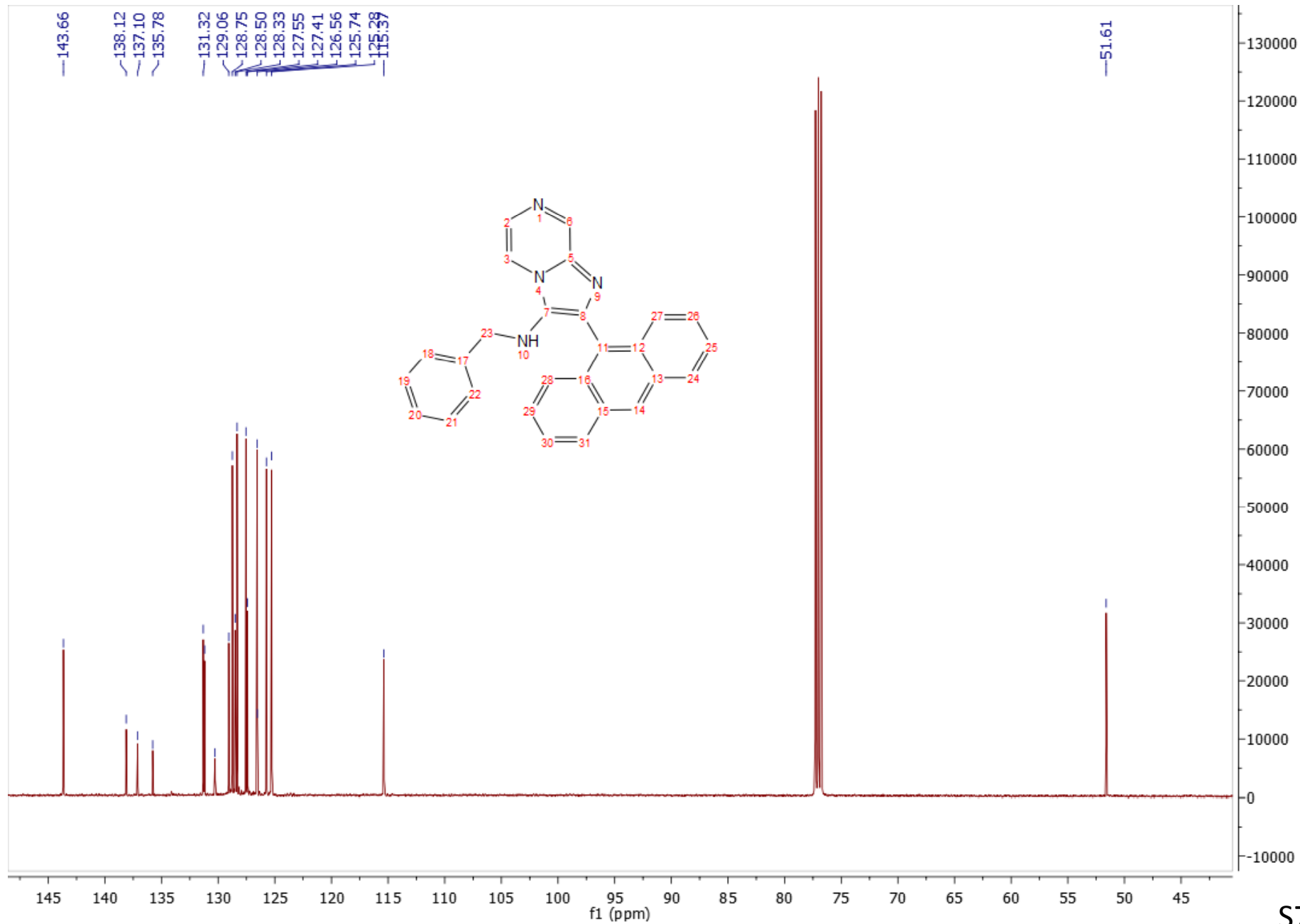
3g LC-MS



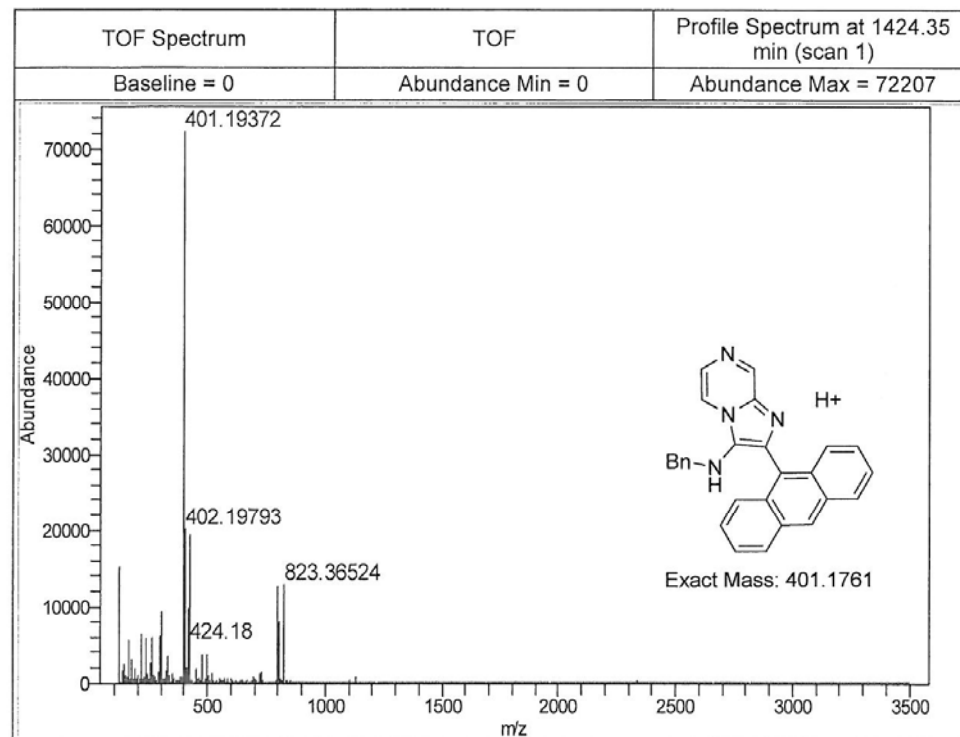
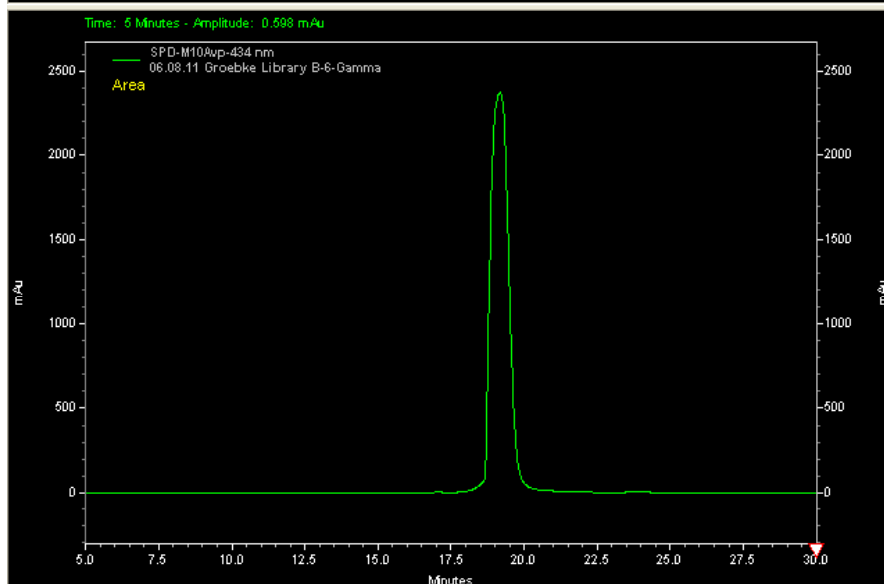
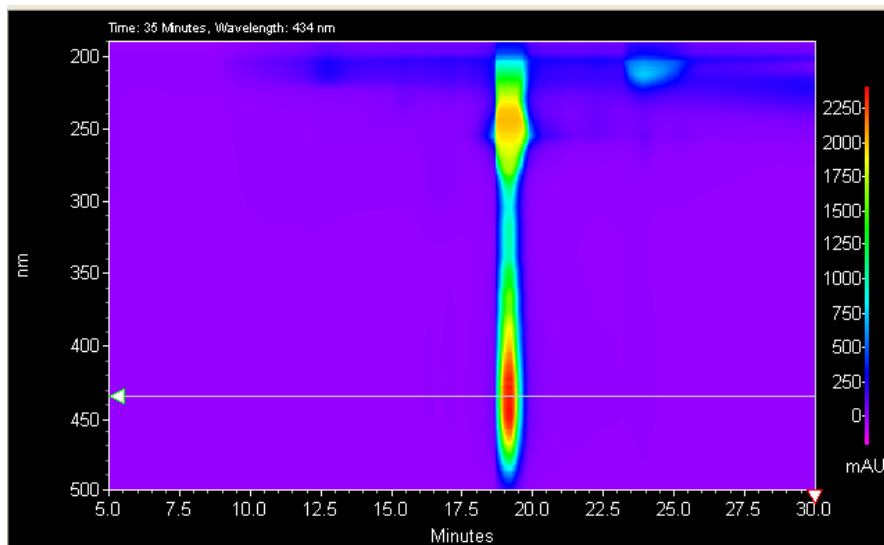
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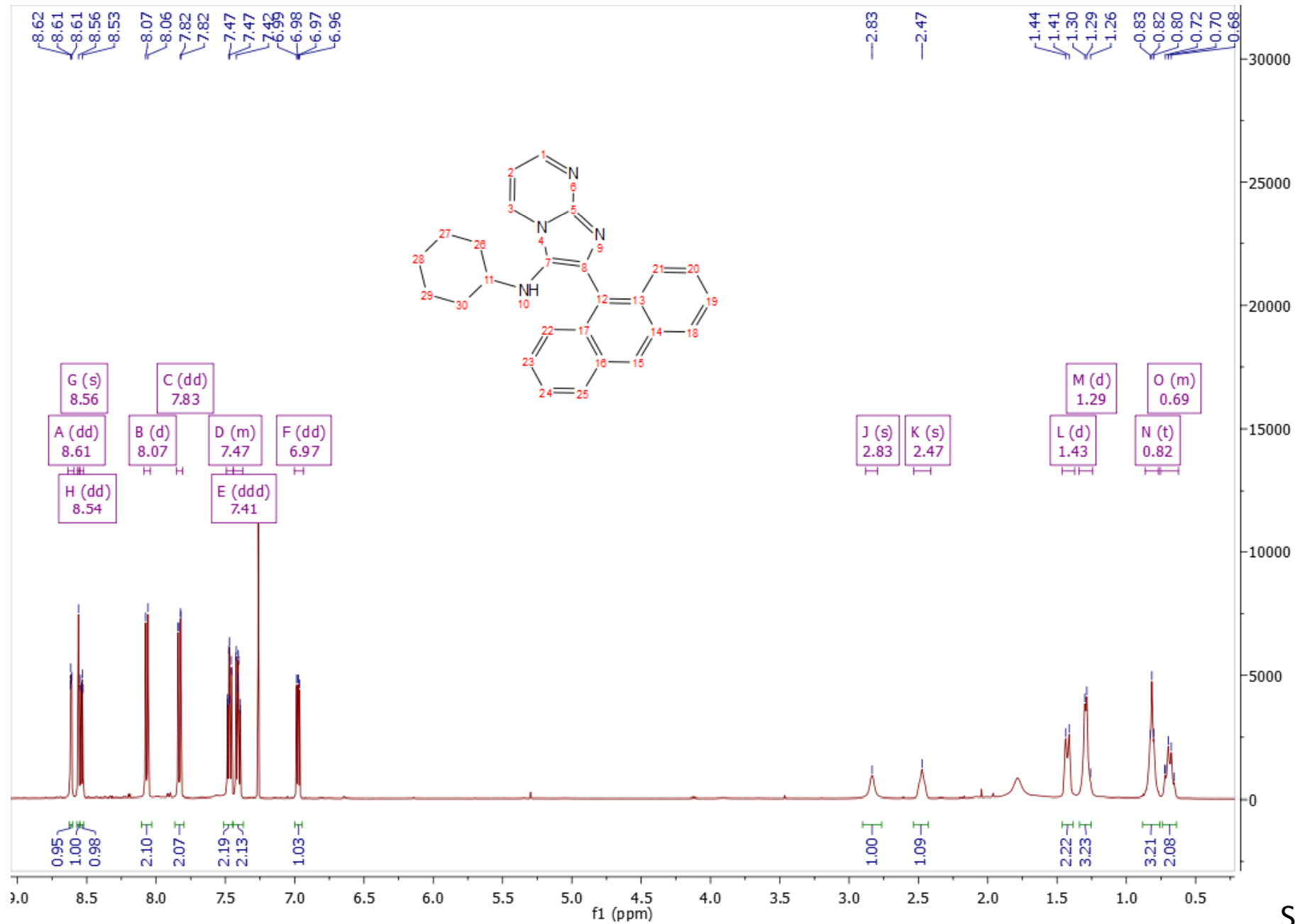
3h ¹³C Spectrum



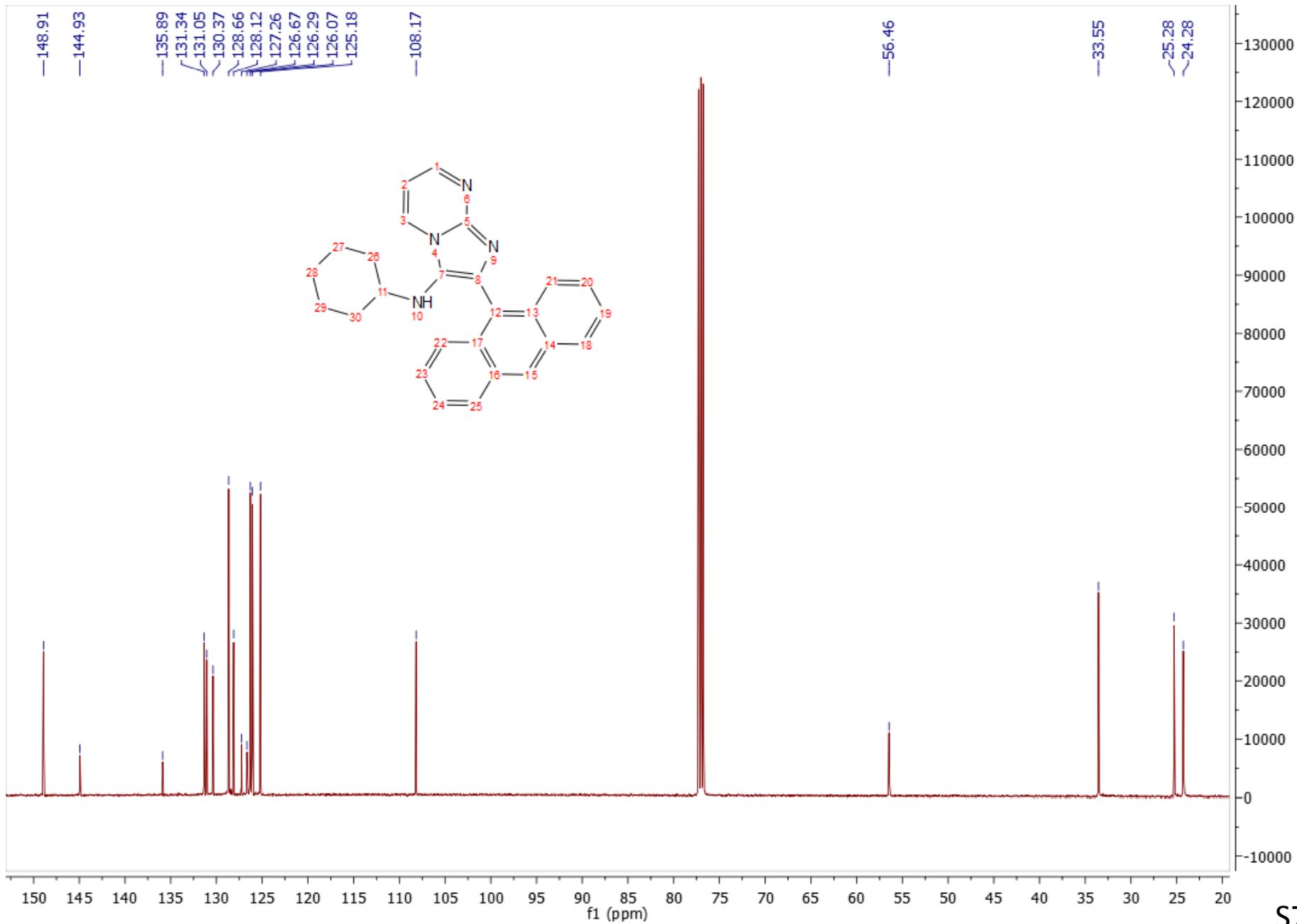
3h LC-MS



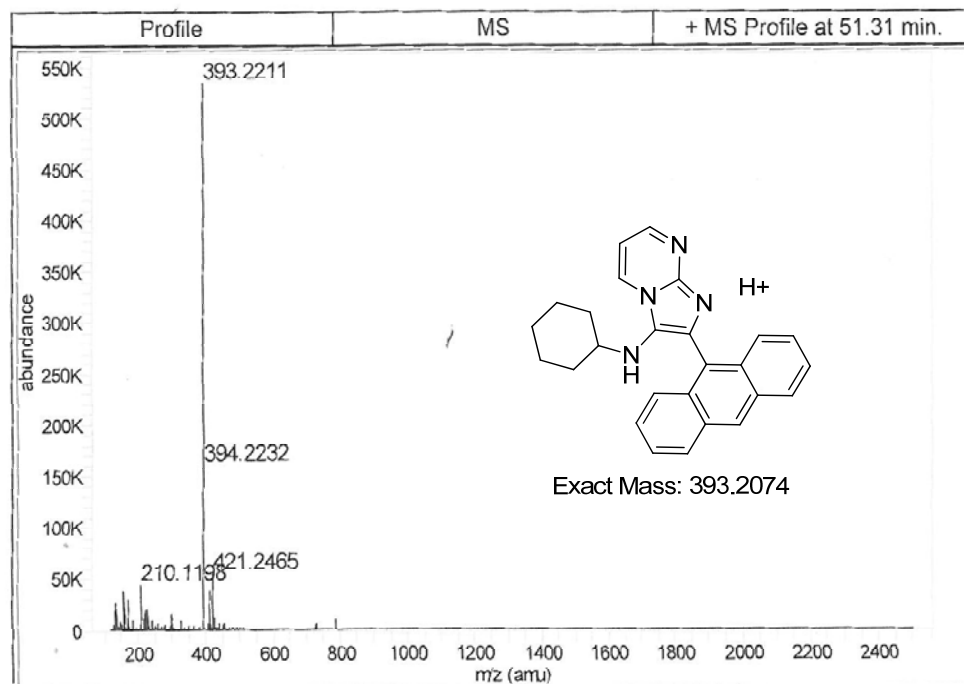
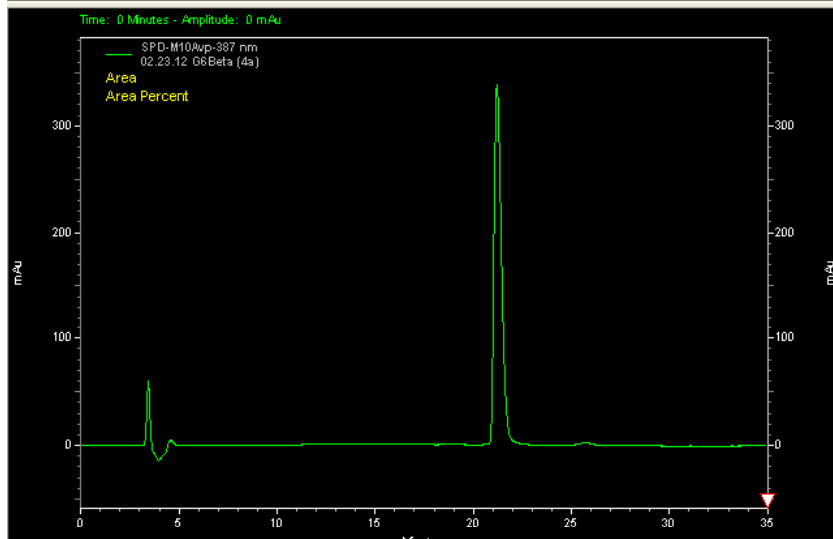
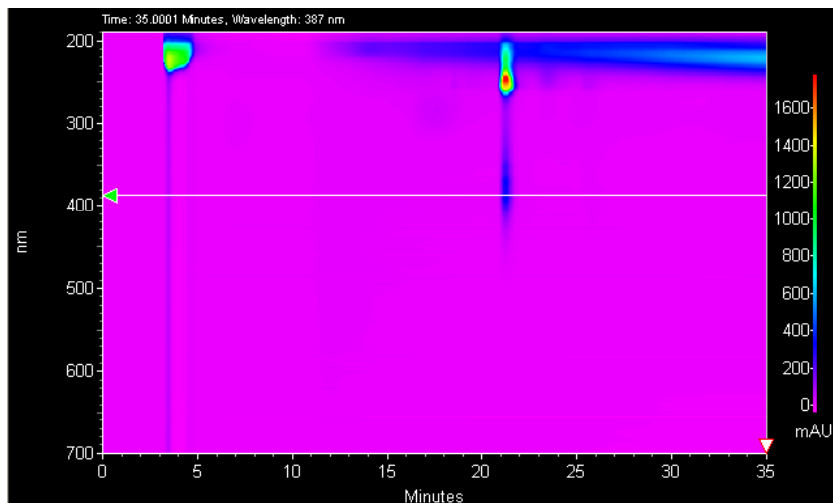
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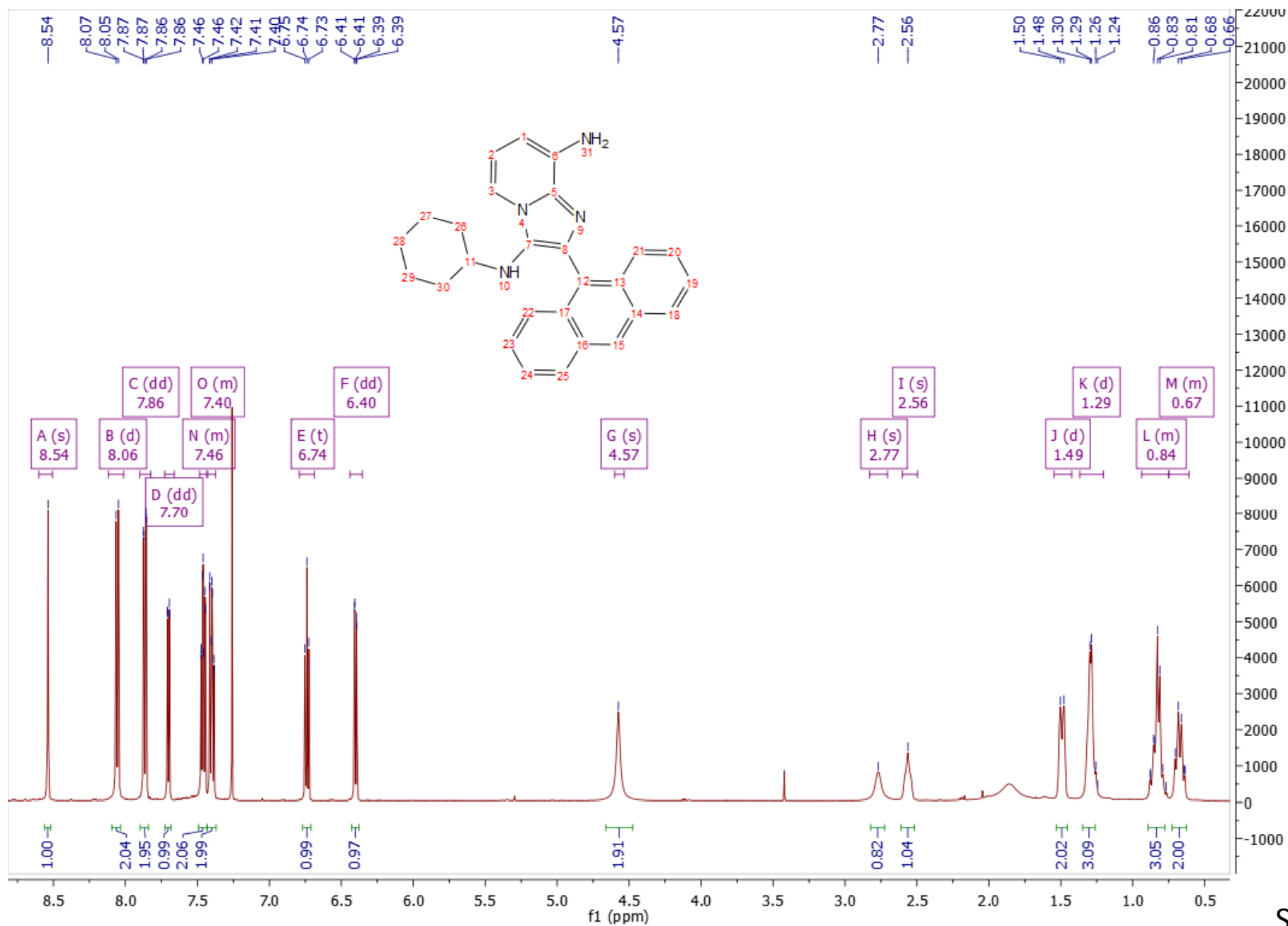
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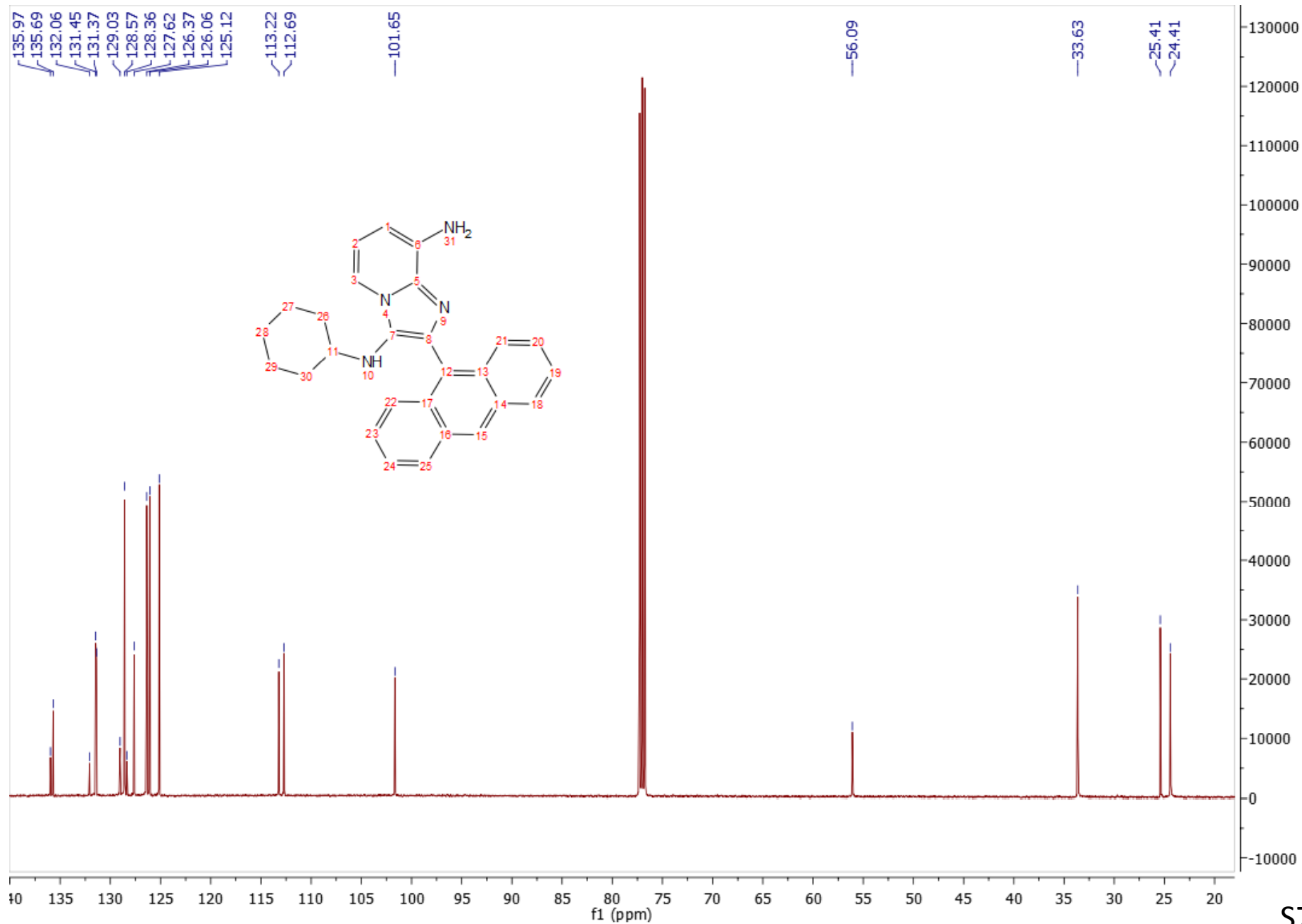
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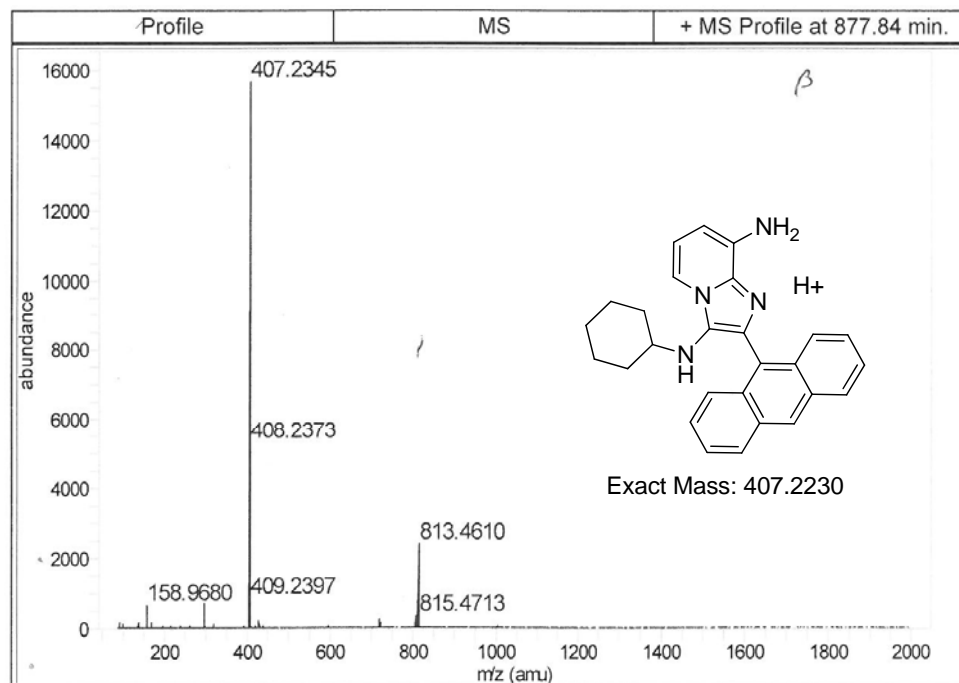
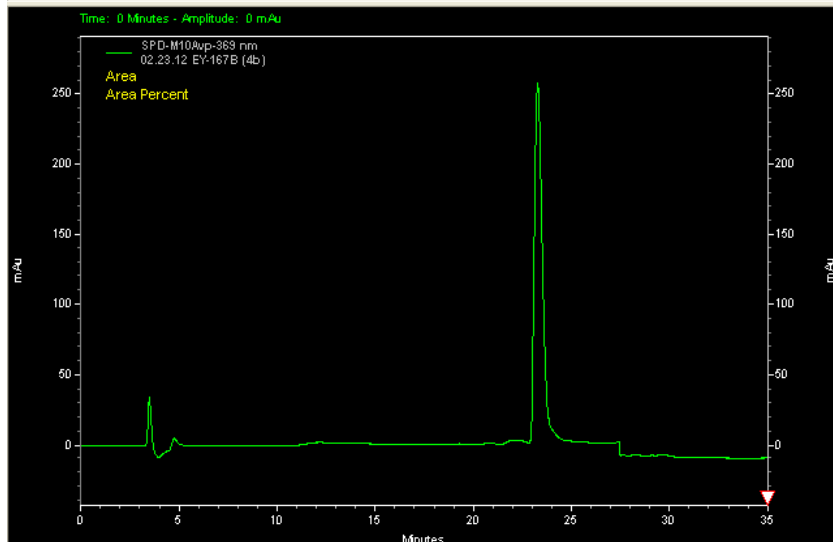
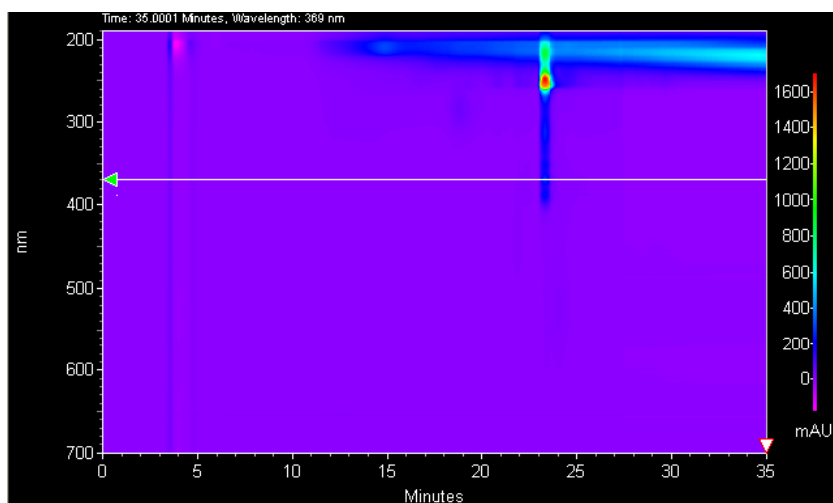
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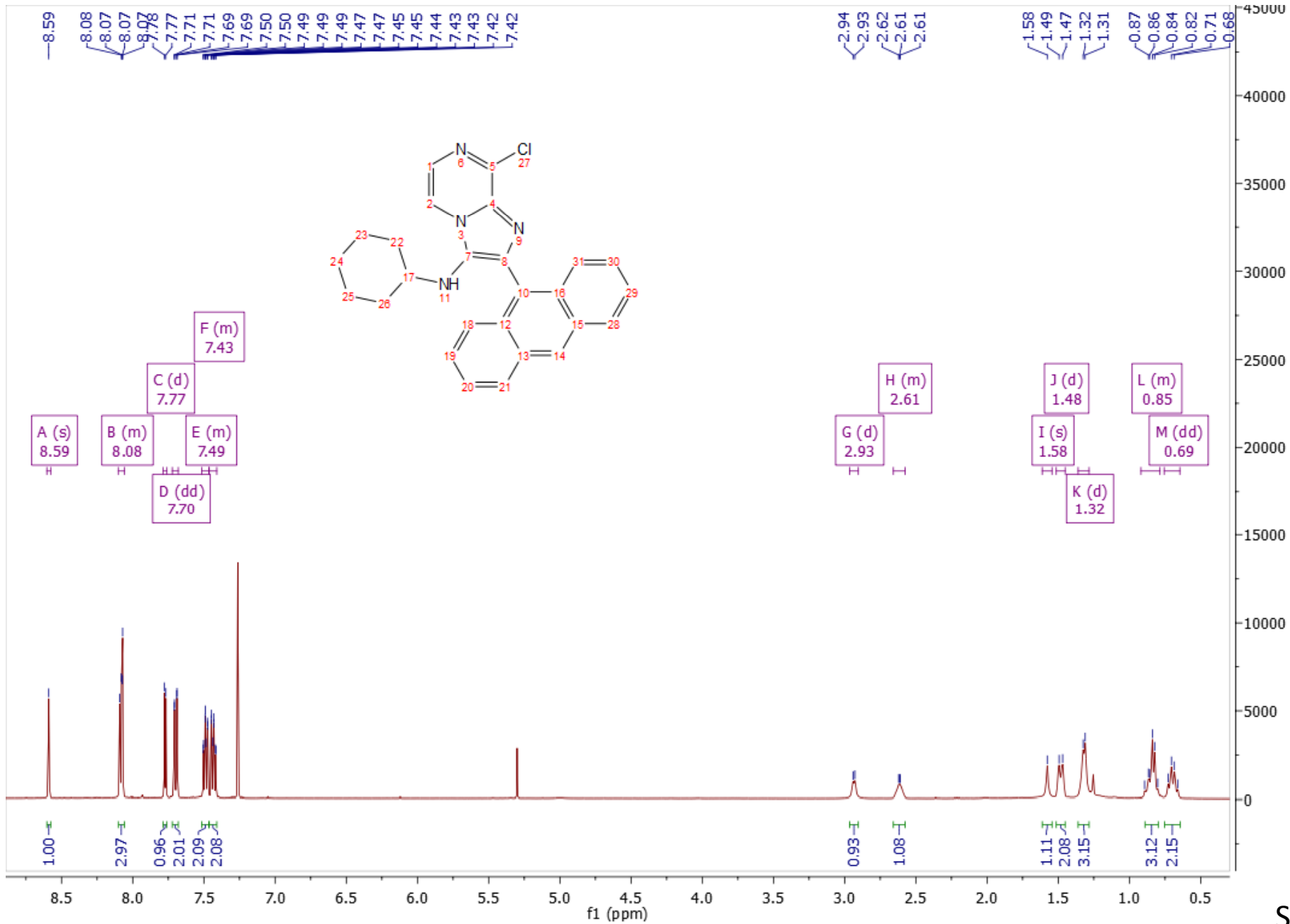
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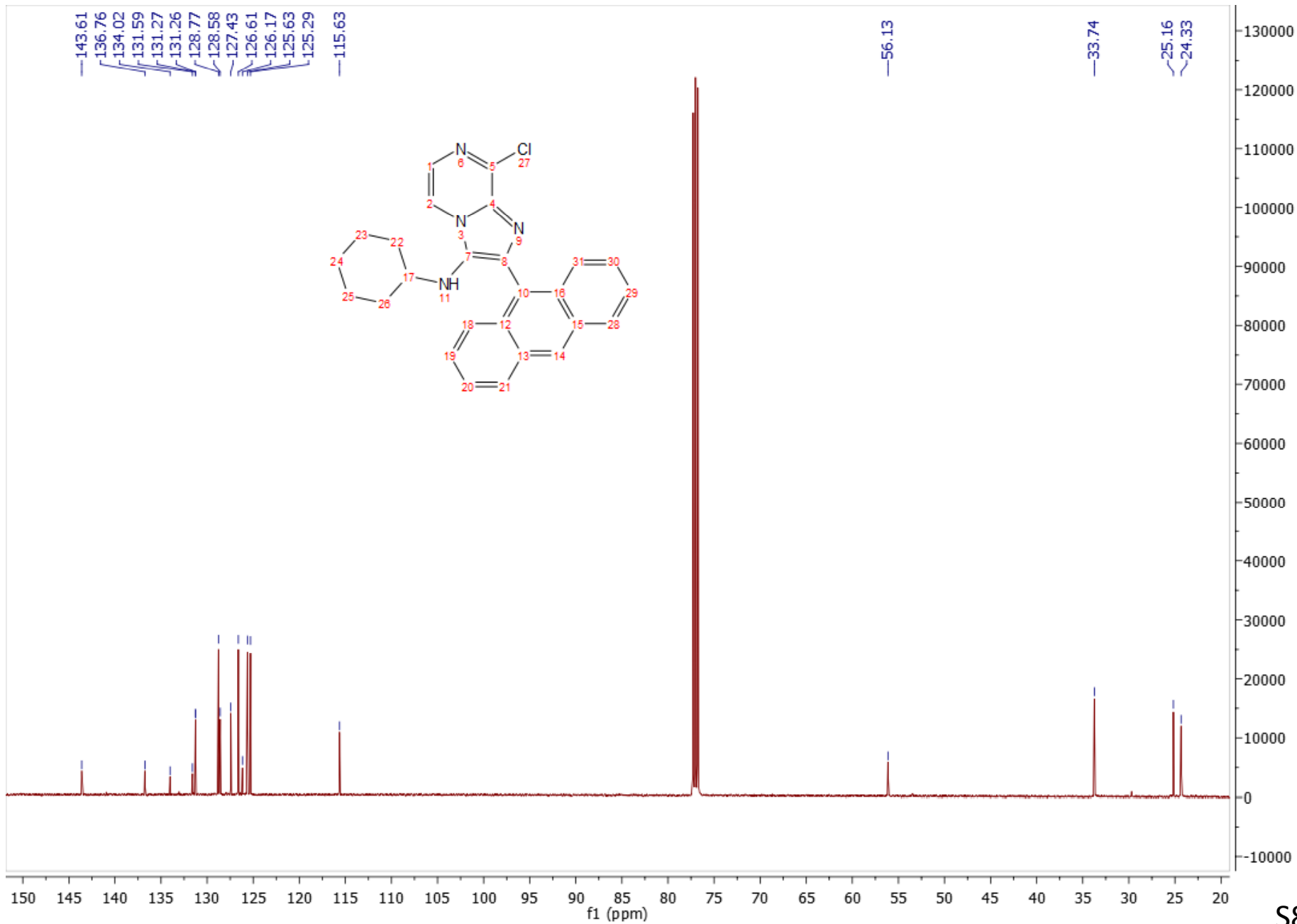
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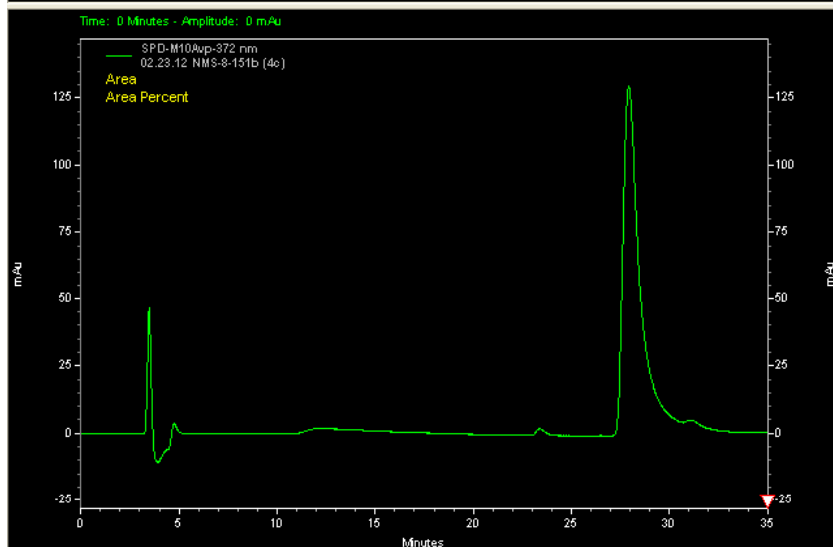
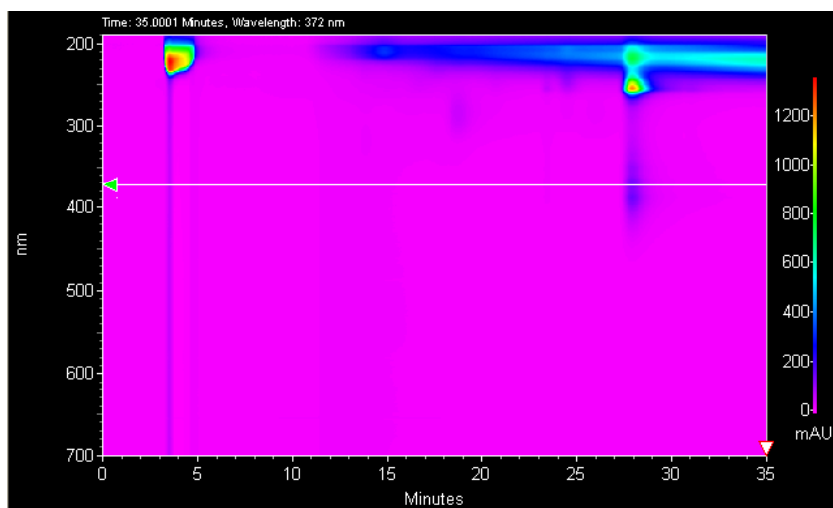
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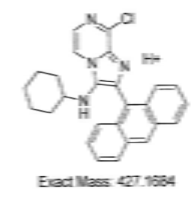
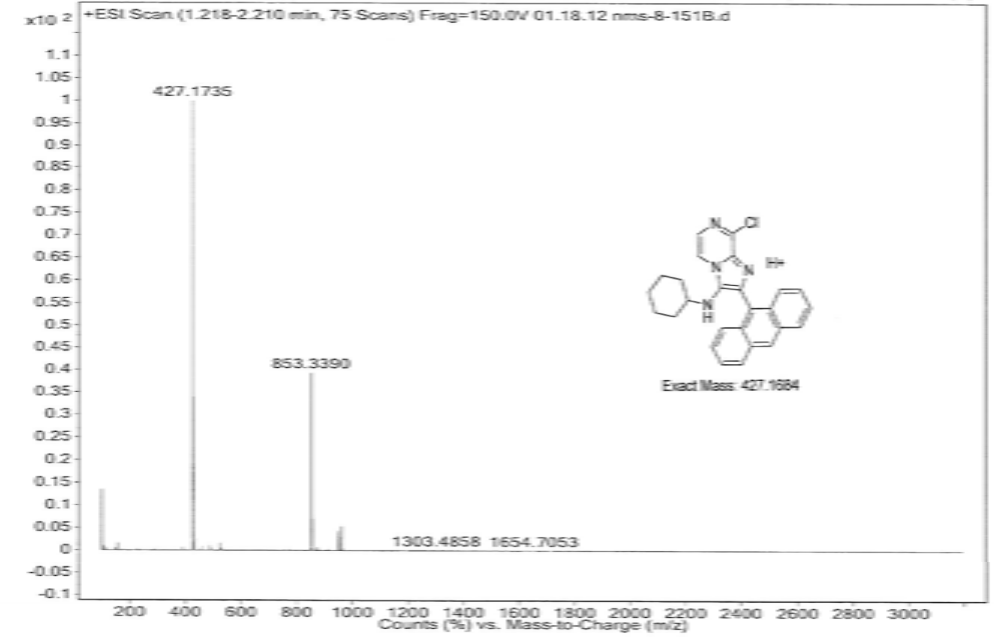
4c ¹³C Spectrum



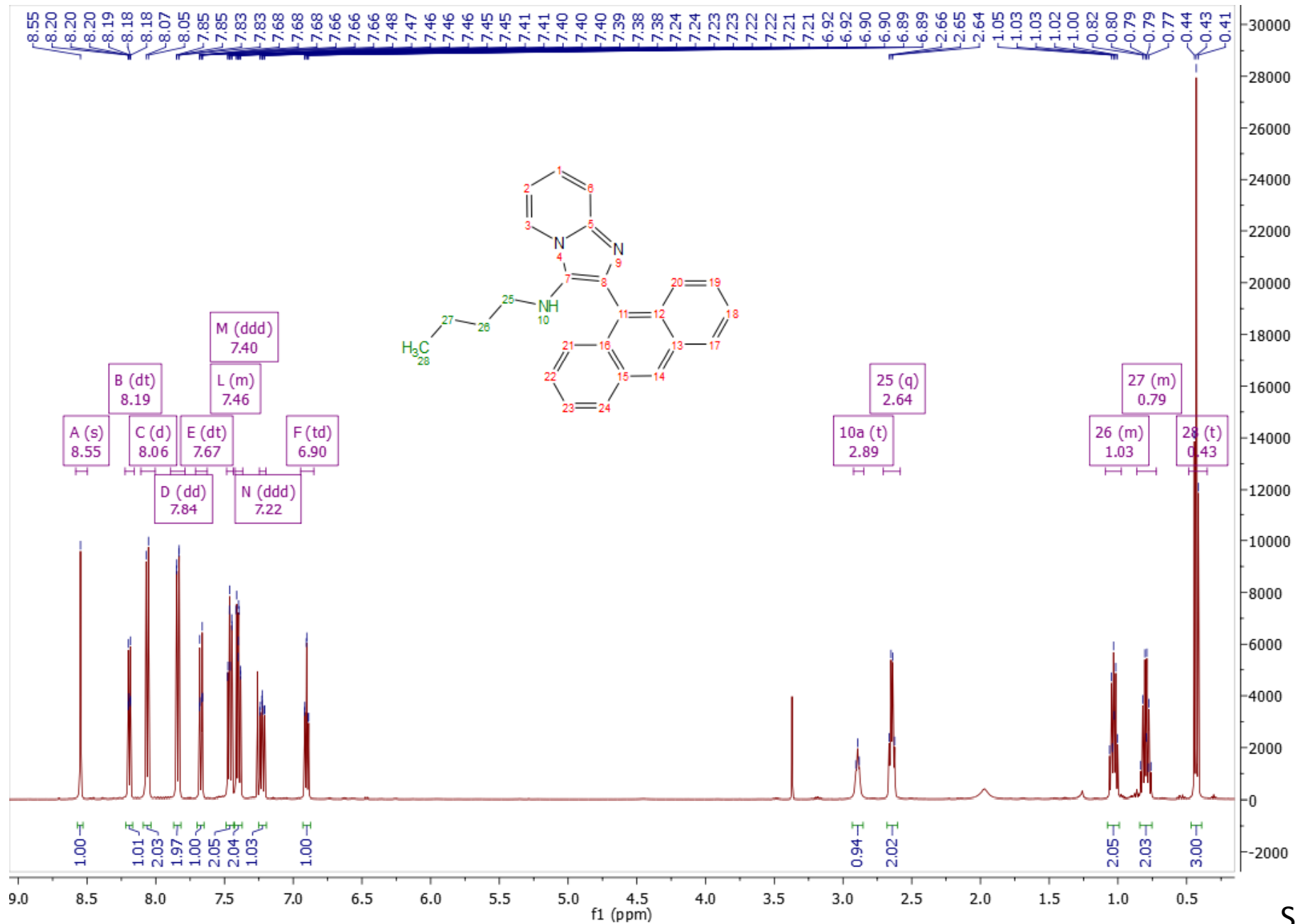
4c LC-MS



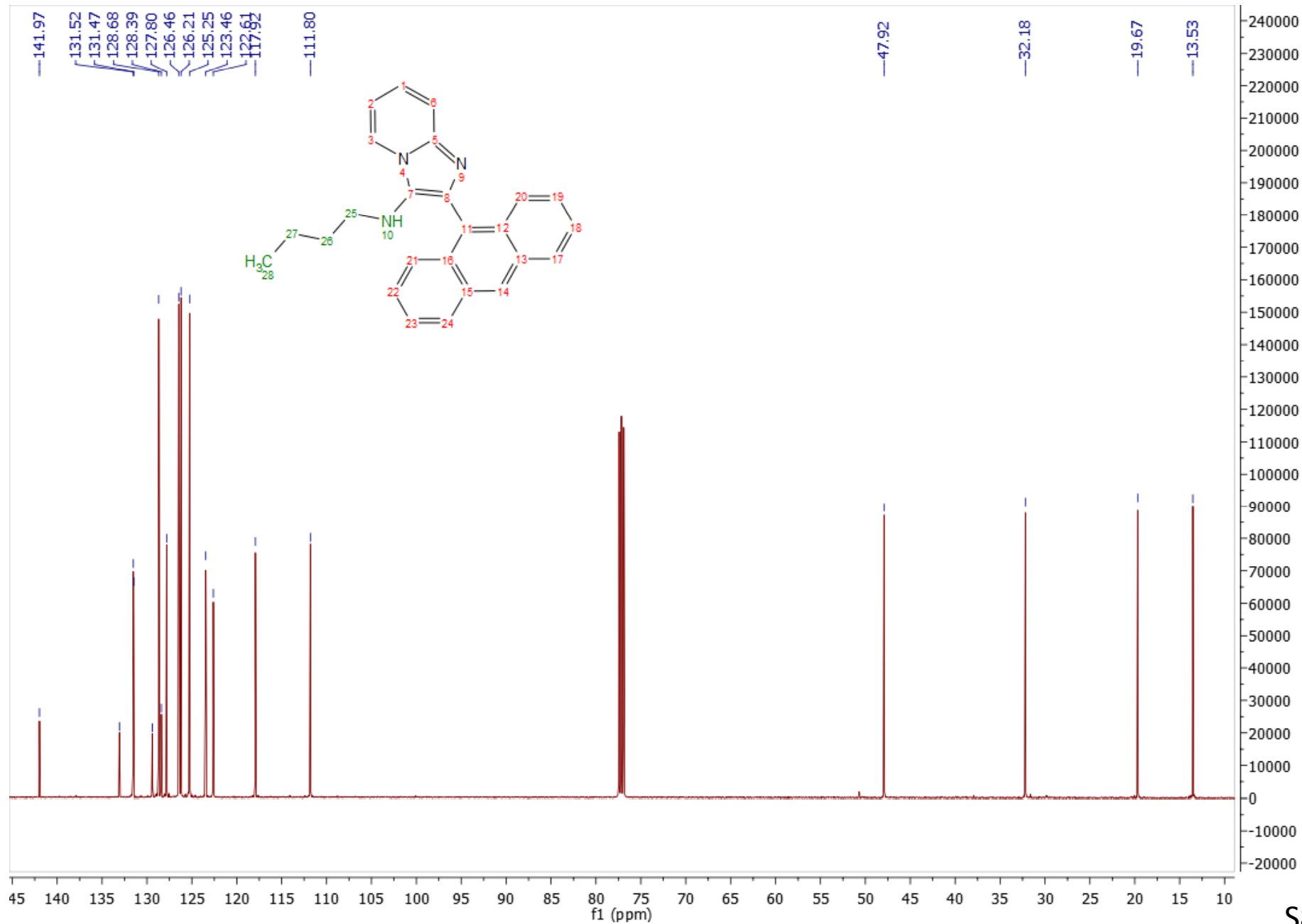
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Dq/Vol	-1	Dq/Position		SampleType	Sample	IRM Calibration Status		1/18/2012 6:29:42
Data Filename	01.18.12 nms-8-151B	ACQ Method	Watz-ACI Infusion M	Comment		Acquired Time		



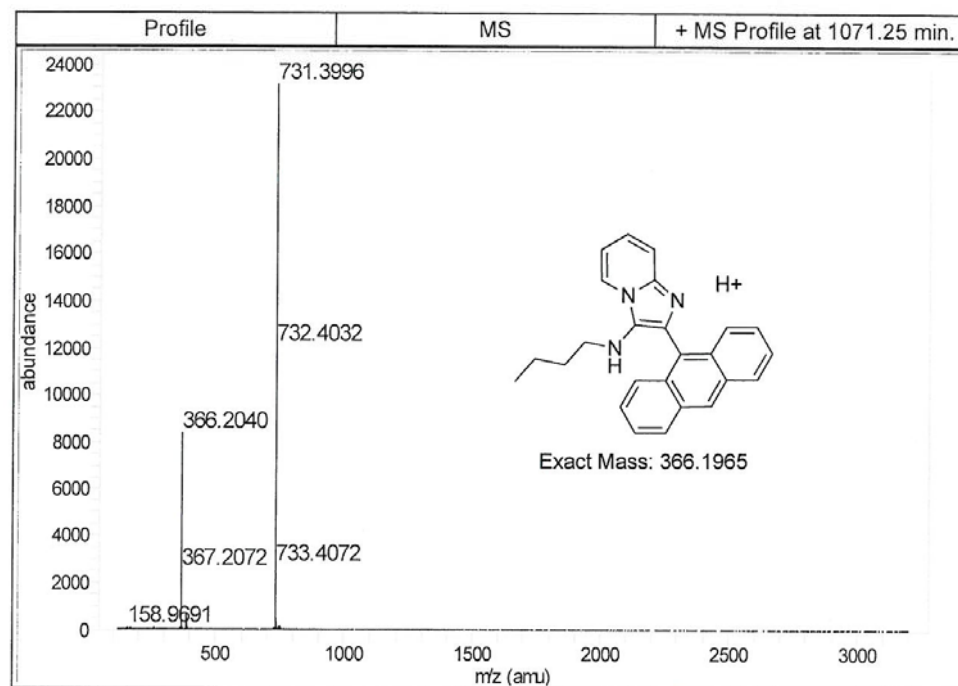
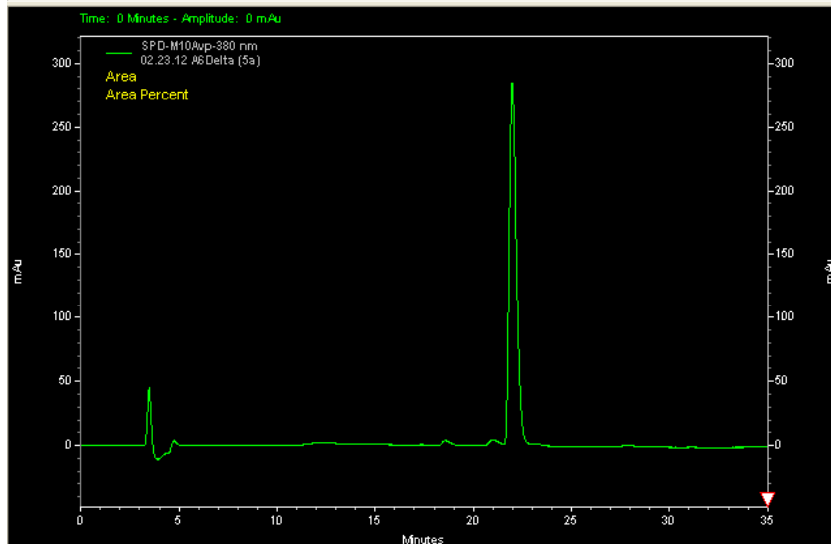
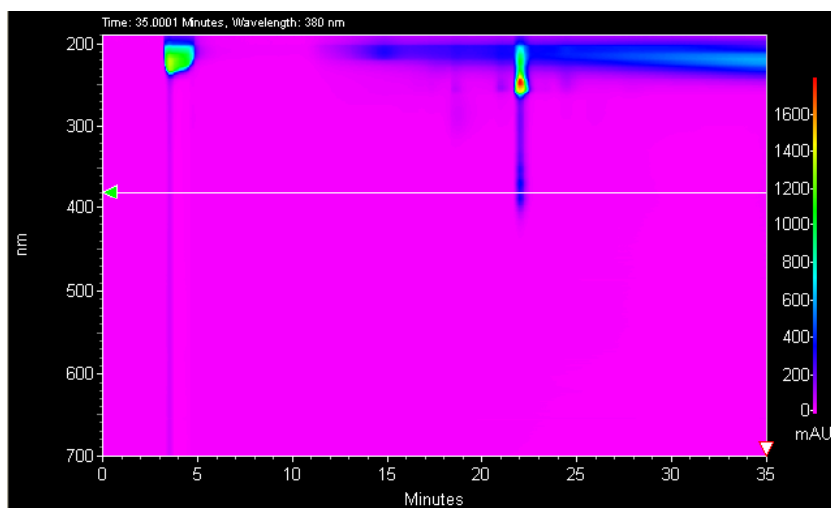
5a ¹H Spectrum



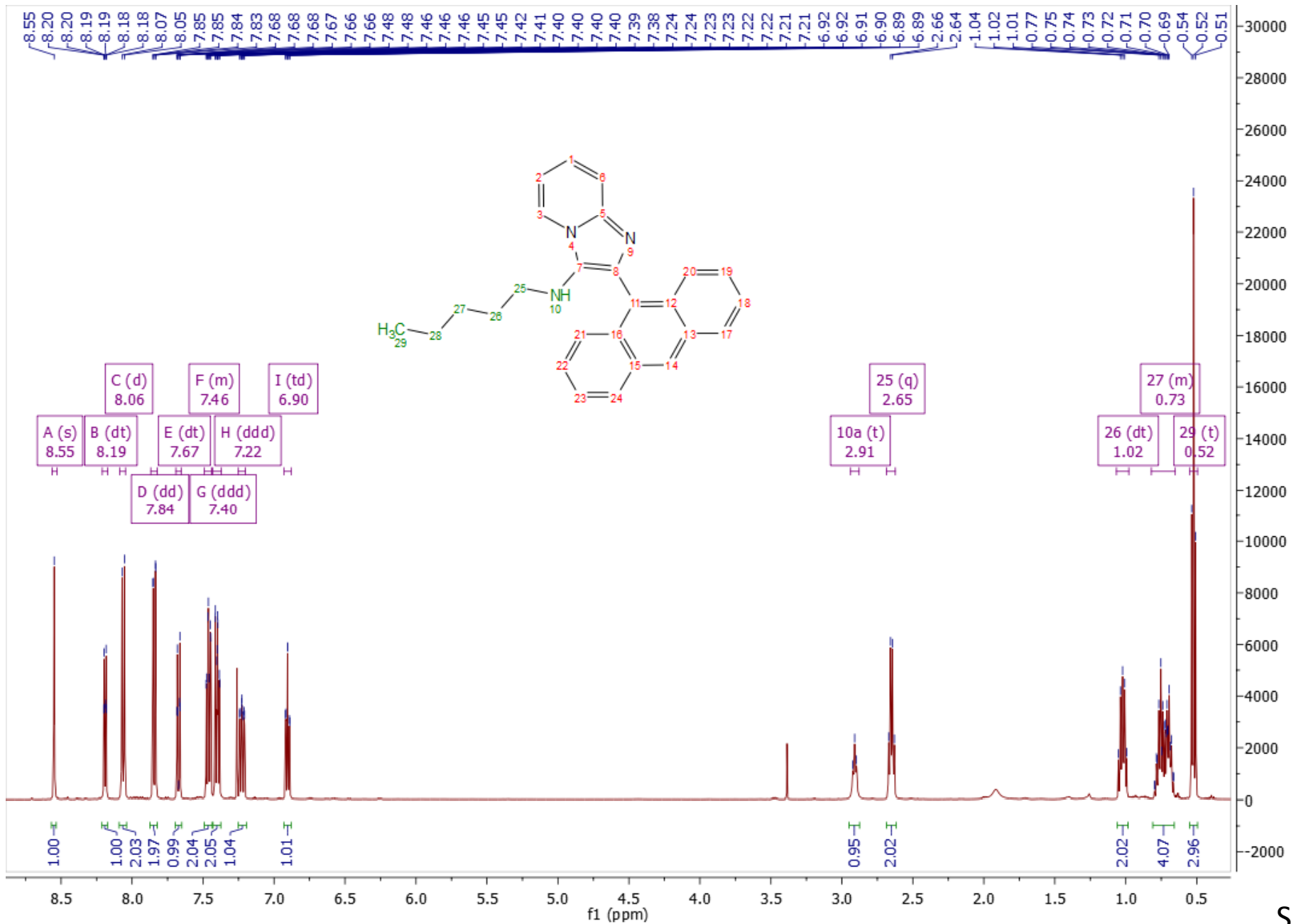
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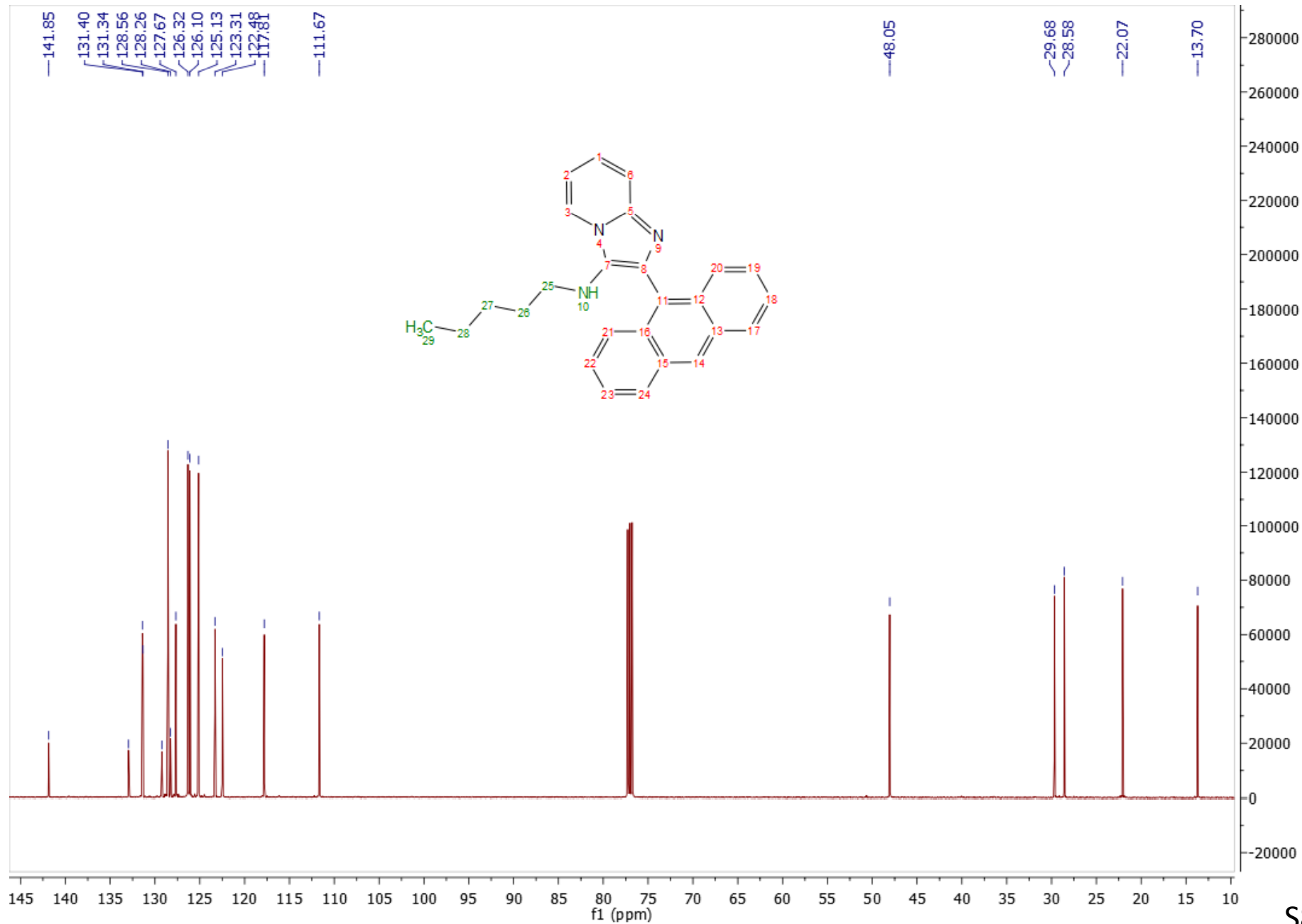
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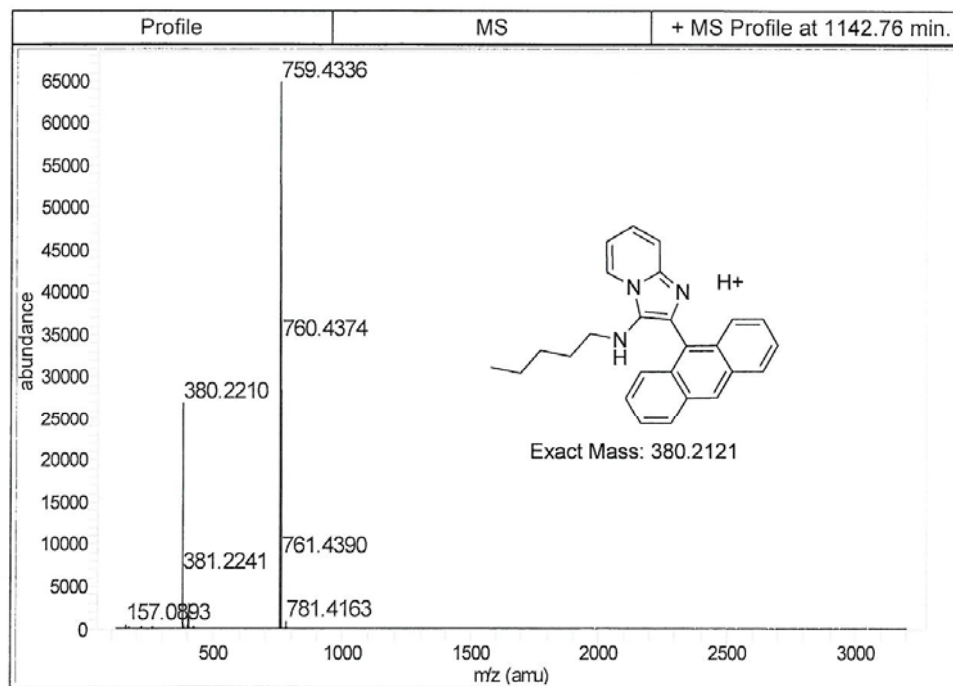
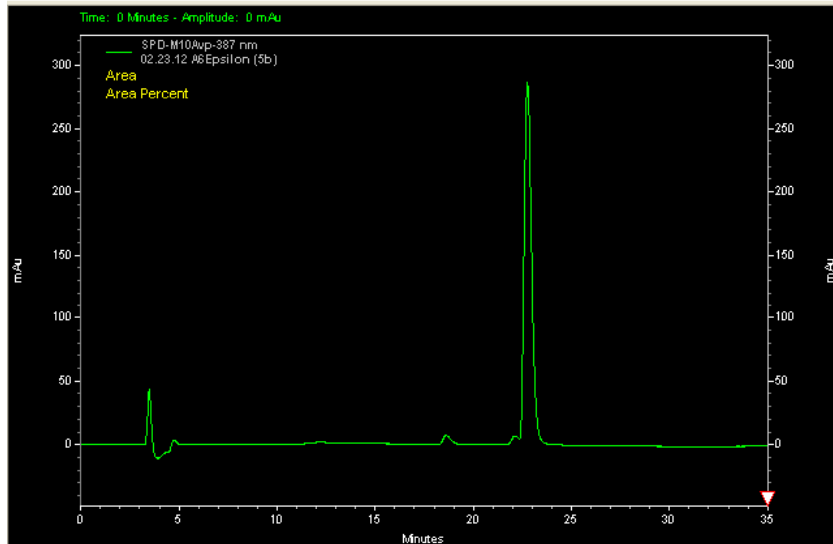
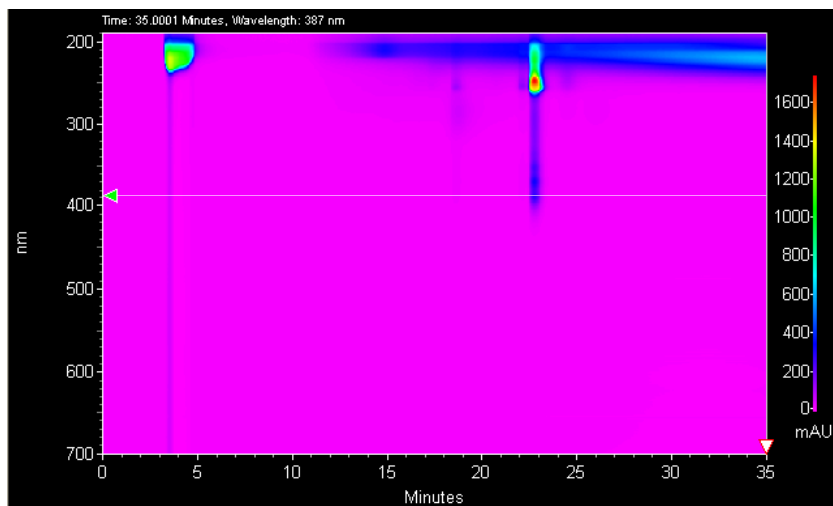
5b ¹H Spectrum



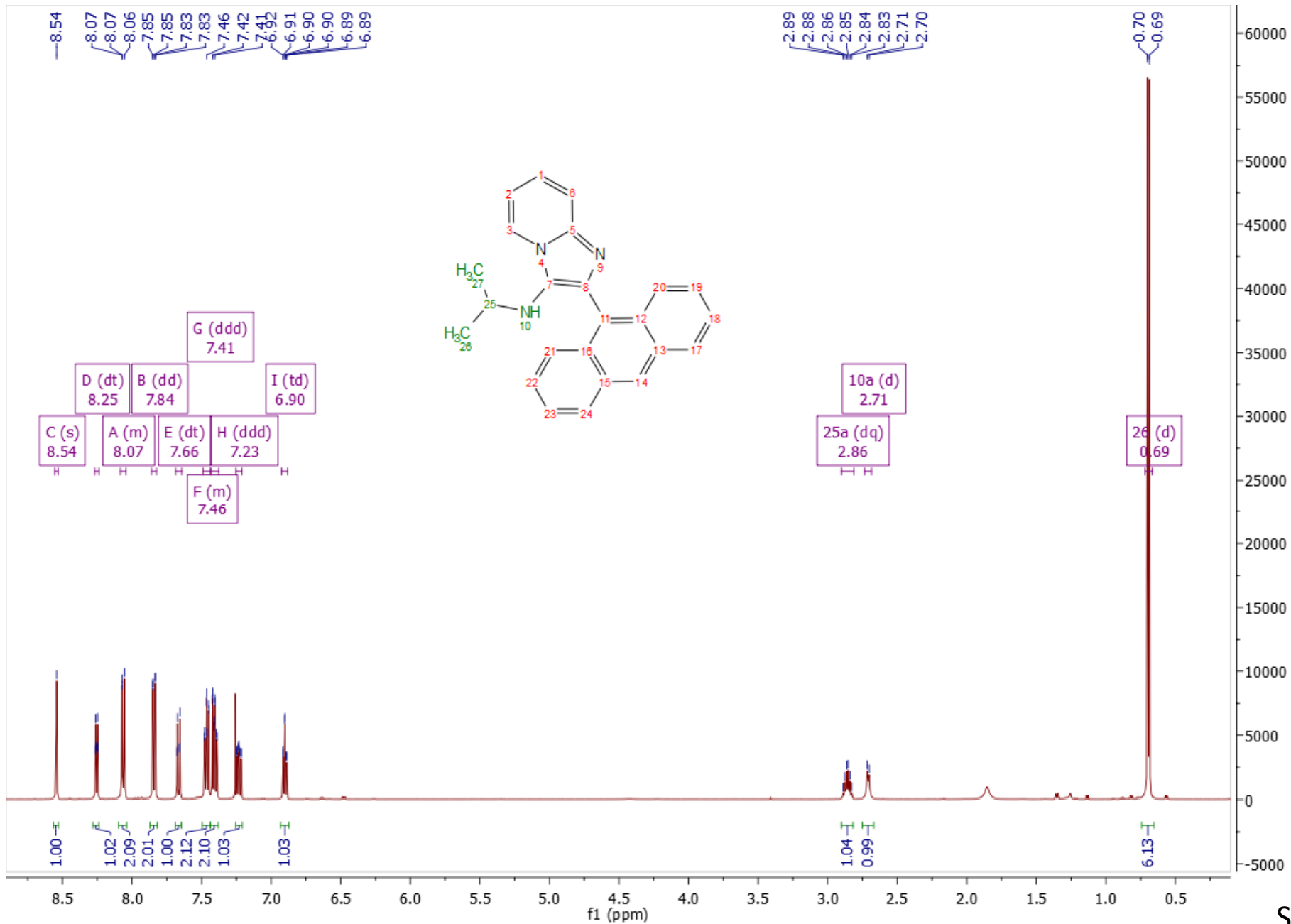
5b ¹³C Spectrum



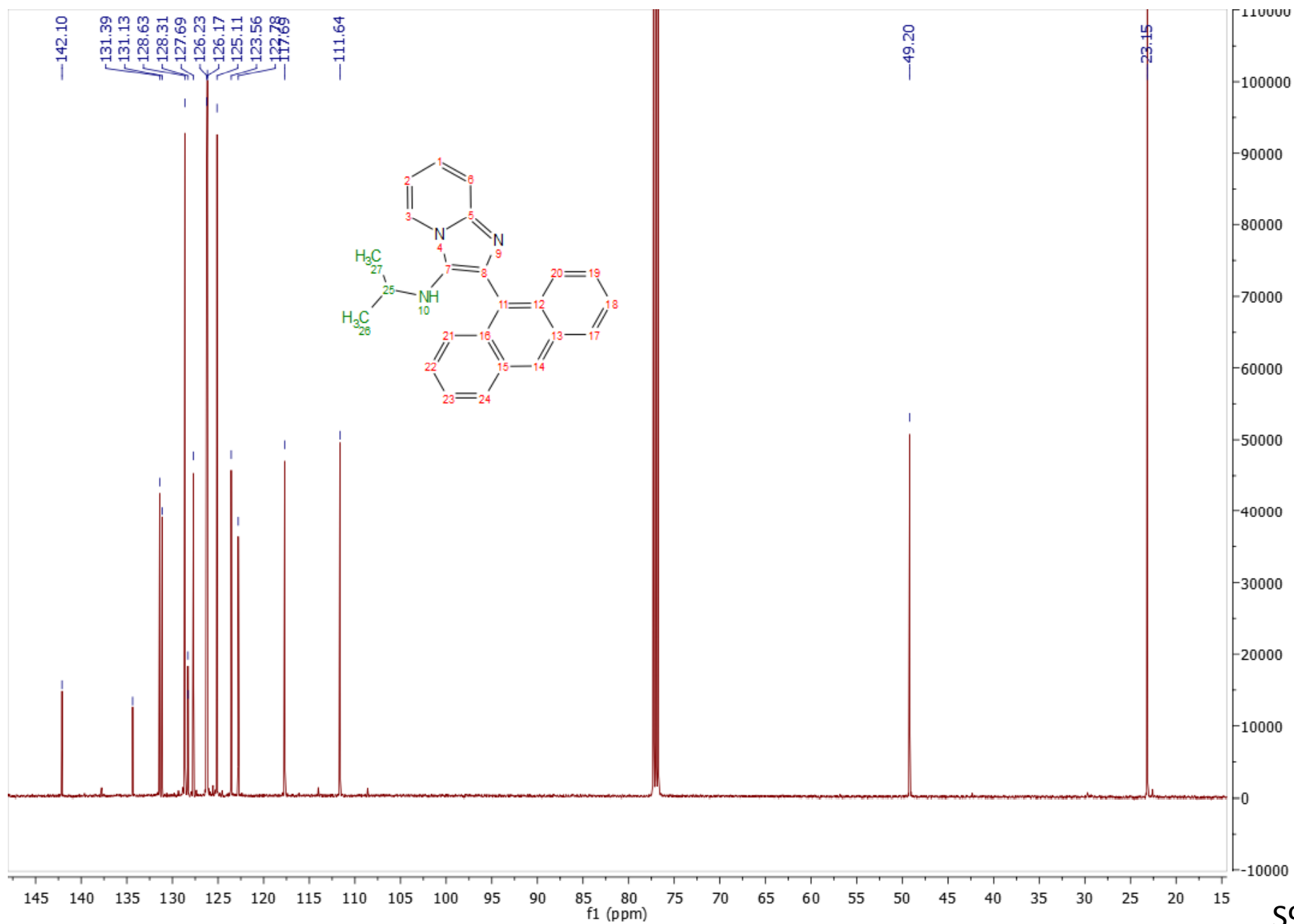
5b LC-MS



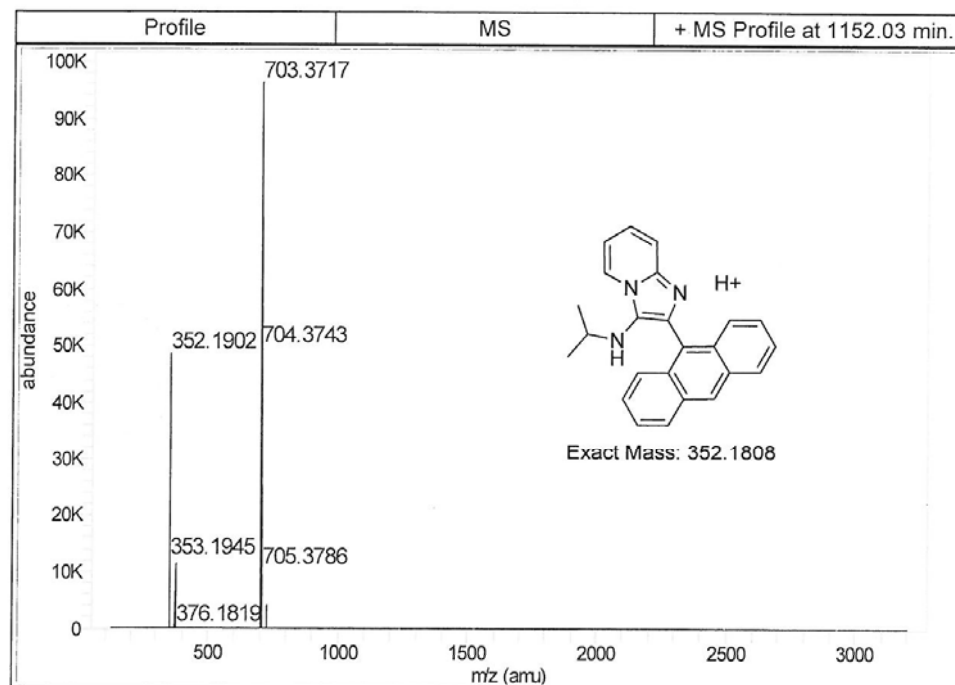
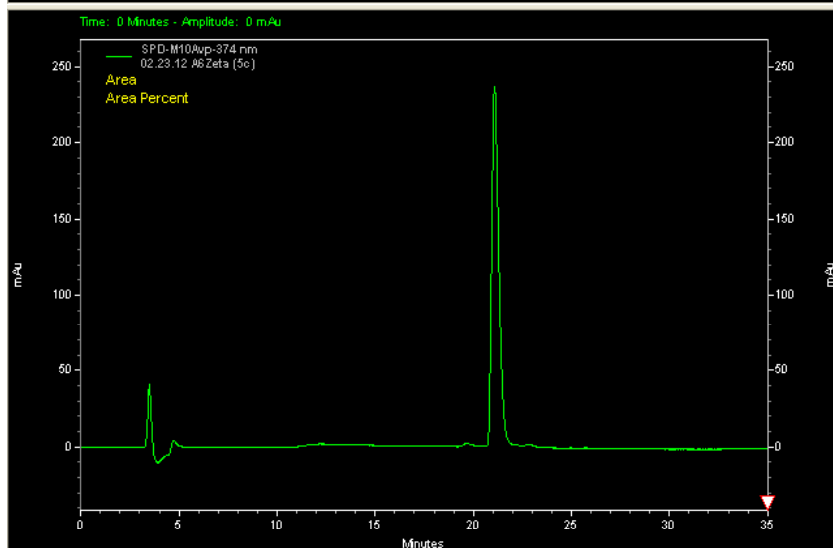
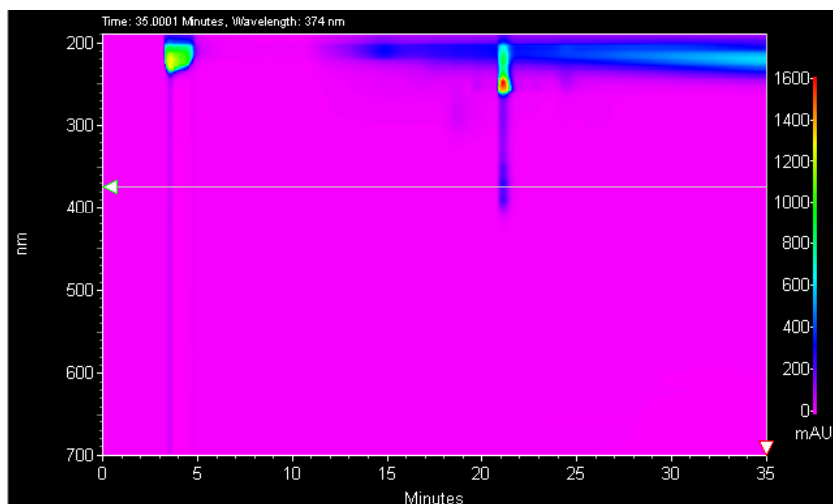
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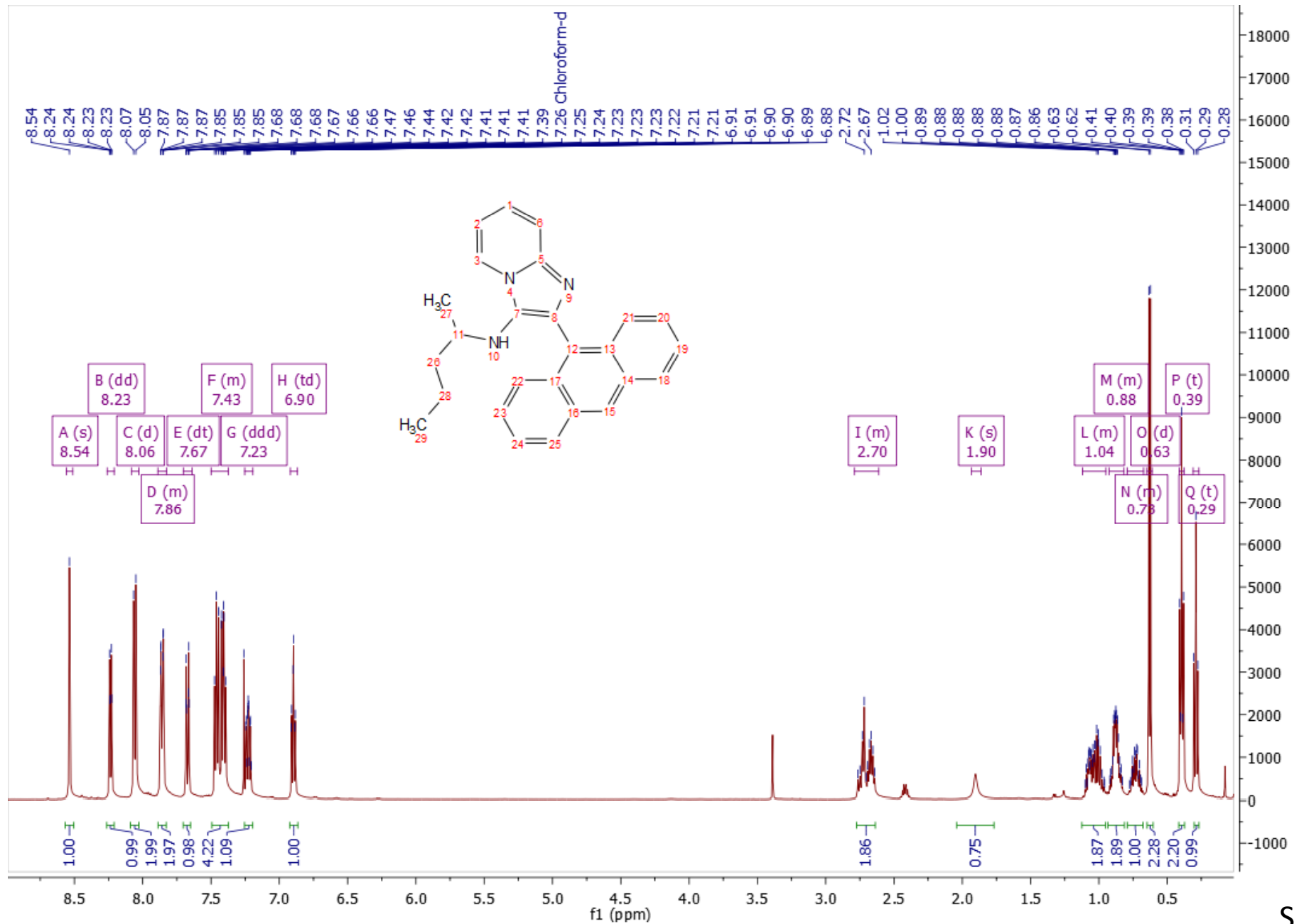
5c ¹³C Spectrum



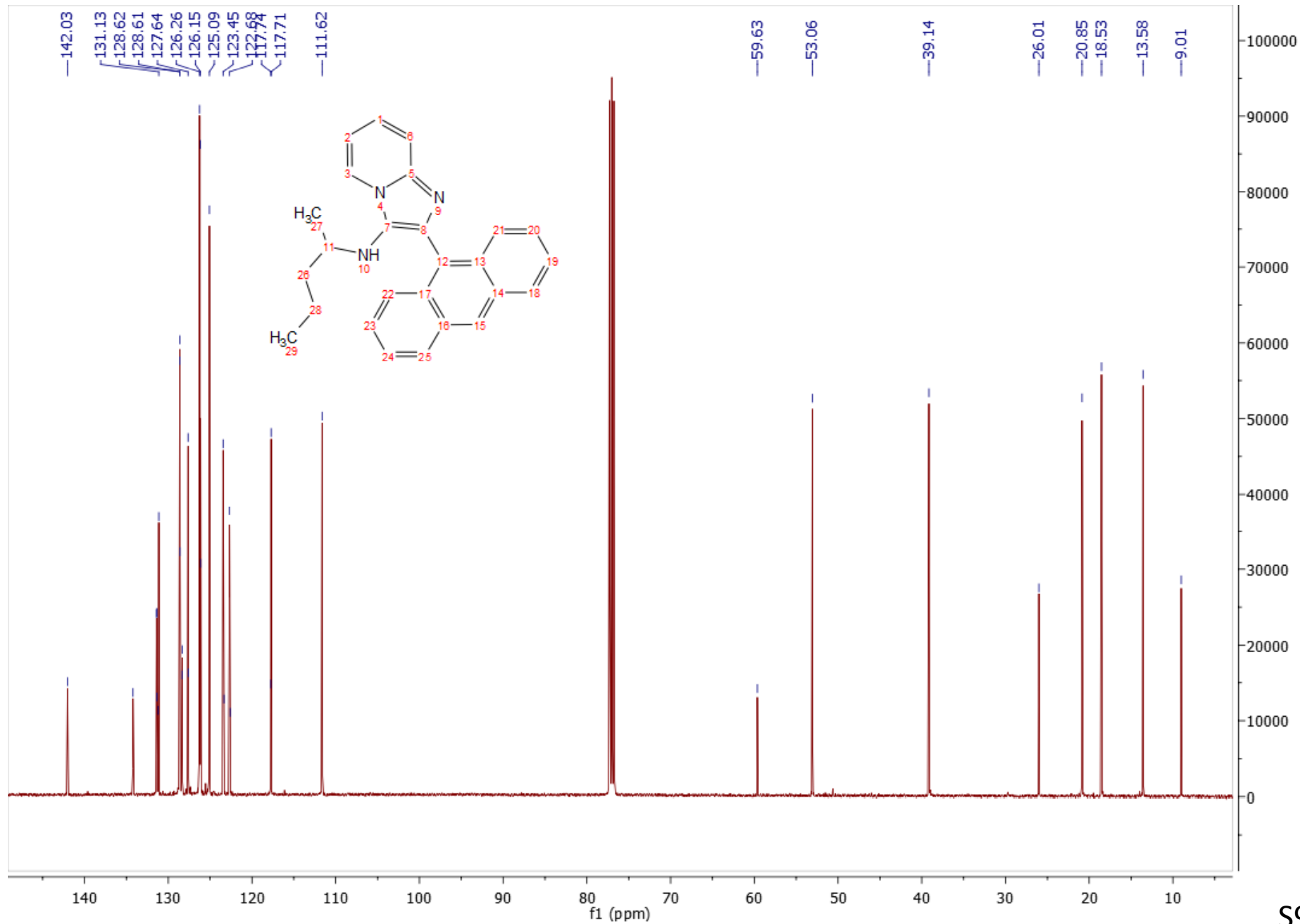
5c LC-MS



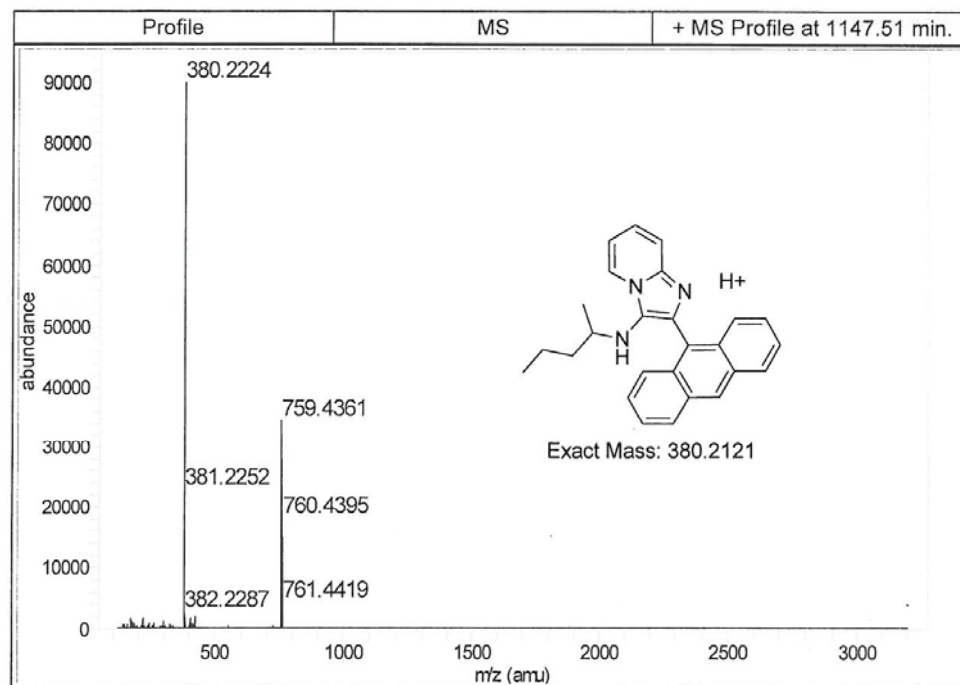
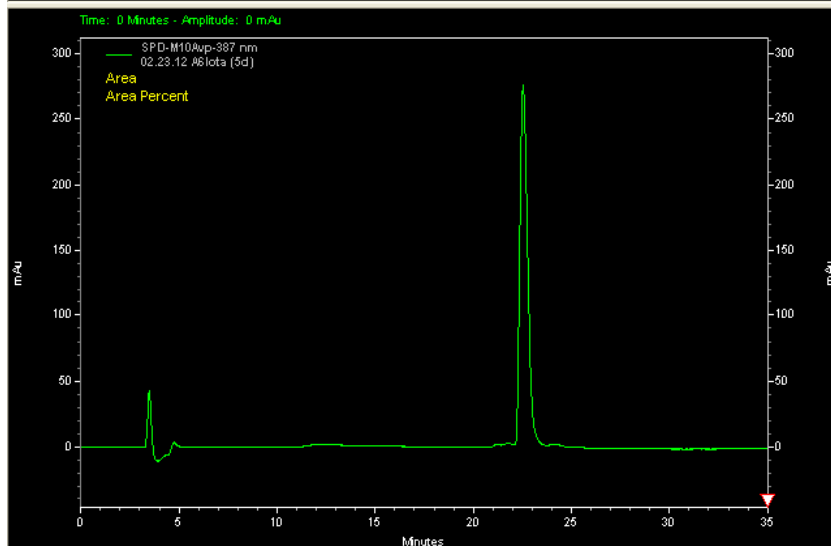
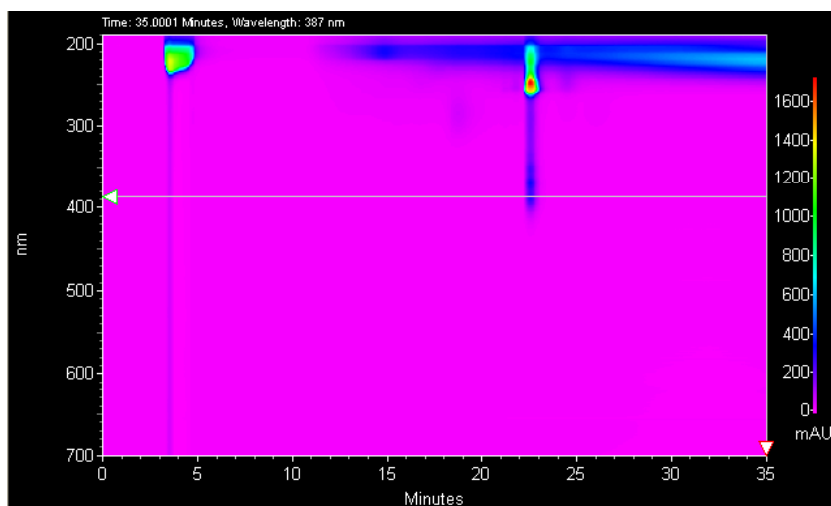
5d ¹H Spectrum



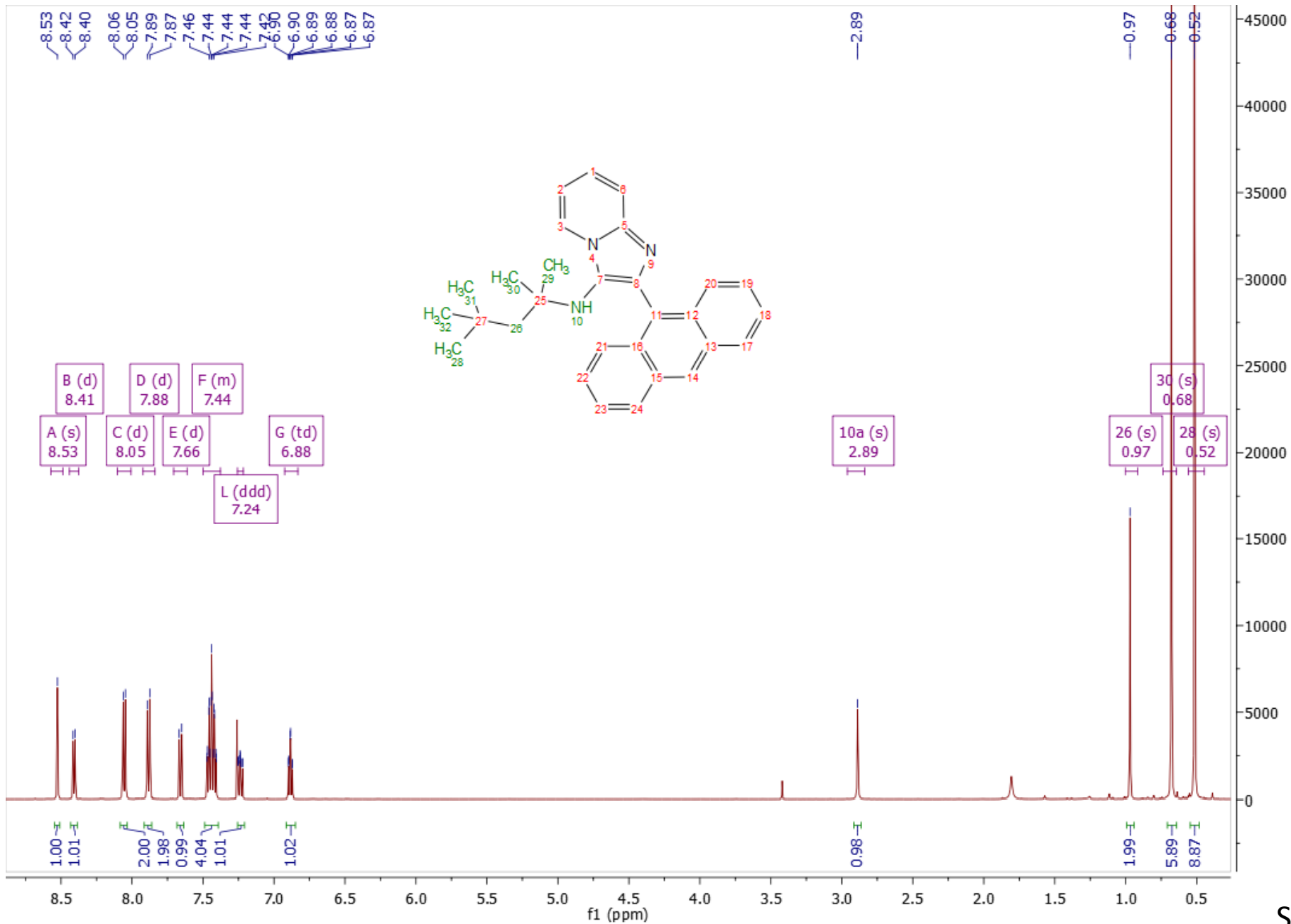
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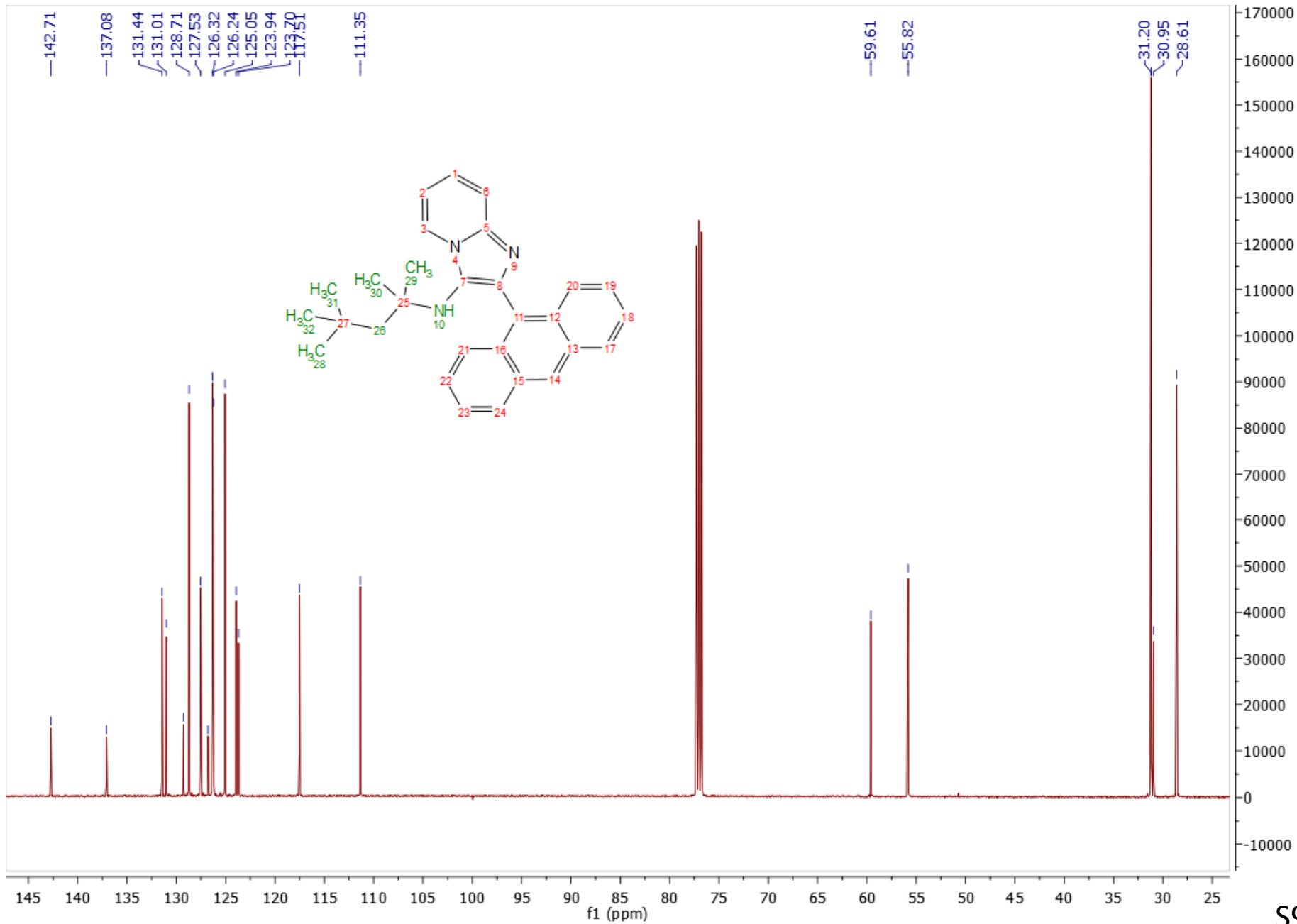
5d LC-MS



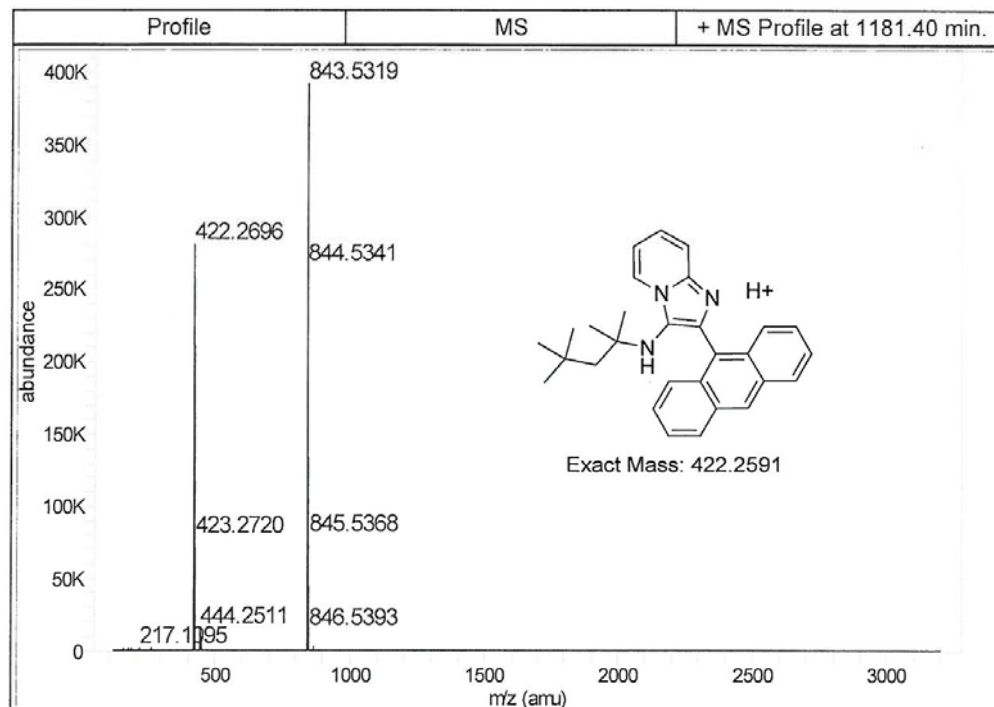
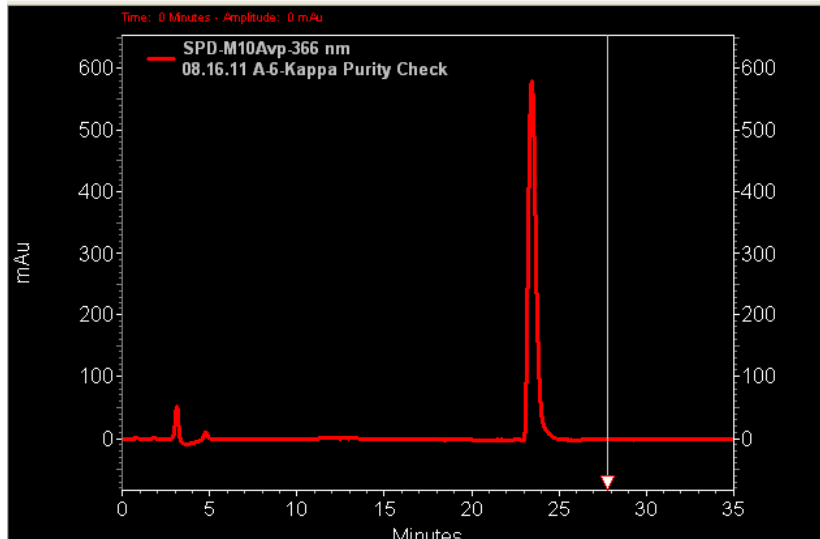
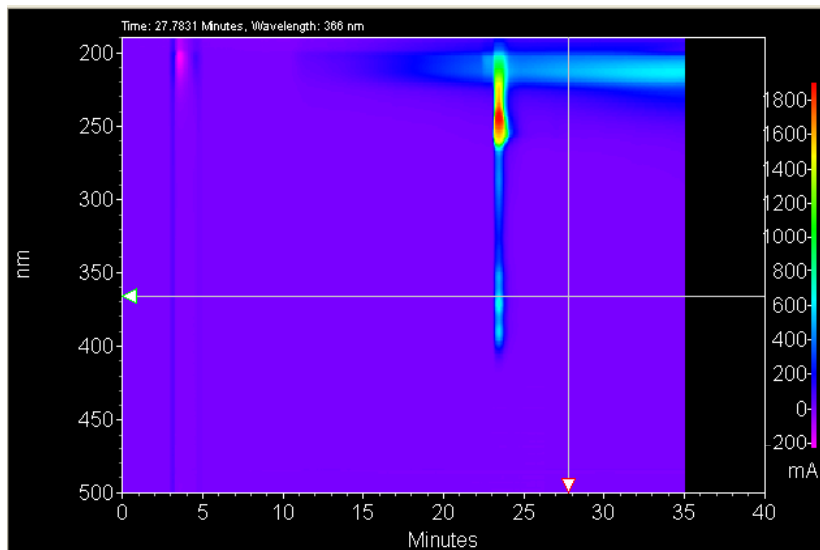
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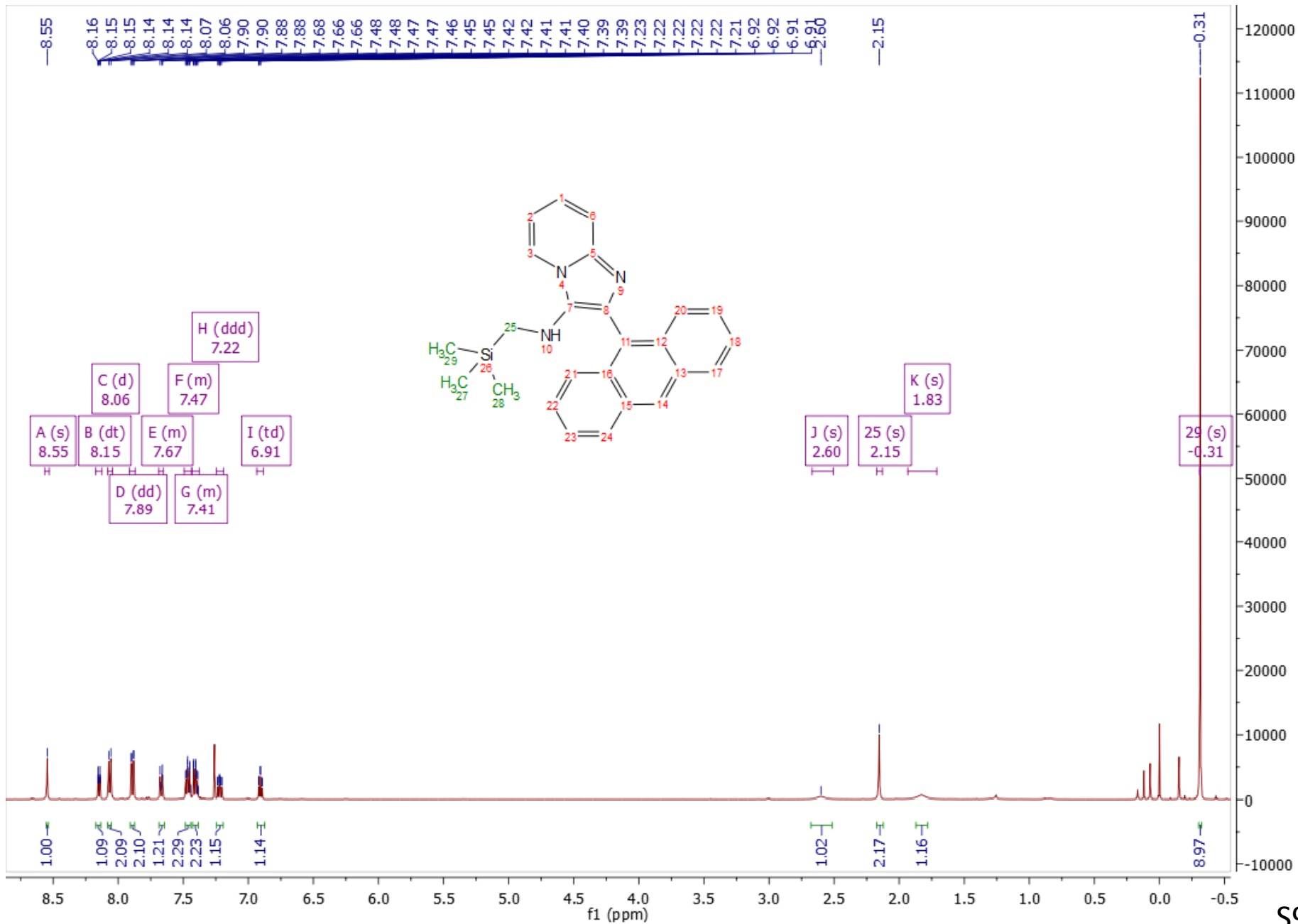
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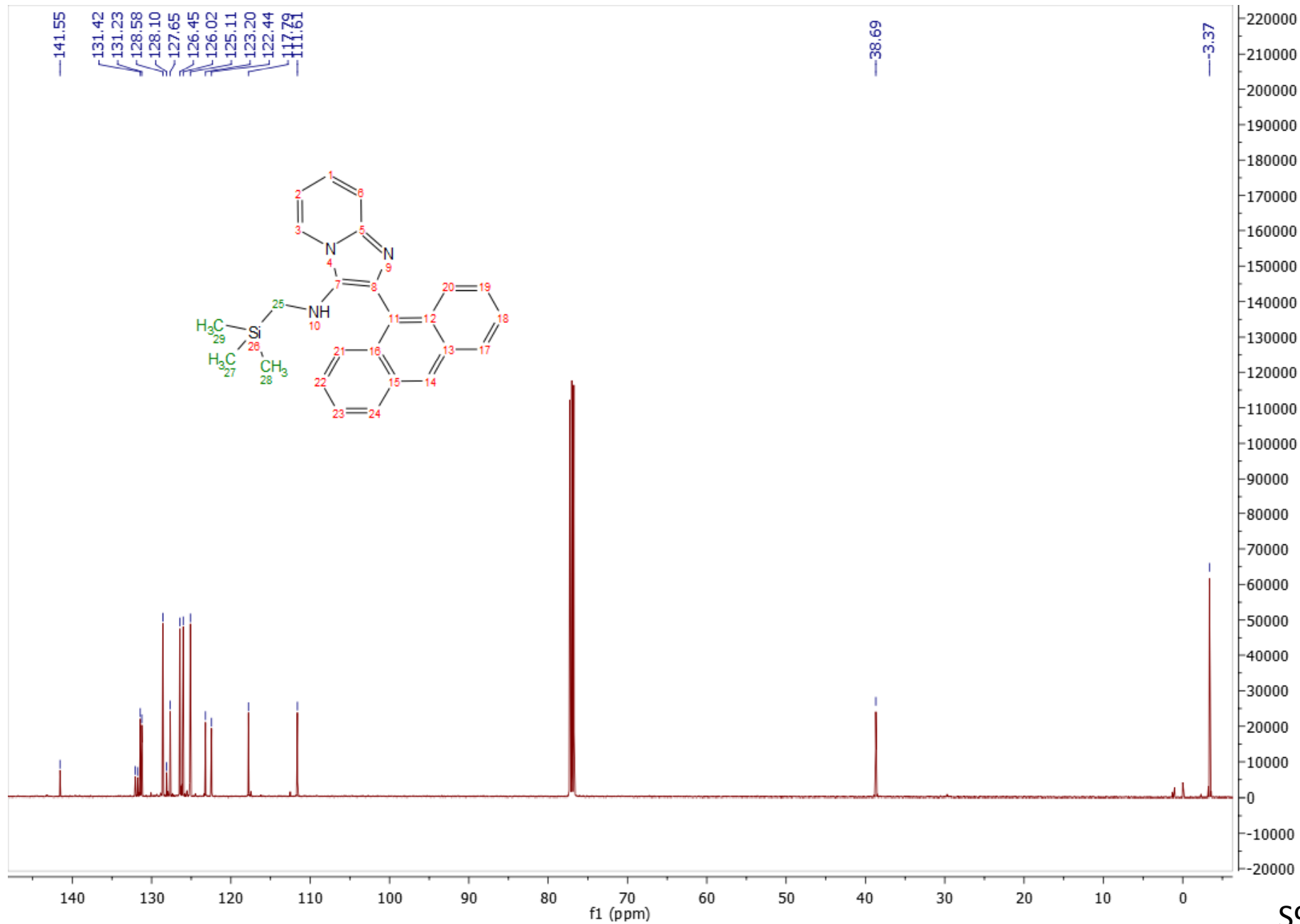
5e LC-MS



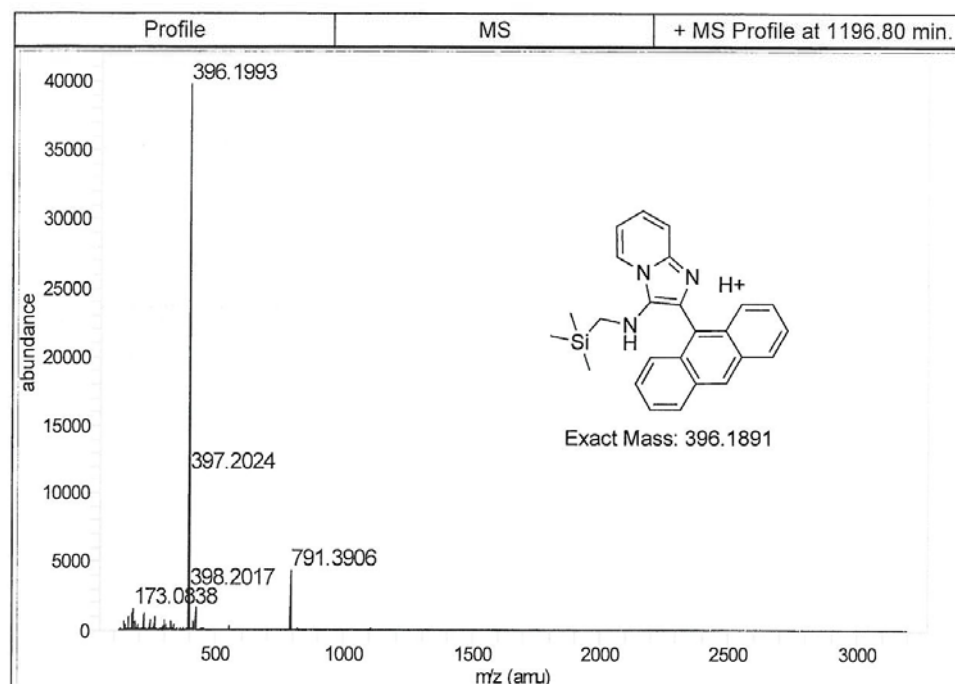
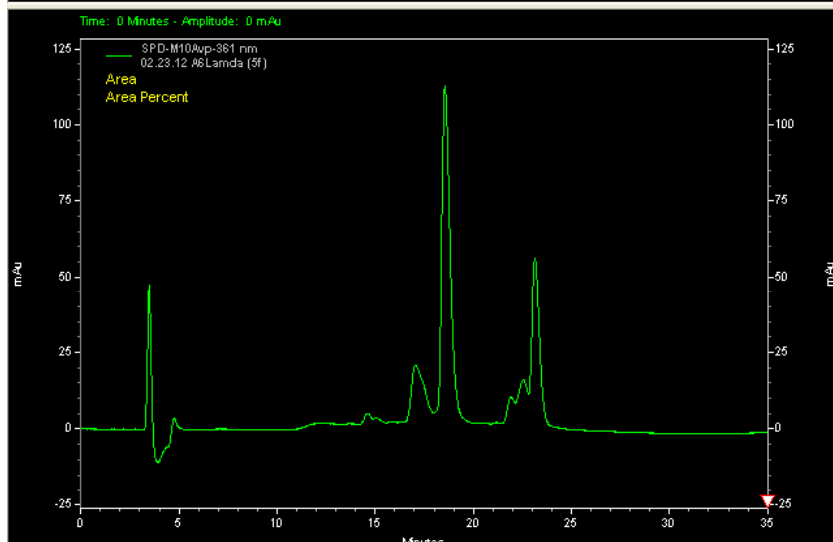
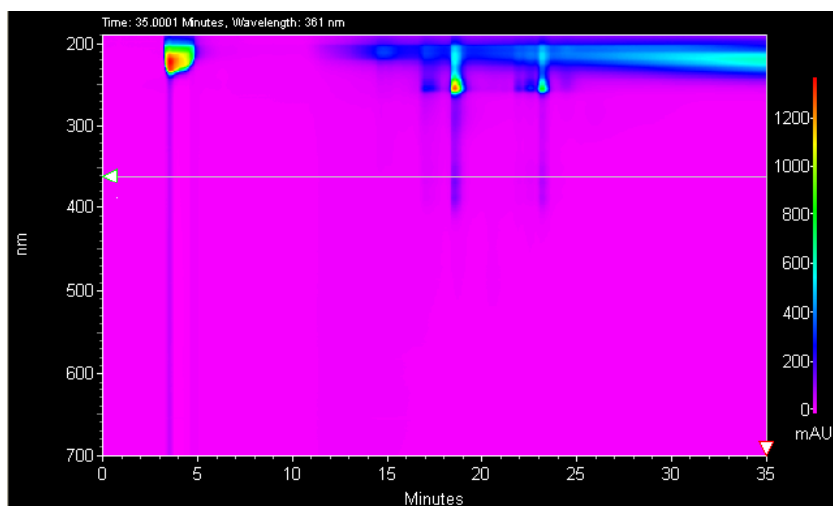
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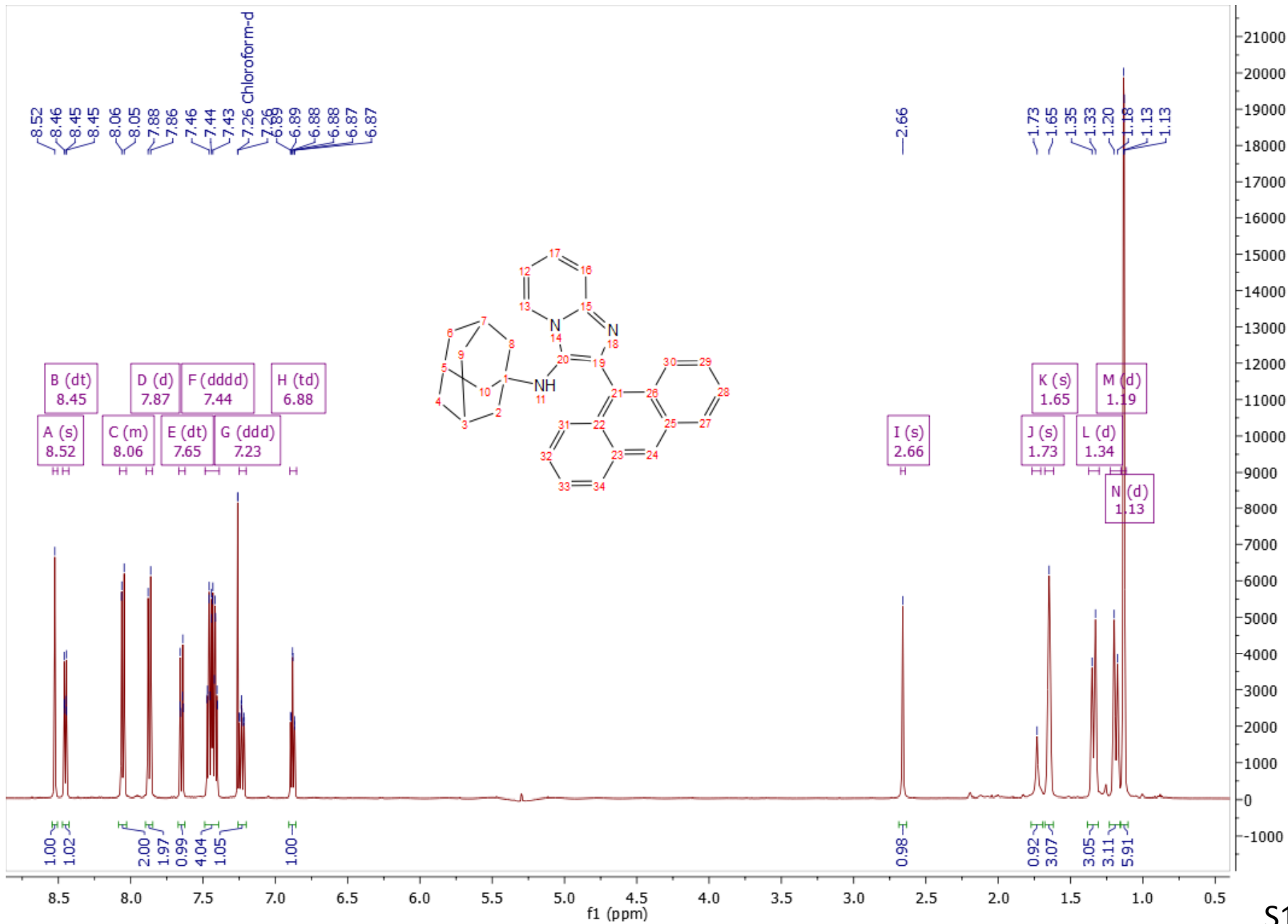
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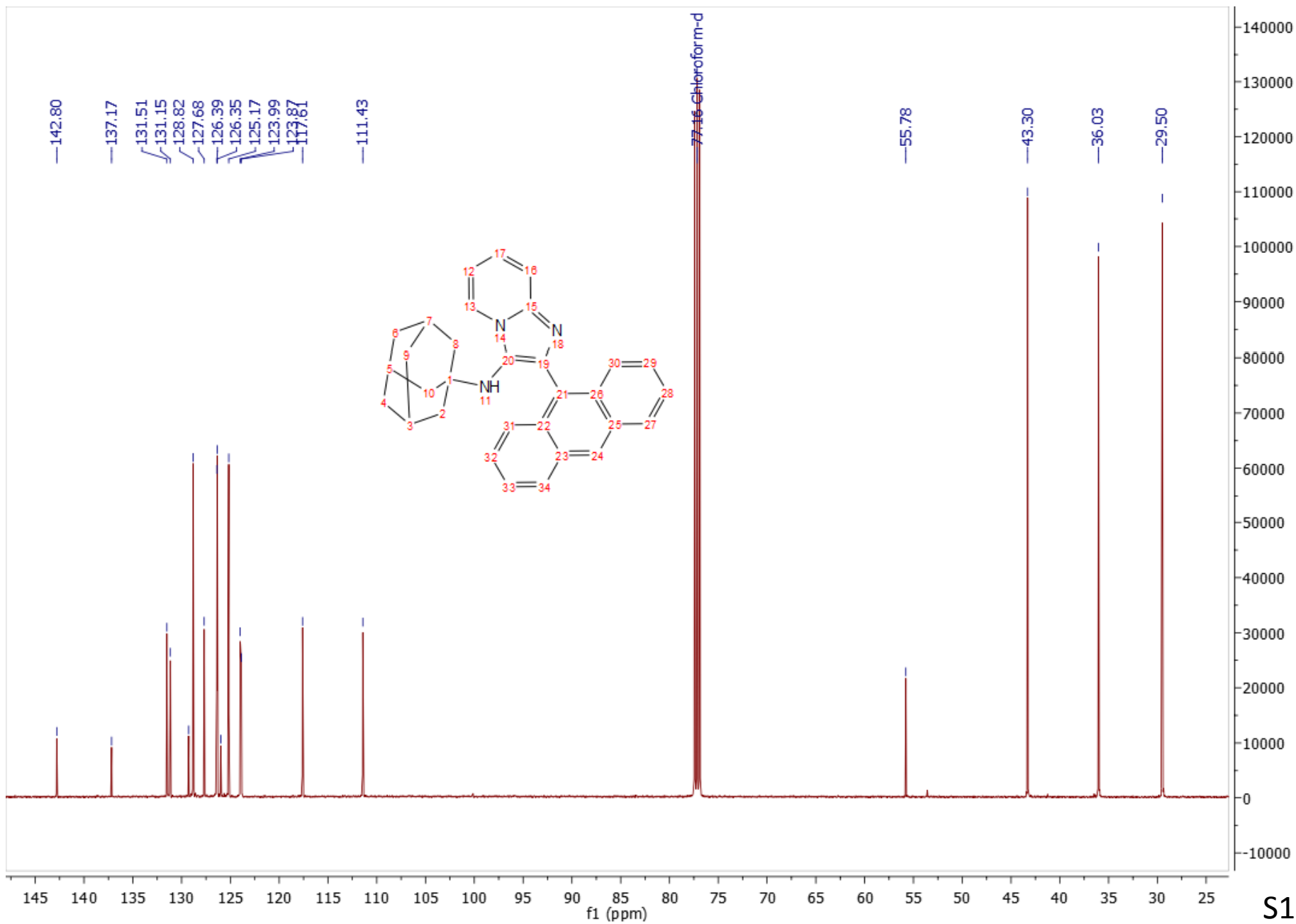
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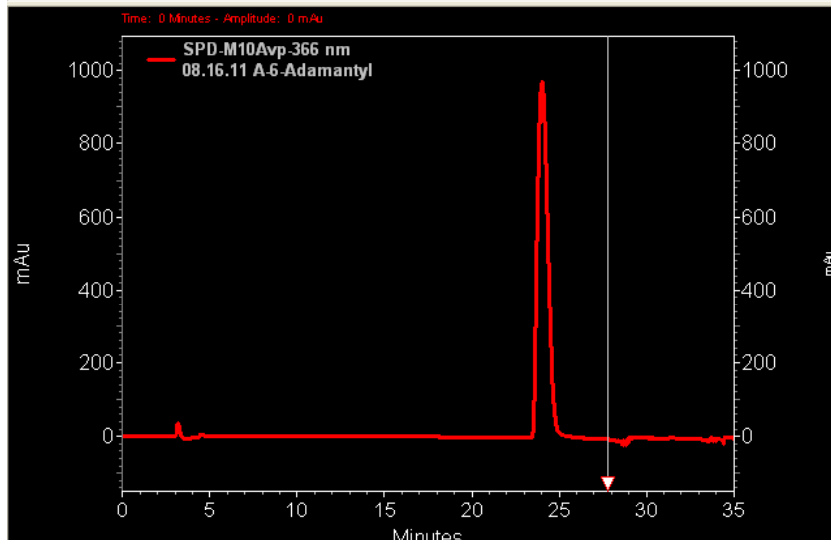
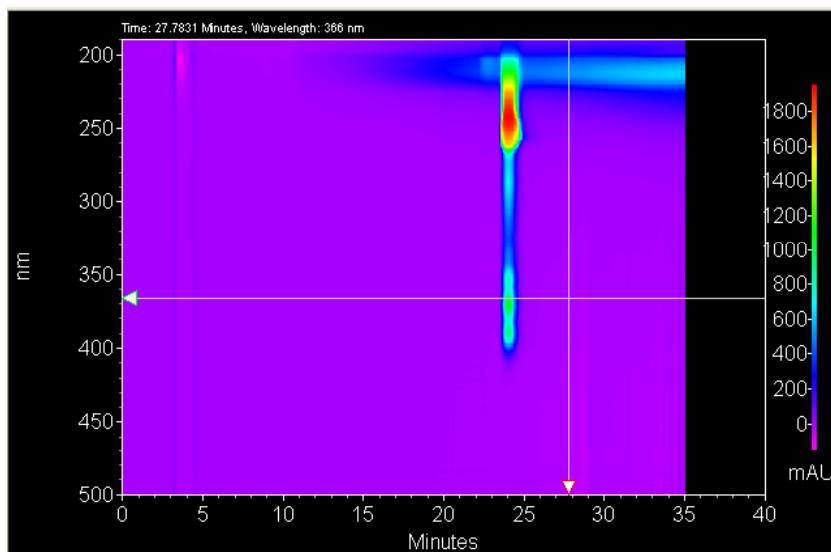
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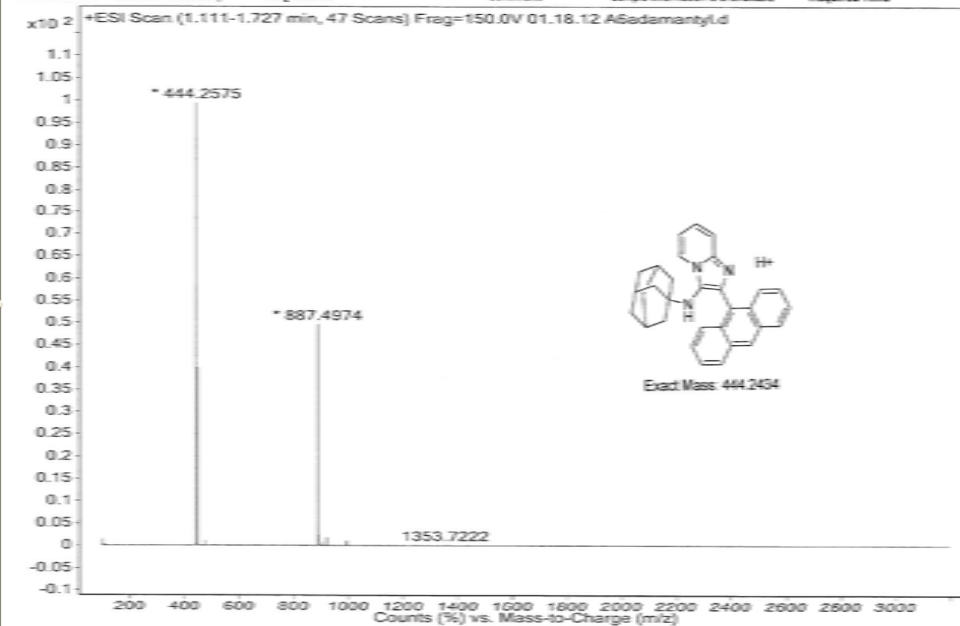
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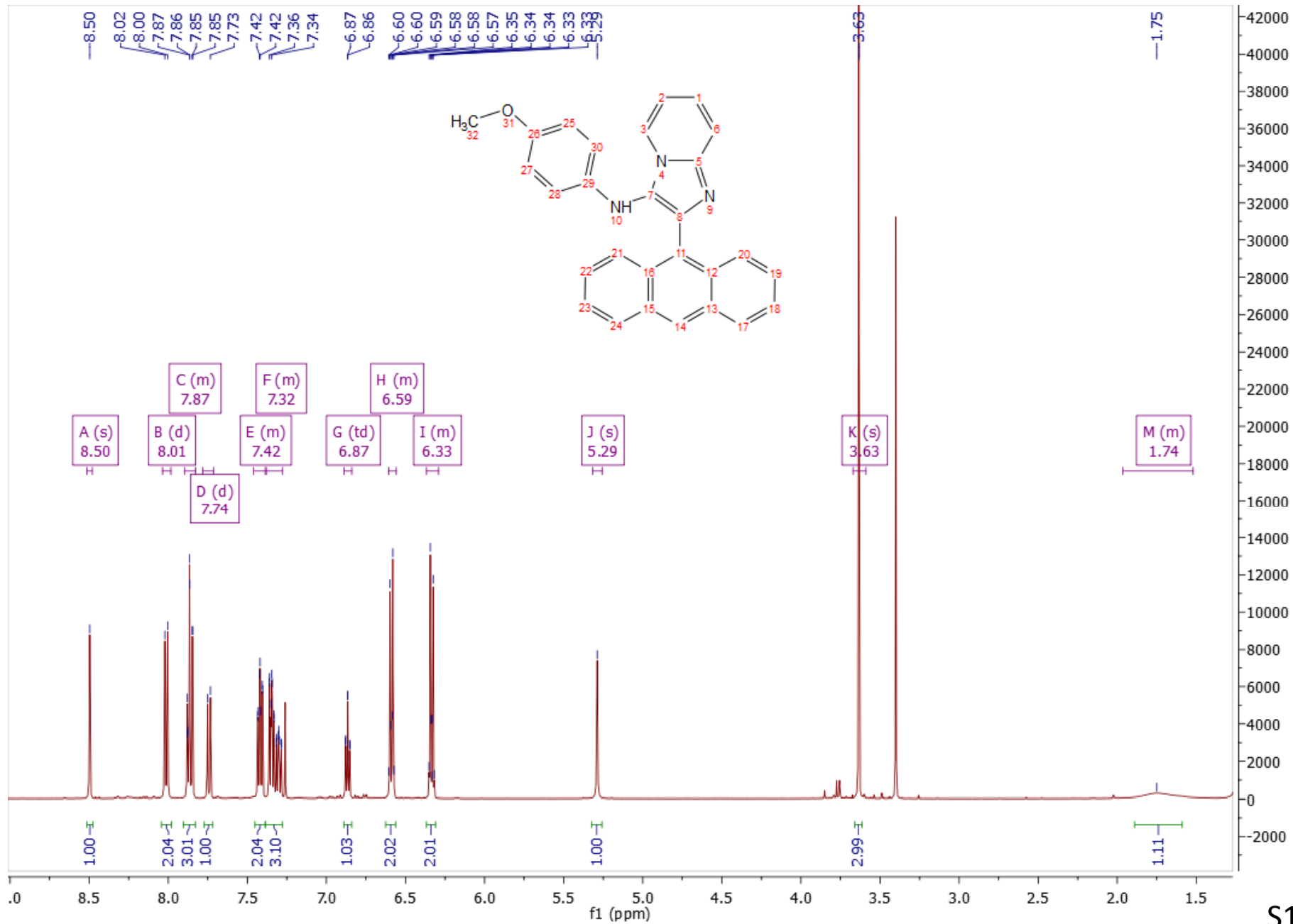
5g LC-MS



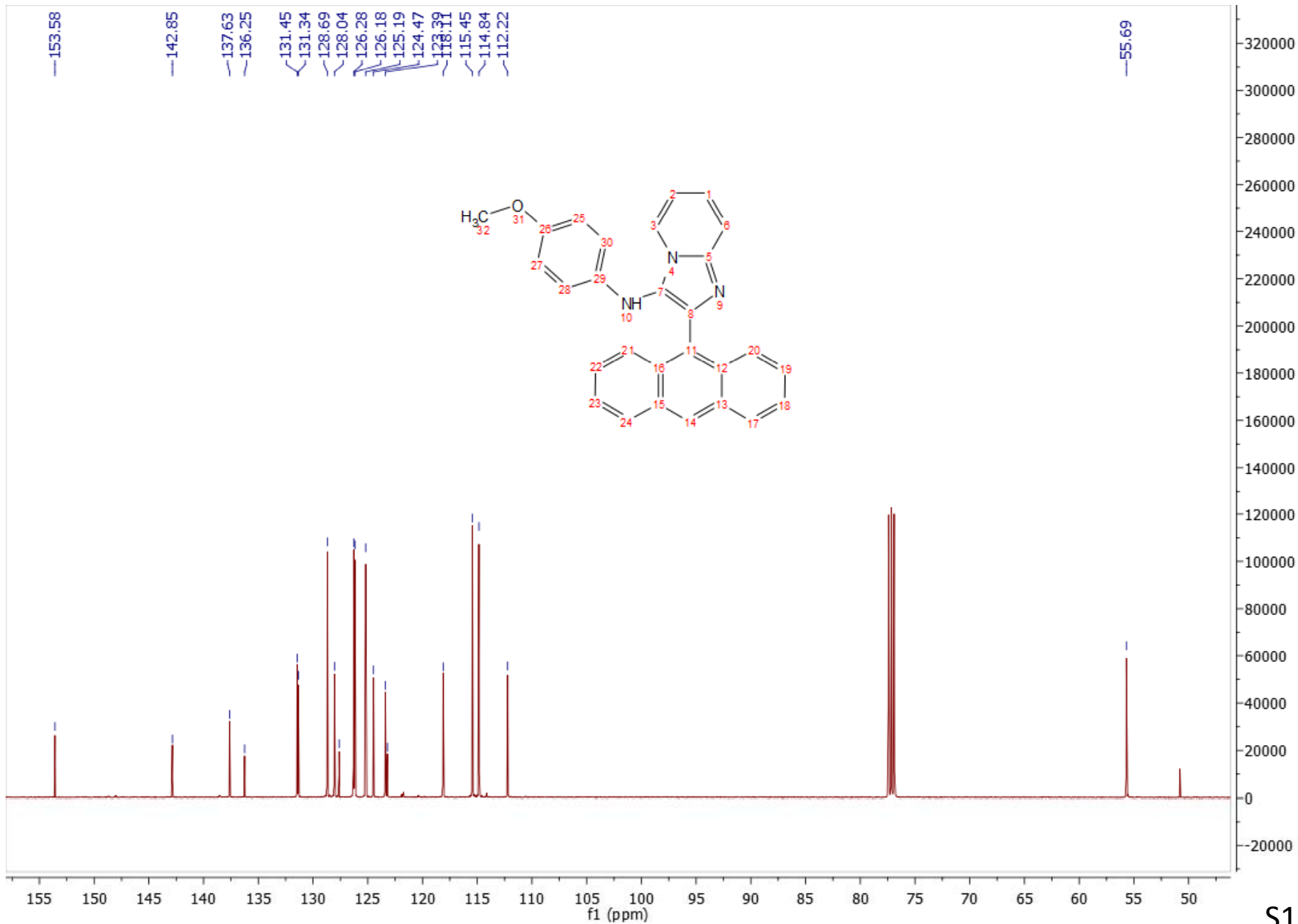
Sample Name	Injection	Position	Injection	Instrument Name	Sample Type	User Name	IRMS Calibration Status	Success
Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable	Unavailable
Data Filename	01.18.12 A6adamantyl	ACQ Method		Comment	Sample information is unavailable	Acquired Time		Unavailable



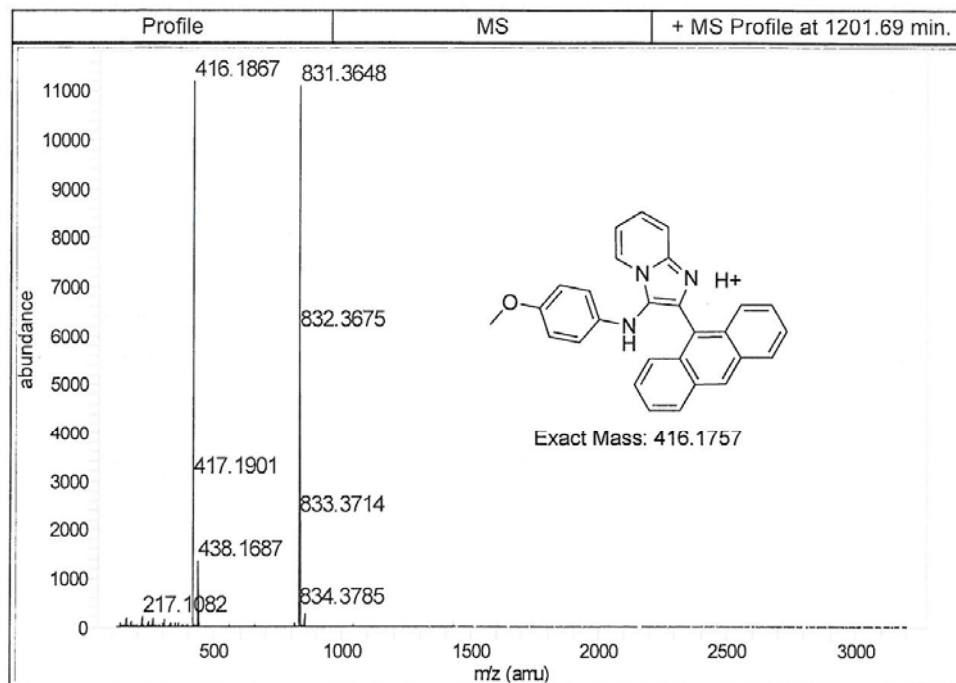
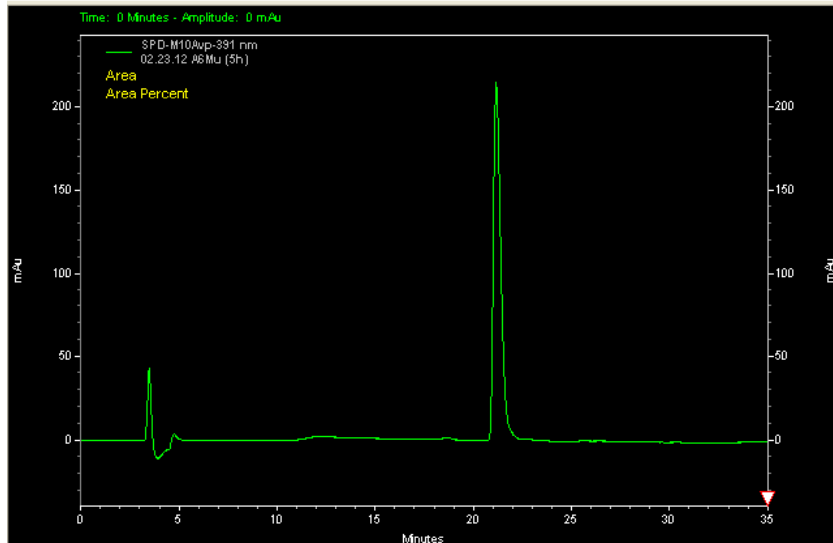
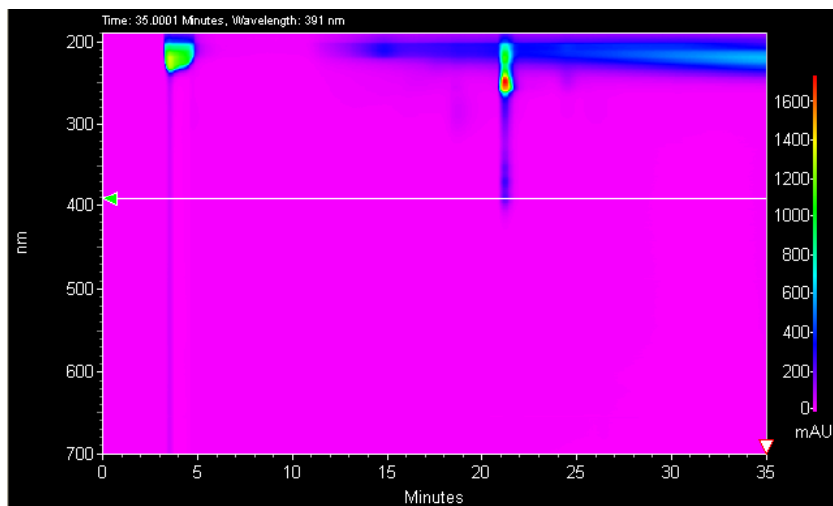
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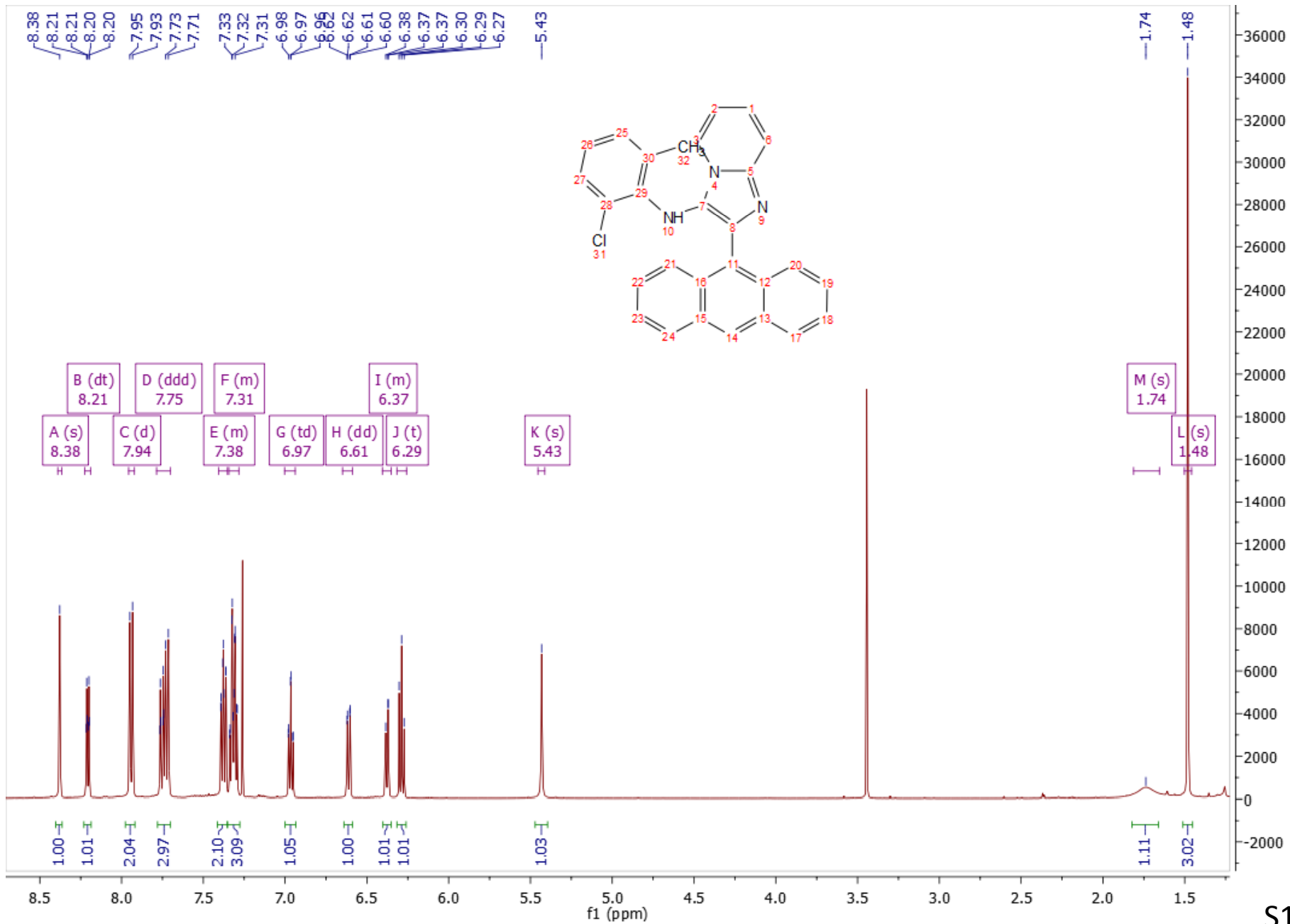
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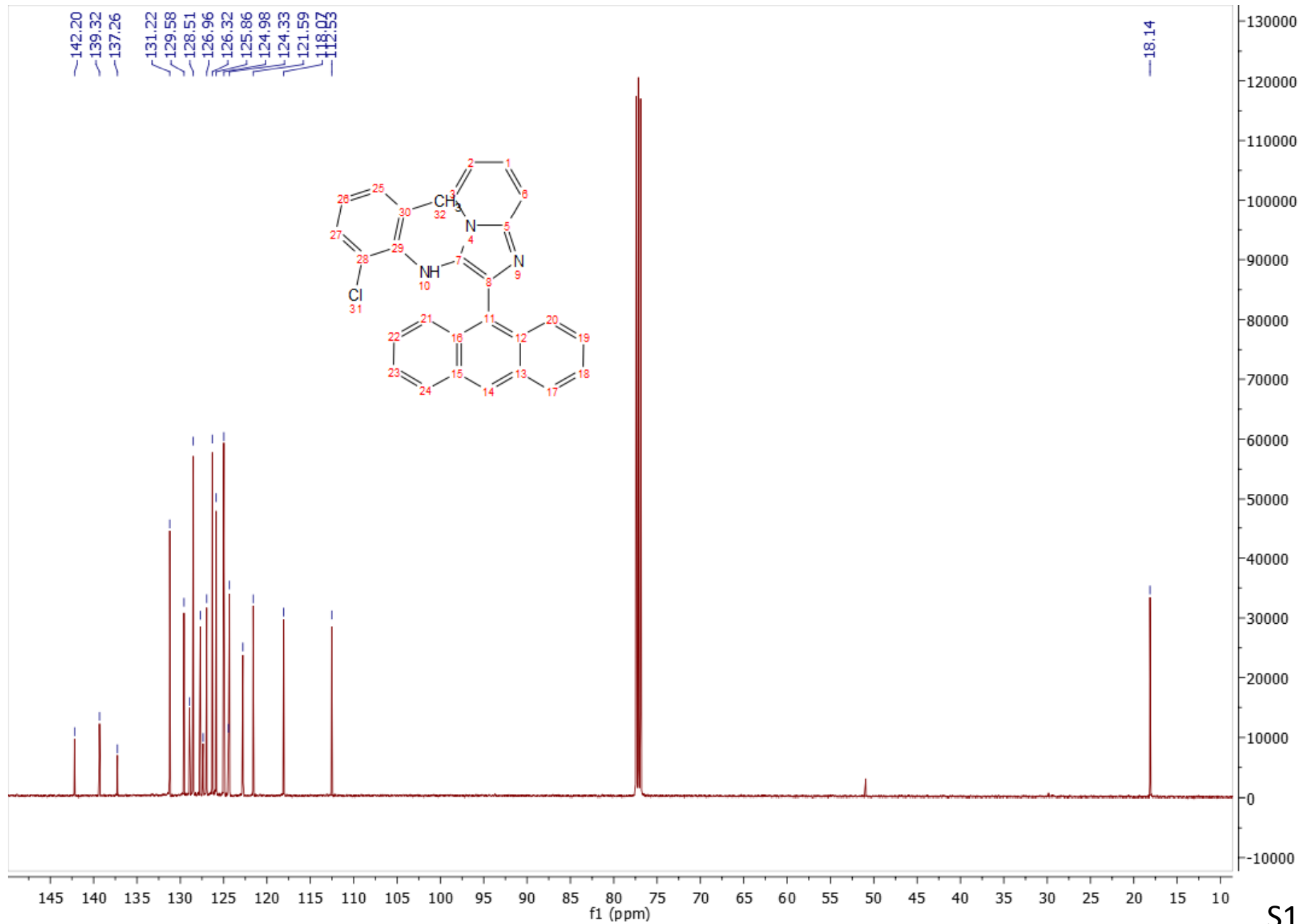
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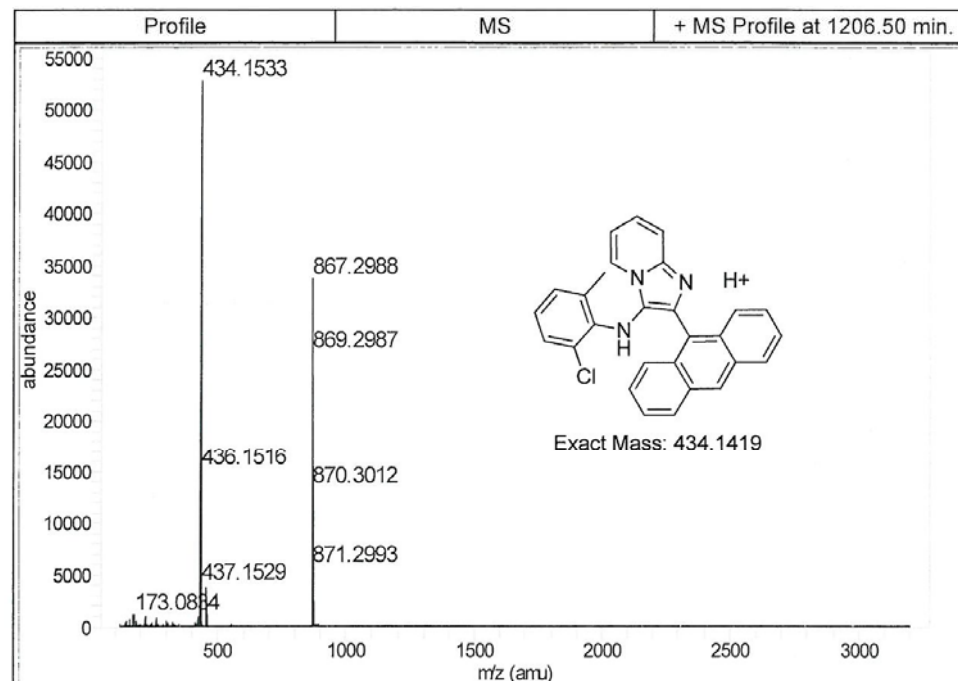
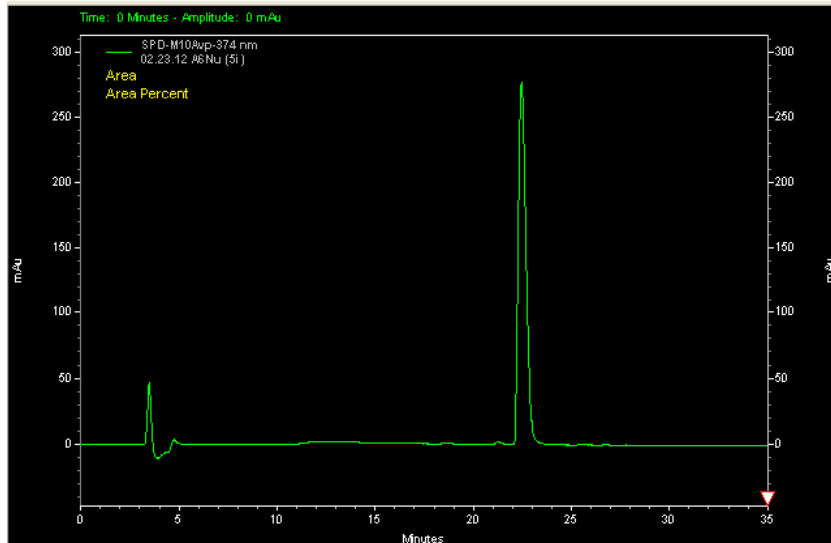
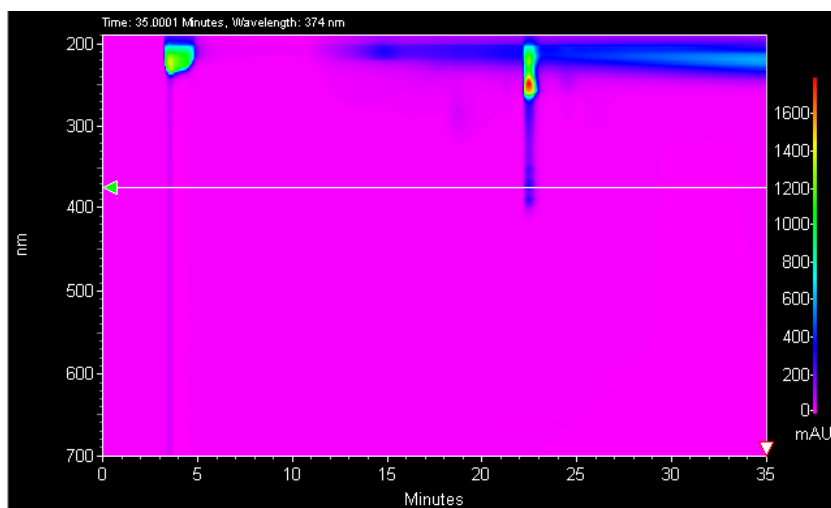
5i ¹H Spectrum



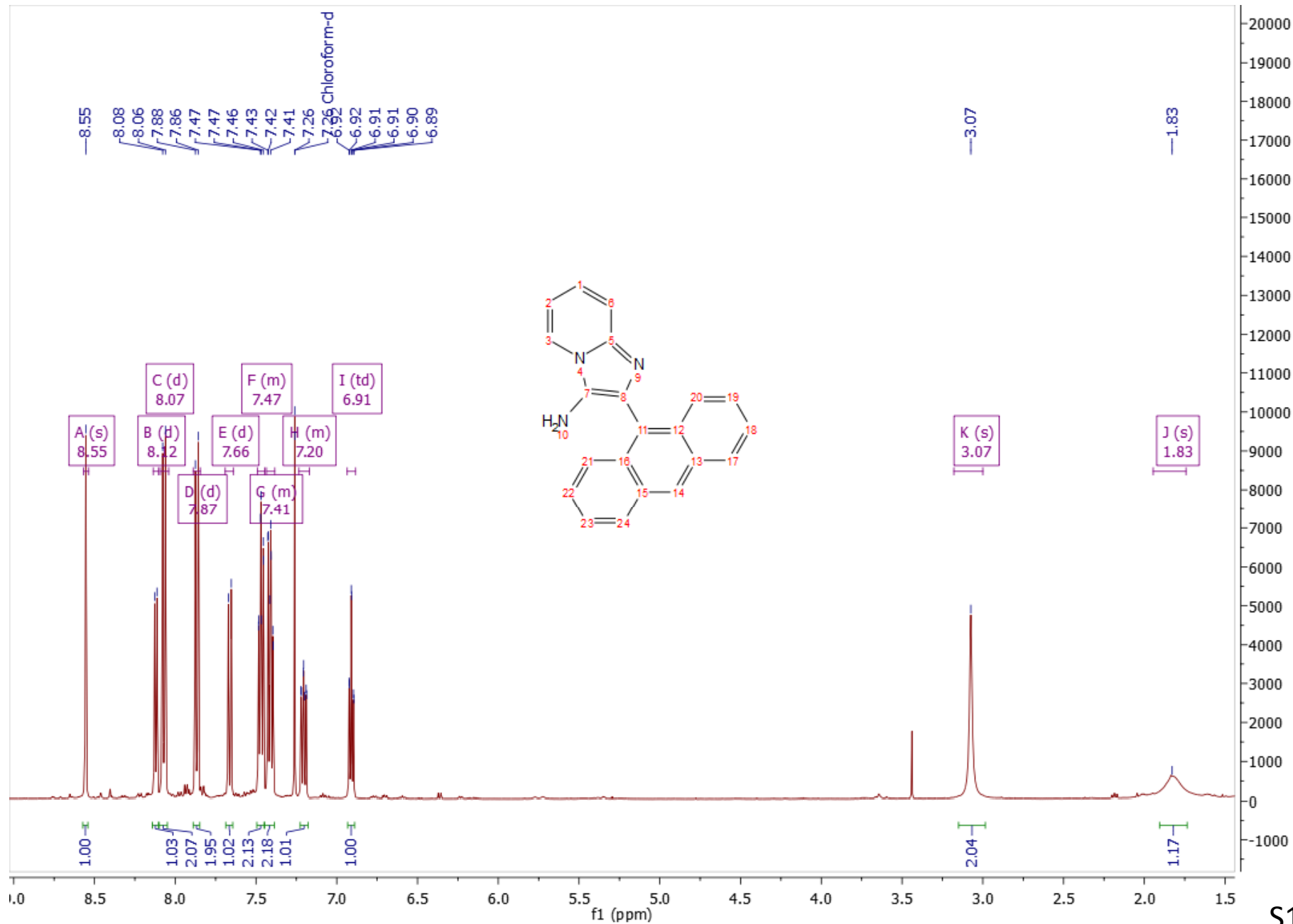
5i ¹³C Spectrum



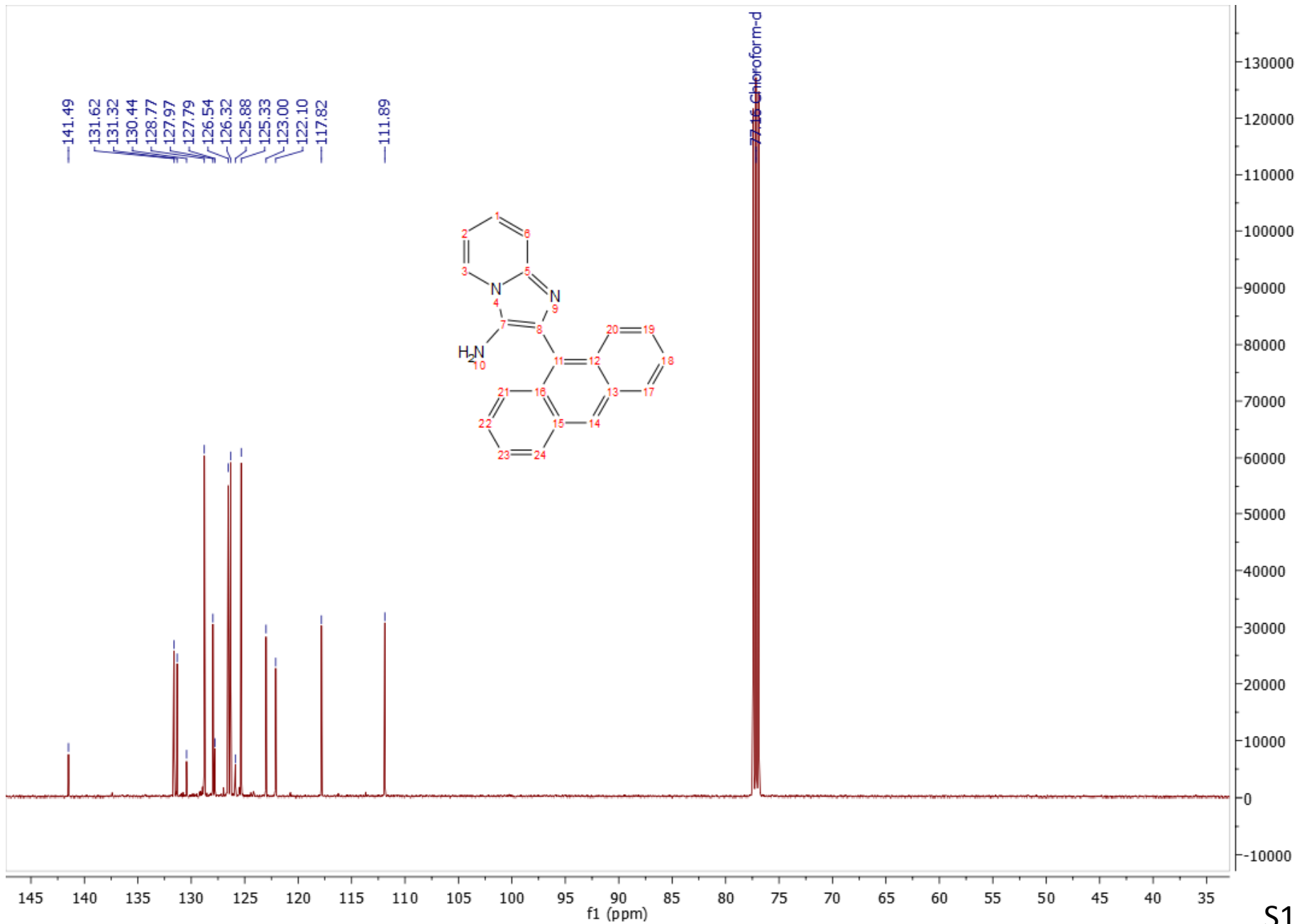
5i LC-MS



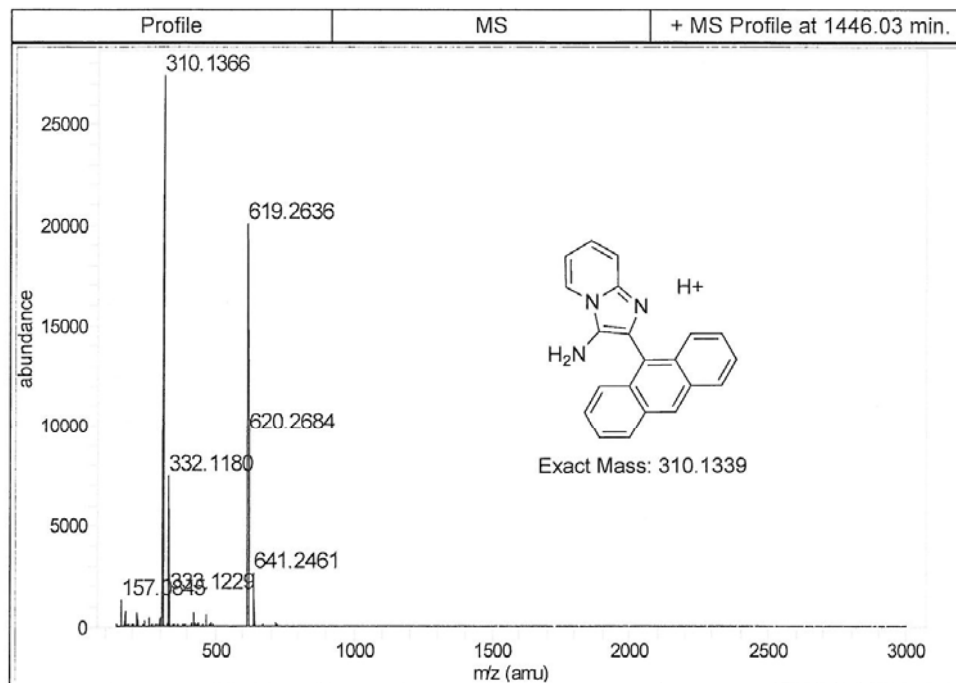
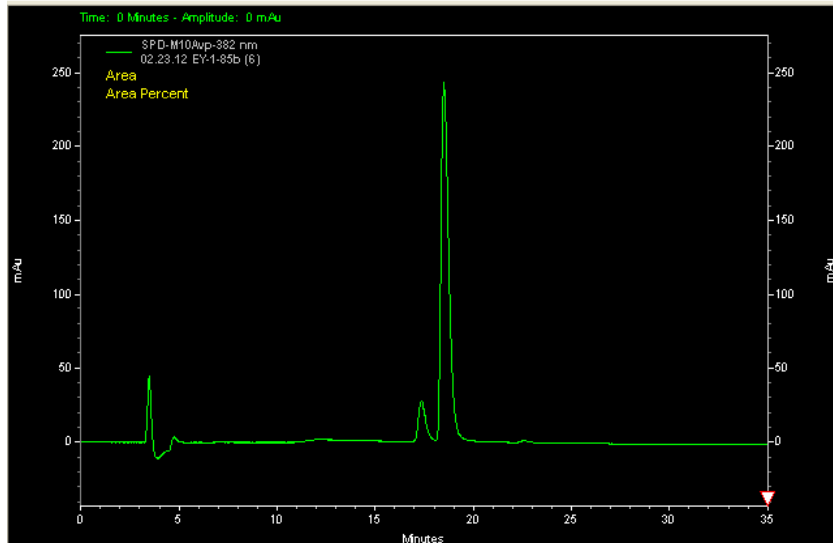
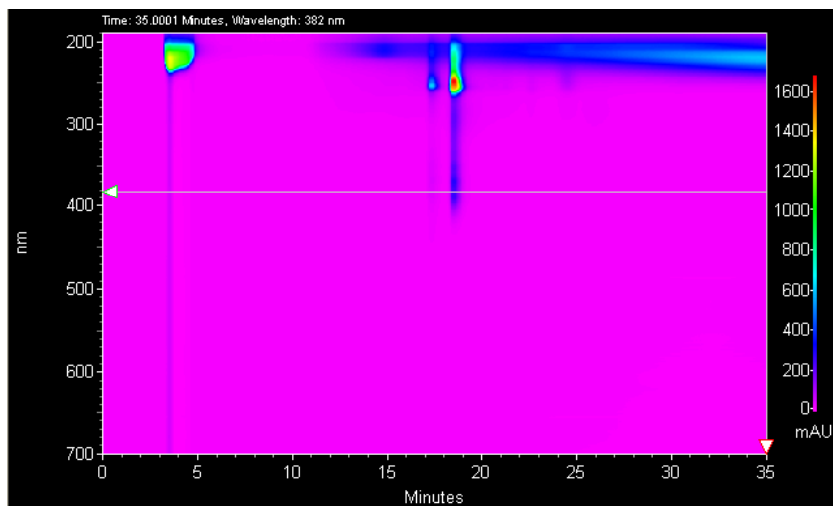
6 ¹H Spectrum



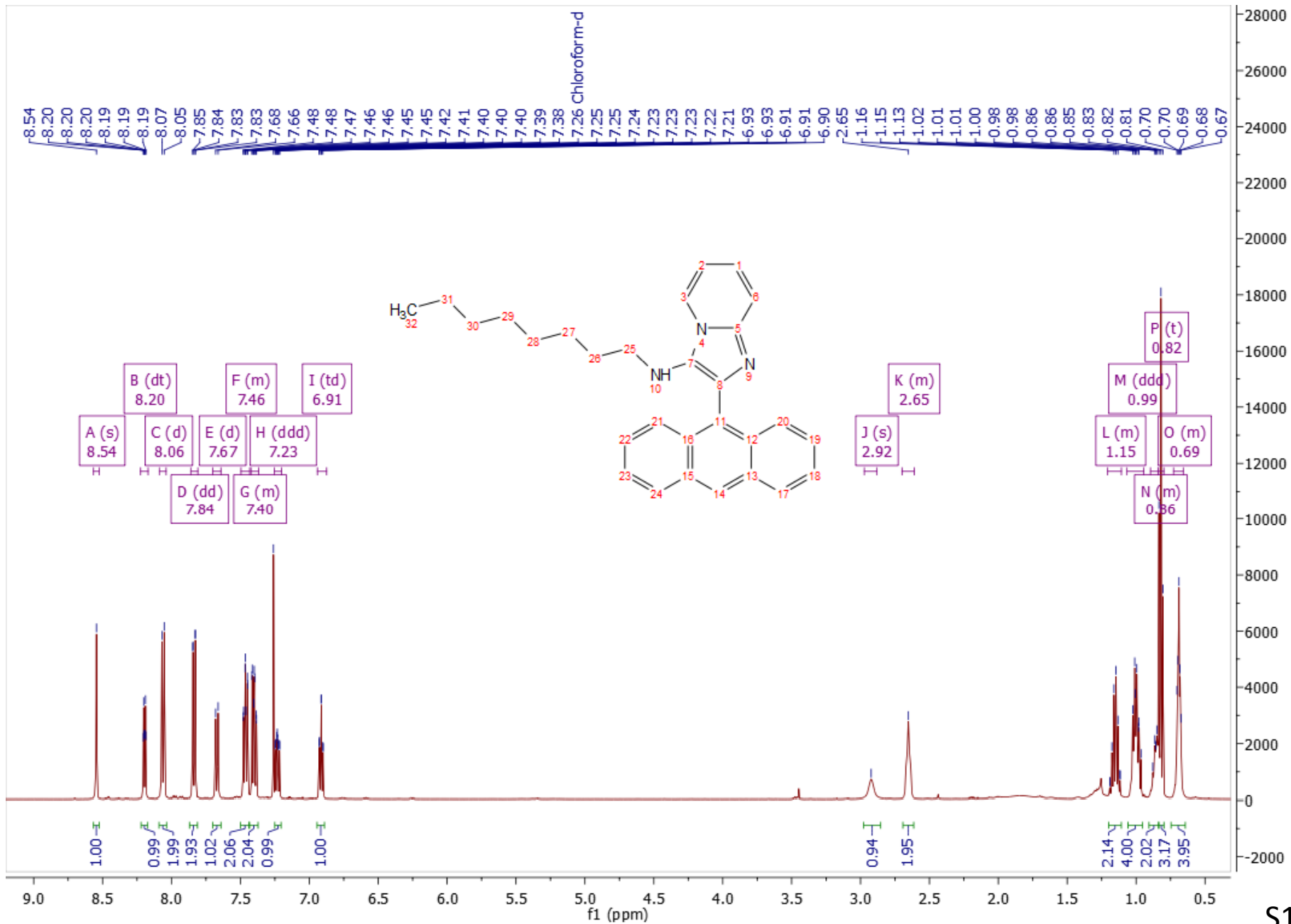
6 ¹³C Spectrum



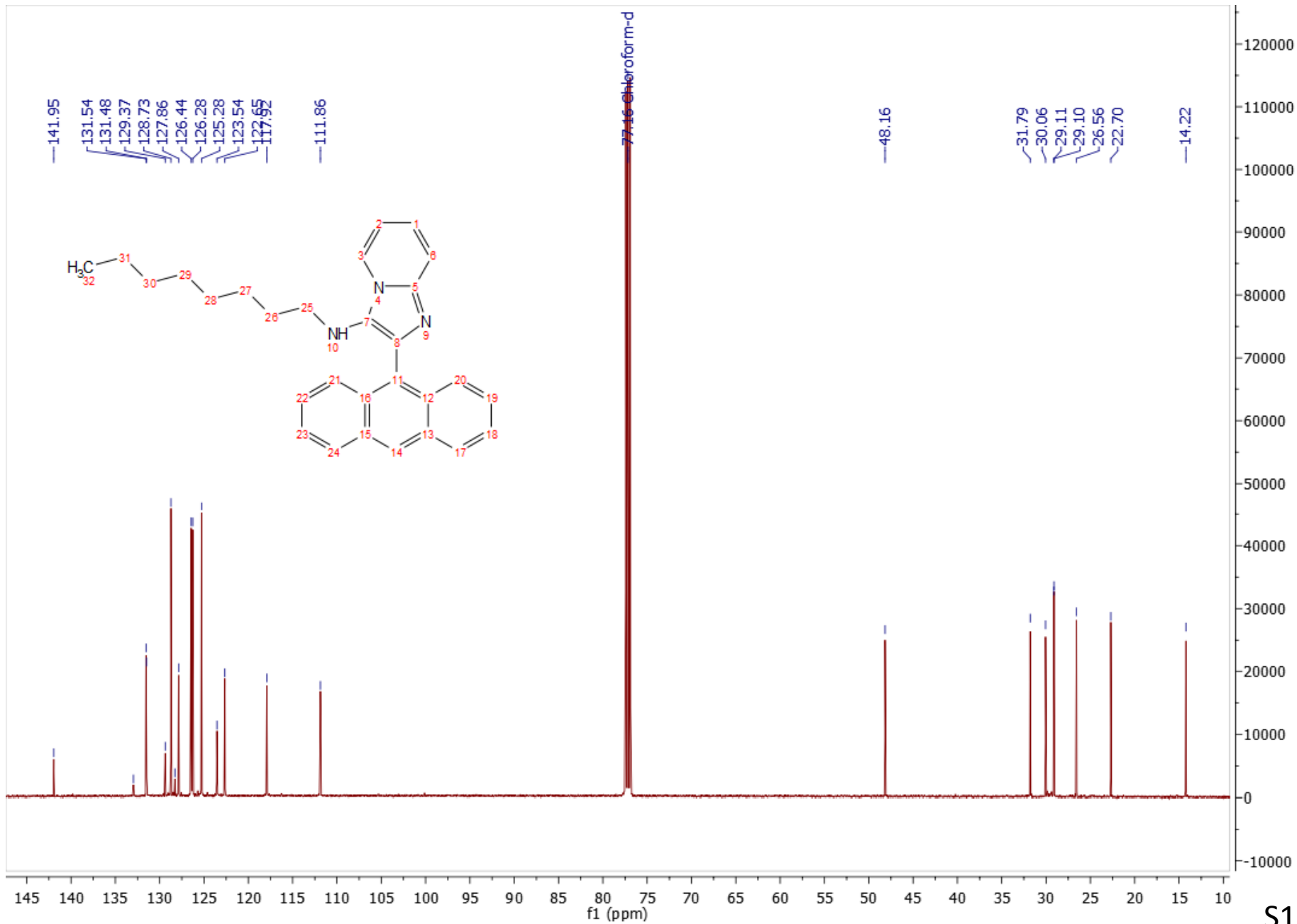
6 LC-MS



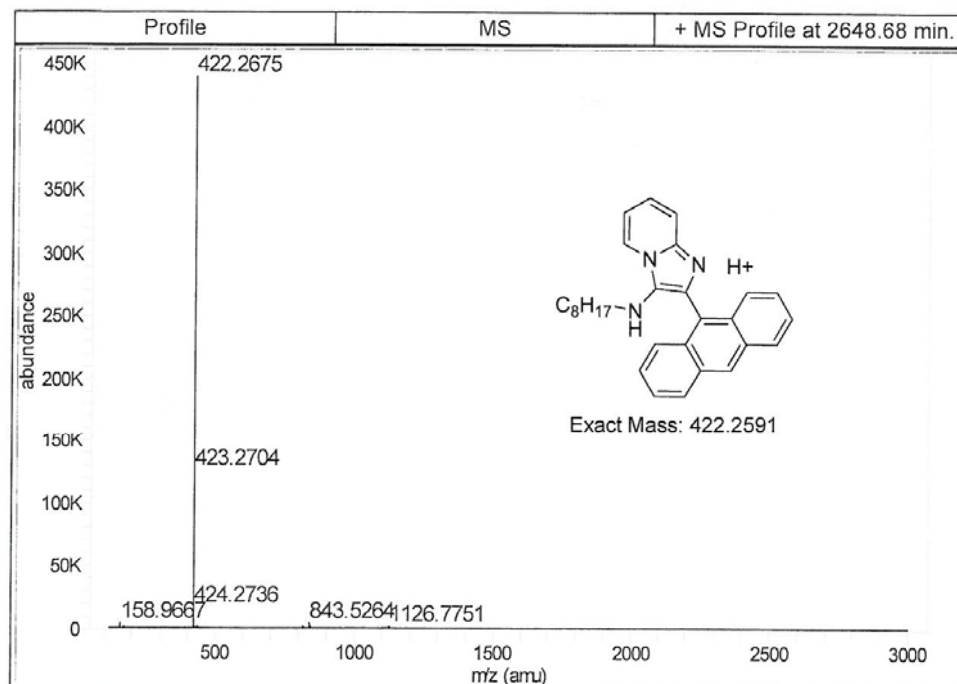
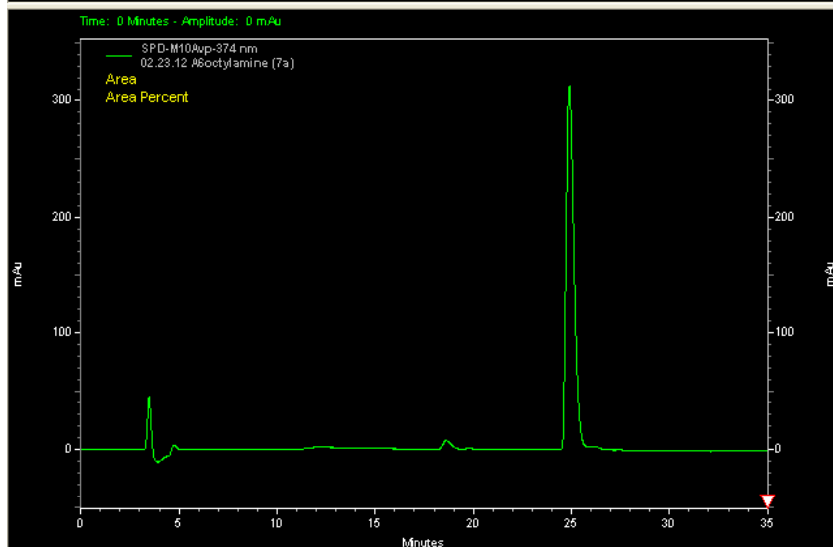
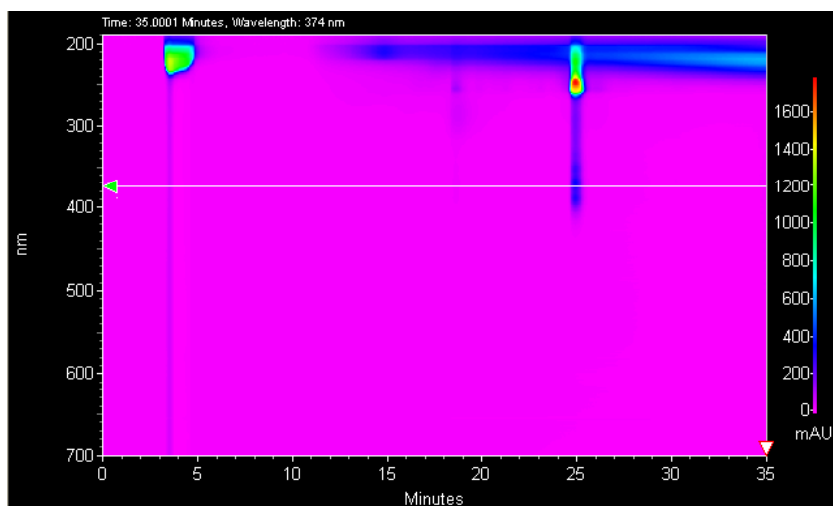
7a ¹H Spectrum



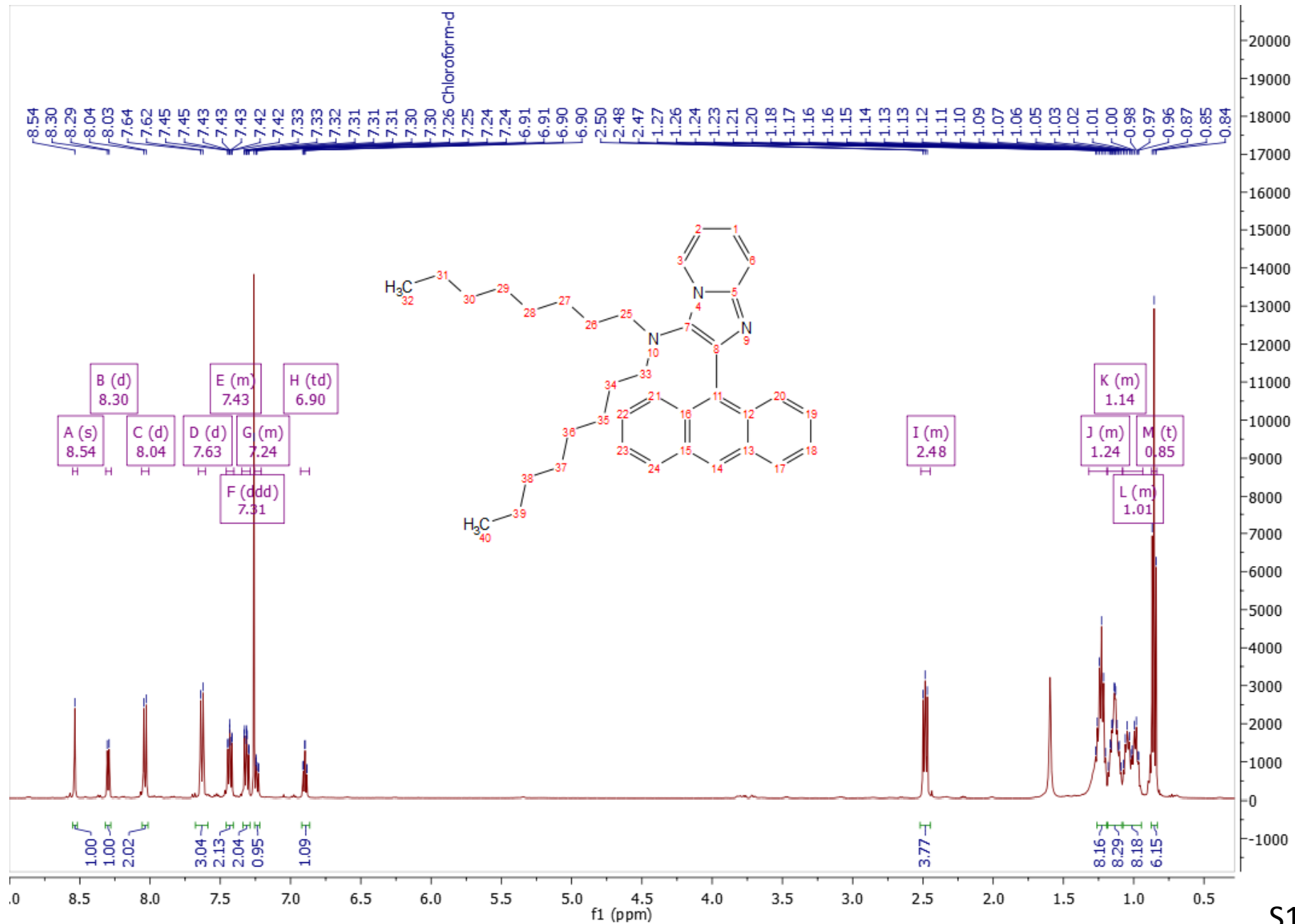
7a ¹³C Spectrum



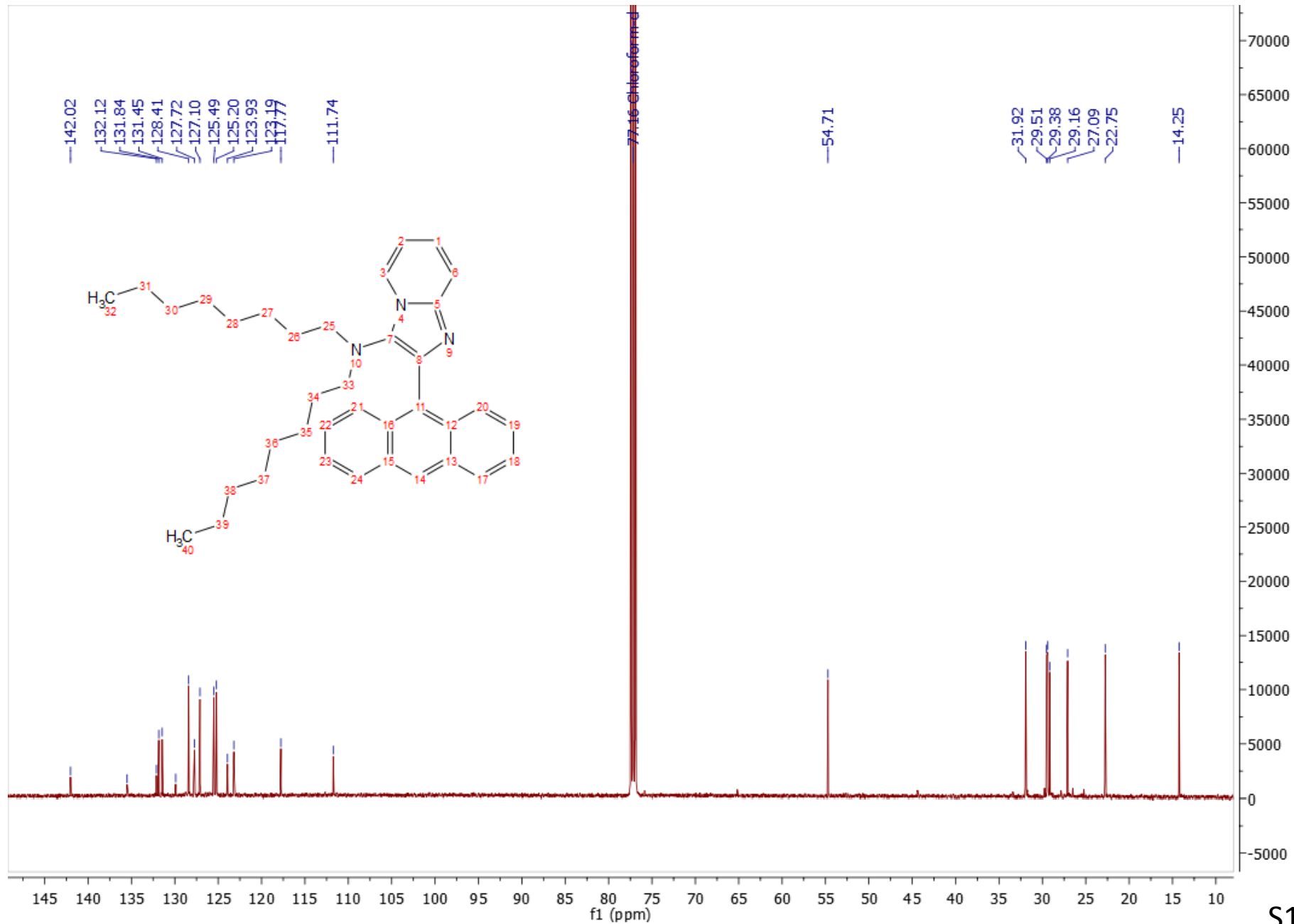
7a LC-MS



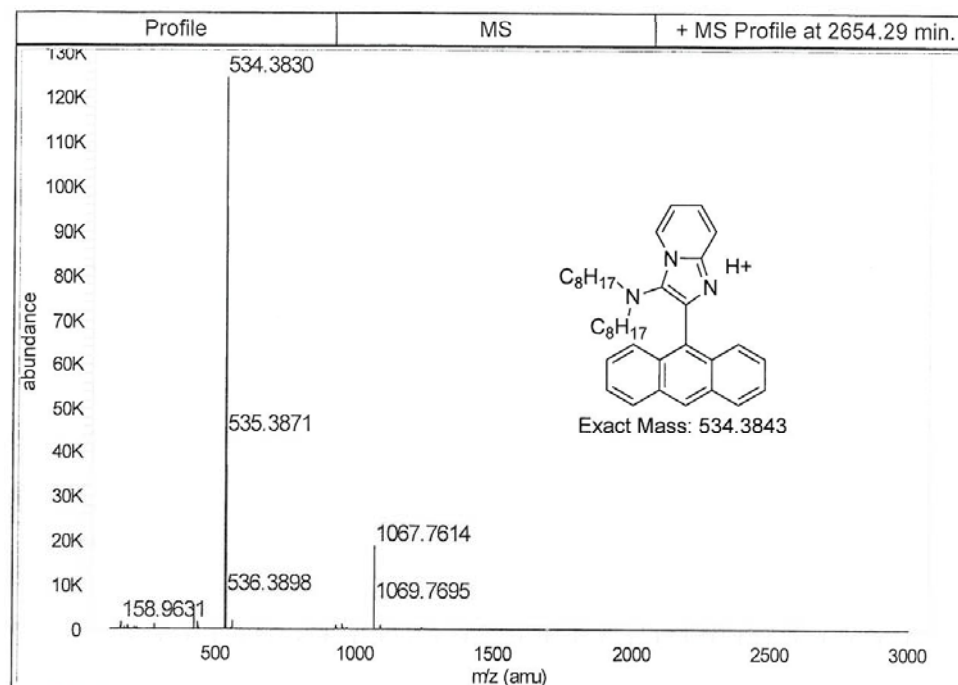
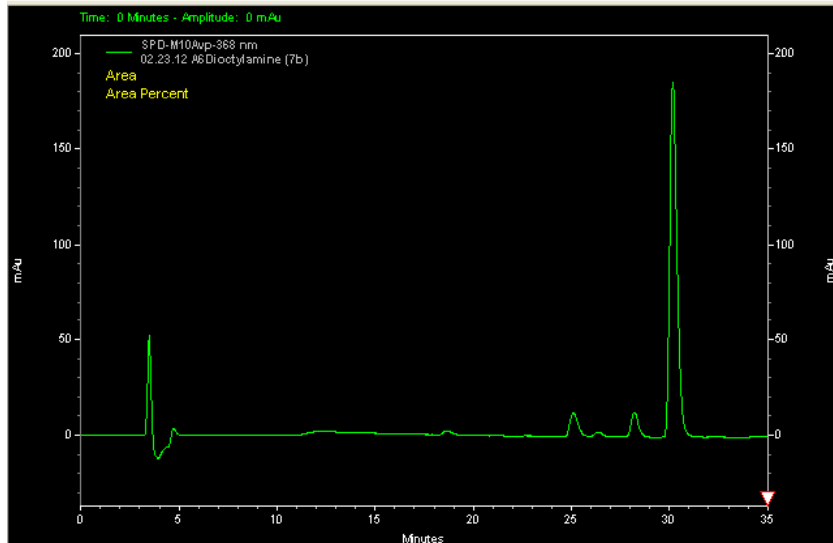
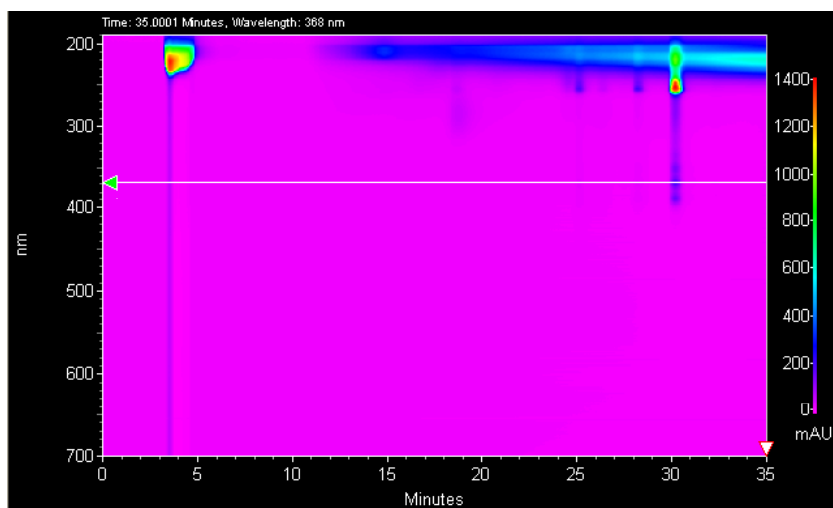
7b ¹H Spectrum



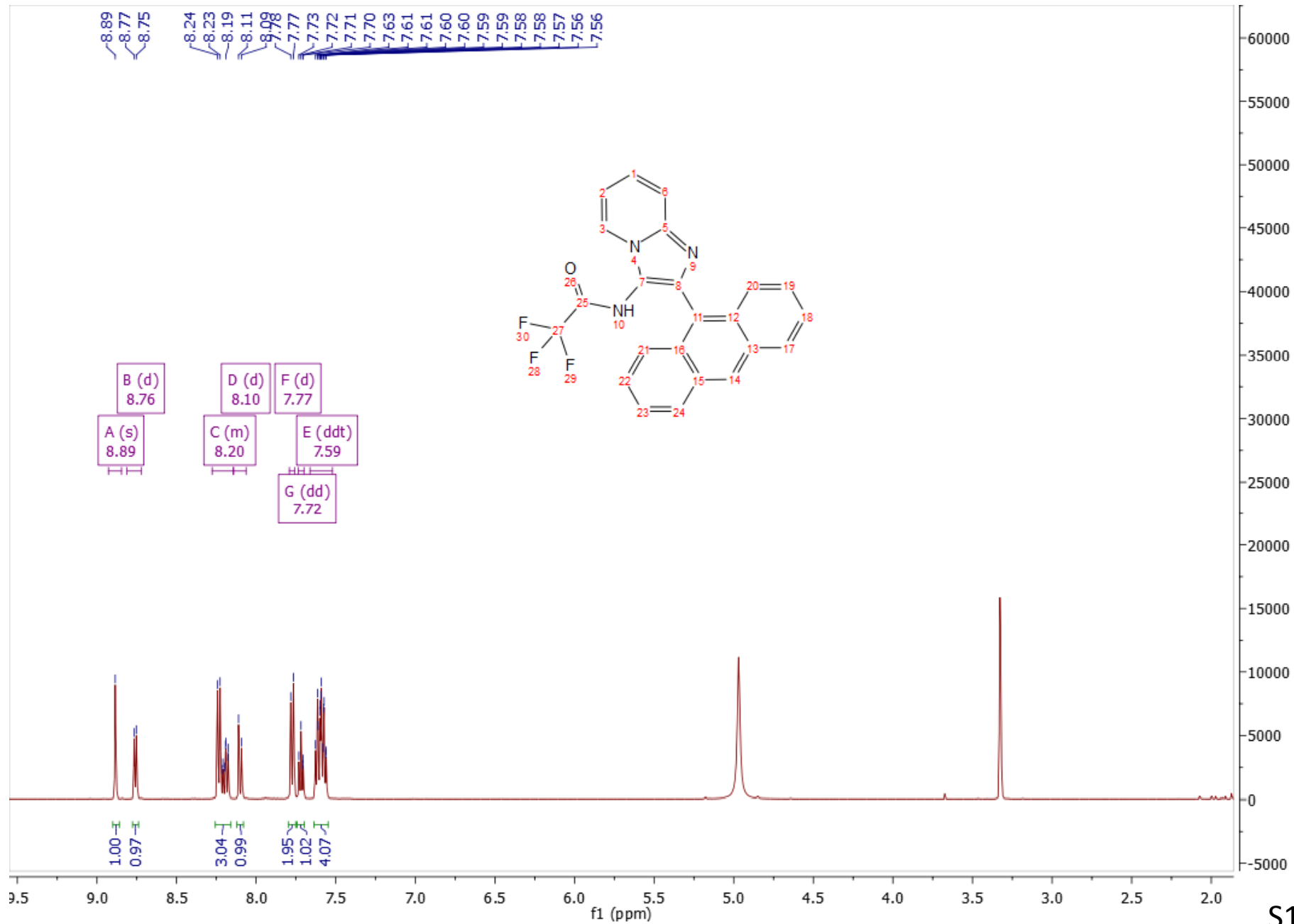
7b ¹³C Spectrum



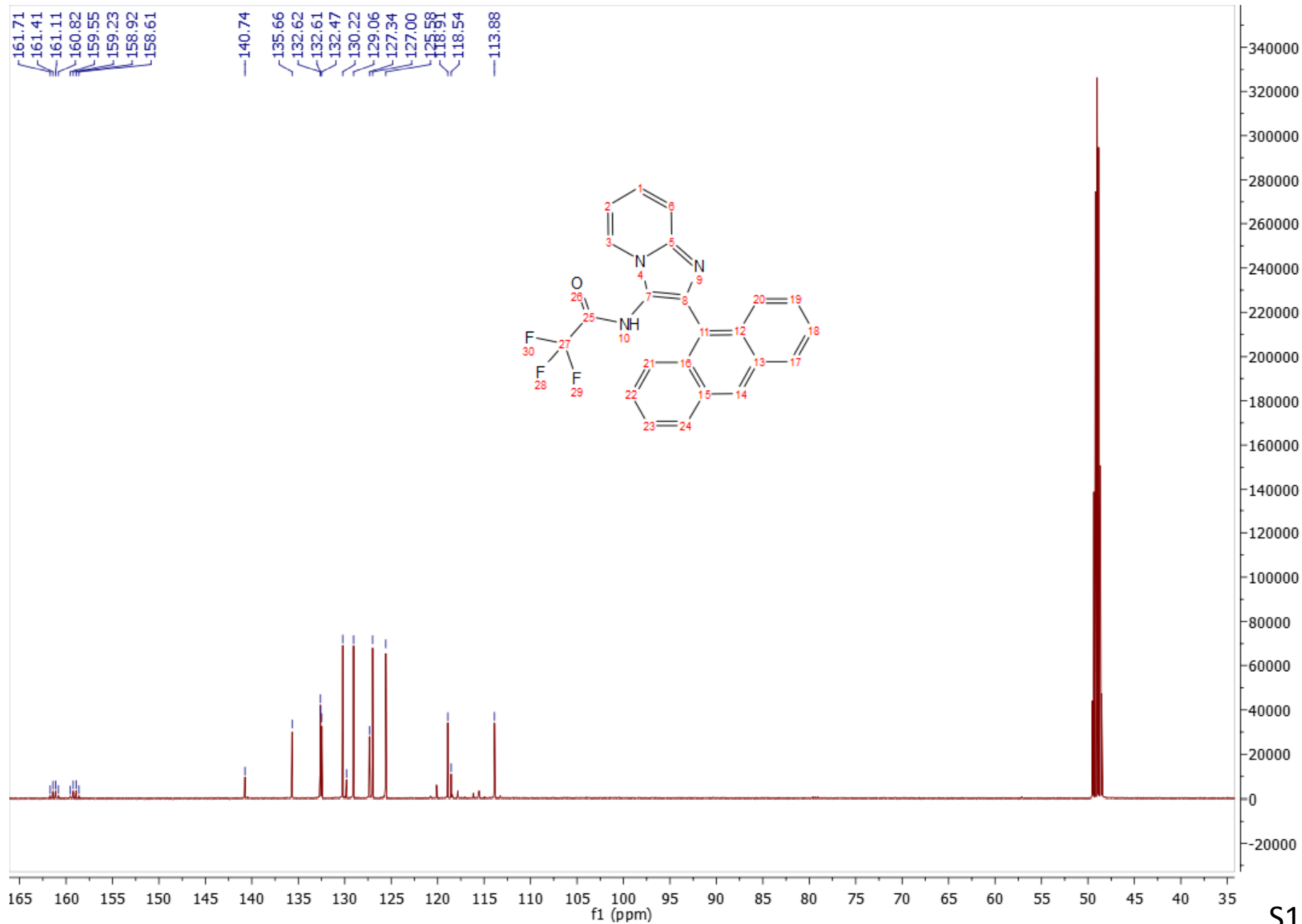
7b LC-MS



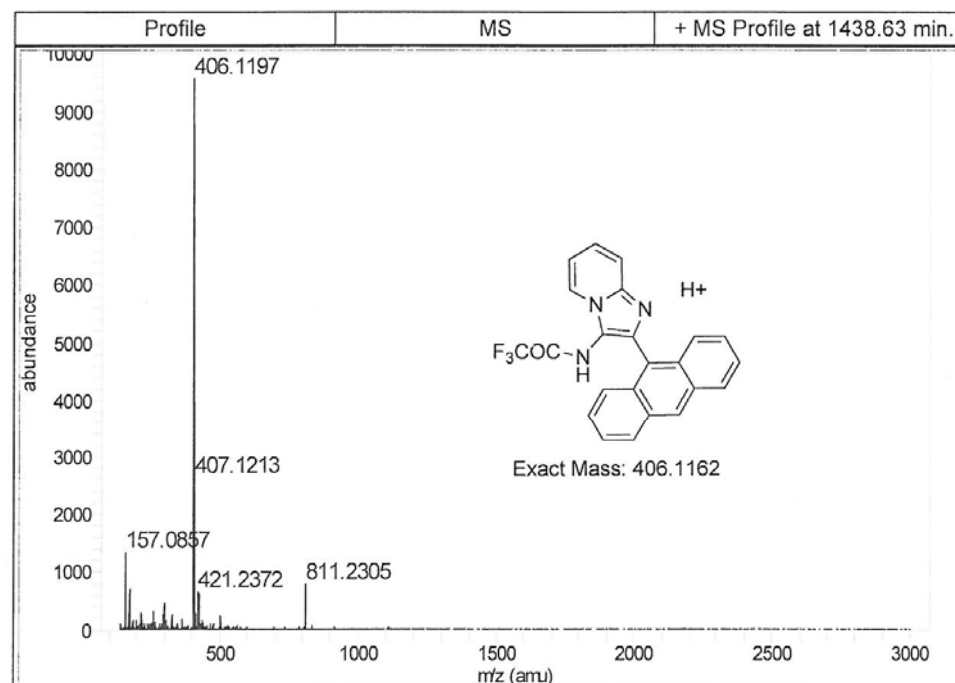
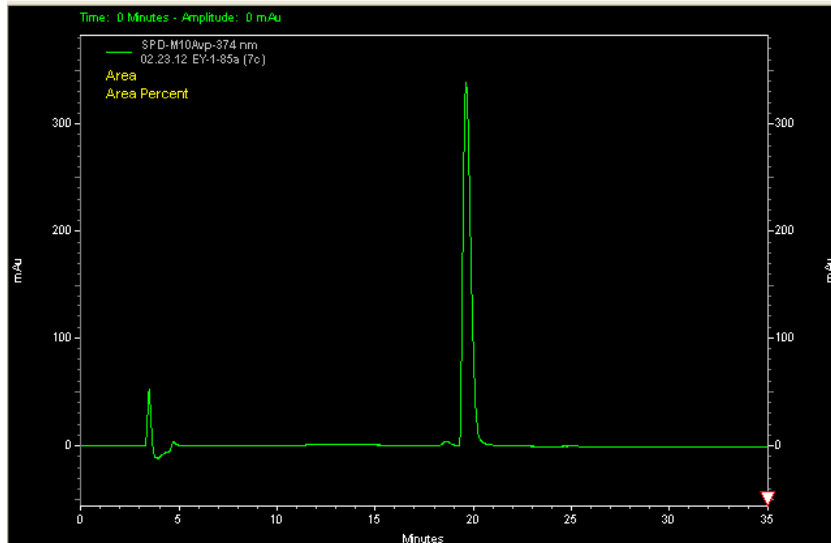
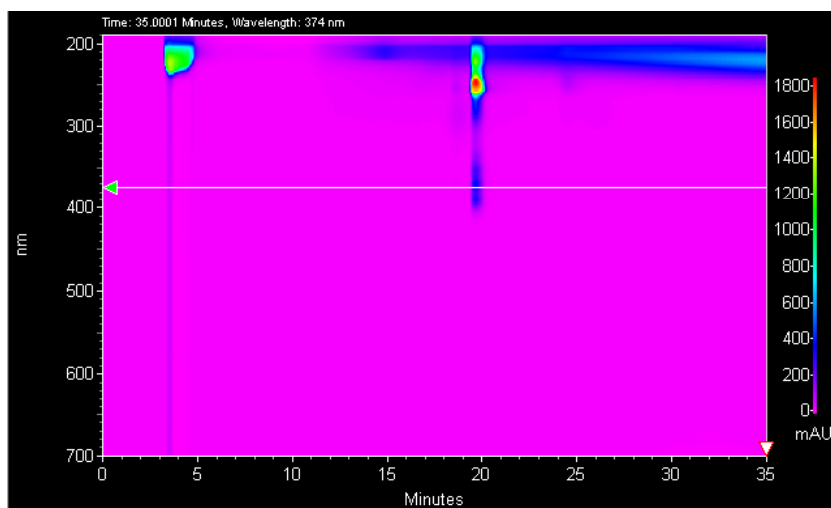
7c ¹H Spectrum



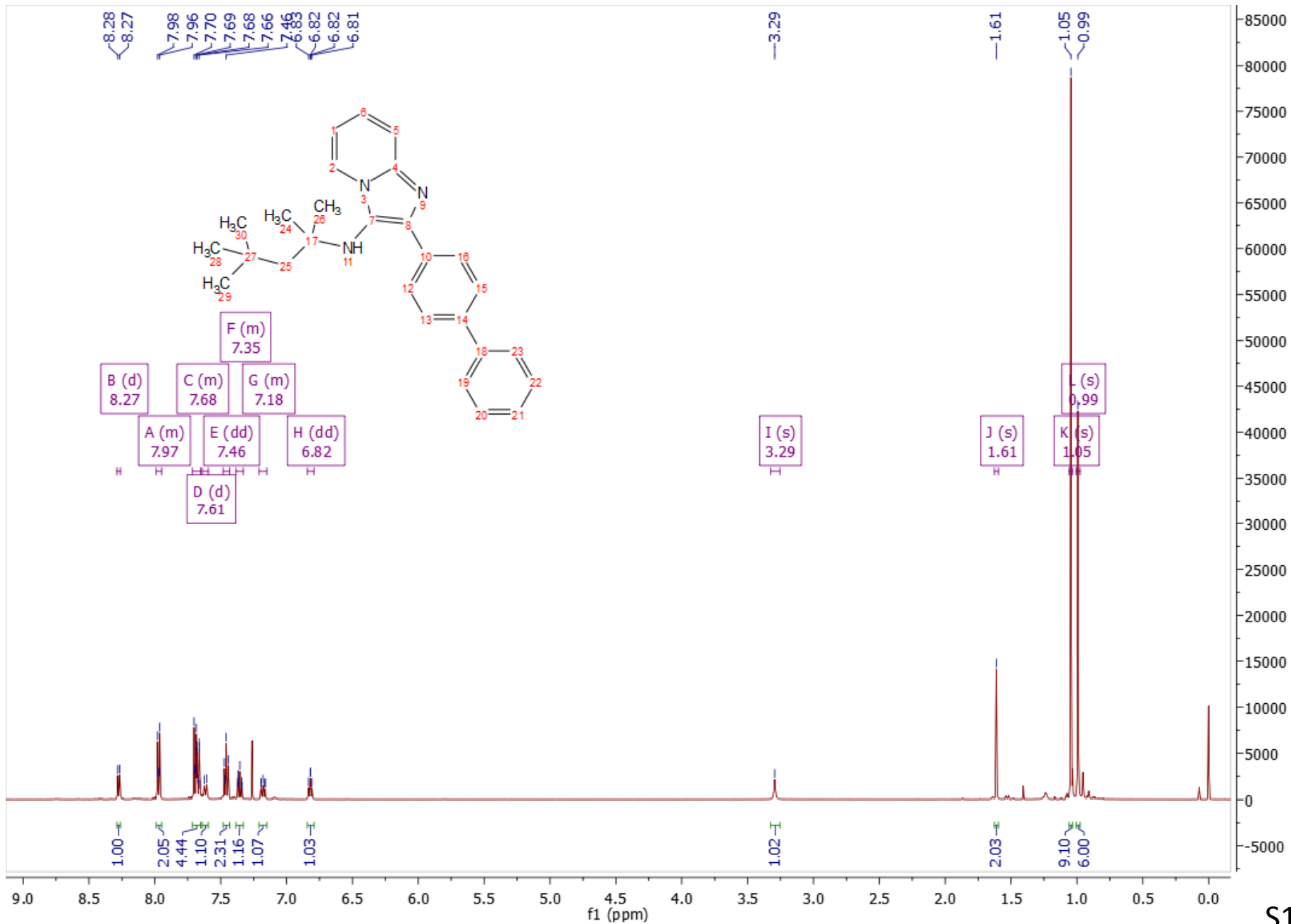
7c ¹³C Spectrum



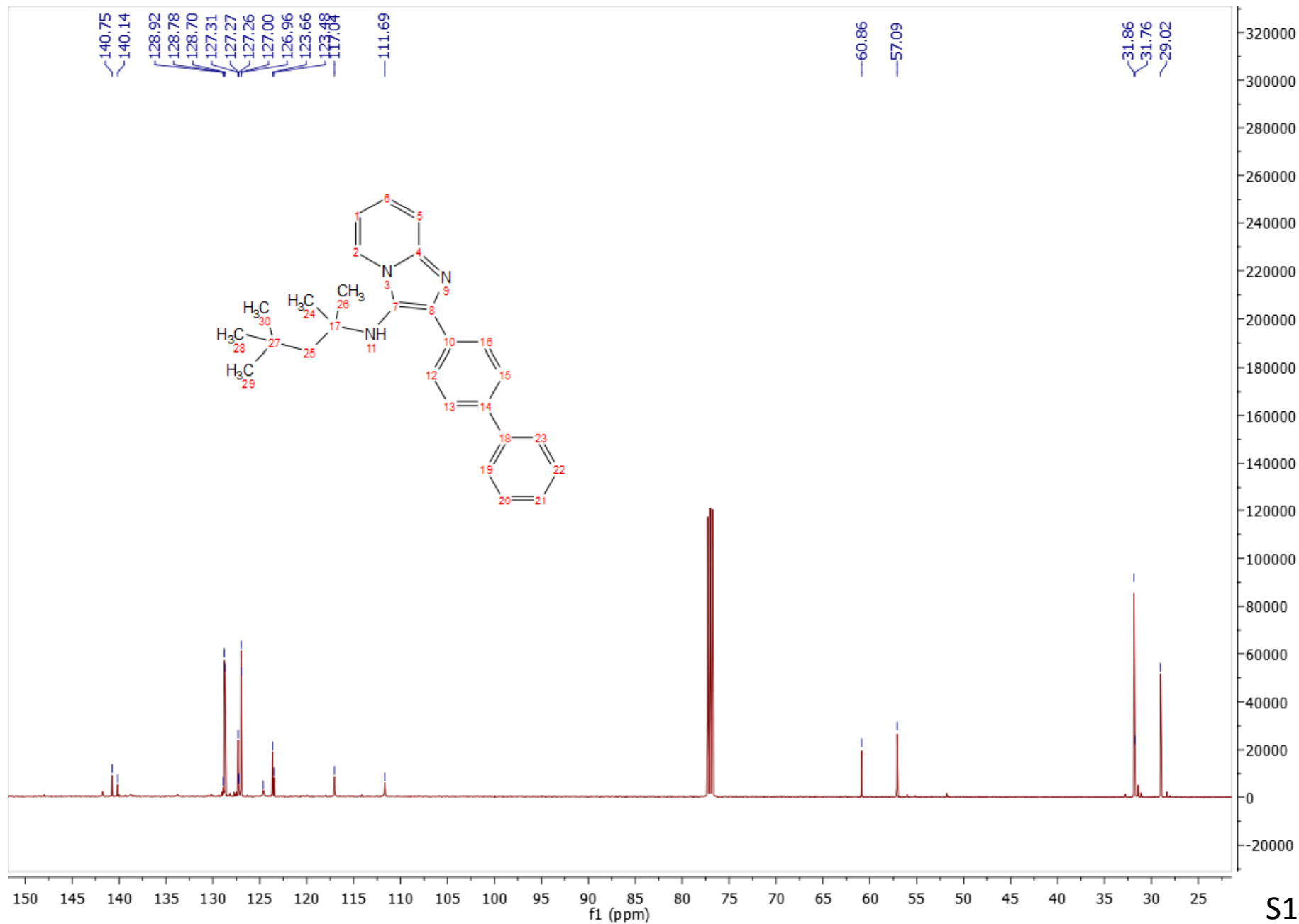
7c LC-MS



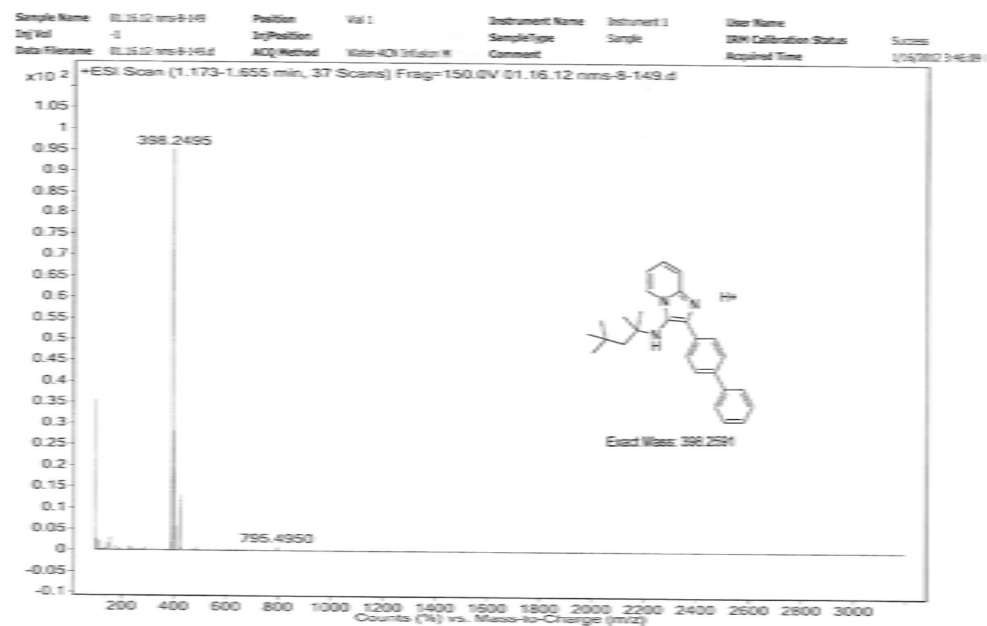
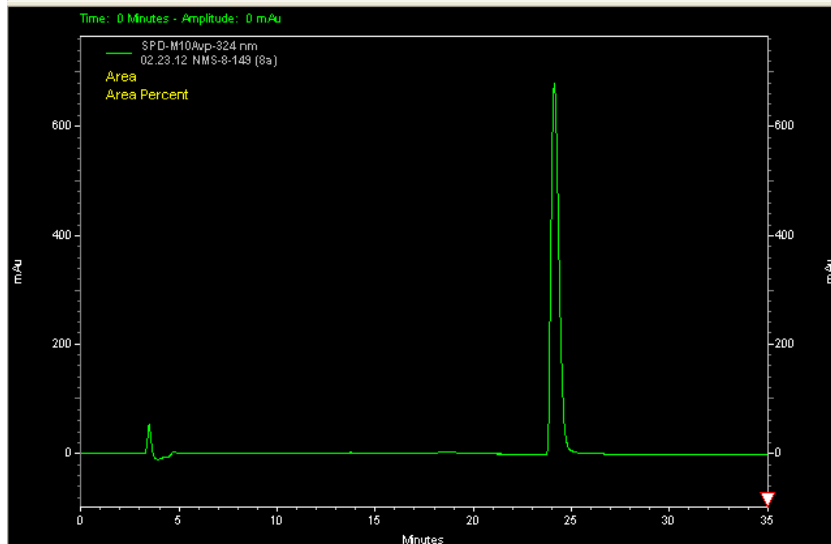
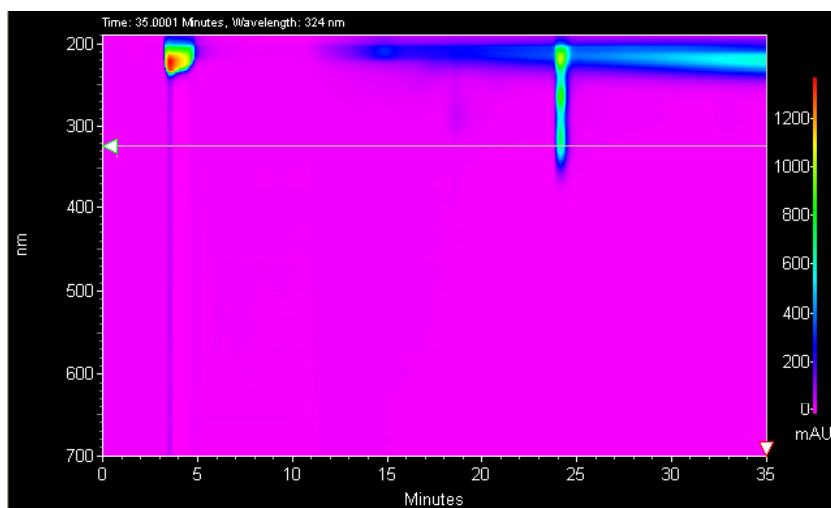
8a ¹H Spectrum



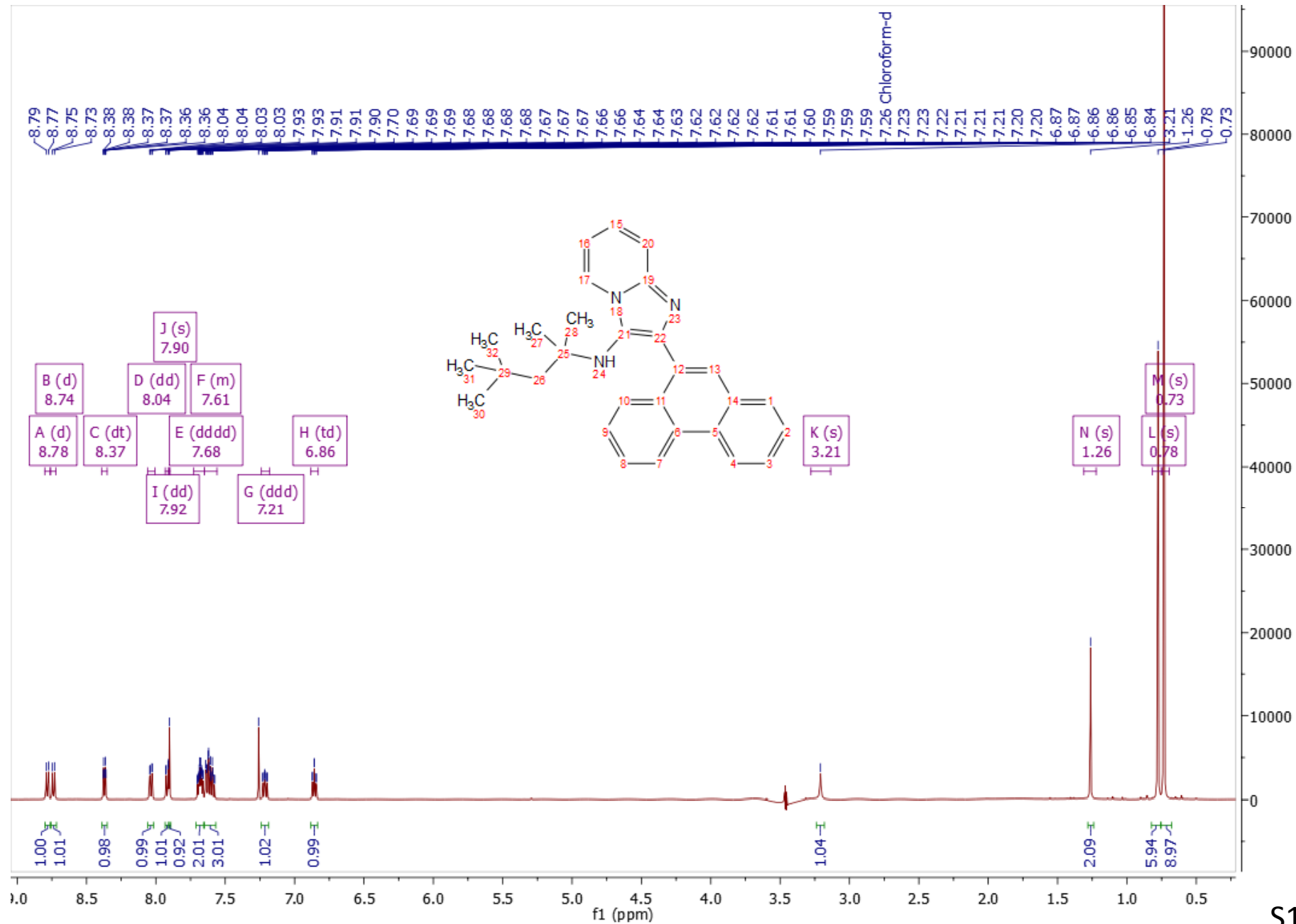
8a ¹³C Spectrum



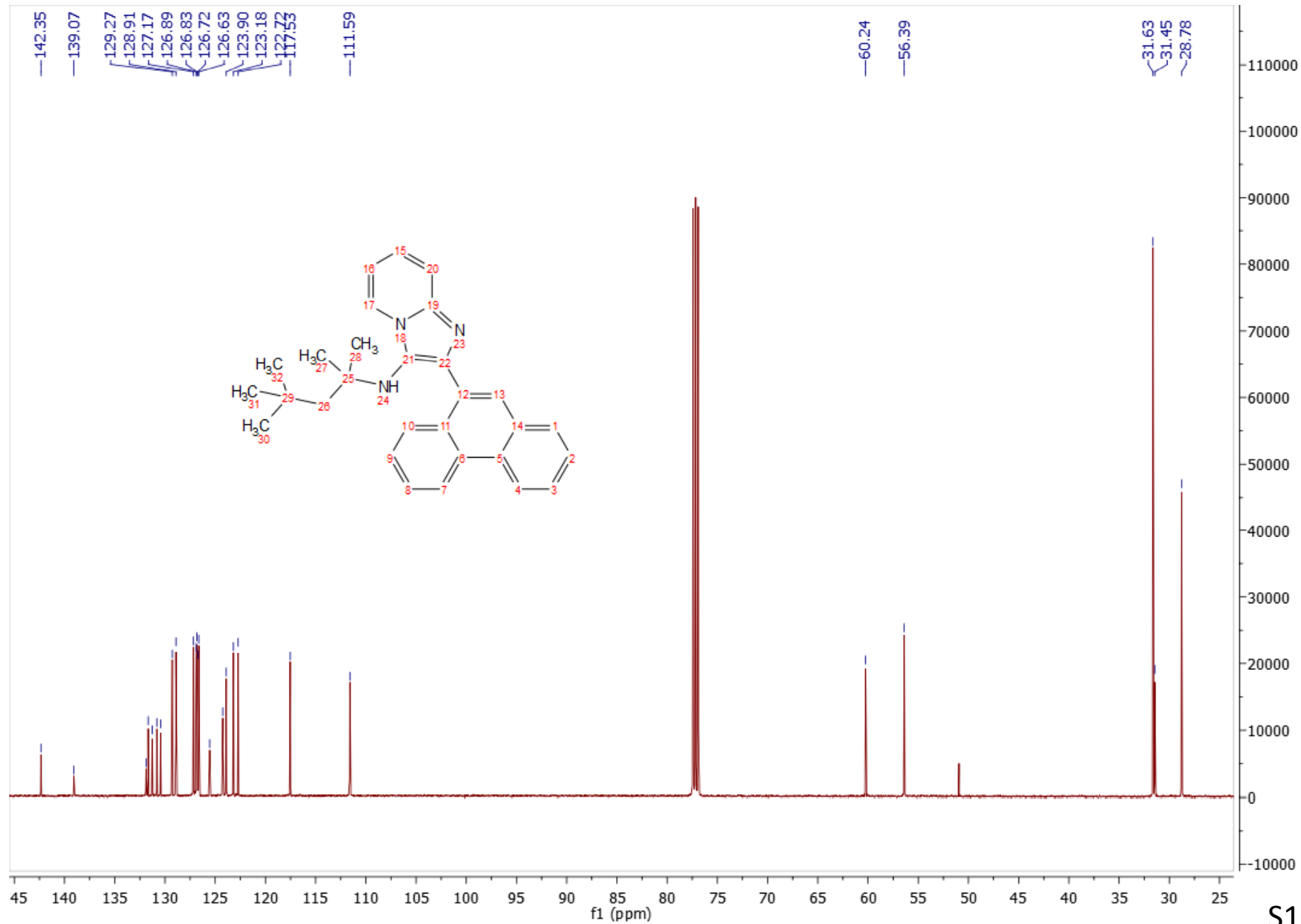
8a LC-MS



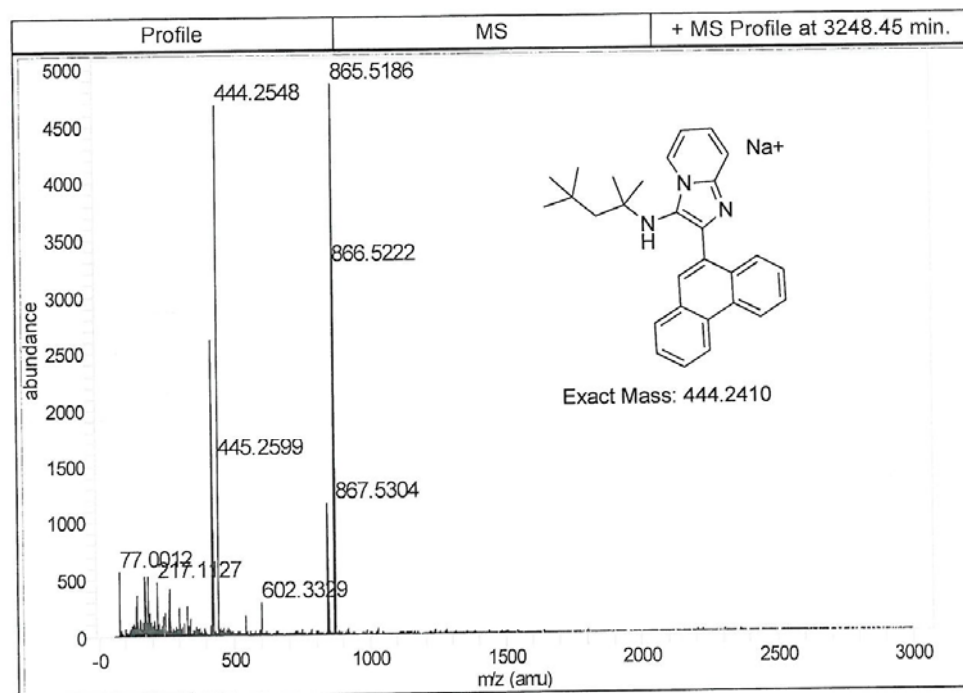
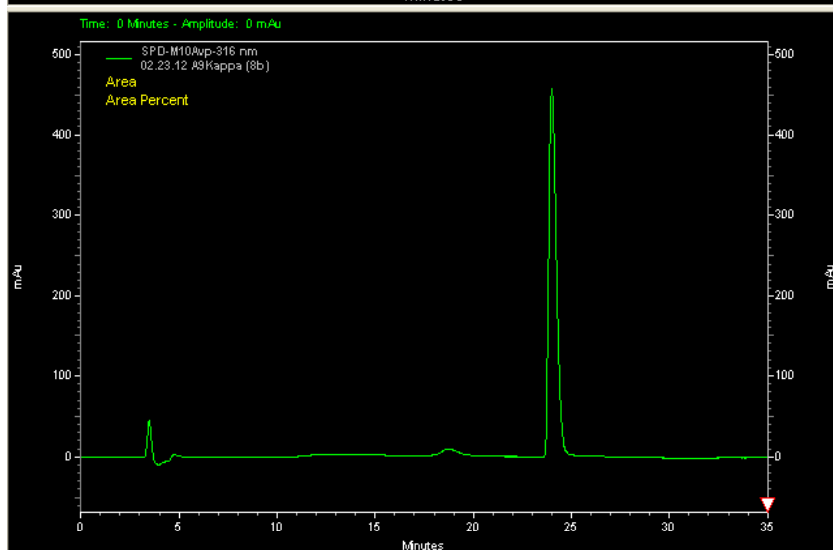
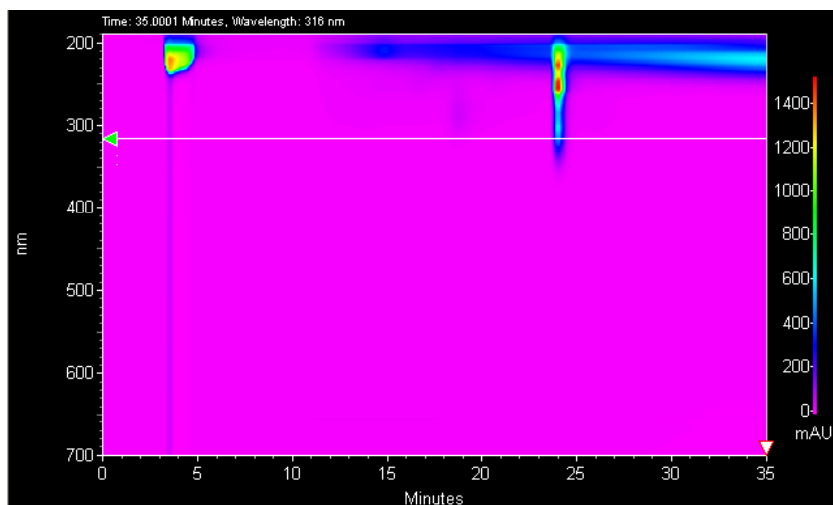
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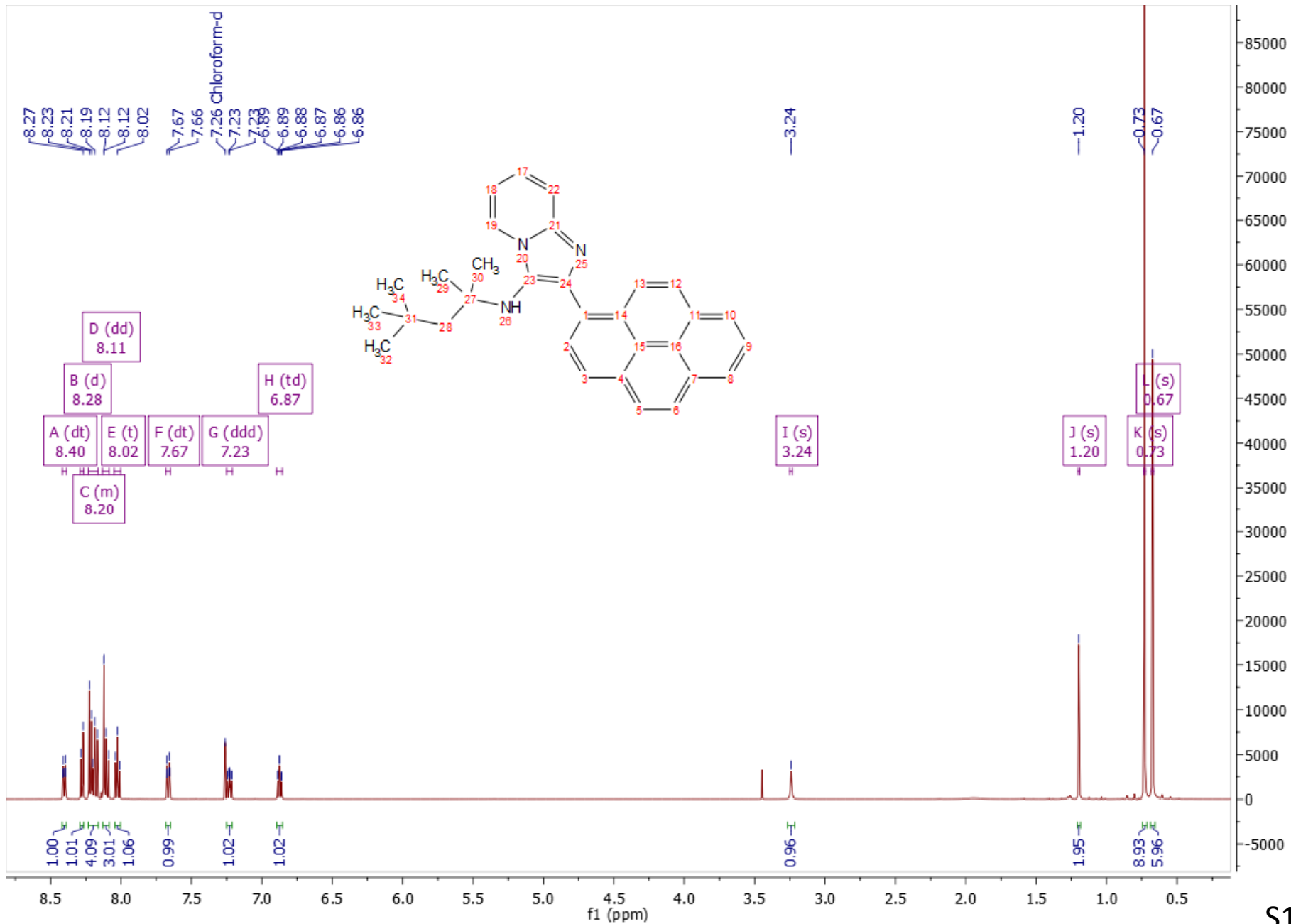
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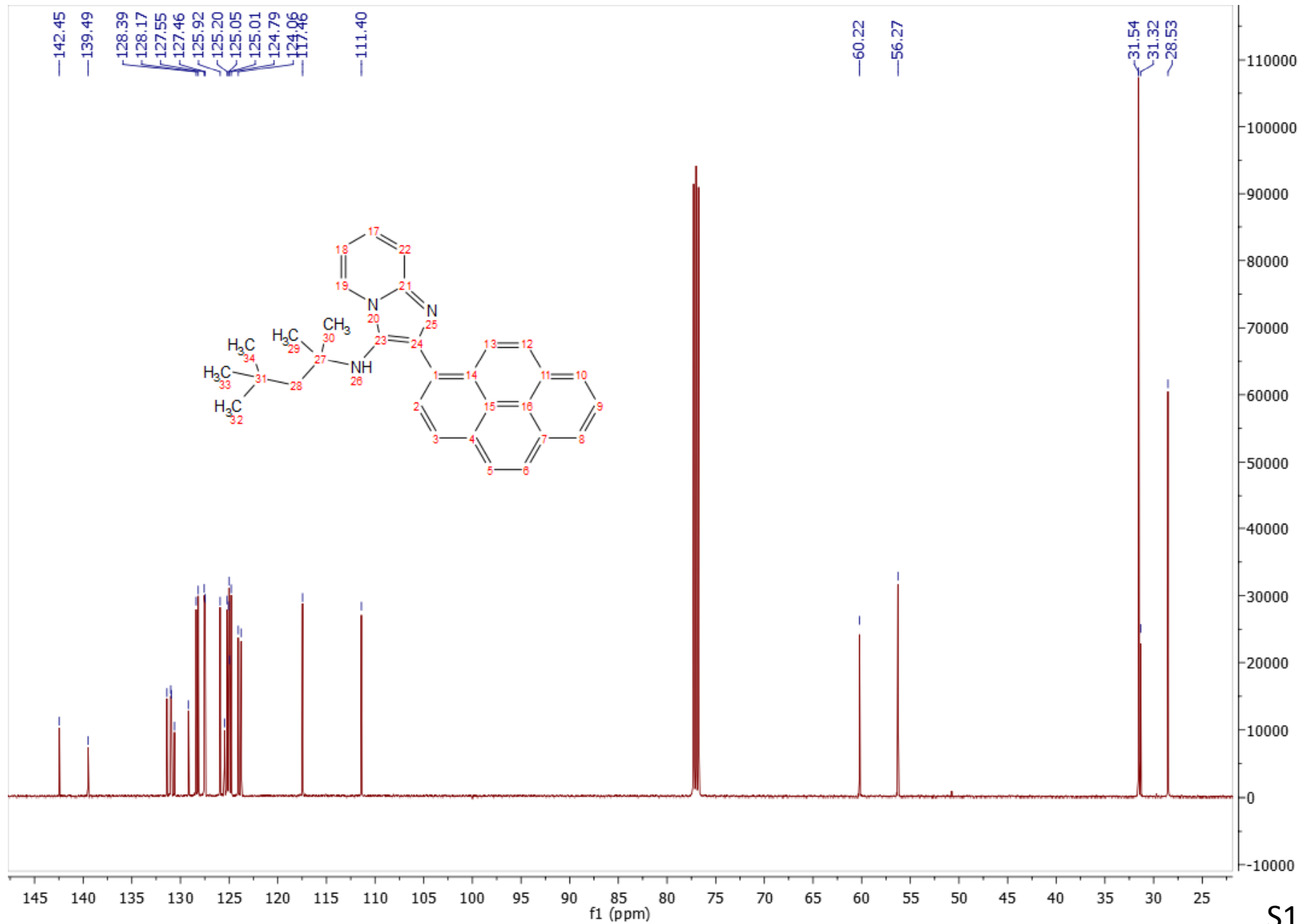
8b LC-MS



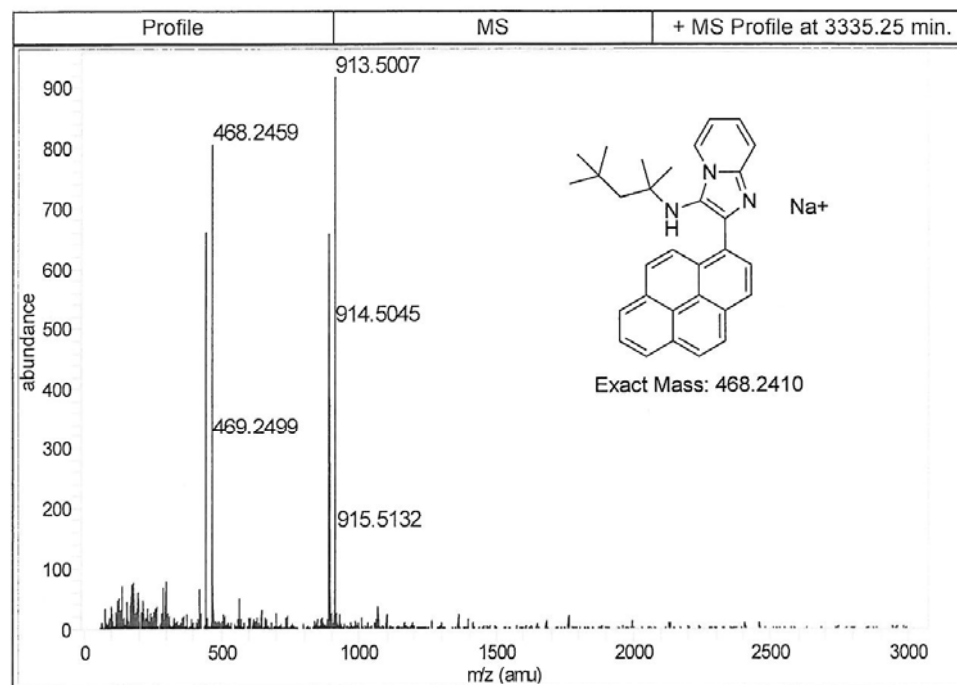
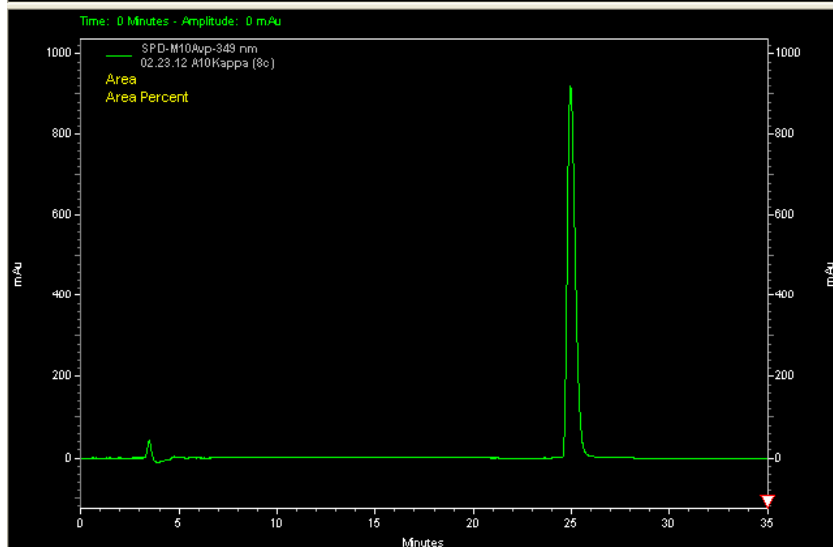
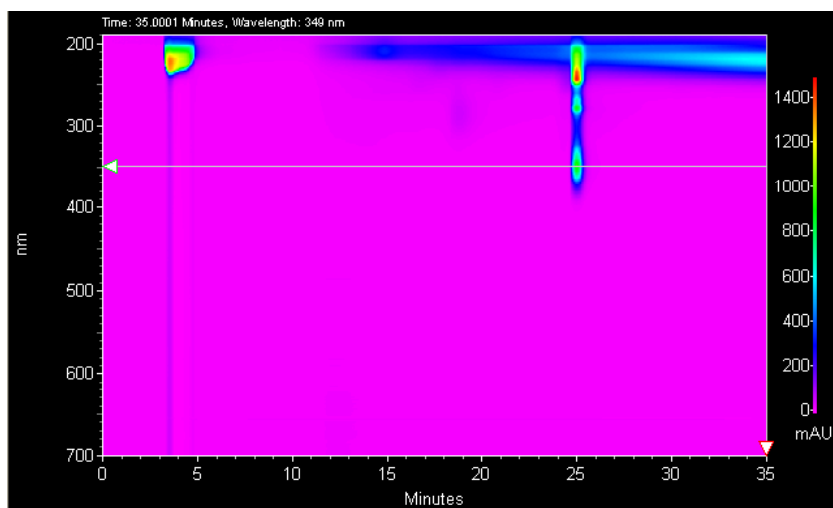
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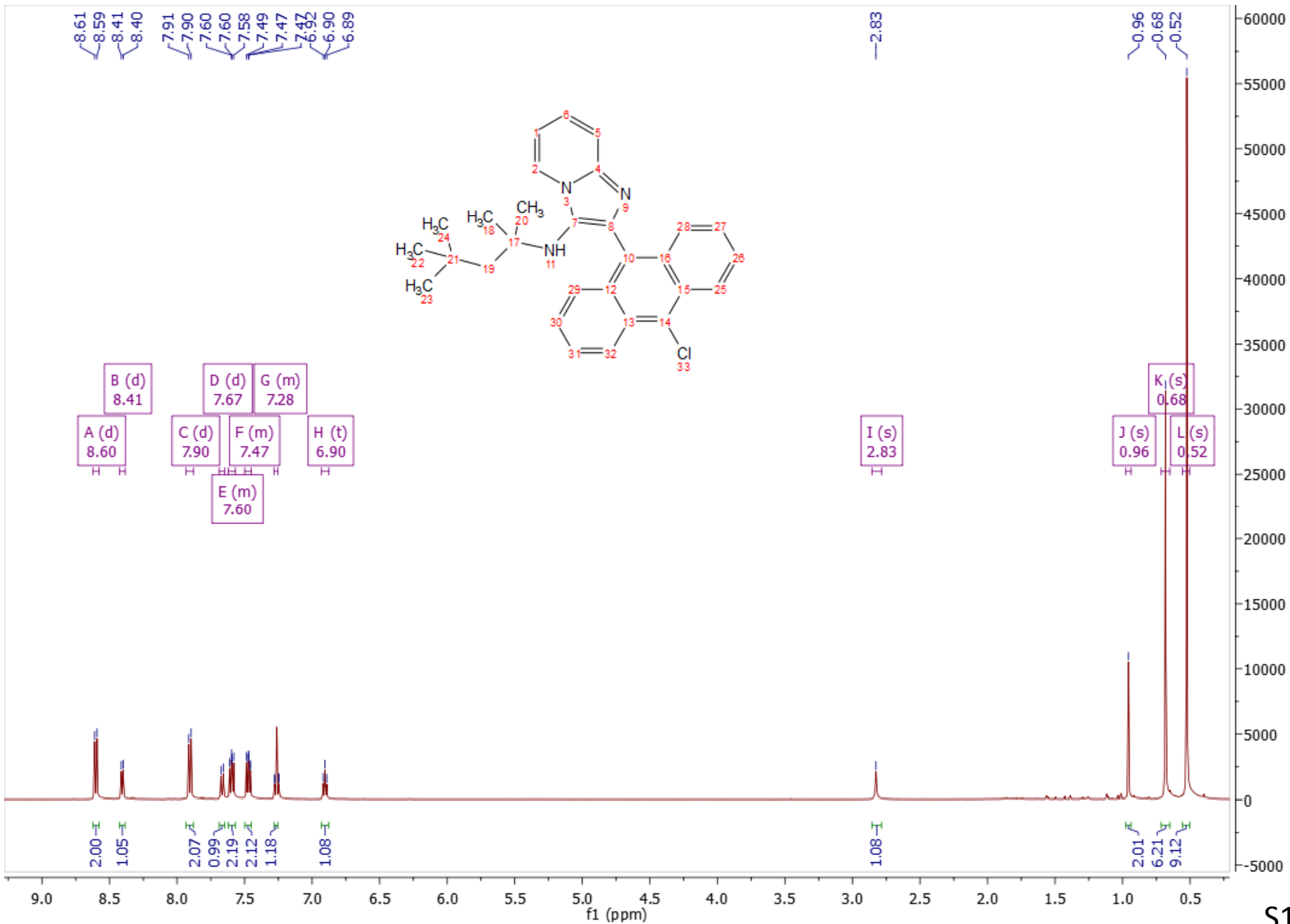
8c ¹³C Spectrum



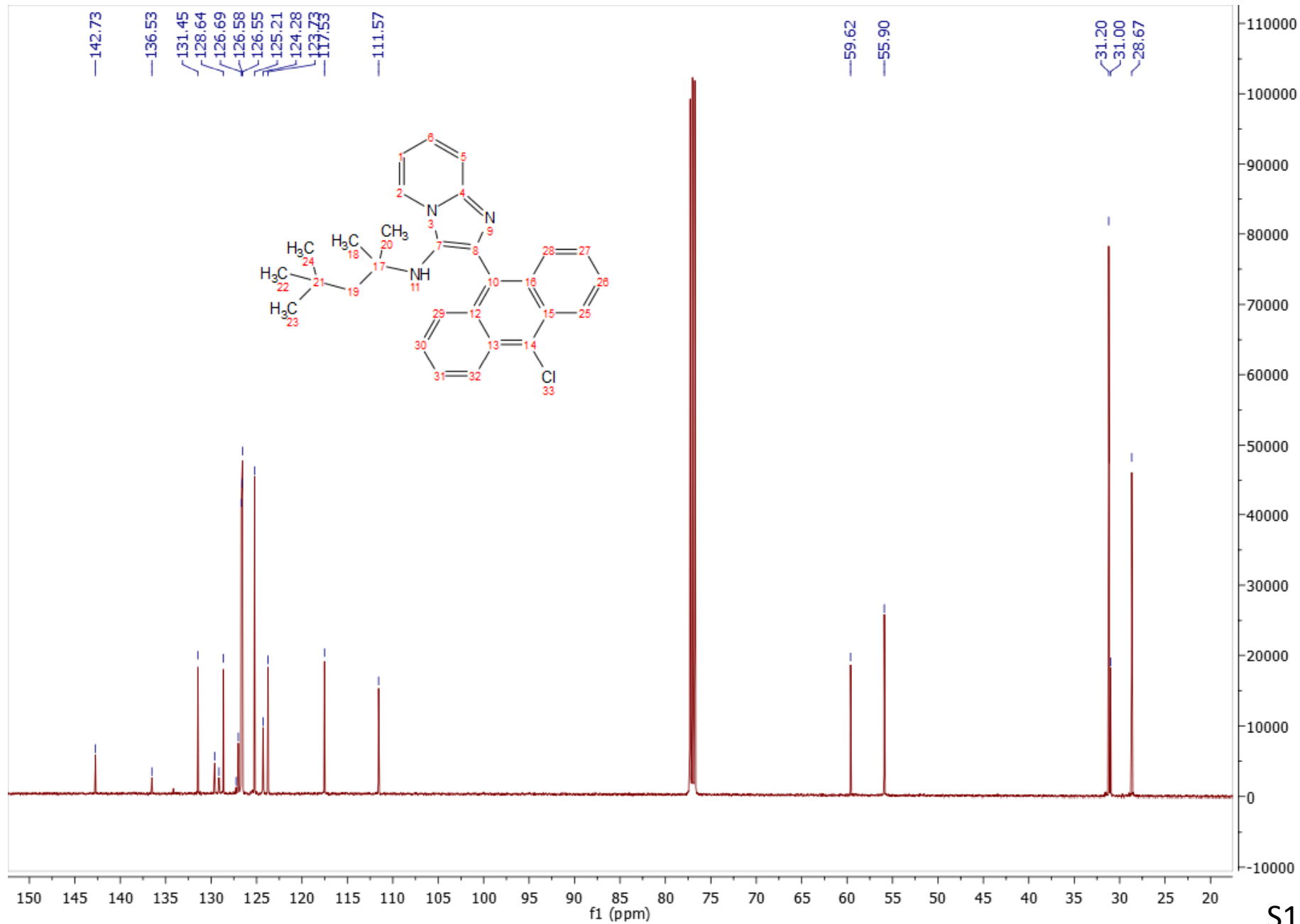
8c LC-MS



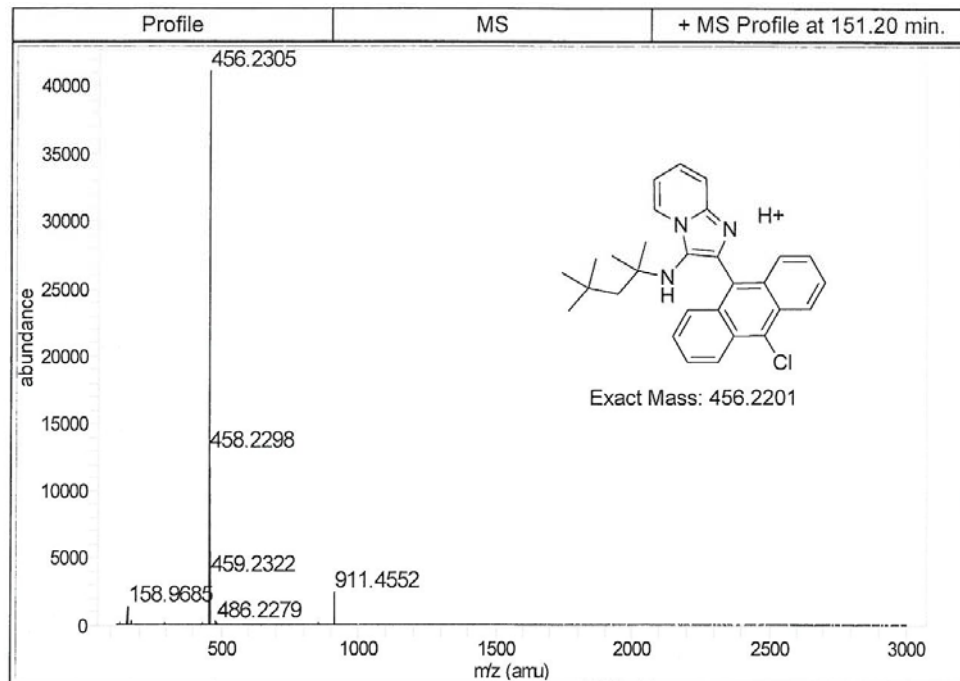
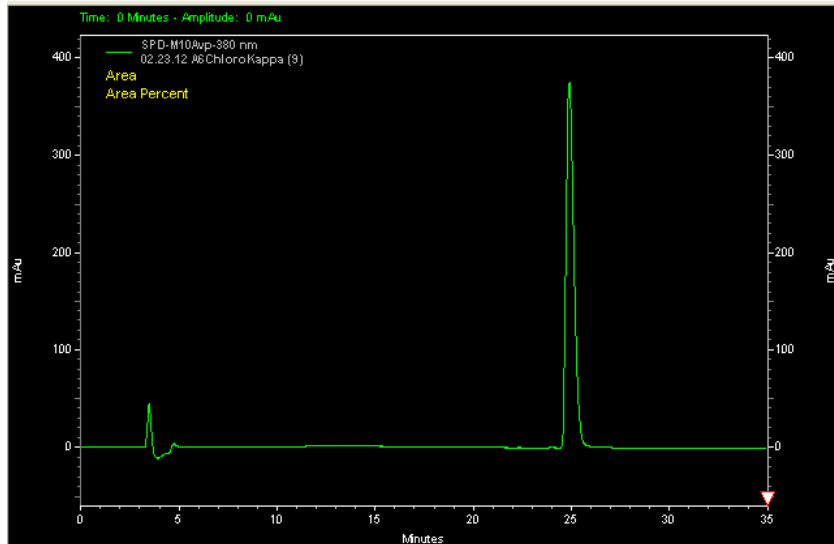
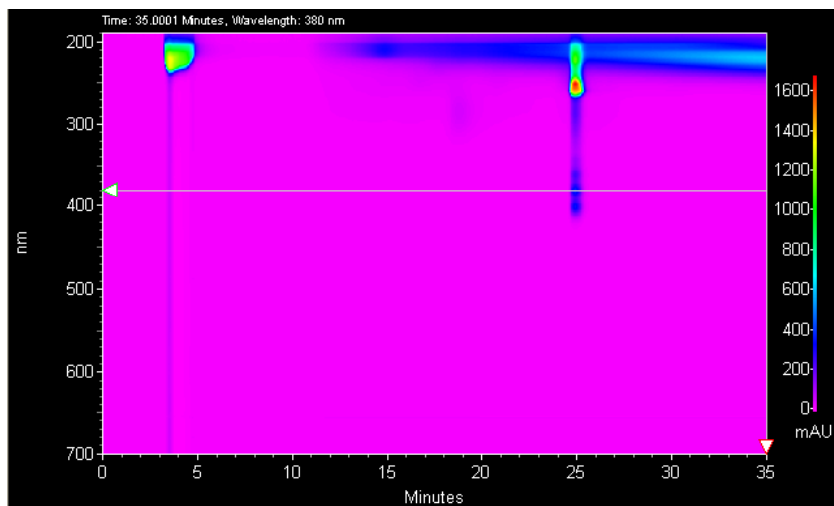
9 ¹H Spectrum



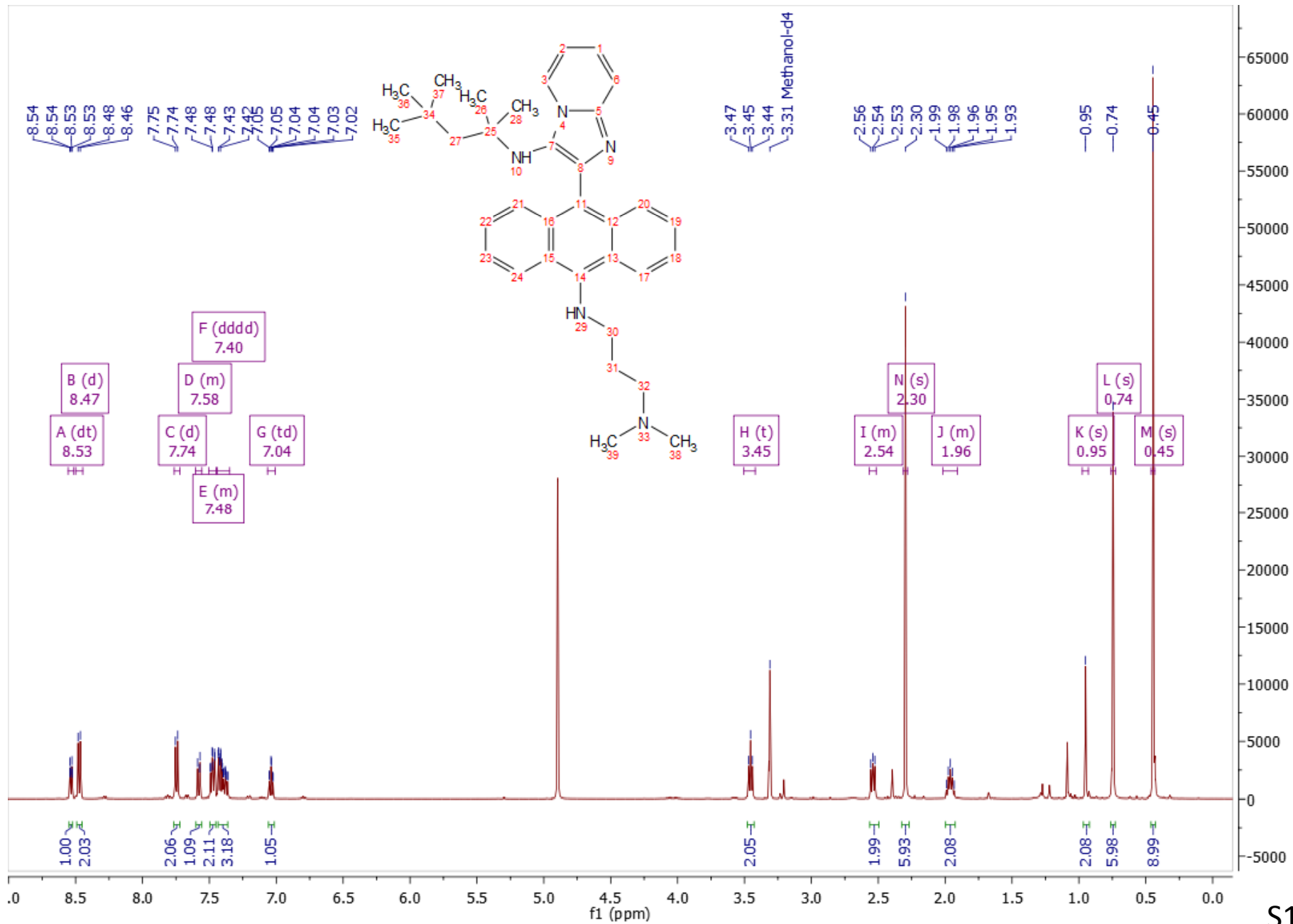
9 ¹³C Spectrum



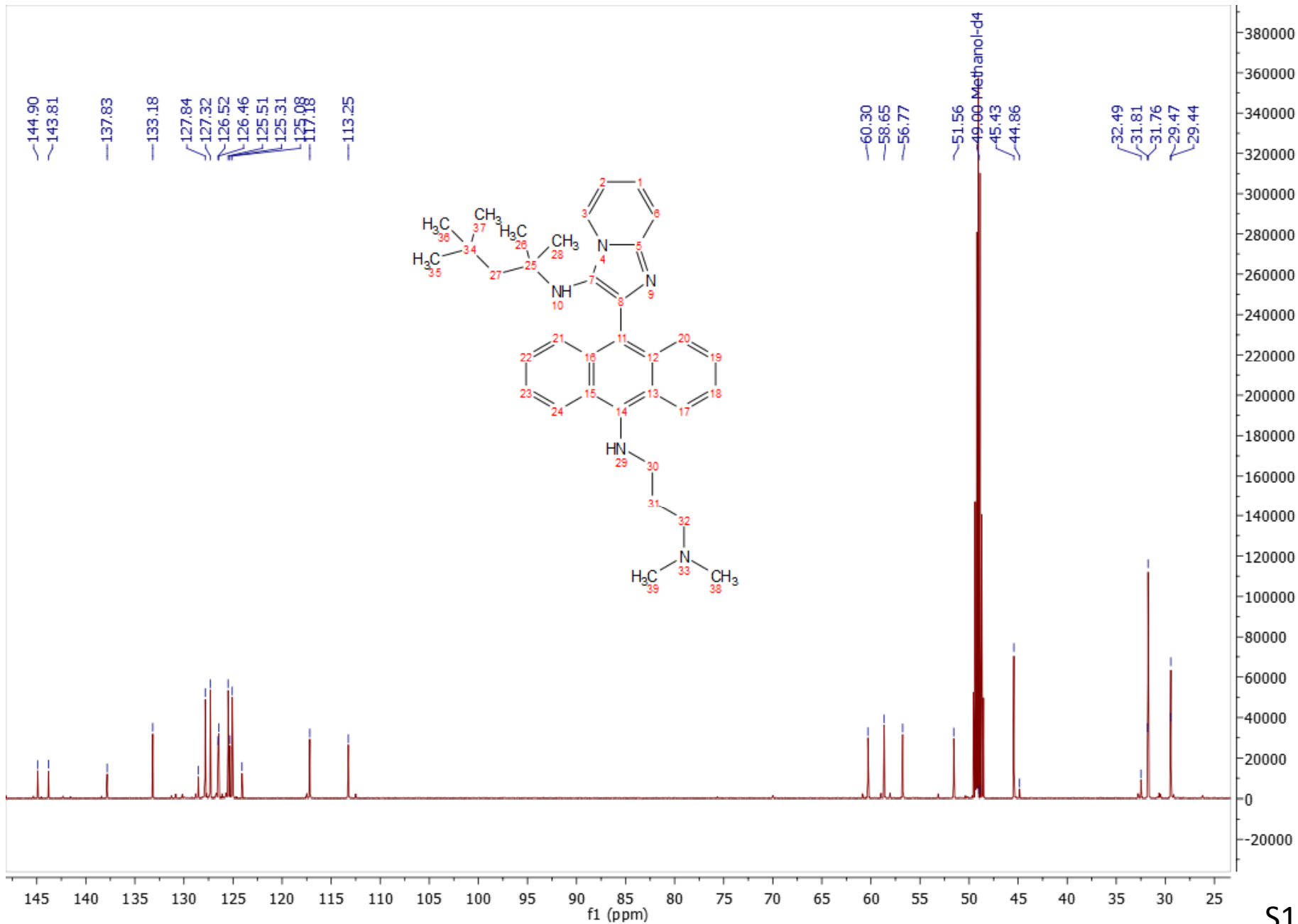
9 LC-MS



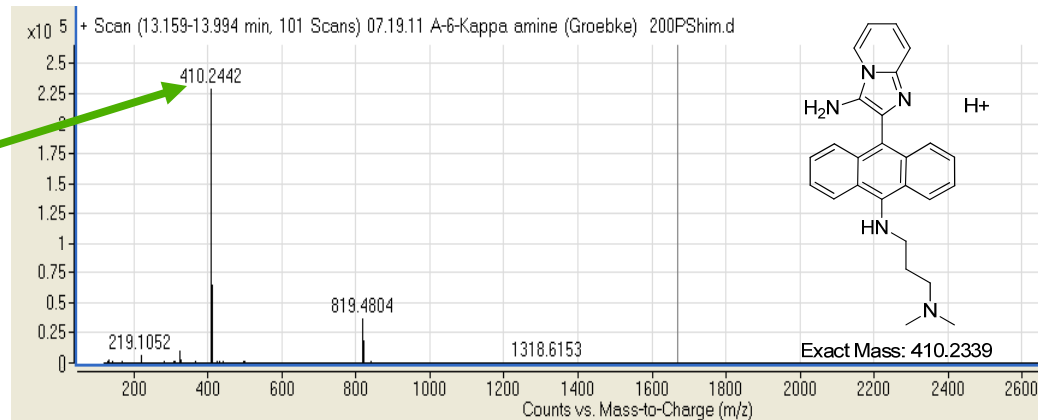
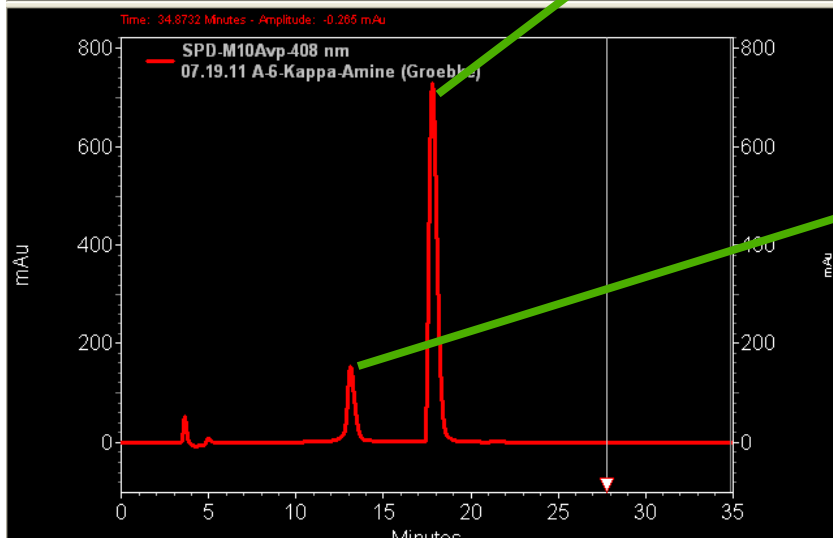
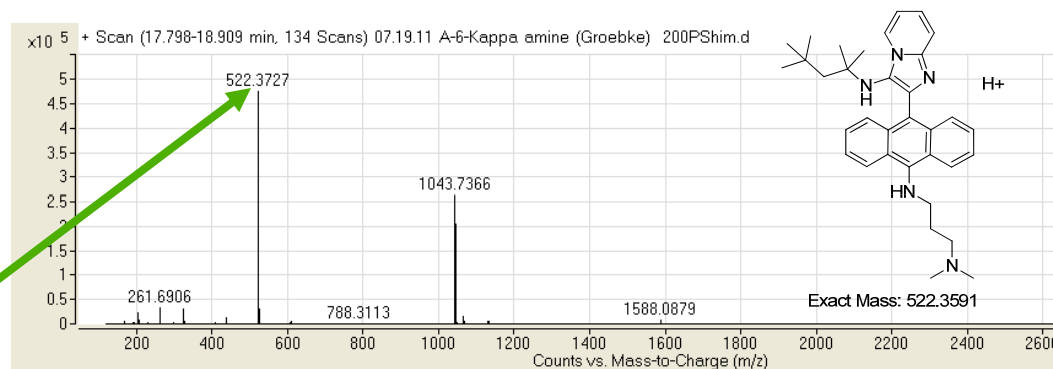
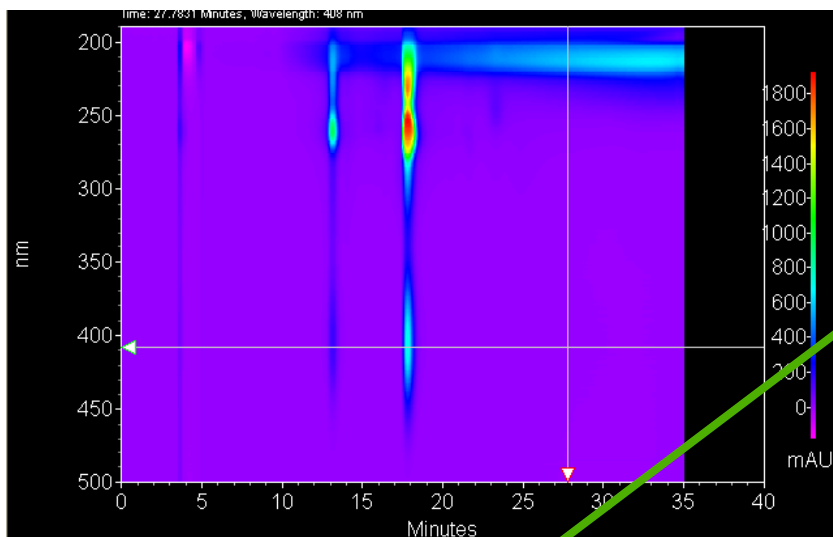
10 ¹H Spectrum



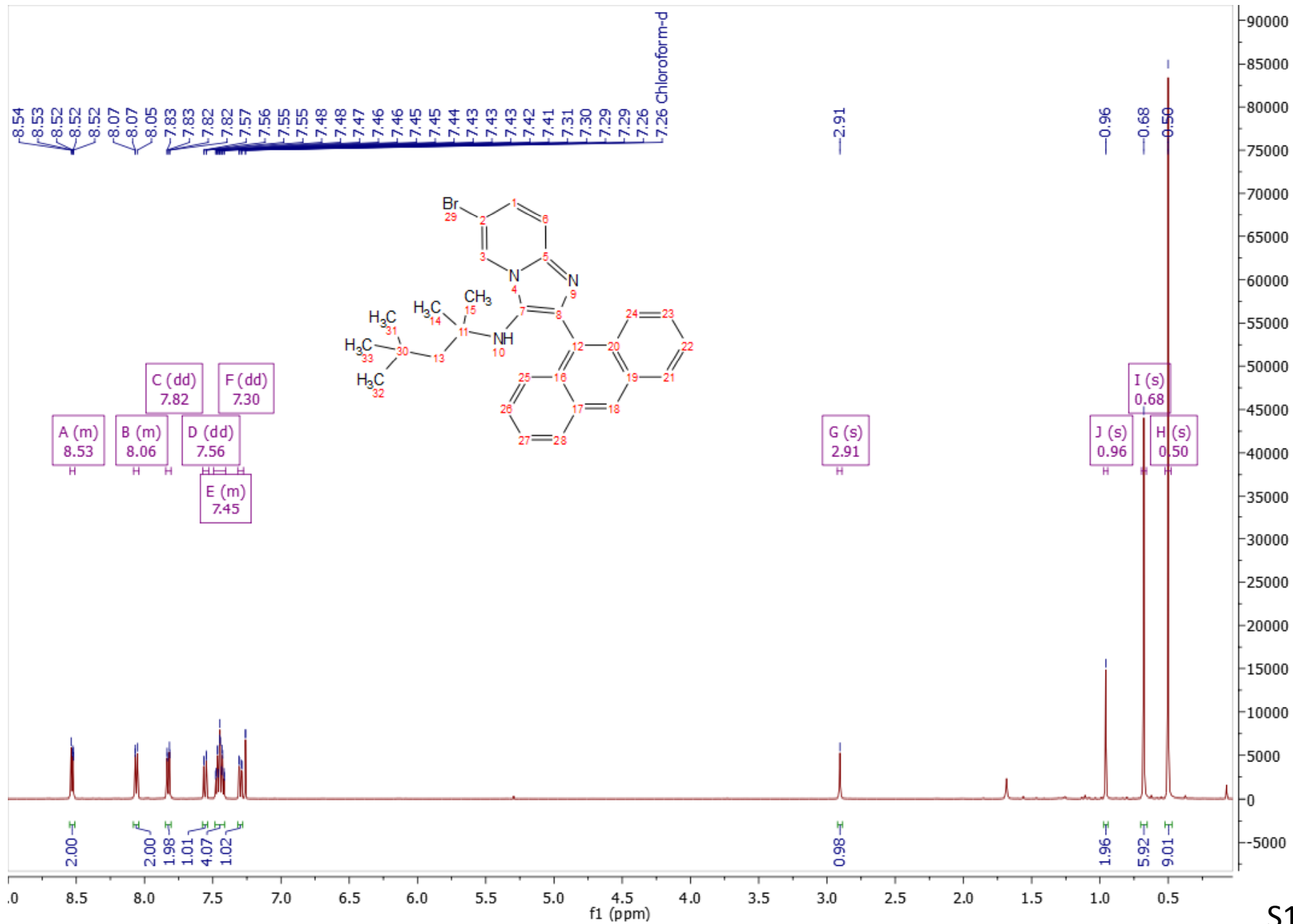
10 ¹³C Spectrum



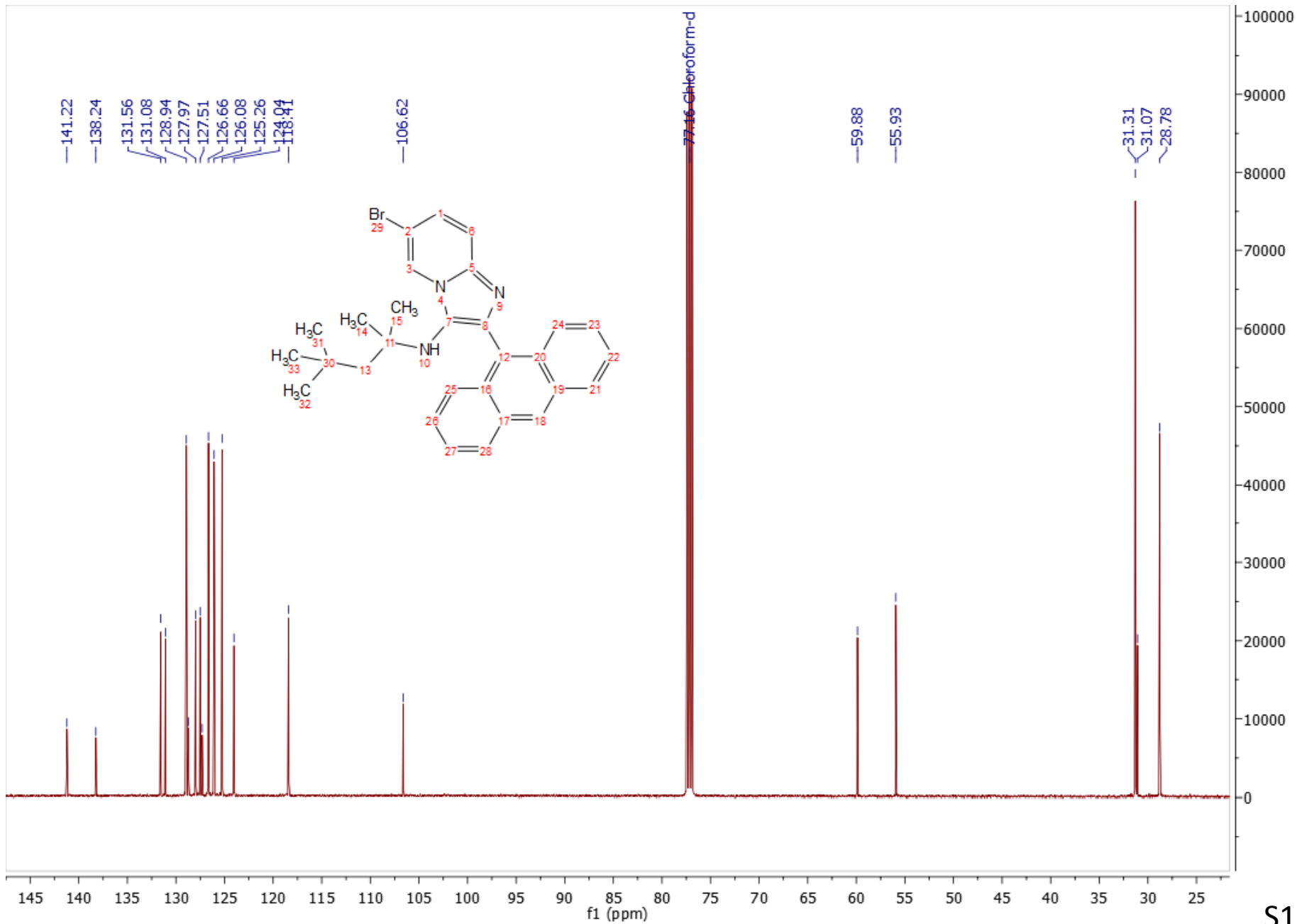
10 LC-MS



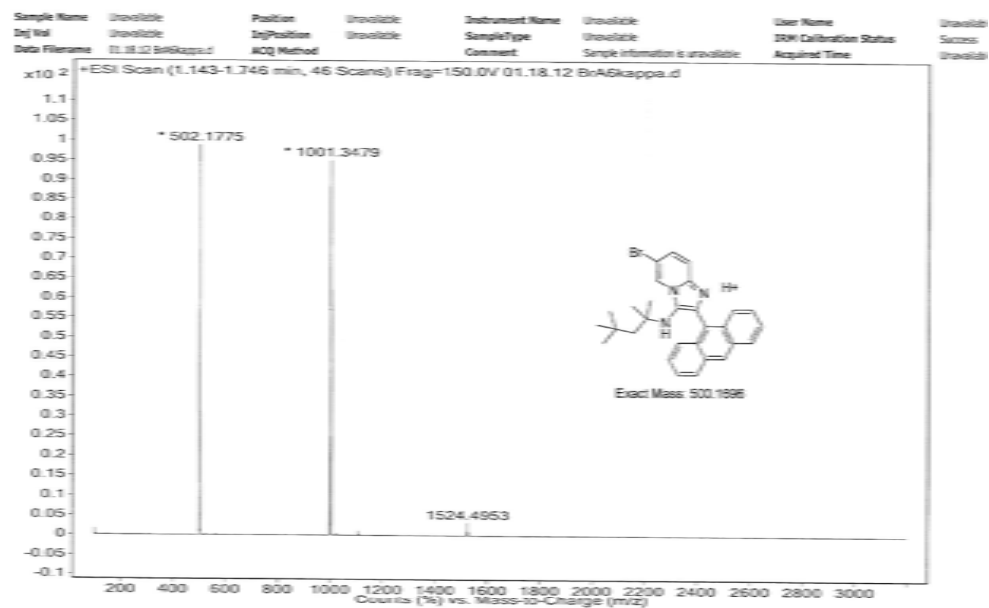
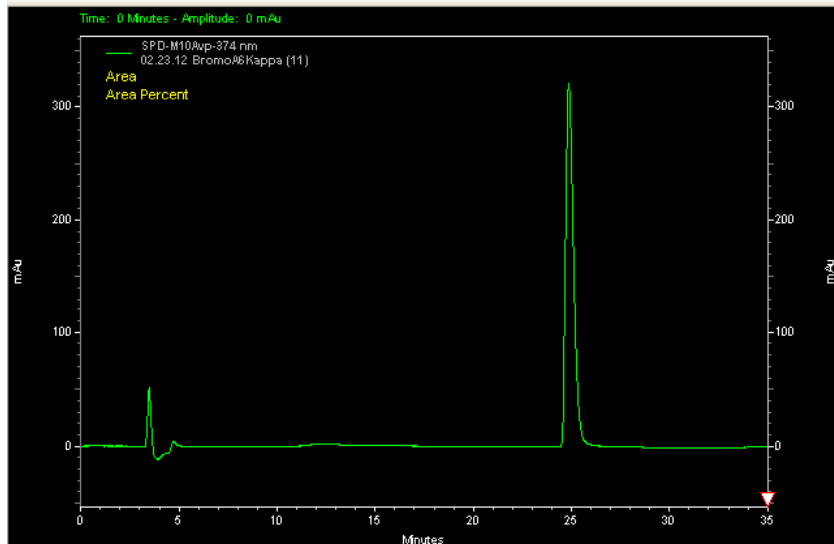
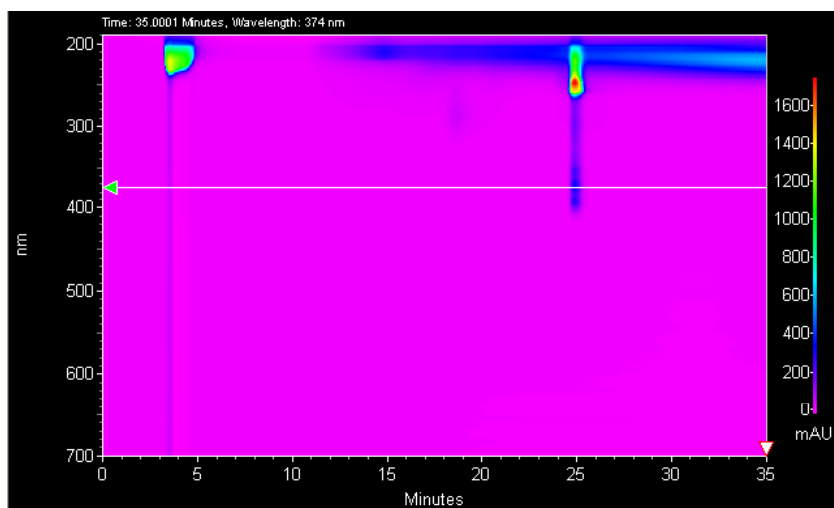
11 ¹H Spectrum



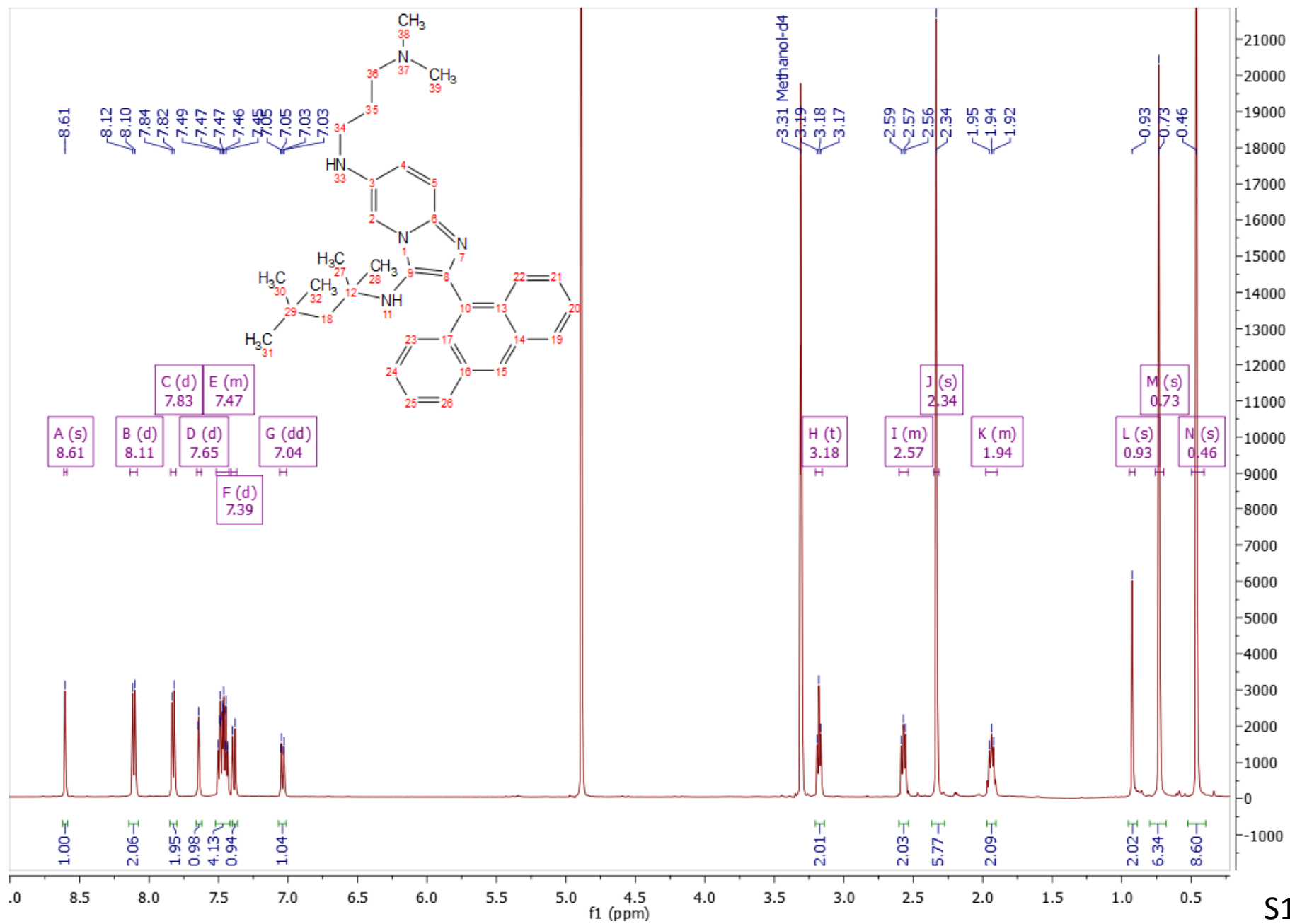
11 ¹³C Spectrum



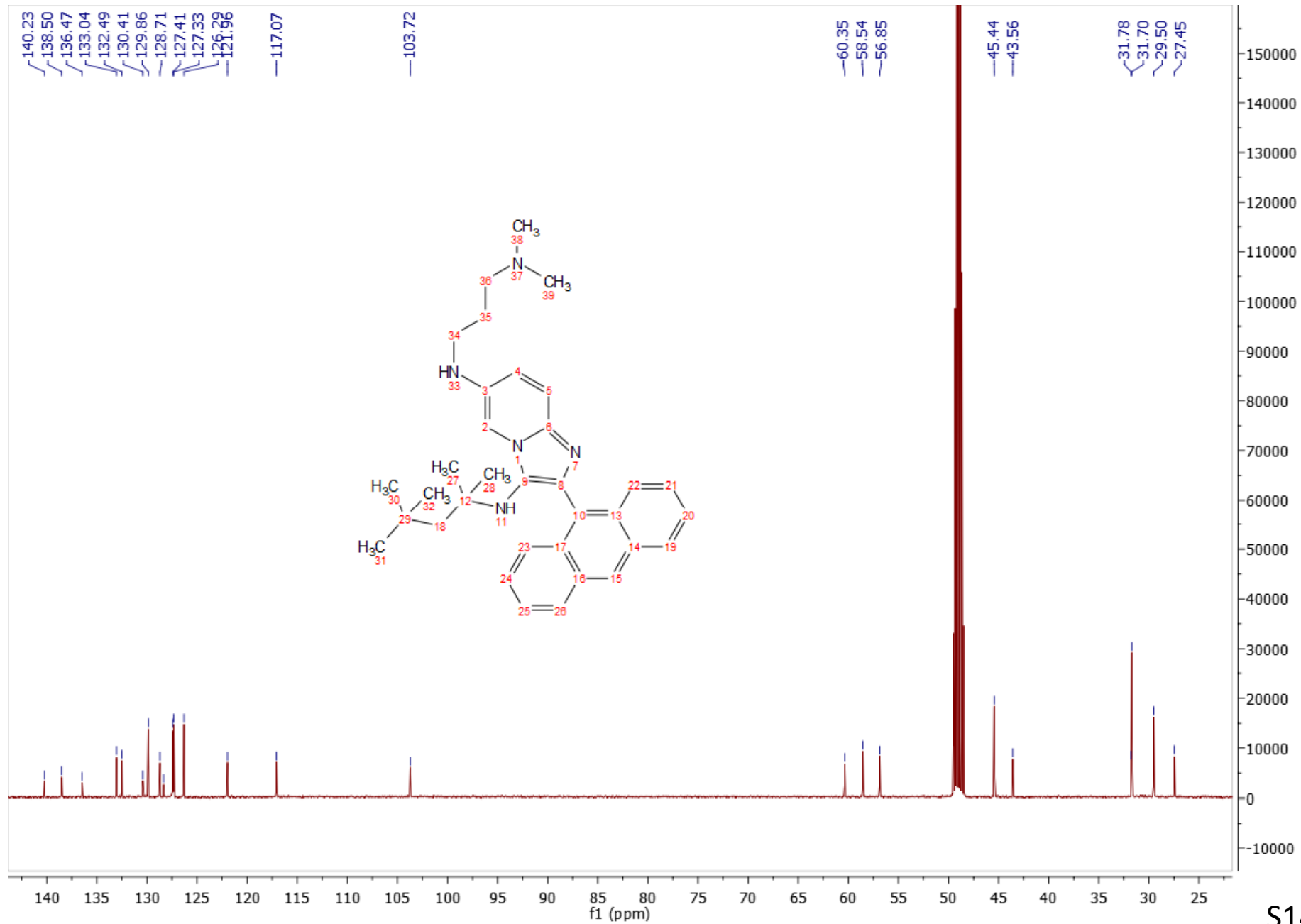
11 LC-MS



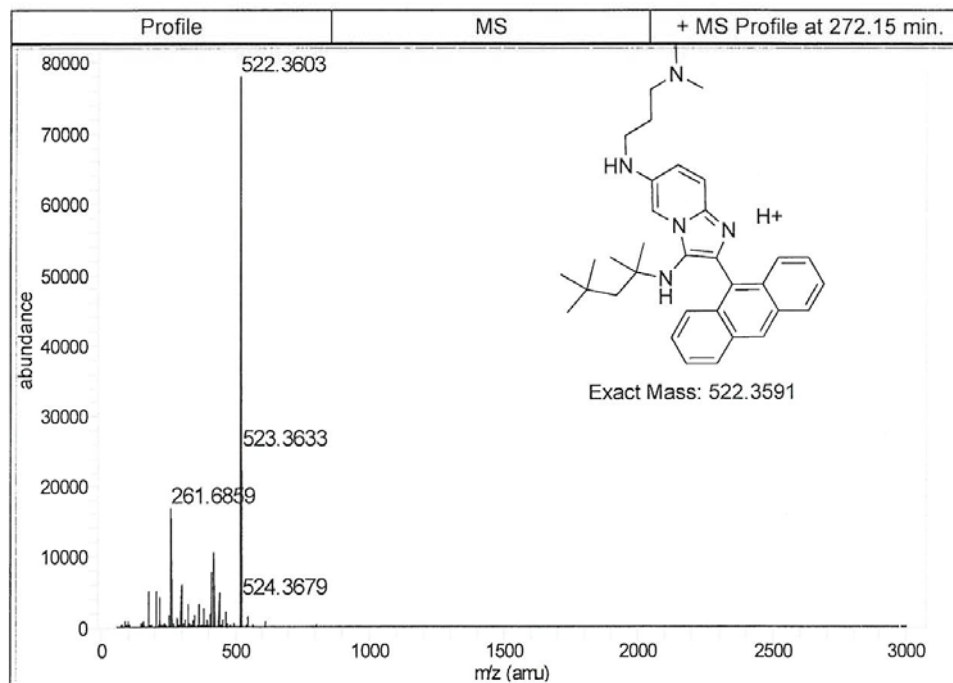
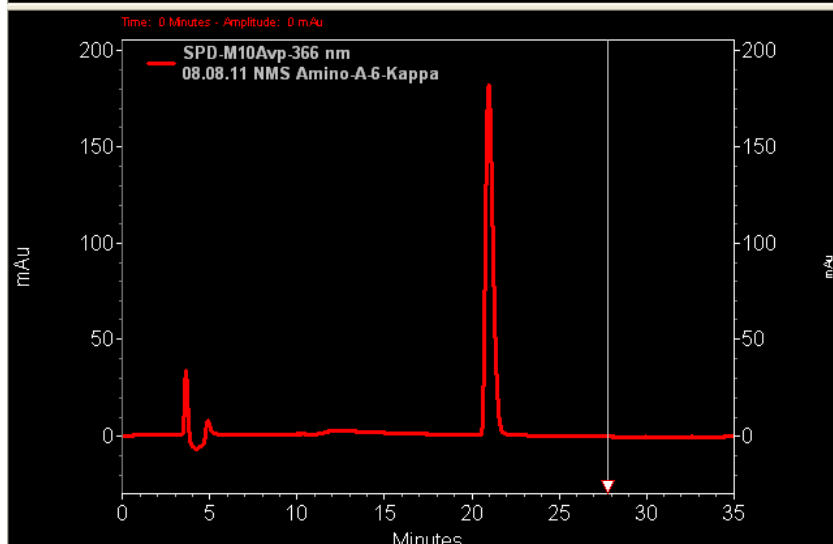
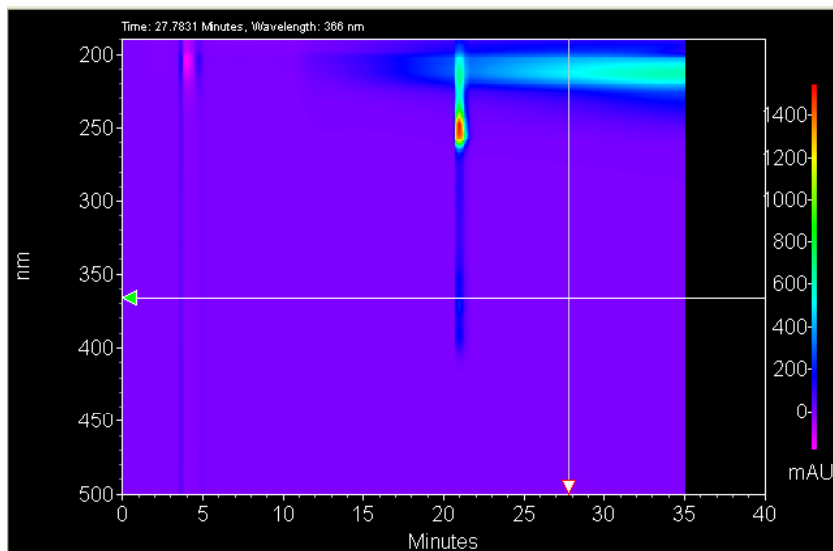
12 ¹H Spectrum



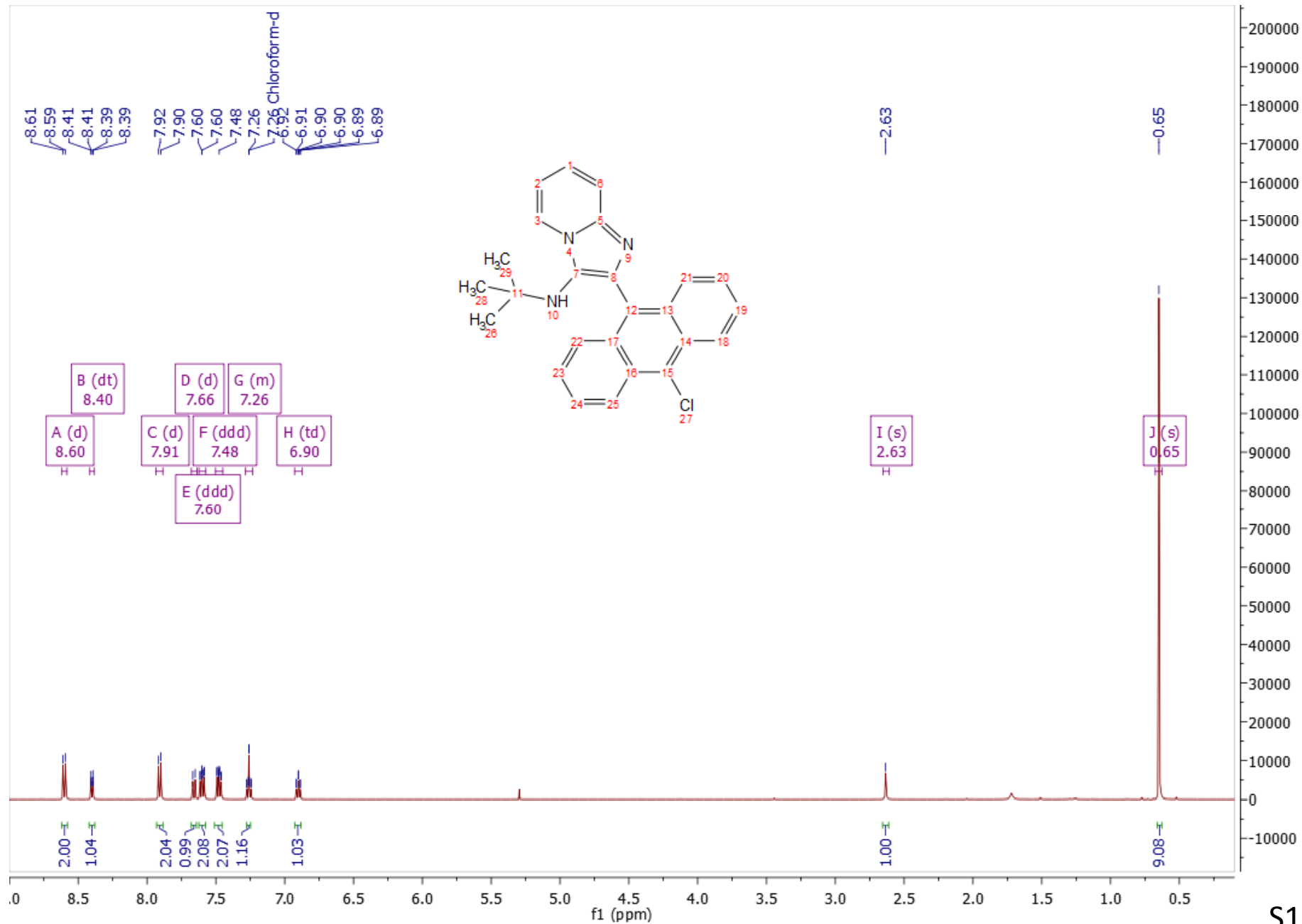
12 ¹³C Spectrum



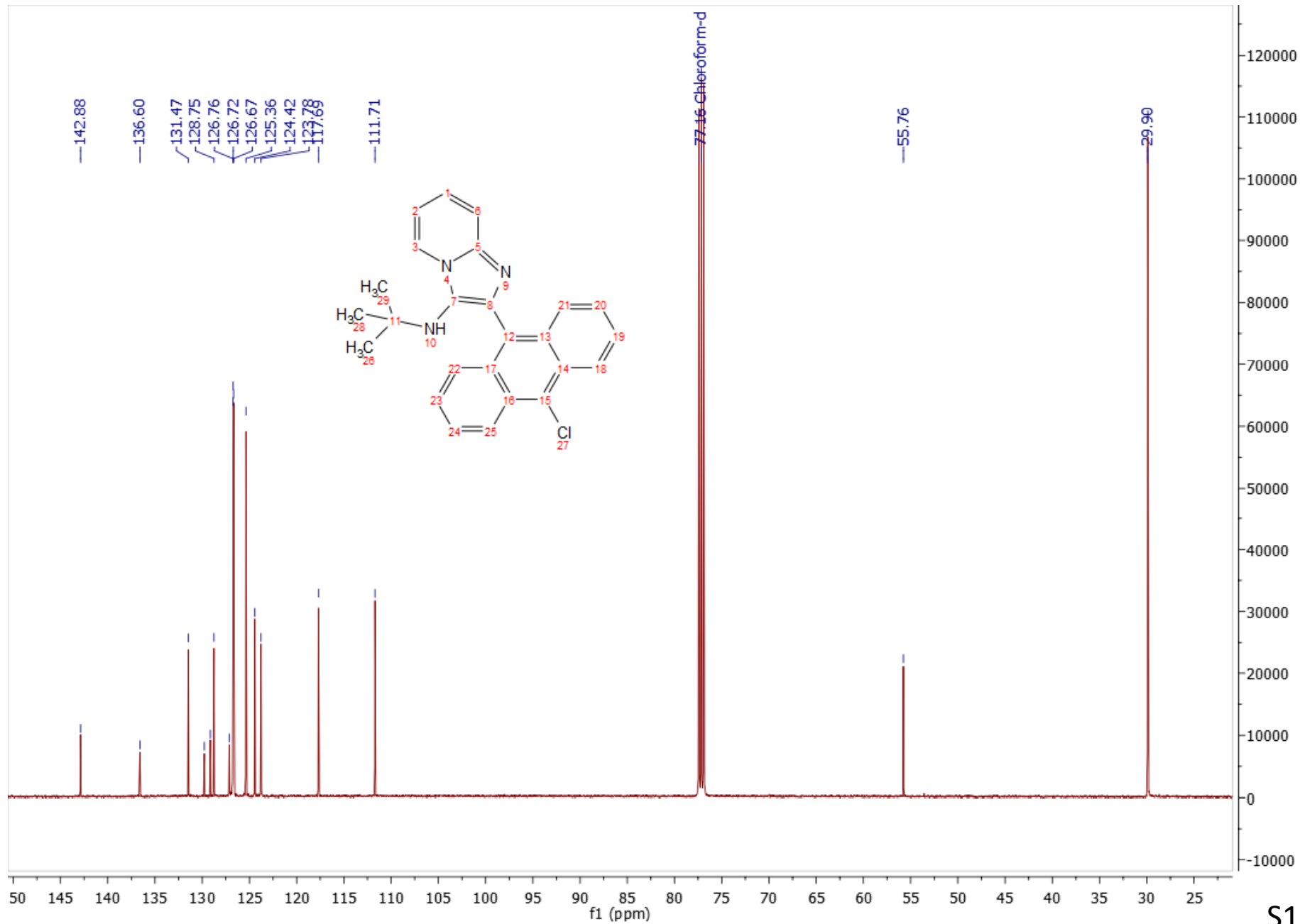
12 LC-MS



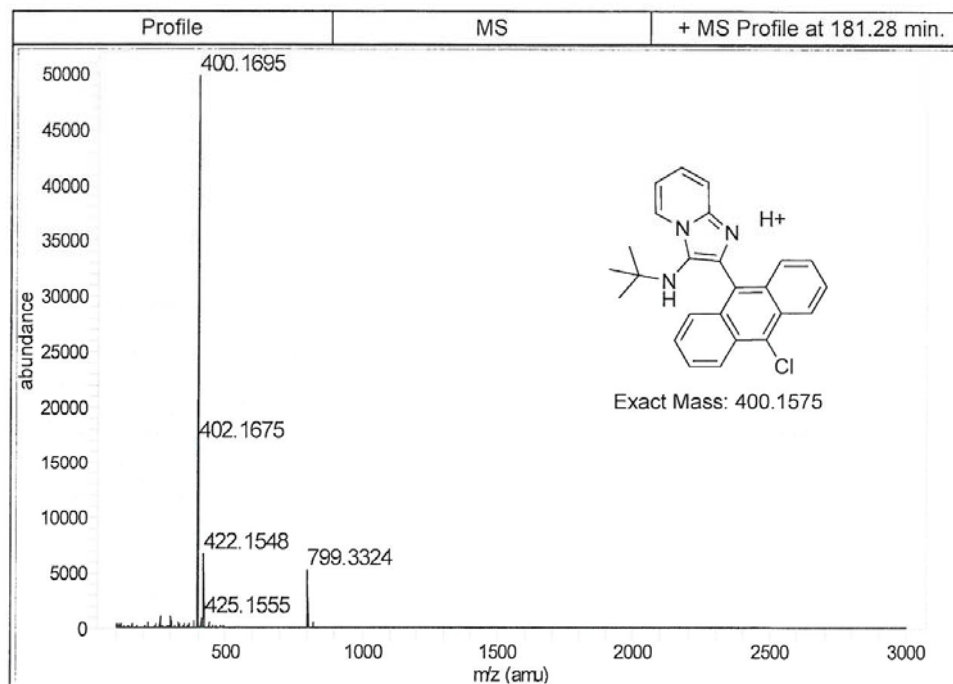
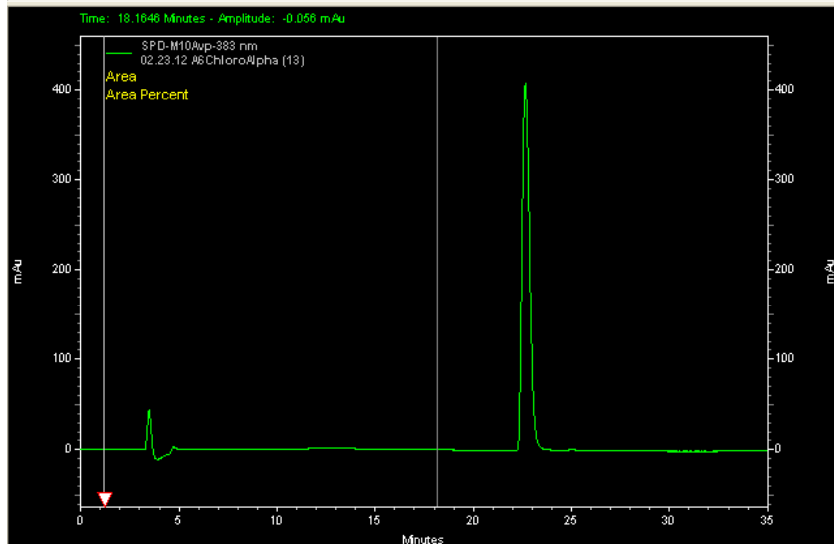
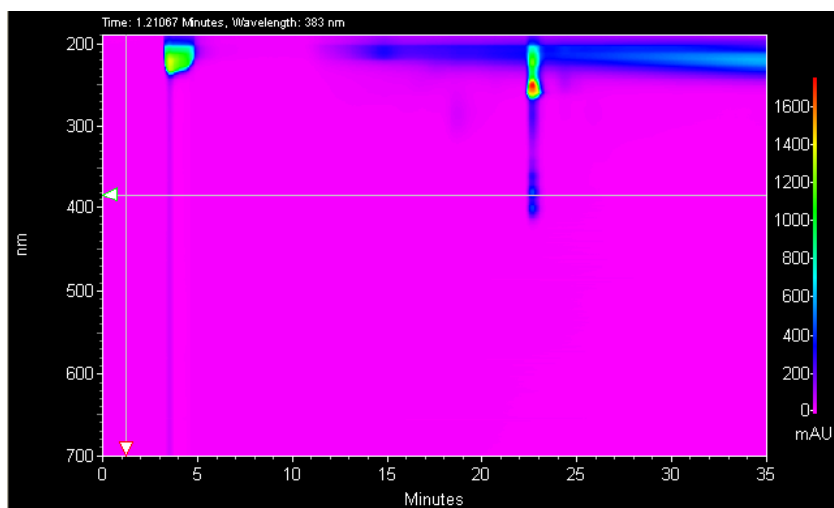
13 ¹H Spectrum



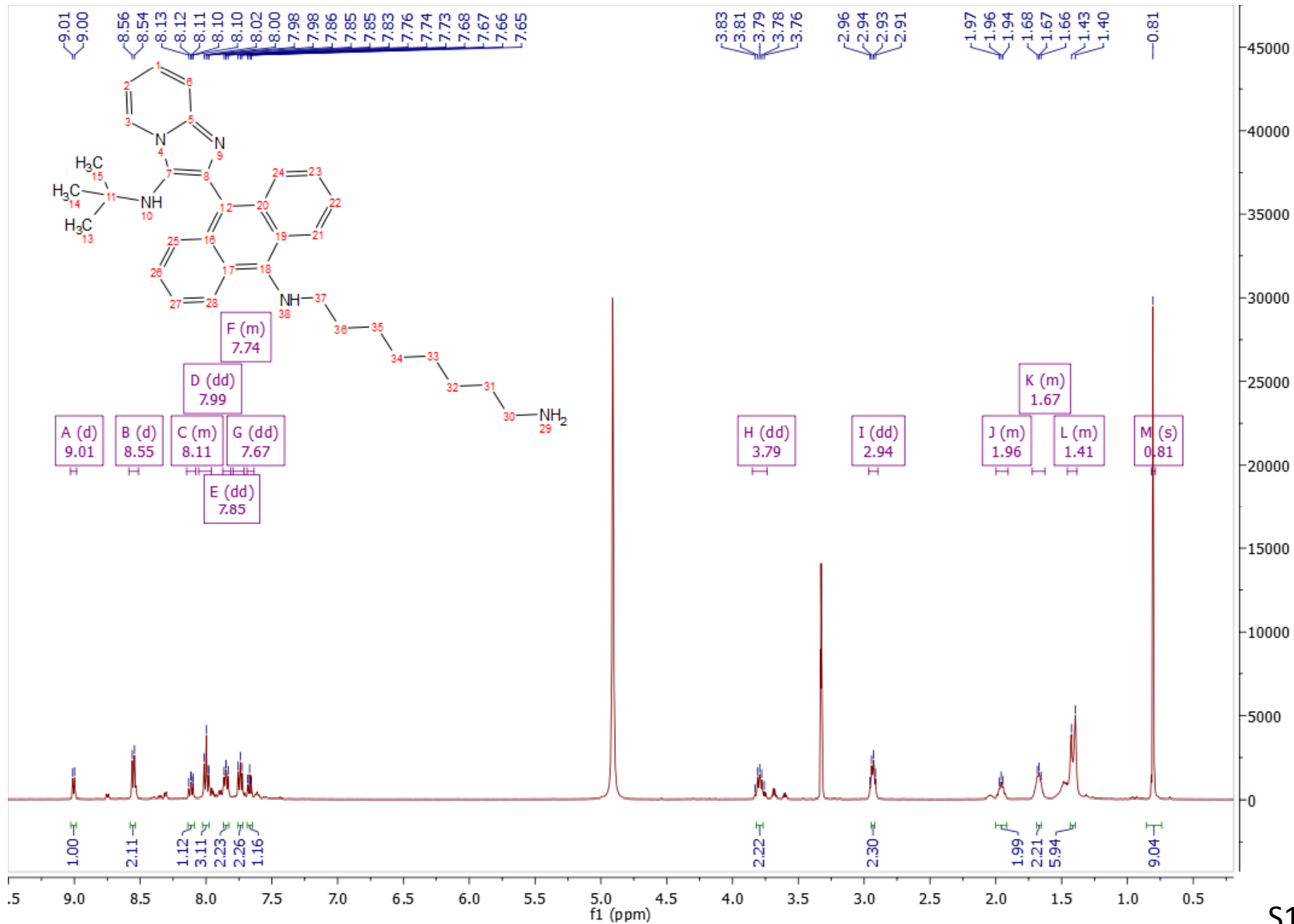
13

¹³C Spectrum

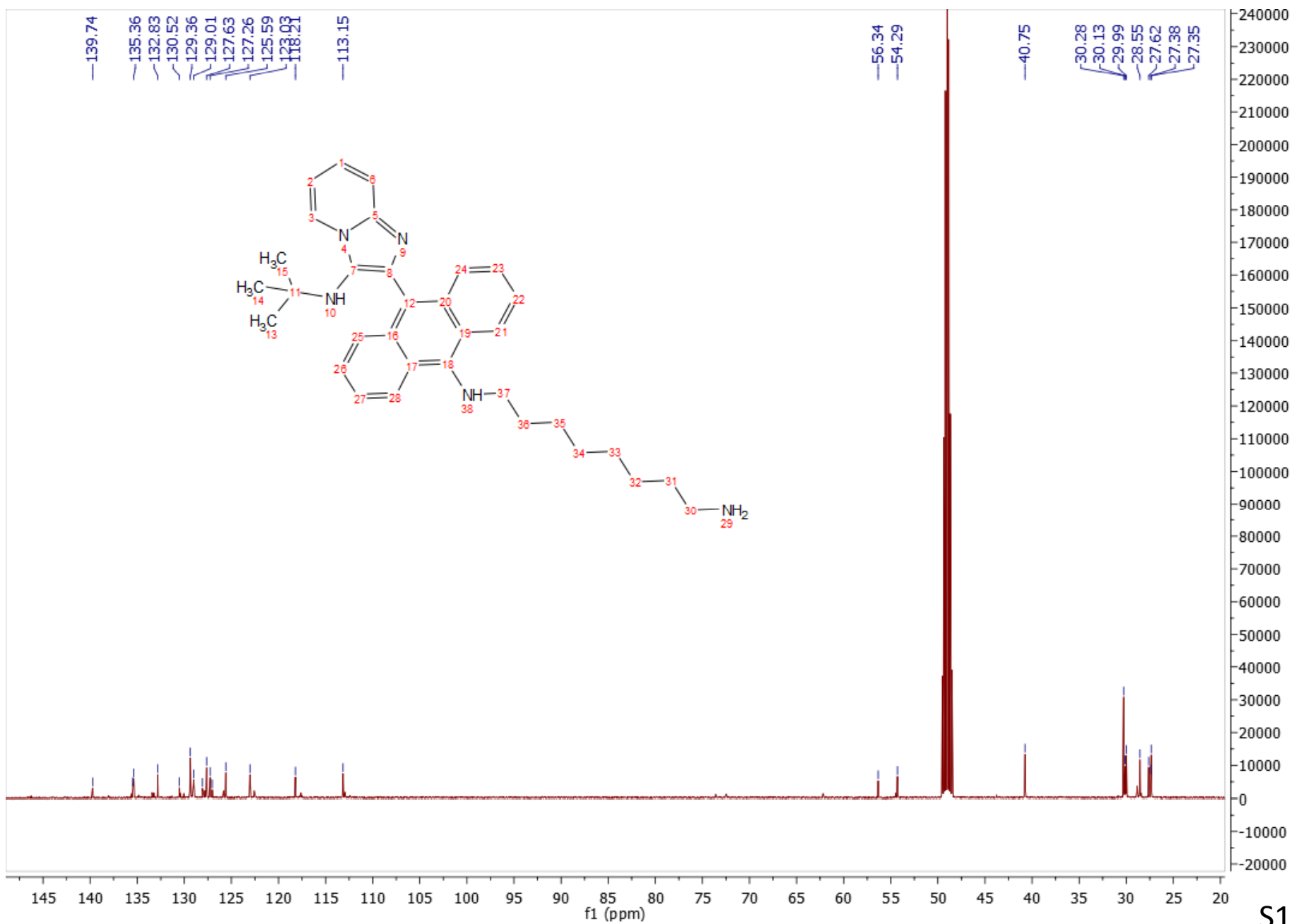
13 LC-MS



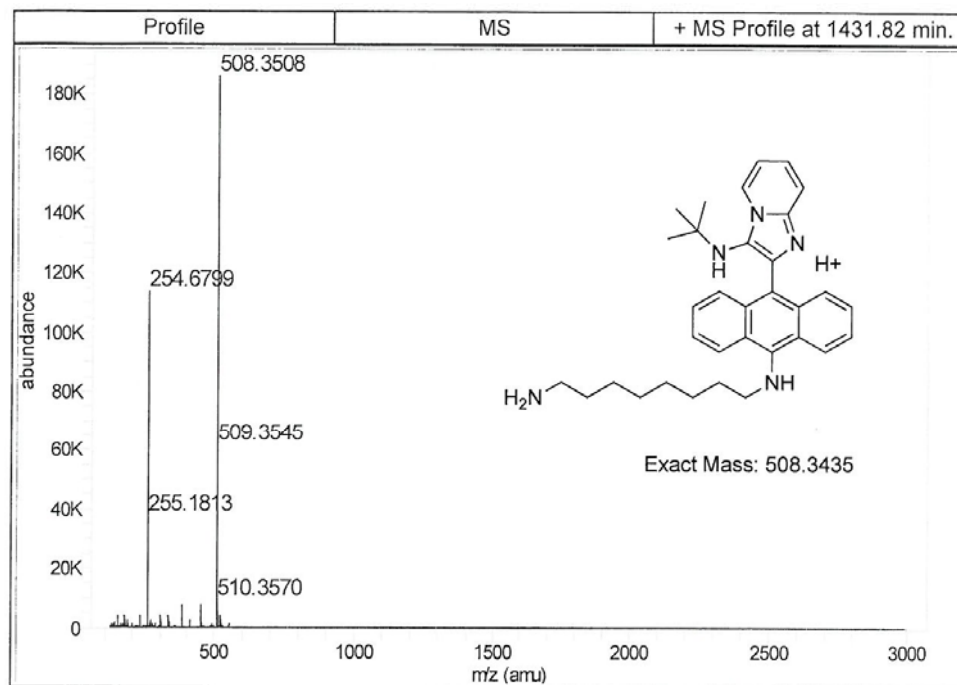
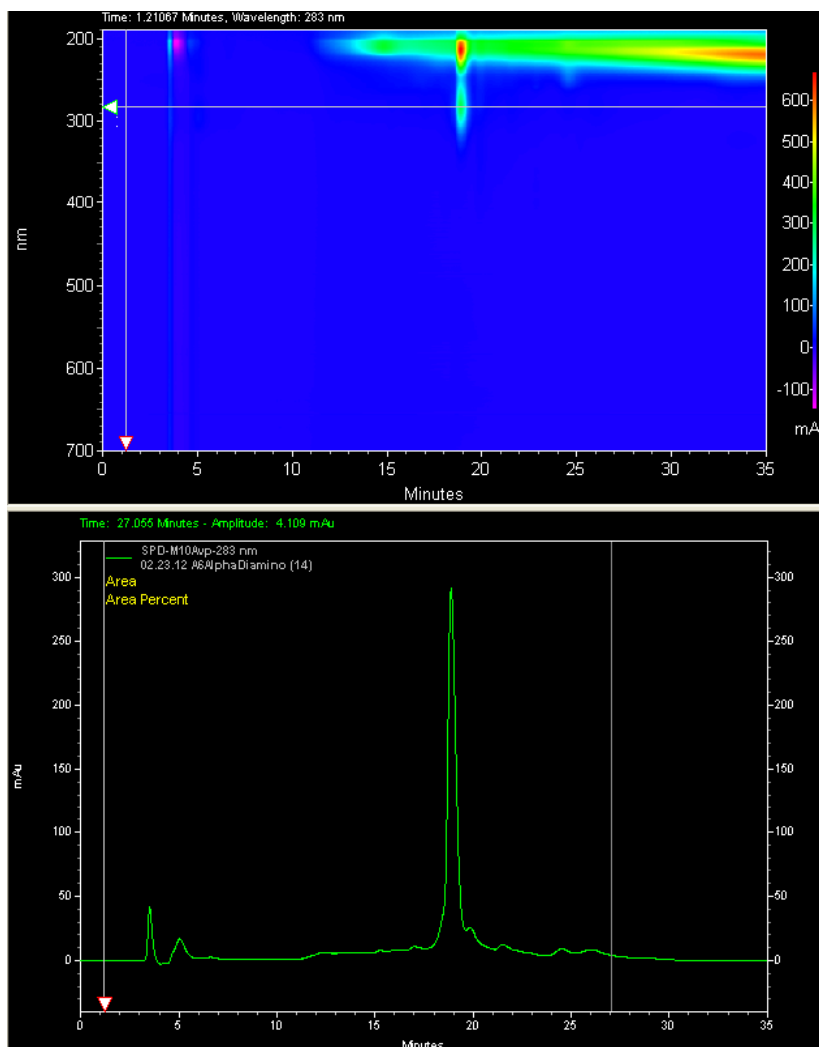
14 ¹H Spectrum



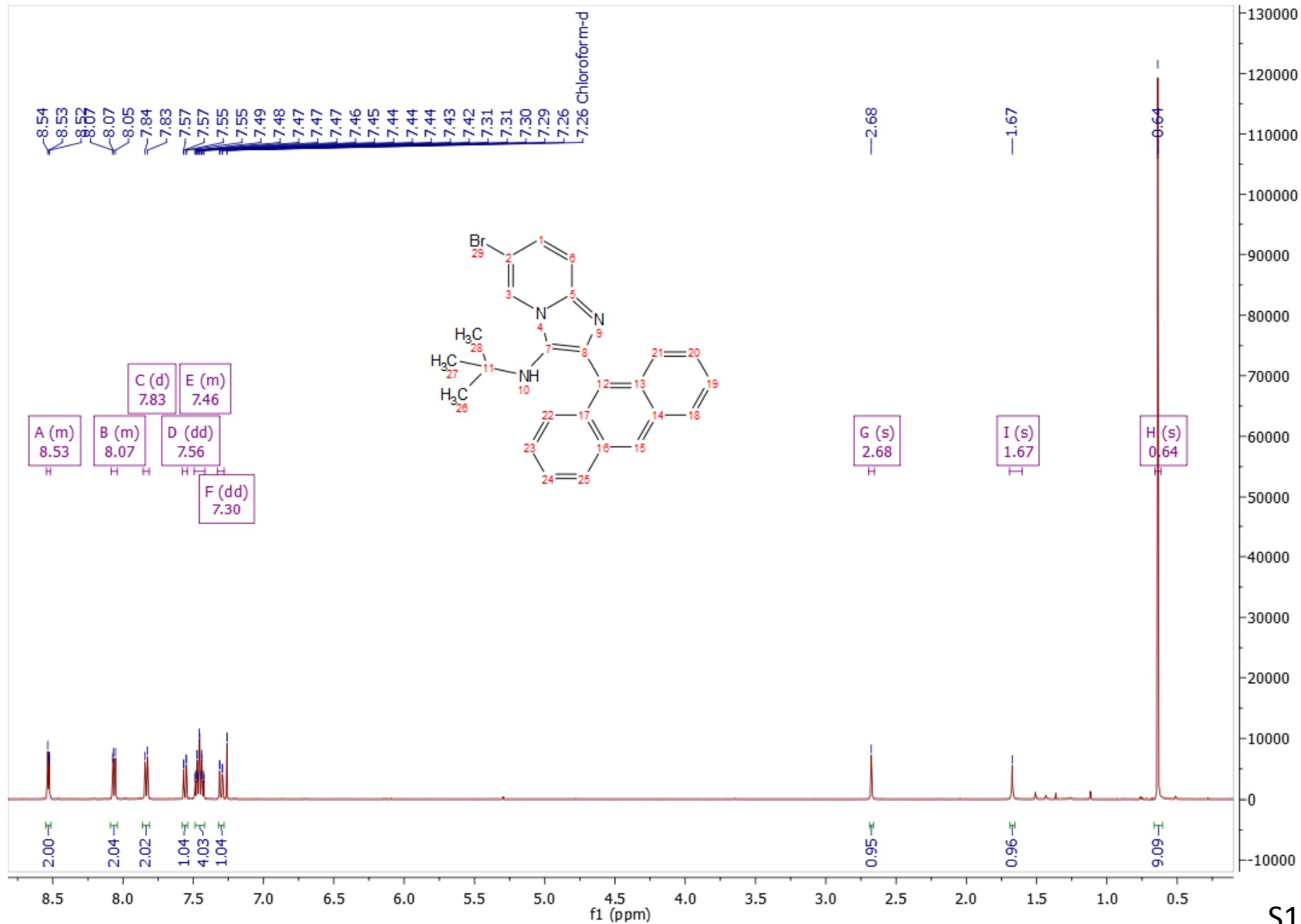
14 ¹³C Spectrum



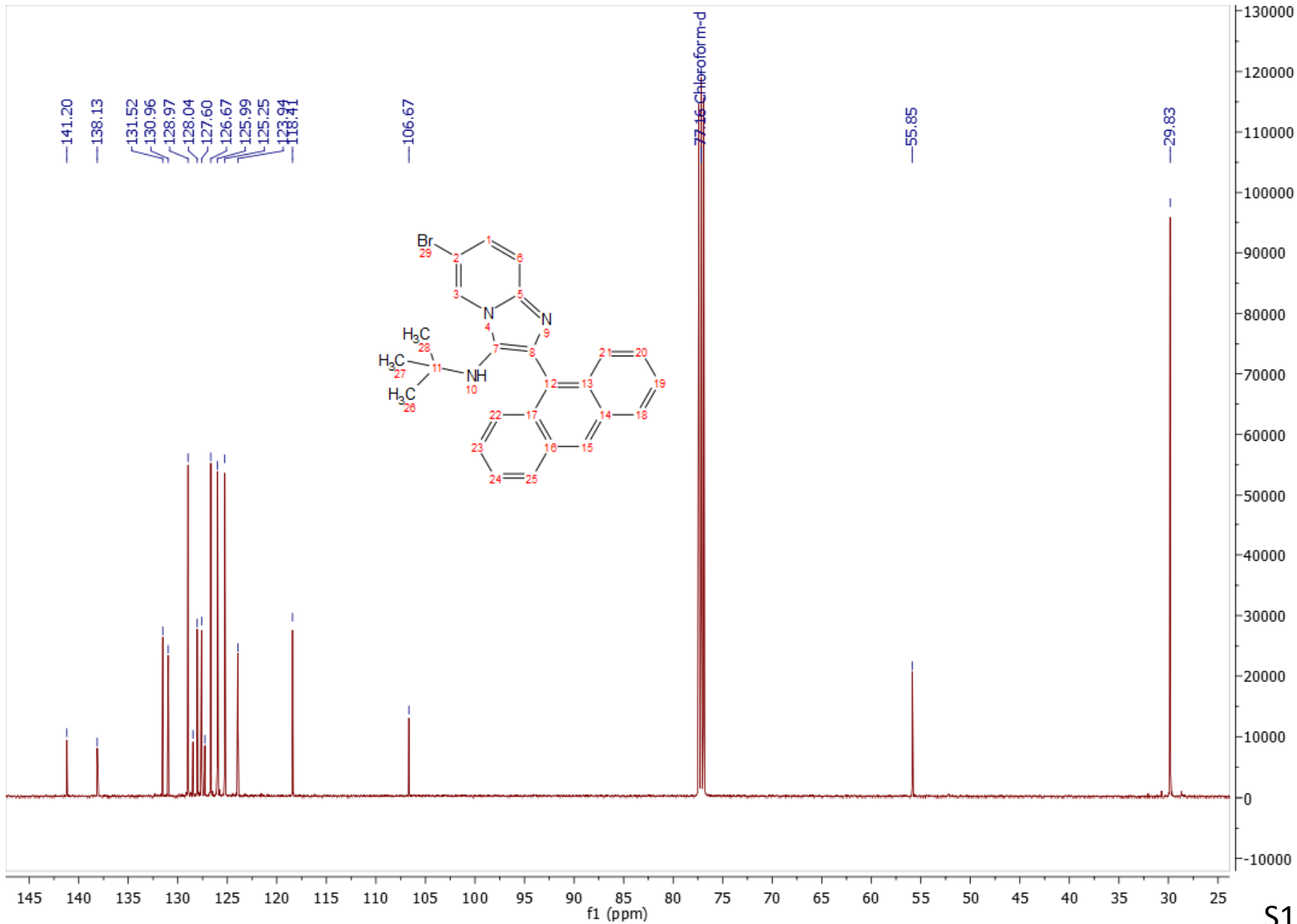
14 LC-MS



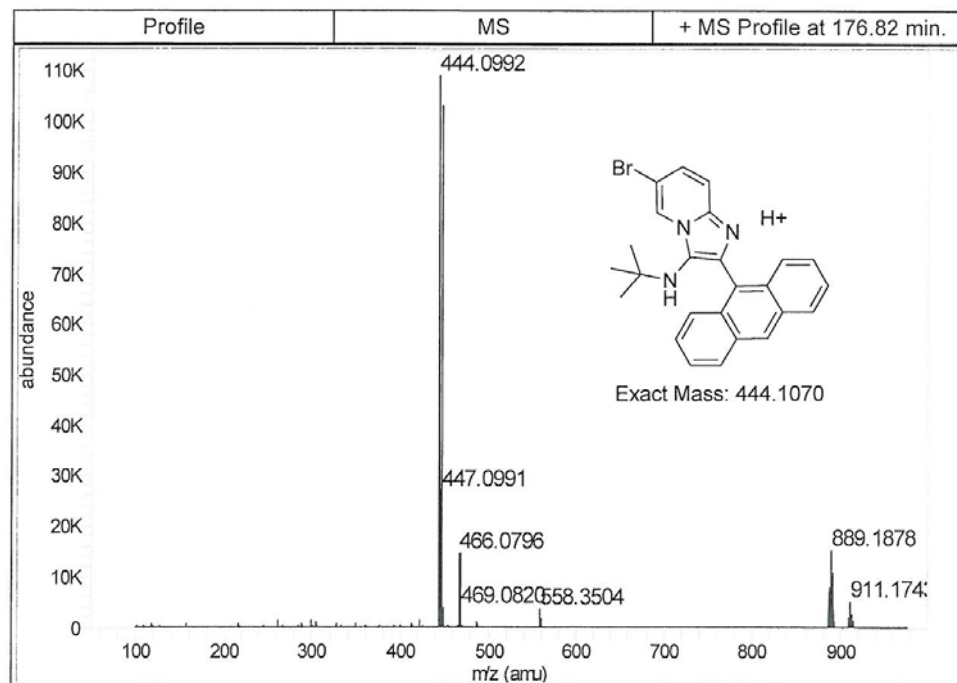
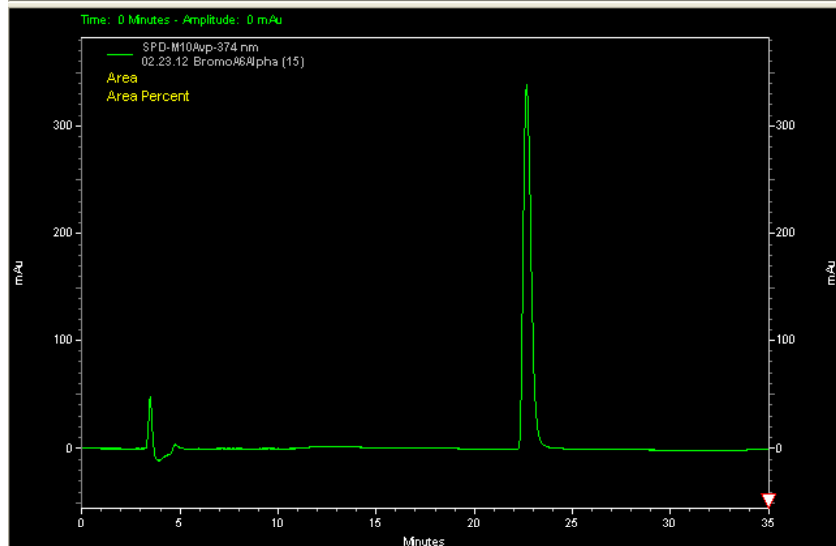
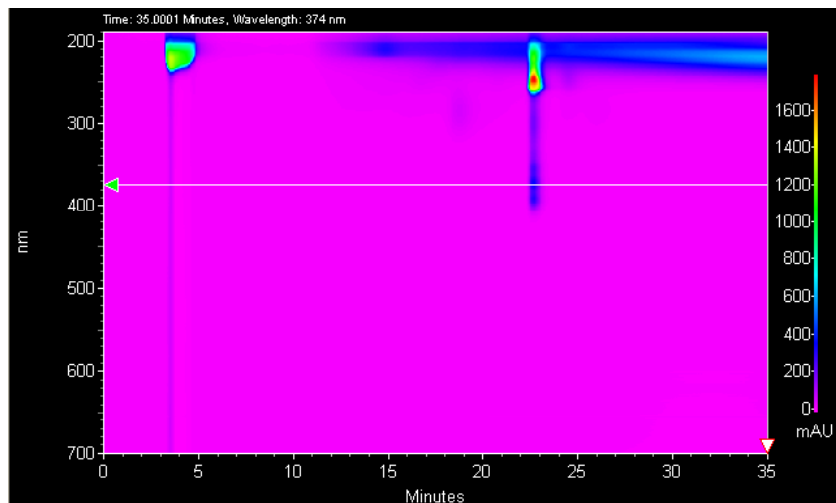
15 ¹H Spectrum



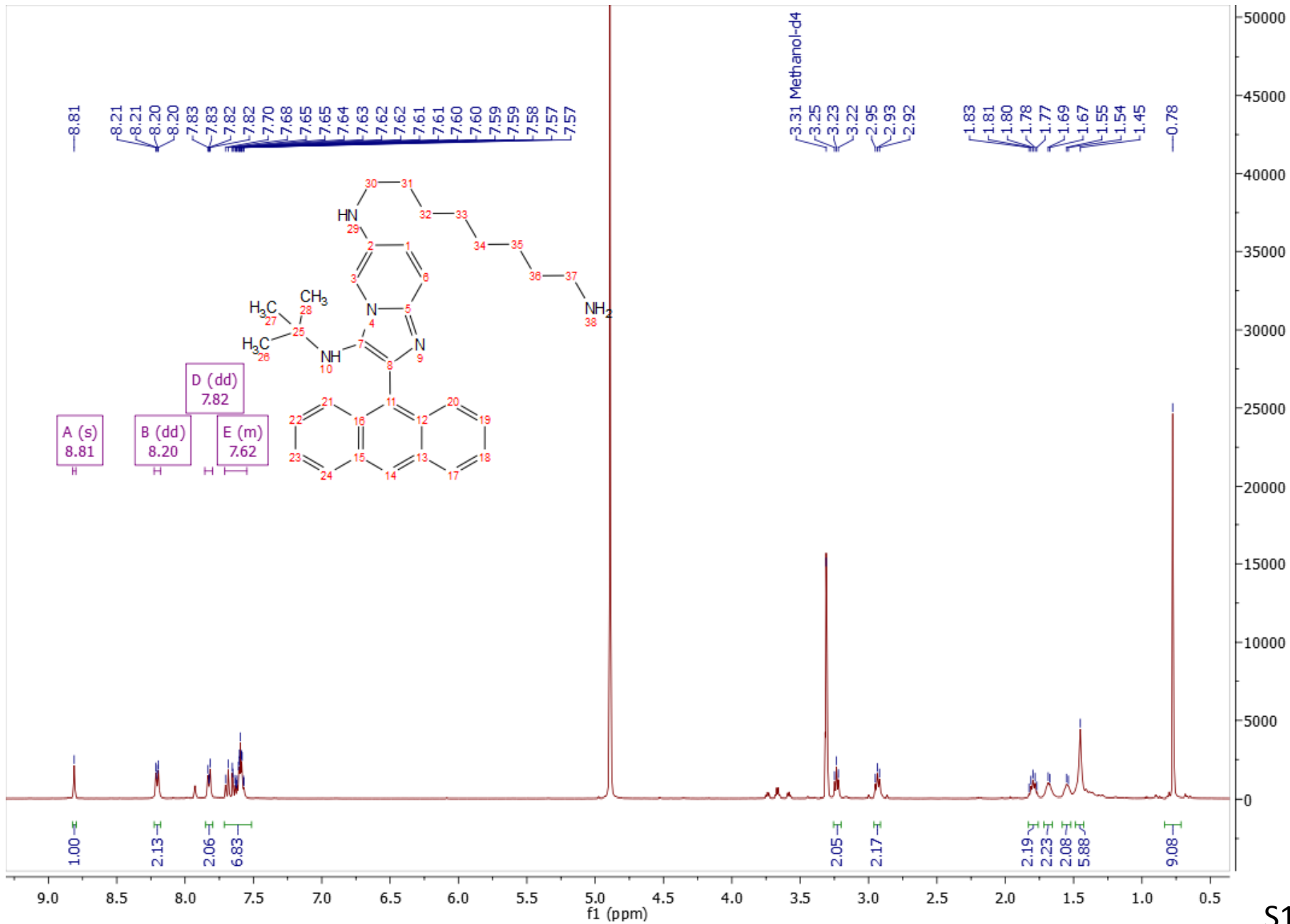
15 ¹³C Spectrum



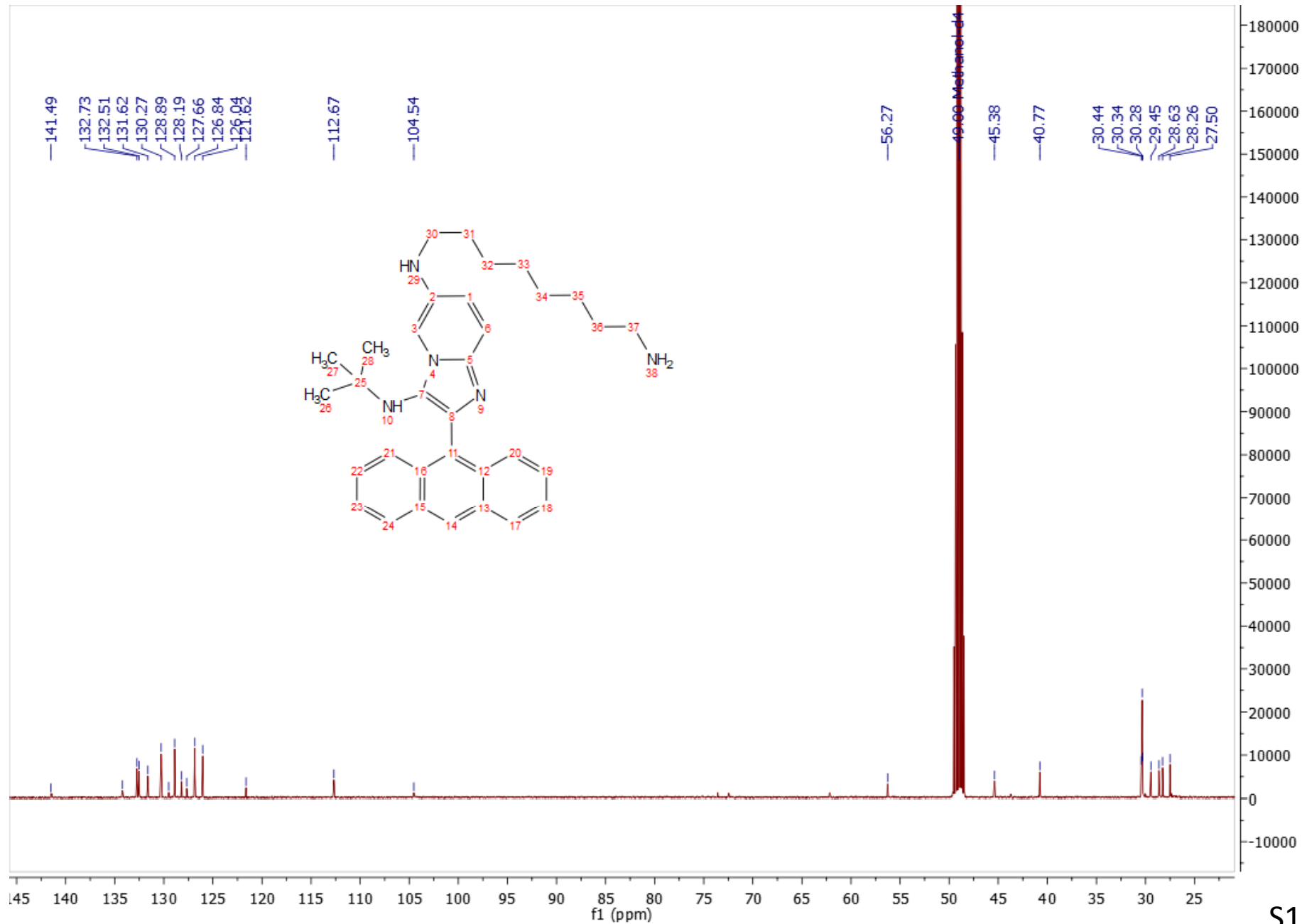
15 LC-MS



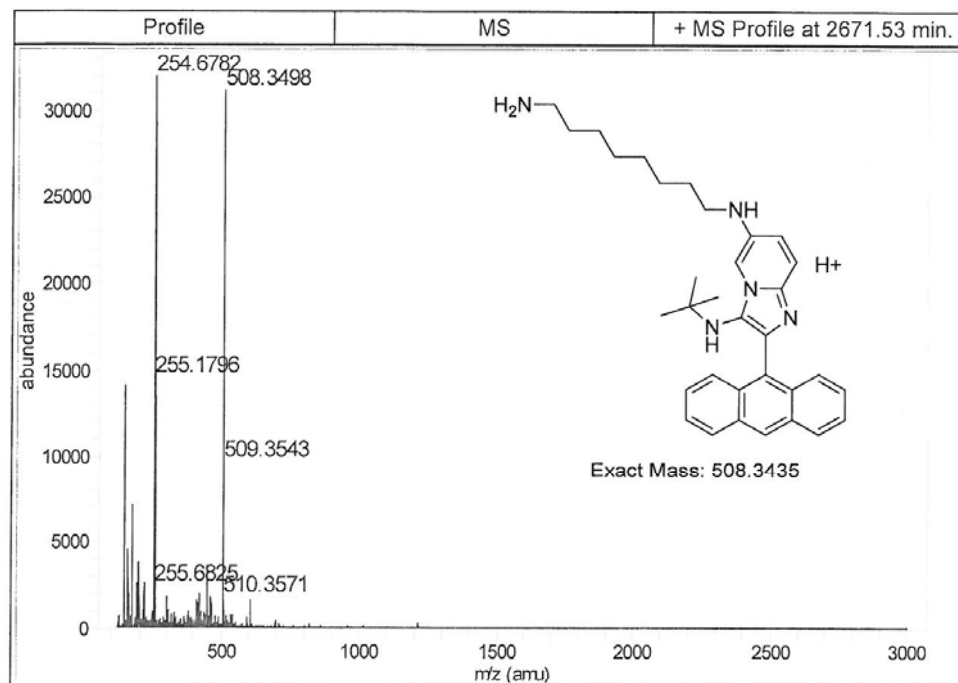
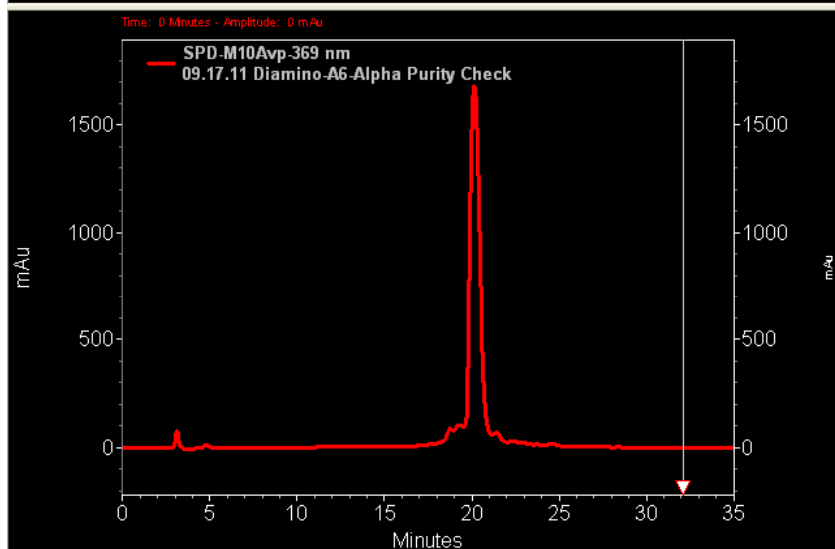
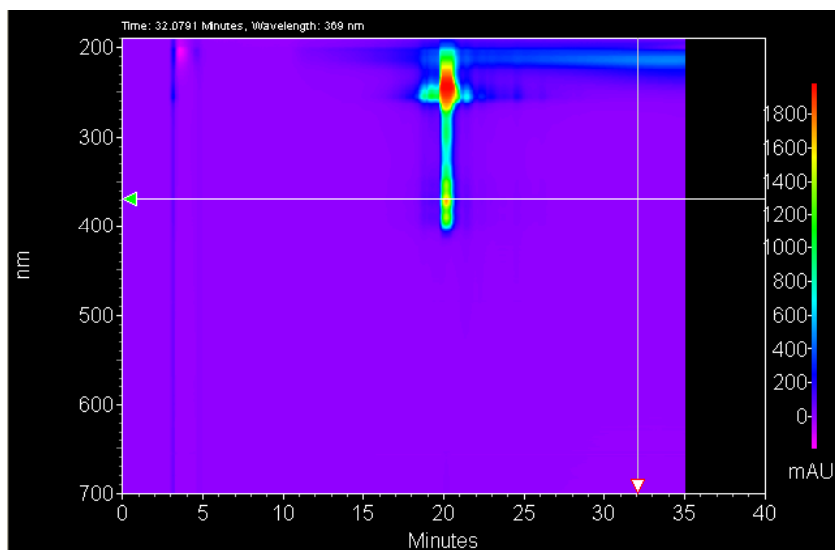
16 ¹H Spectrum



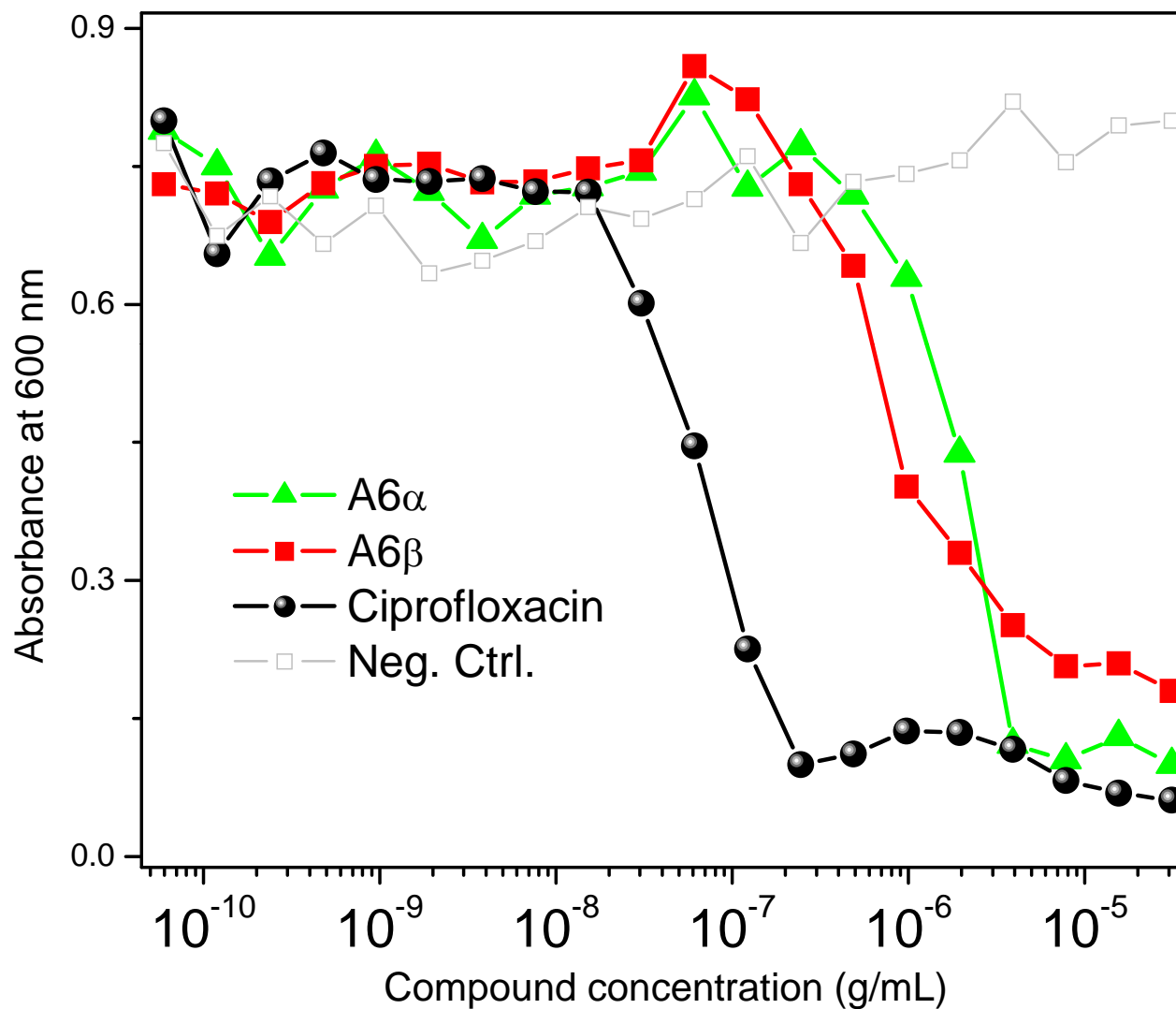
16 ¹³C Spectrum



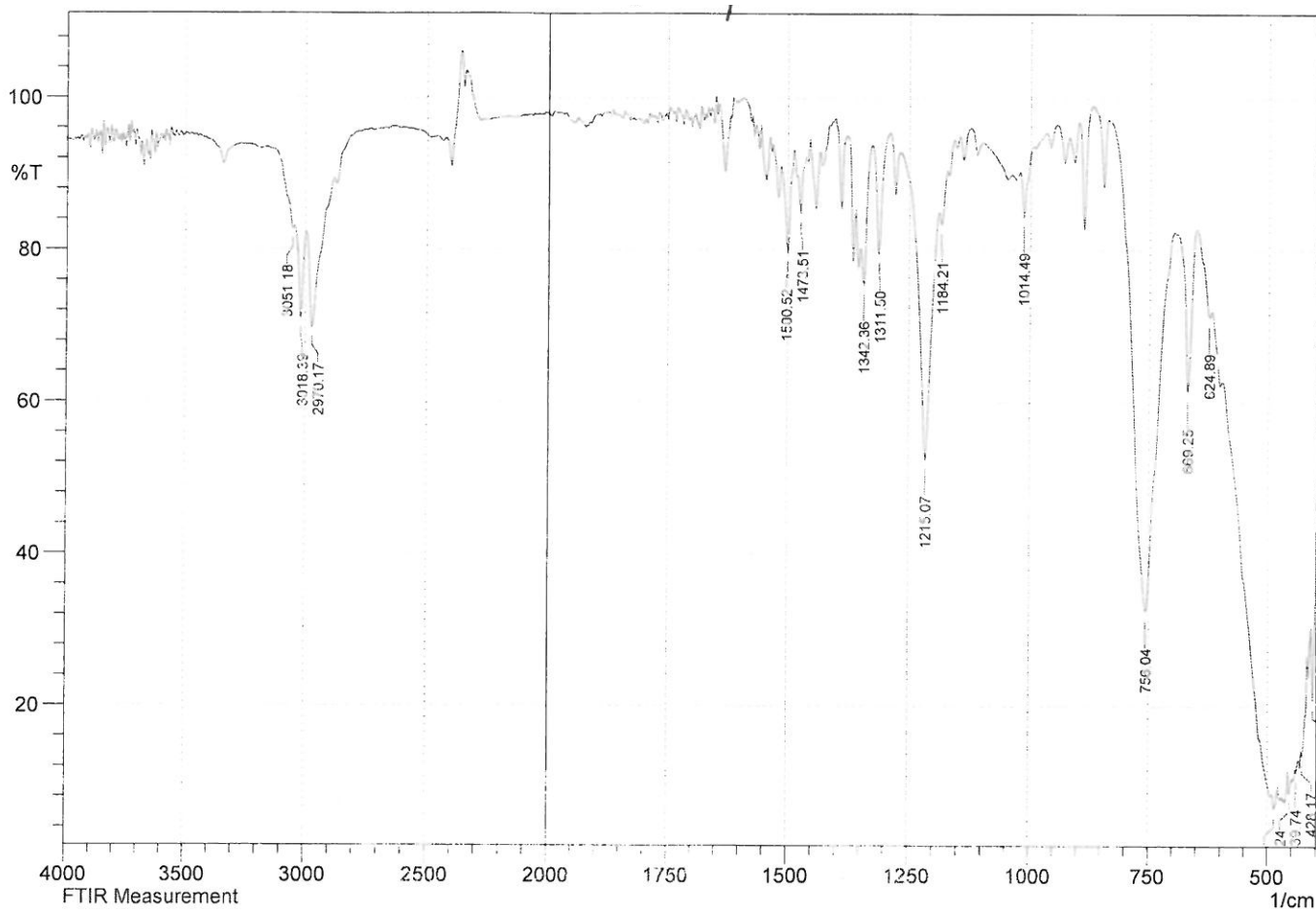
16 LC-MS



MIC of compounds **1g** and **2g** using
Coagulase Negative Staphylococcus (*S.epidermidis*) ATCC: 35983

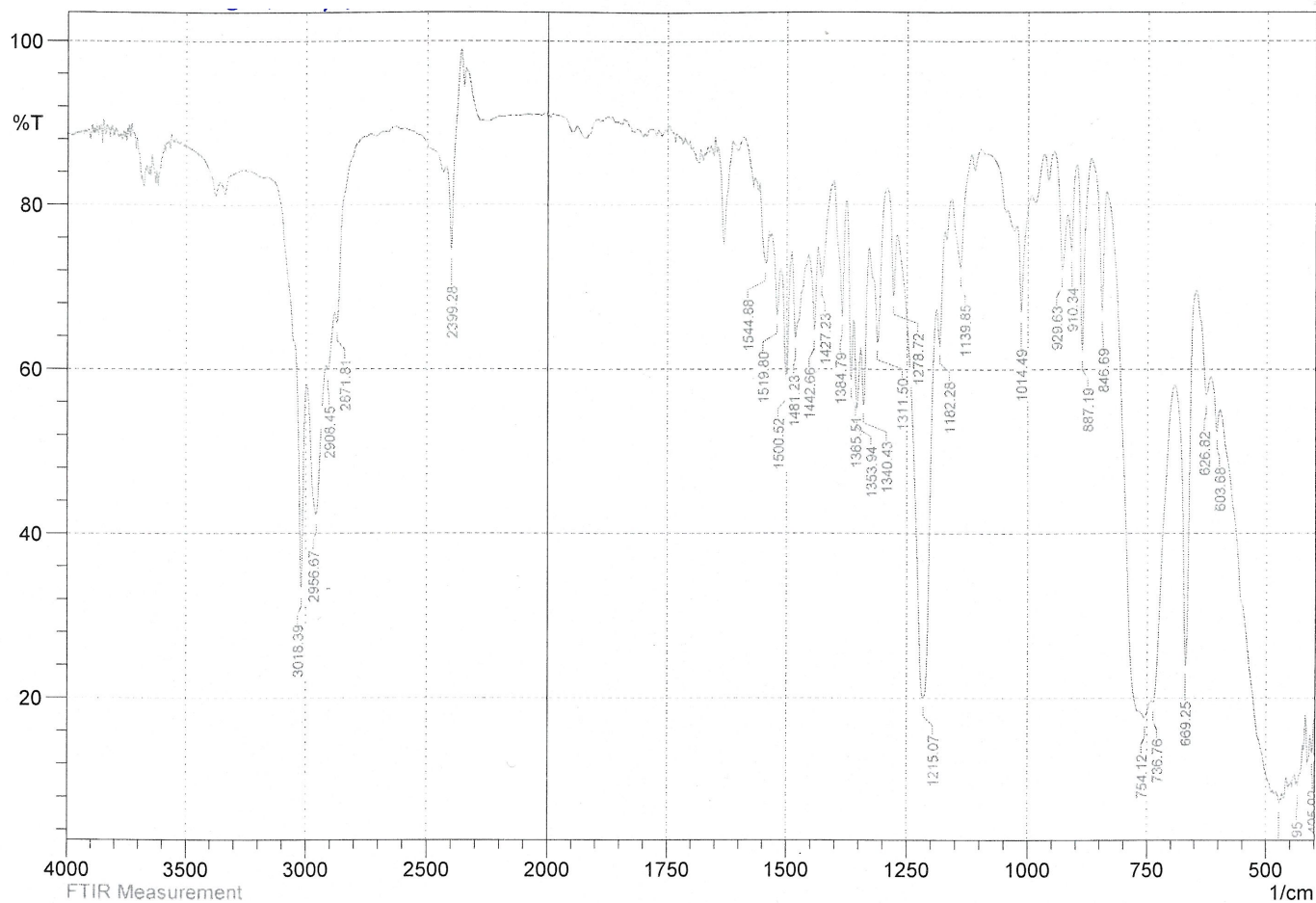


Compound 1g



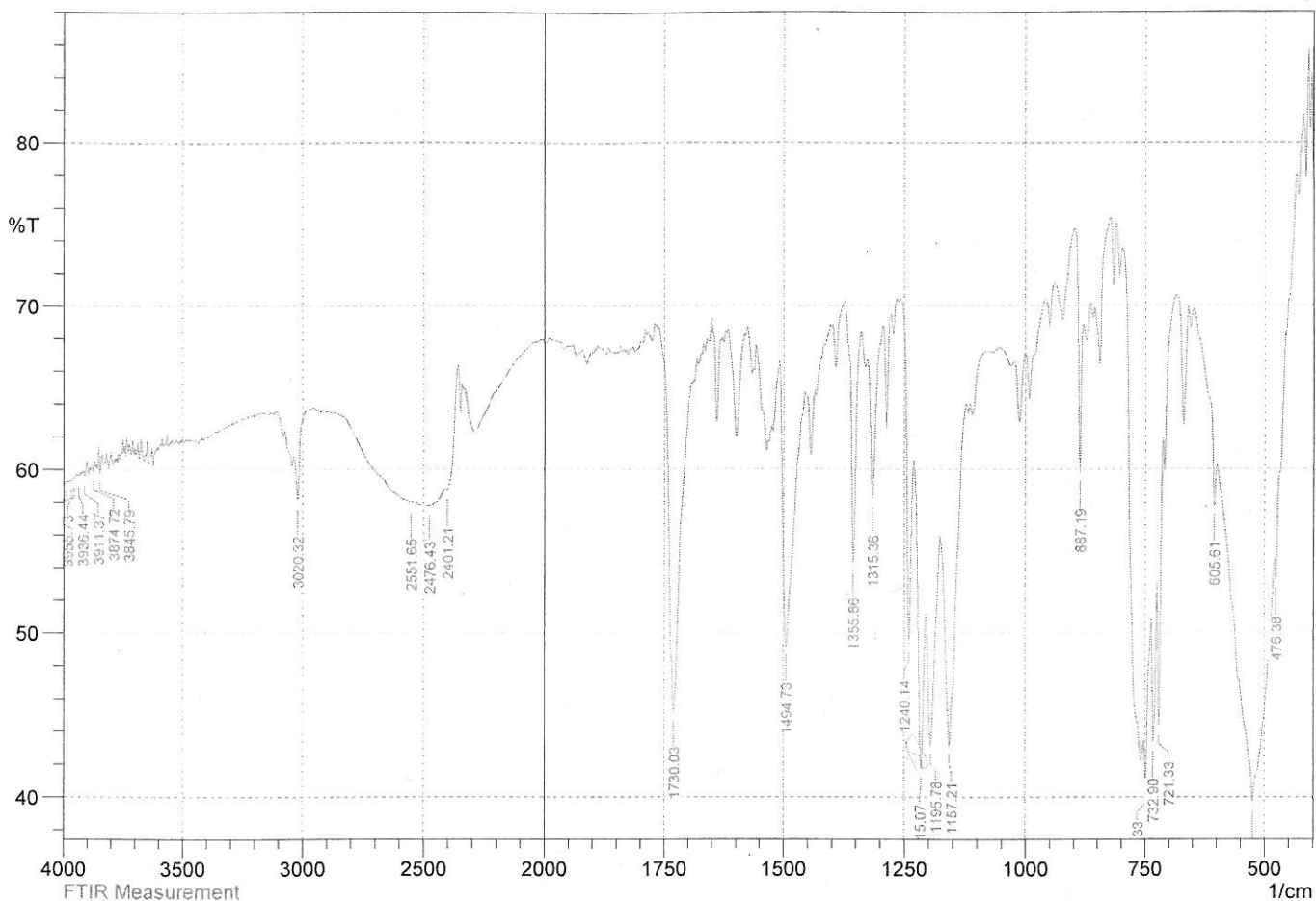
	Peak	Height	Corr. Height	Base (H)	Base (L)	Area	Corr. Area
1	406.95	79.101	15.91	410.81	399.24	6.091	1.544
2	428.17	86.357	2.592	430.1	418.52	8.715	0.751
3	439.74	89.585	1.305	443.6	435.88	7.07	0.023
4	453.24	91.339	2.299	457.1	449.38	7.94	0.493
5	486.03	93.435	1.992	489.89	480.24	10.908	0.597
6	624.89	28.776	2.655	651.89	619.11	3.825	0.133
7	669.25	38.563	20.924	690.47	653.82	4.814	1.722
8	756.04	67.461	56.001	837.05	698.18	27.035	20.269
9	1014.49	15.562	6.386	1020.27	995.2	1.215	0.298
10	1184.21	16.669	3.046	1188.07	1172.64	0.98	0.127
11	1215.07	47.508	34.959	1267.14	1190	9.363	5.326
12	1311.5	20.583	14.967	1325.01	1290.29	1.702	0.867
13	1342.36	24.571	8.366	1348.15	1326.93	1.534	0.316
14	1473.51	15.27	7.827	1487.01	1461.94	1.21	0.368
15	1500.52	20.349	11.595	1512.09	1488.94	1.516	0.601
16	2970.17	30.249	13.912	2993.32	2881.45	10.805	3.333
17	3018.39	29.063	11.697	3043.46	2995.25	5.214	1.22
18	3051.18	17.32	1.013	3128.32	3045.39	4.444	0.056

Compound 5e



	Peak	Height	Corr. Height	Base (H)	Base (L)	Area	Corr. Area
1	405.02	86.723	2.32	406.95	401.17	4.781	0.237
2	433.95	90.583	2.715	439.74	424.31	14.908	1.07
3	472.53	92.673	1.26	478.31	466.74	12.759	0.412
4	603.68	47.489	3.261	617.18	599.82	4.43	0.16
5	626.82	43.128	5.018	646.11	619.11	5.668	0.358
6	669.25	76.009	40.155	692.4	648.04	14.296	5.668
7	736.76	80.475	3.301	740.61	694.33	20.152	0.488
8	754.12	82.407	1.355	765.69	740.61	18.413	0.35
9	846.69	33.009	15.447	867.91	838.98	3.082	0.784
10	887.19	37.809	23.019	898.77	869.84	3.289	1.294
11	910.34	25.653	6.591	916.12	900.7	1.548	0.224
12	929.63	27.873	9.771	946.98	918.05	2.987	0.558
13	1014.49	33.062	11.497	1022.2	993.27	3.503	0.609
14	1139.85	27.649	10.753	1157.21	1118.64	3.996	0.965
15	1182.28	36.984	7.849	1188.07	1172.64	2.517	0.362
16	1215.07	80.009	50.186	1269.07	1190	27.372	15.883
17	1278.72	31.111	9.781	1290.29	1271	2.367	0.389
18	1311.5	36.628	14.419	1326.93	1292.22	4.873	1.199
19	1340.43	44.293	9.155	1344.29	1328.86	2.961	0.451
20	1353.94	44.905	9.202	1359.72	1346.22	3.101	0.467
21	1365.51	41.256	11.334	1375.15	1361.65	2.413	0.477
22	1384.79	33.544	14.715	1402.15	1377.08	3.185	0.964
23	1427.23	28.755	4.831	1433.01	1404.08	3.309	0.324
24	1442.66	35.345	9.829	1454.23	1434.94	2.945	0.473
25	1481.23	36.287	9.969	1488.94	1461.94	4.527	0.87
26	1500.52	41.492	14.368	1512.09	1490.87	3.784	0.868
27	1519.8	33.421	7.016	1529.45	1514.02	2.338	0.303
28	1544.88	27.064	6.151	1556.45	1537.16	2.362	0.422
29	2399.28	25.528	15.114	2420.5	2358.78	3.911	1.611
30	2871.81	34.336	2.516	2879.52	2756.09	10.737	0.156
31	2908.45	40.106	1.66	2914.24	2881.45	6.589	0.195
32	2956.67	57.668	16.933	2995.25	2916.17	23.608	5.669
33	3018.39	66.734	28.12	3161.11	2997.17	28.516	4.746

Compound 7c



	Peak	Height	Corr. Height	Base (H)	Base (L)	Area	Corr. Area
1	476.38	46.798	2.389	478.31	435.88	7.612	0.094
2	524.6	60.294	10.072	551.6	480.24	24.93	3.839
3	605.61	42.238	3.654	648.04	599.82	9.057	0.125
4	721.33	55.628	7.695	723.26	713.61	2.725	0.344
5	732.9	56.646	8.204	736.76	725.18	3.789	0.511
6	748.33	59.288	4.604	752.19	738.69	4.653	0.234
7	887.19	40.203	11.25	896.84	881.41	2.658	0.404
8	1157.21	56.863	15.215	1174.57	1124.42	14.131	2.879
9	1195.78	56.787	8.696	1203.5	1176.5	8.504	1.108
10	1215.07	58.2	12.928	1230.5	1205.43	7.689	1.231
11	1240.14	50.656	14.079	1255.57	1232.43	5.233	0.864
12	1315.36	41.832	9.159	1325.01	1294.15	5.927	0.715
13	1355.86	45.641	14.757	1371.29	1340.43	6.072	1.109
14	1494.73	50.802	16.906	1508.23	1456.16	12.62	3.087
15	1730.03	54.718	21.657	1760.89	1695.31	15.712	4.2
16	2401.21	41.341	1.067	2407	2360.71	9.867	0.444
17	2476.43	42.223	0.069	2480.29	2408.93	16.803	0.086
18	2551.65	42.031	0.034	2565.15	2547.79	4.107	0.004
19	3020.32	41.839	3.497	3035.75	2985.6	10.621	0.326
20	3845.79	40.202	1.37	3851.58	3838.08	2.958	0.07
21	3874.72	40.134	0.572	3882.44	3868.94	2.978	0.025
22	3911.37	40.399	0.464	3915.23	3901.73	3.004	0.032
23	3936.44	40.502	0.242	3940.3	3930.66	2.166	0.011
24	3955.73	40.566	0.099	3959.59	3948.01	2.607	0.005
25	3967.3	40.677	0.059	3971.16	3959.59	2.621	0.004
26	3990.45	40.742	0.011	3992.37	3980.8	2.628	0.001