

New Approach to Stereoselective Synthesis of trans-3-Carbamoyl- β -Lactam Moiety.

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80-233 Gdansk, Poland

*Corresponding Author: mak@pg.gda.pl.

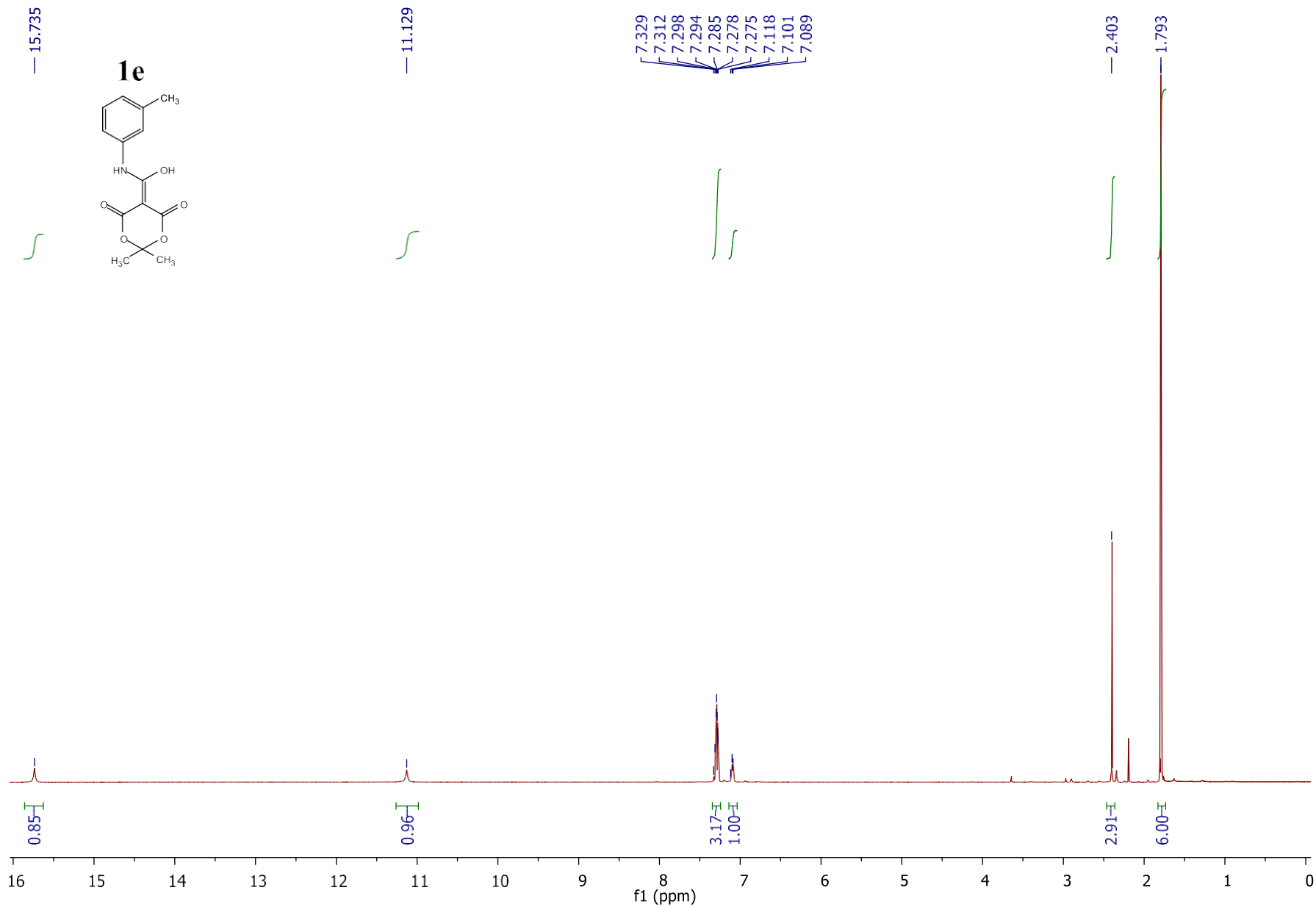
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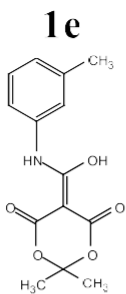
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Page S67-72, Conformational analysis data for 7aea, 8aea, 7cea, 8cea, 7ifa and 8ifa,



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164.312

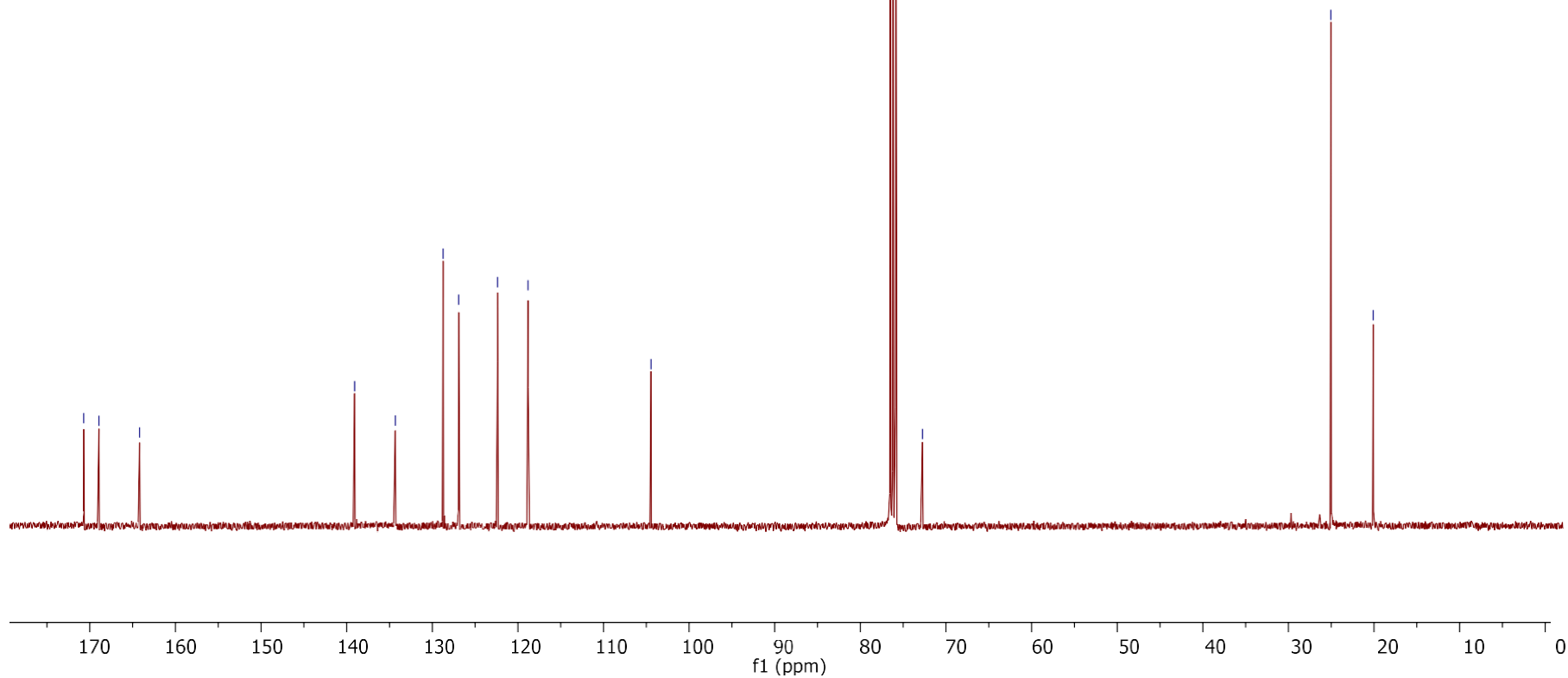


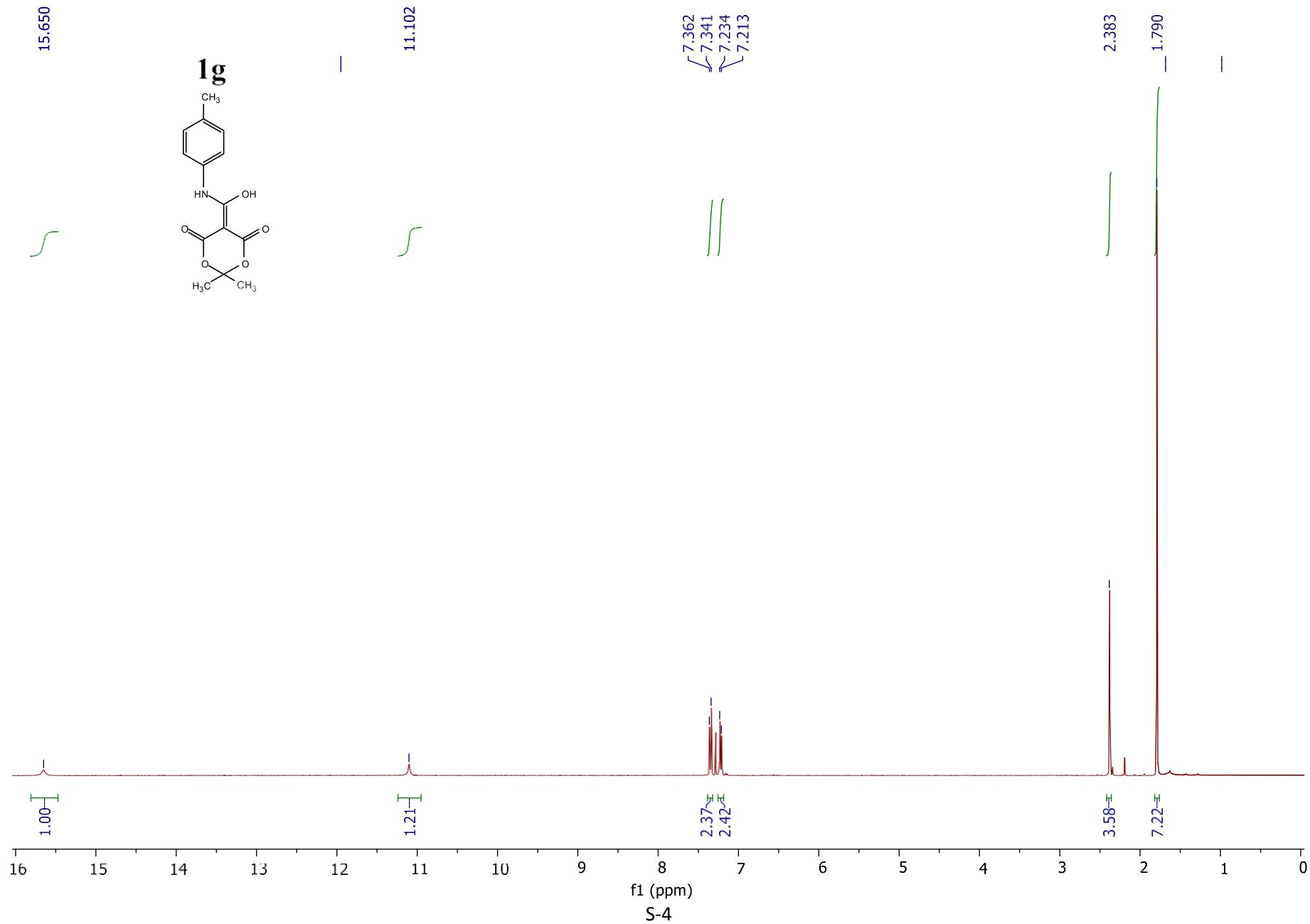
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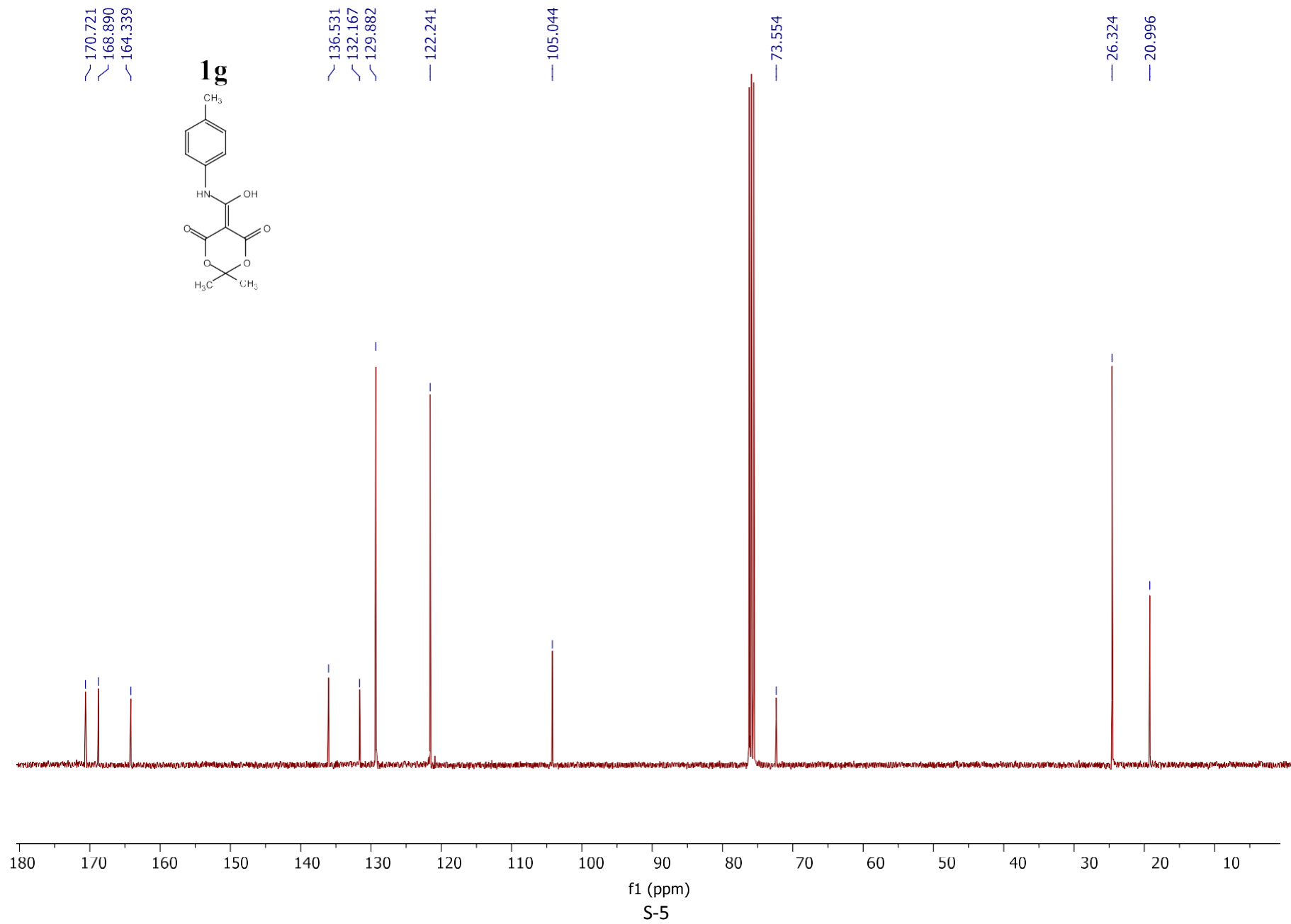
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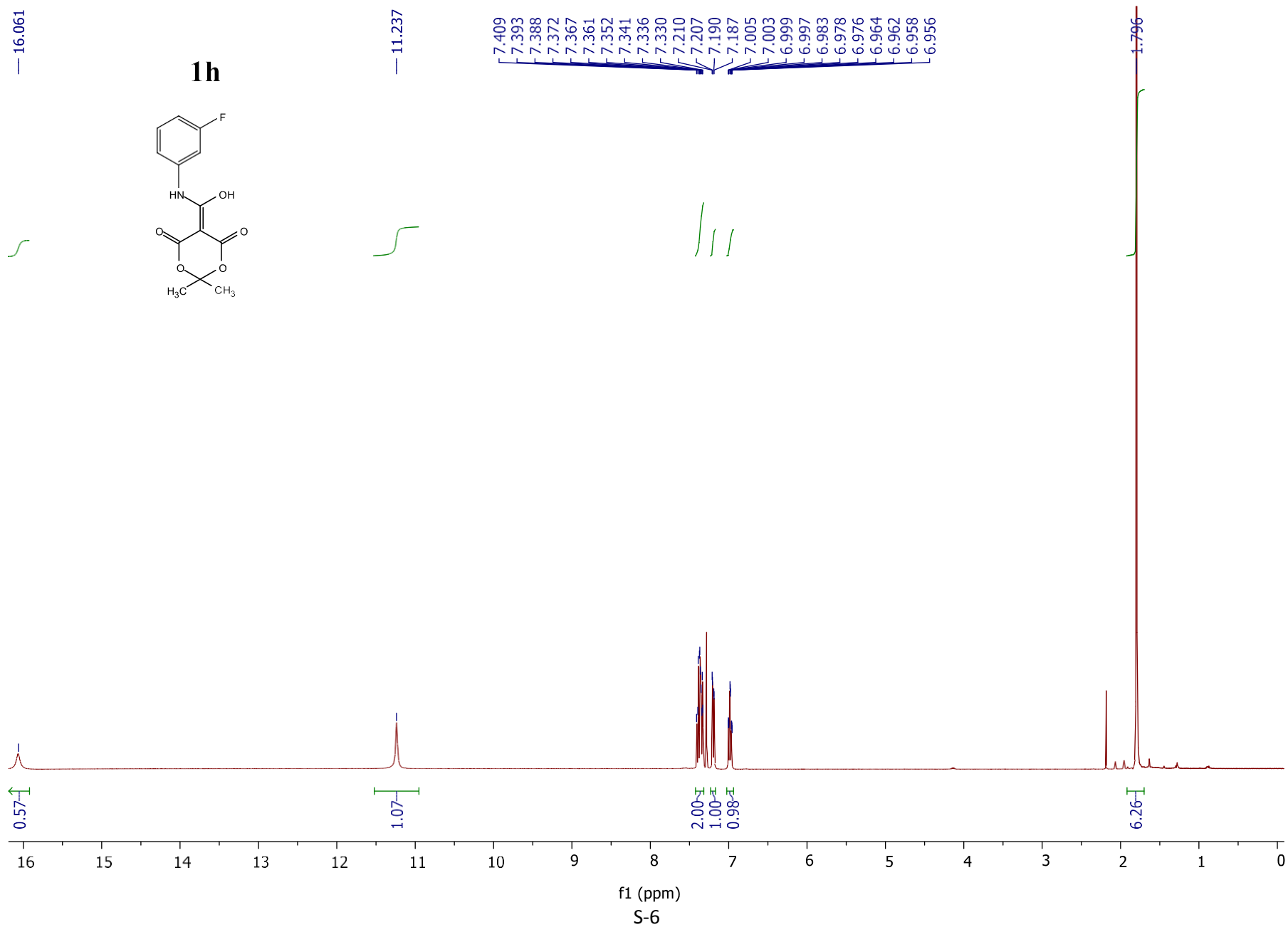
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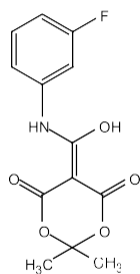
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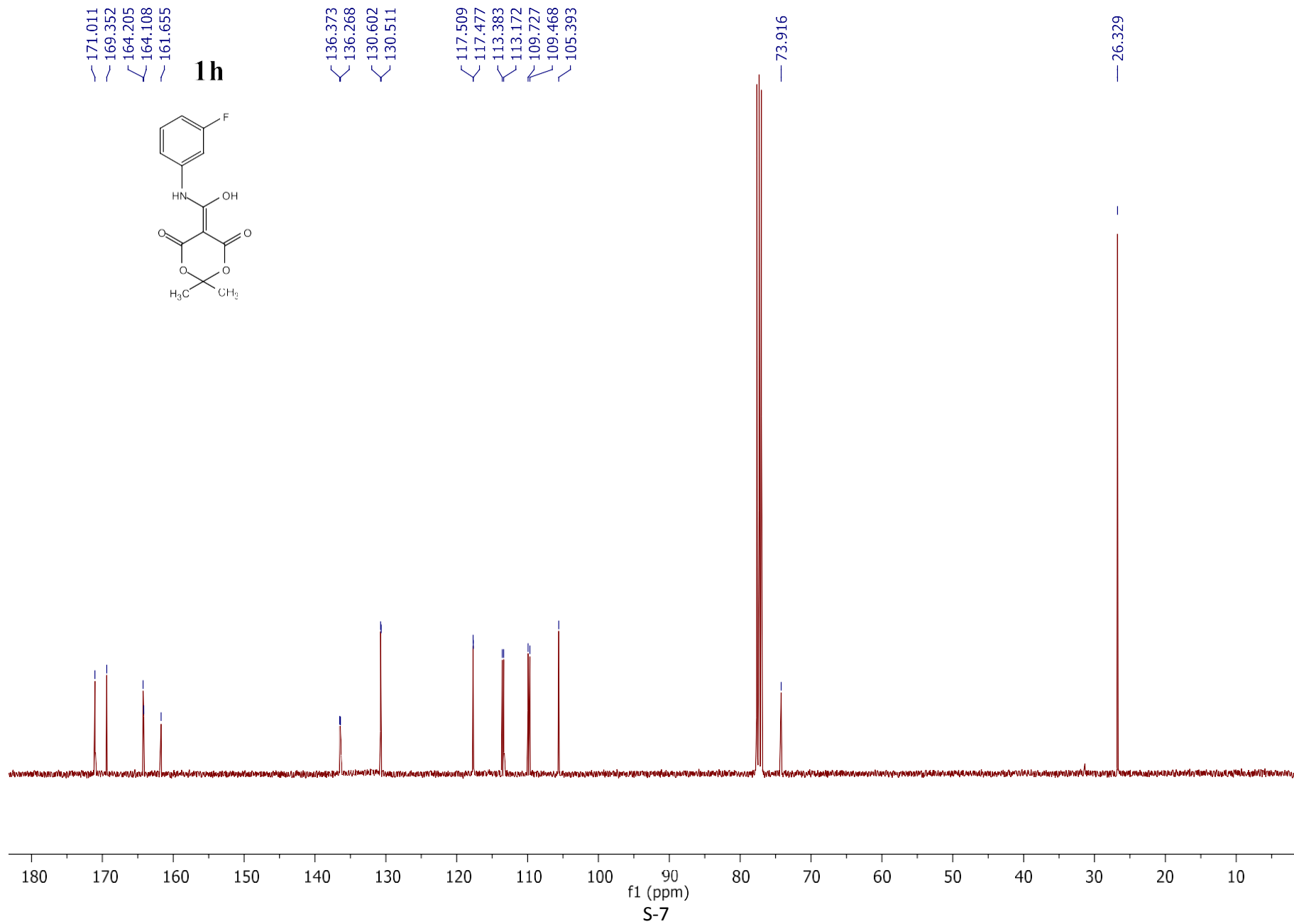


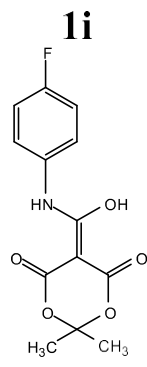
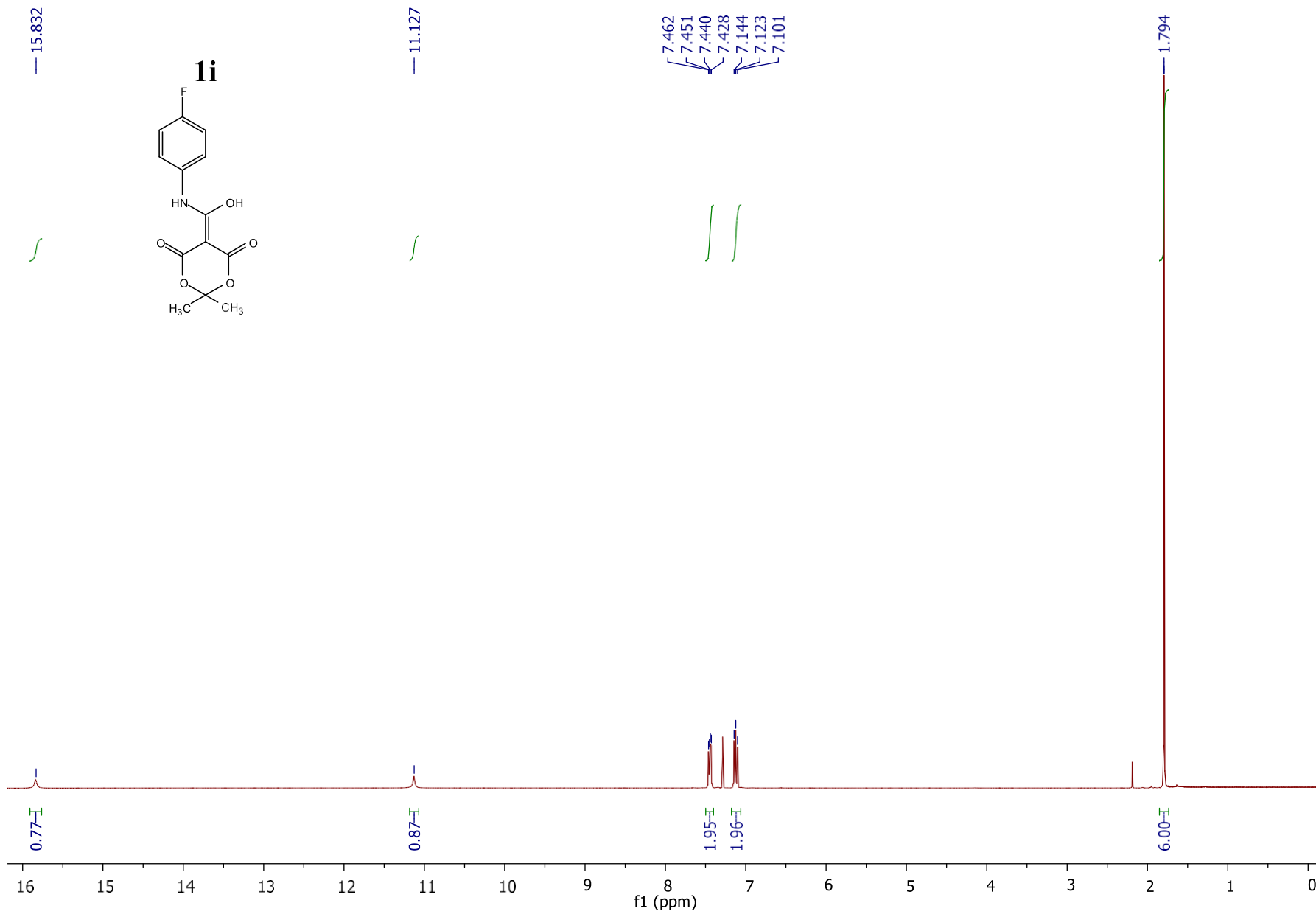


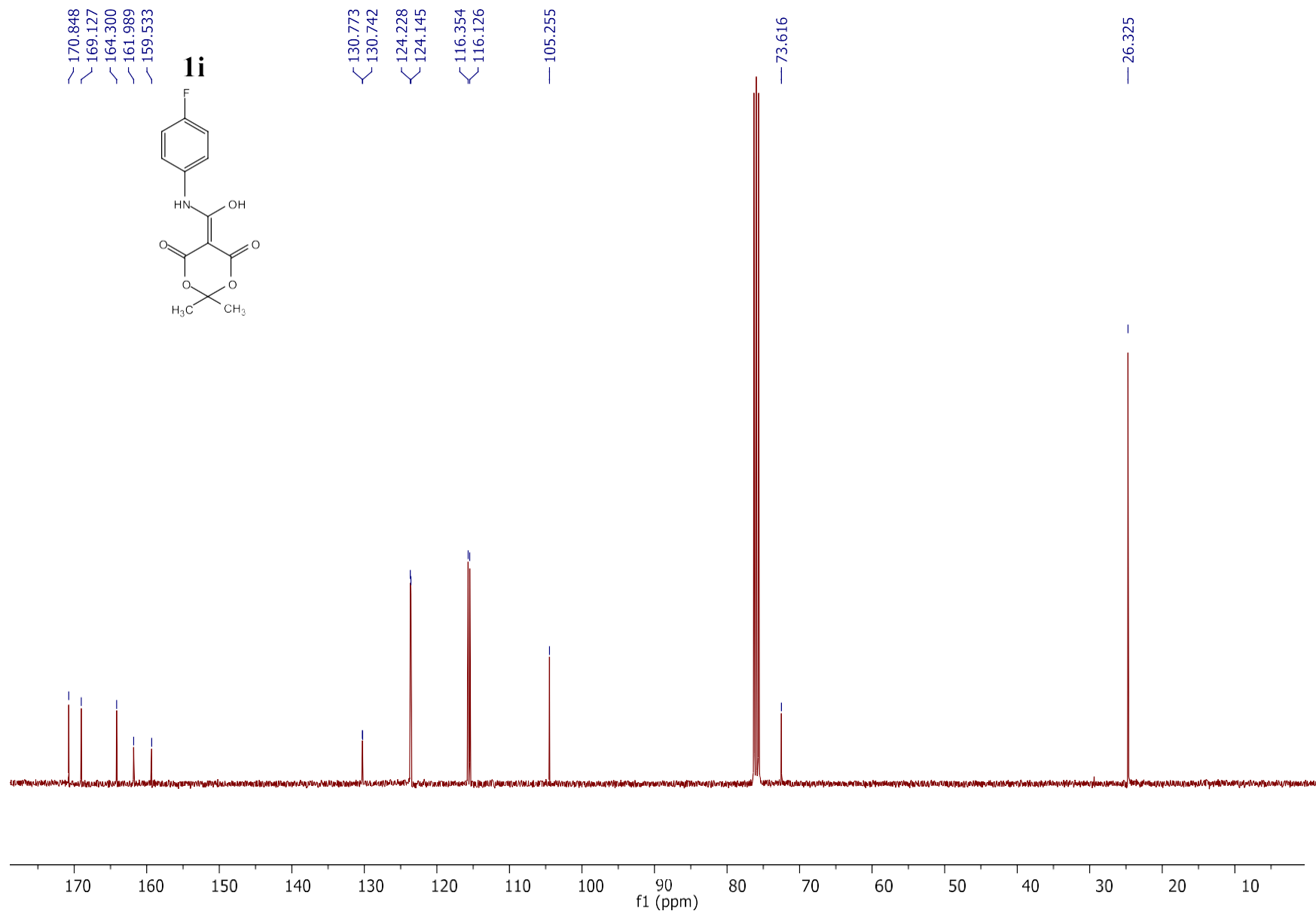


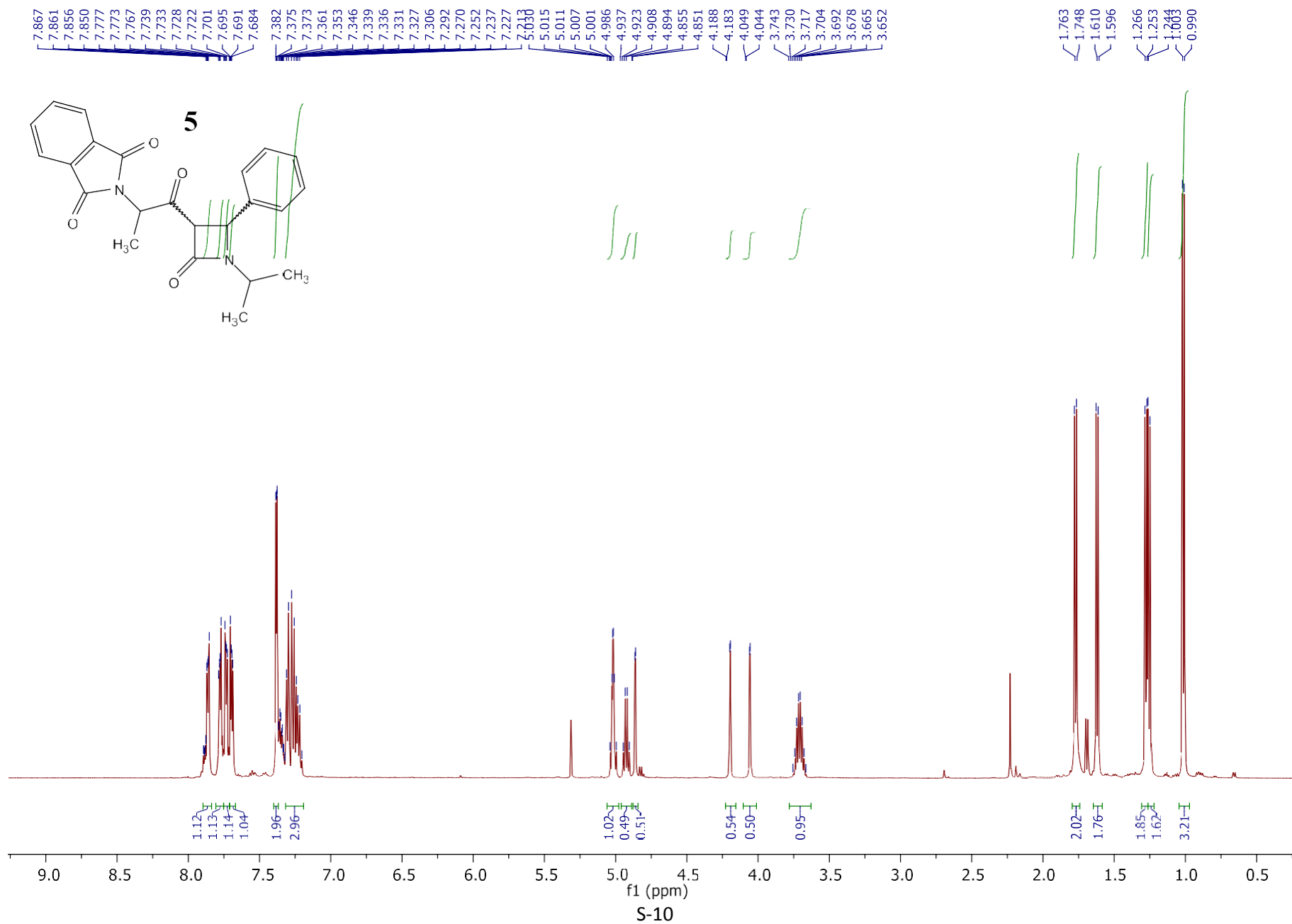


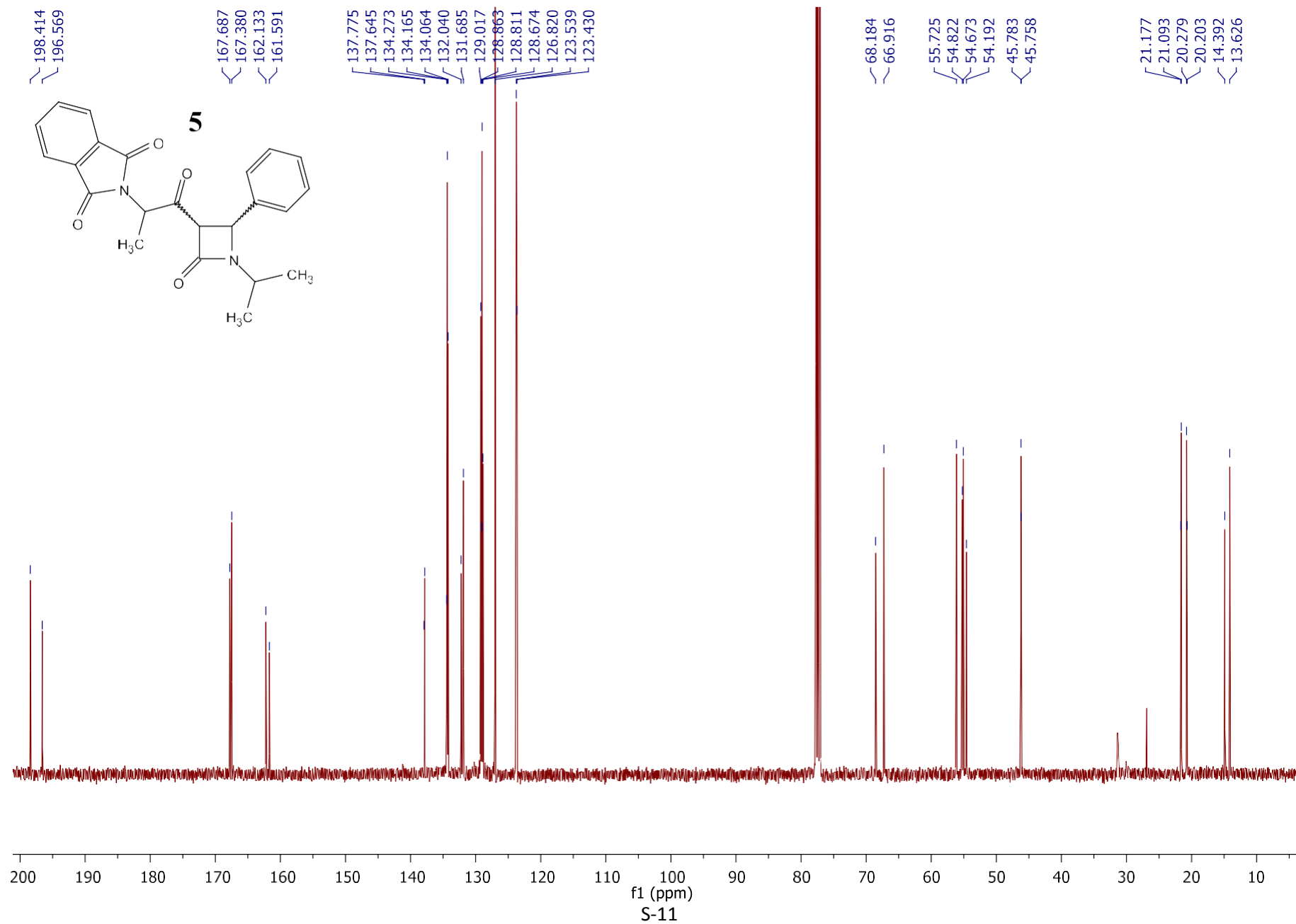
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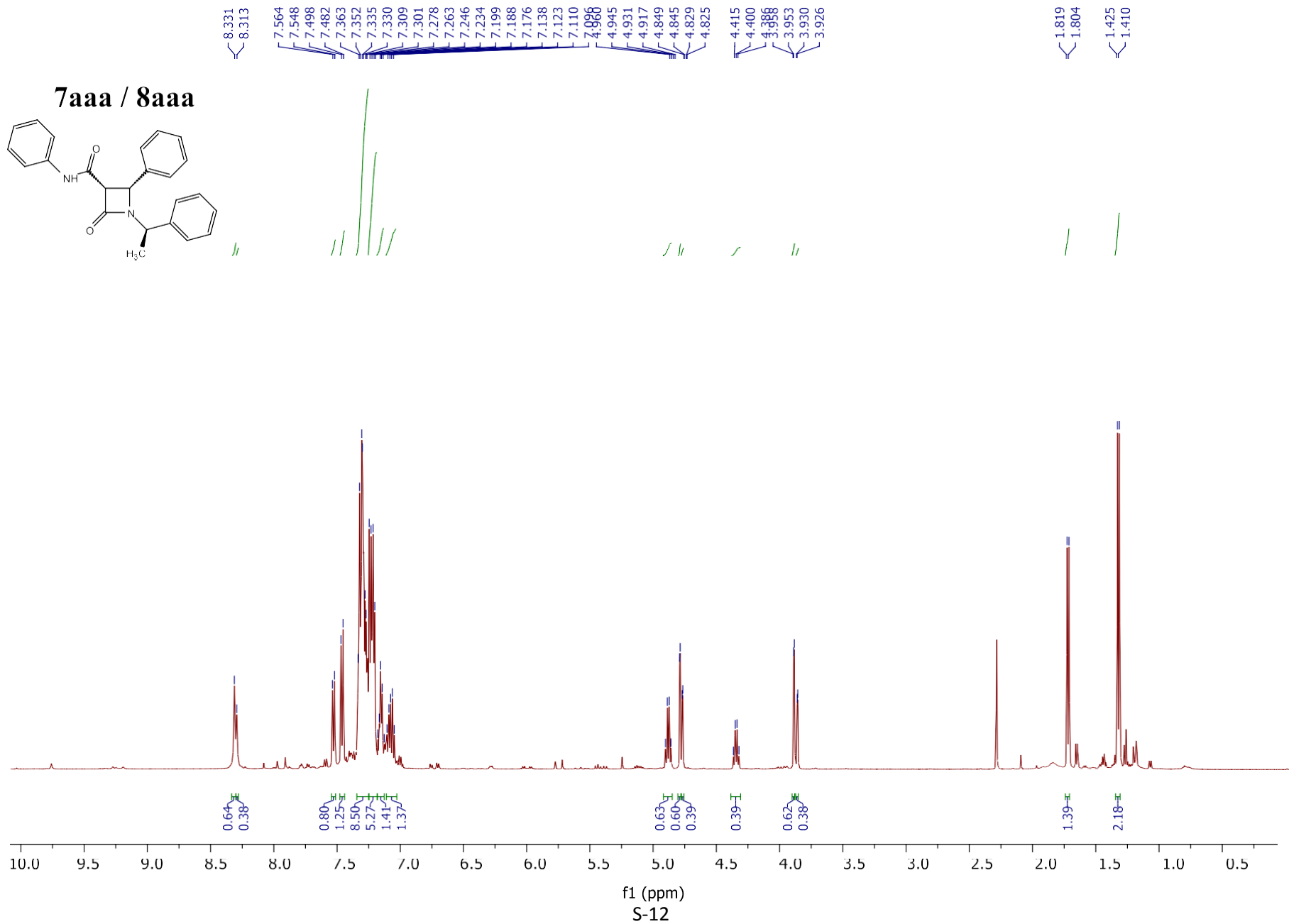
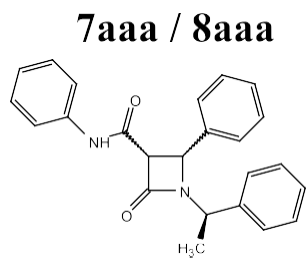




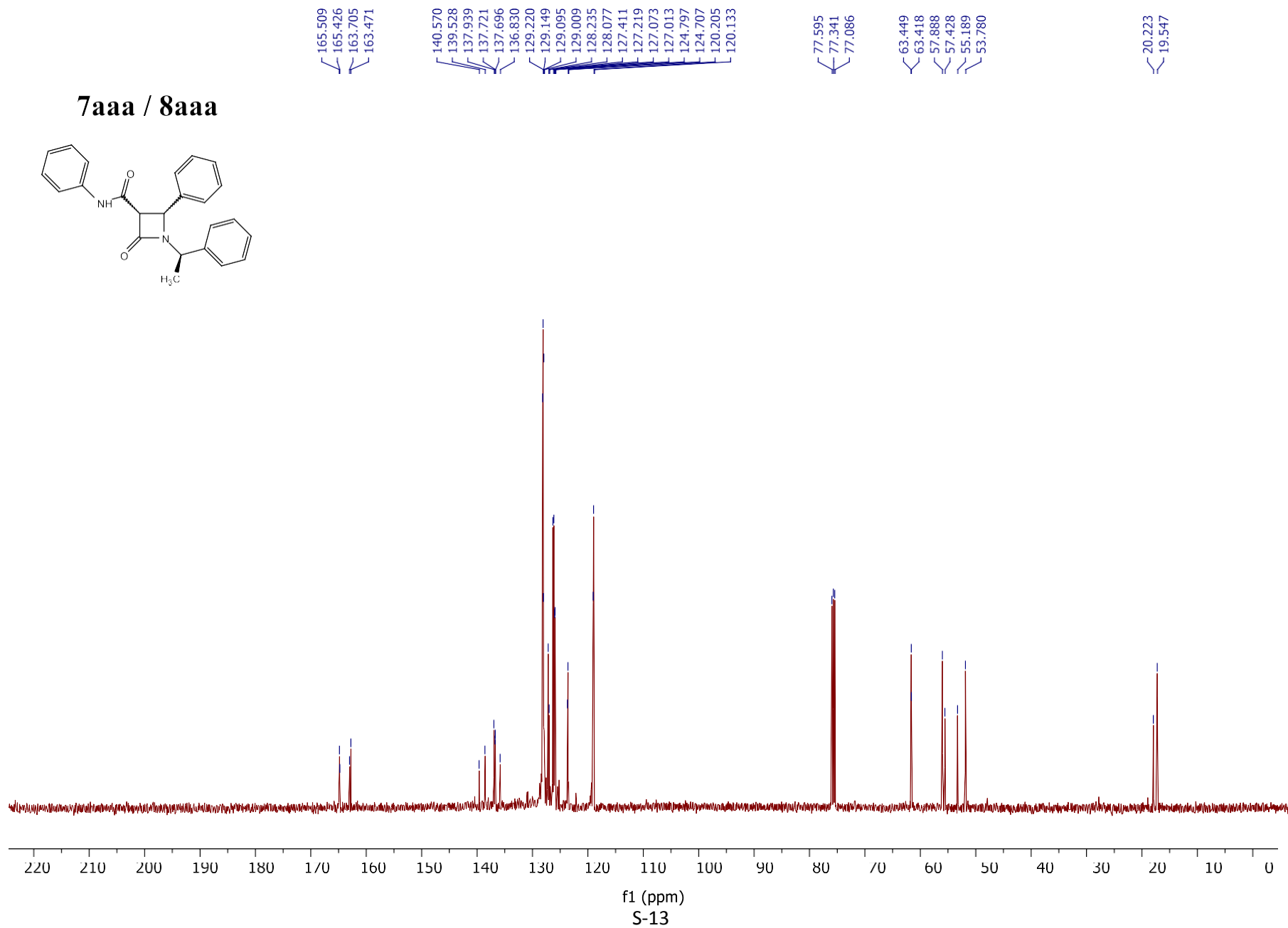
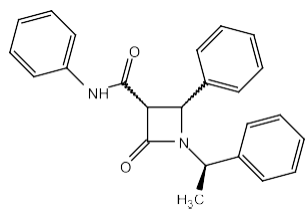




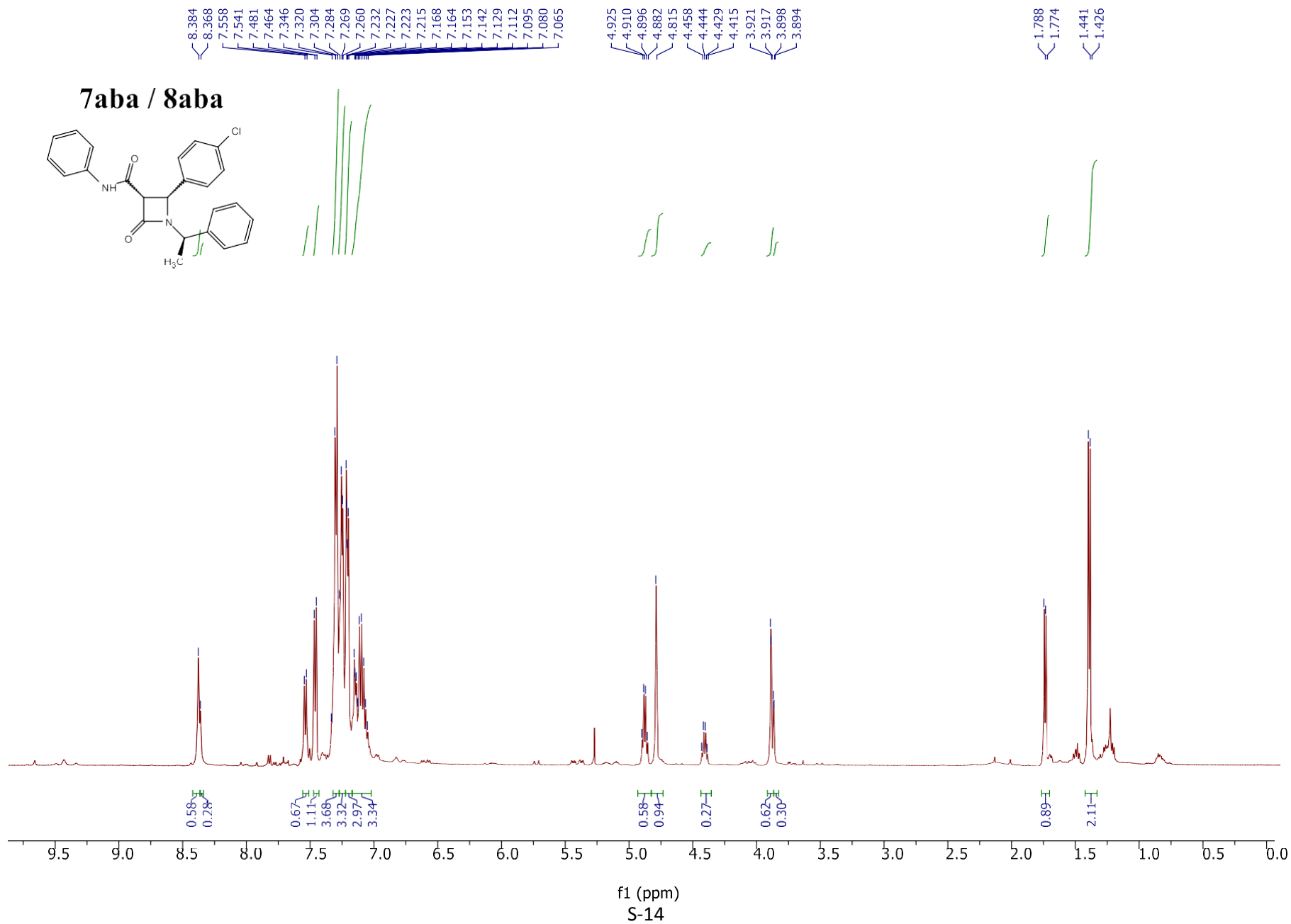
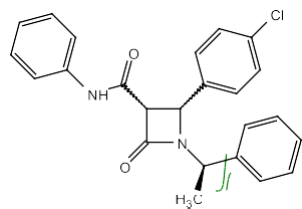




7aaa / 8aaa



7aba / 8aba



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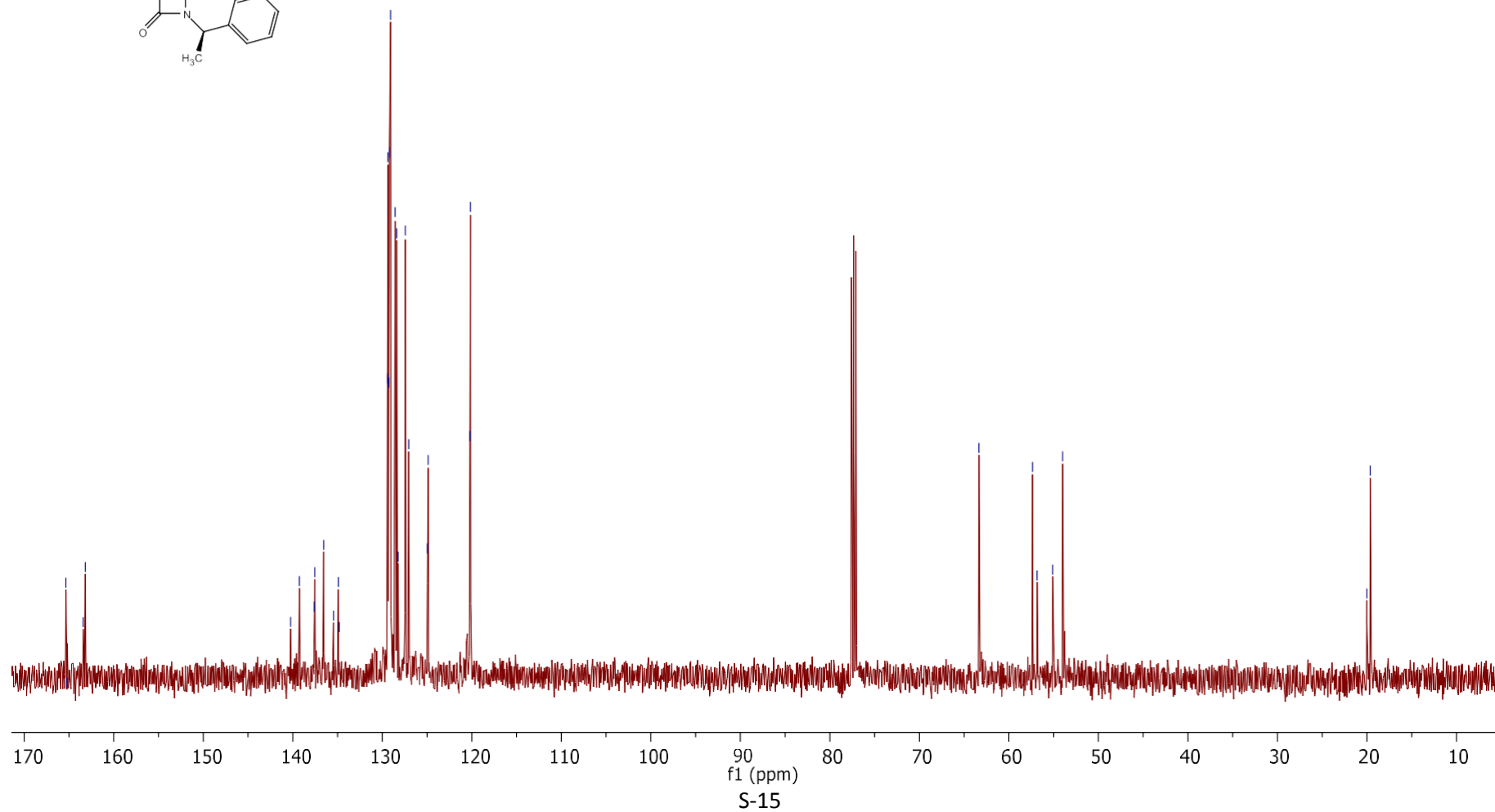
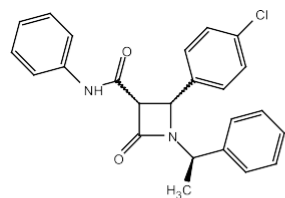
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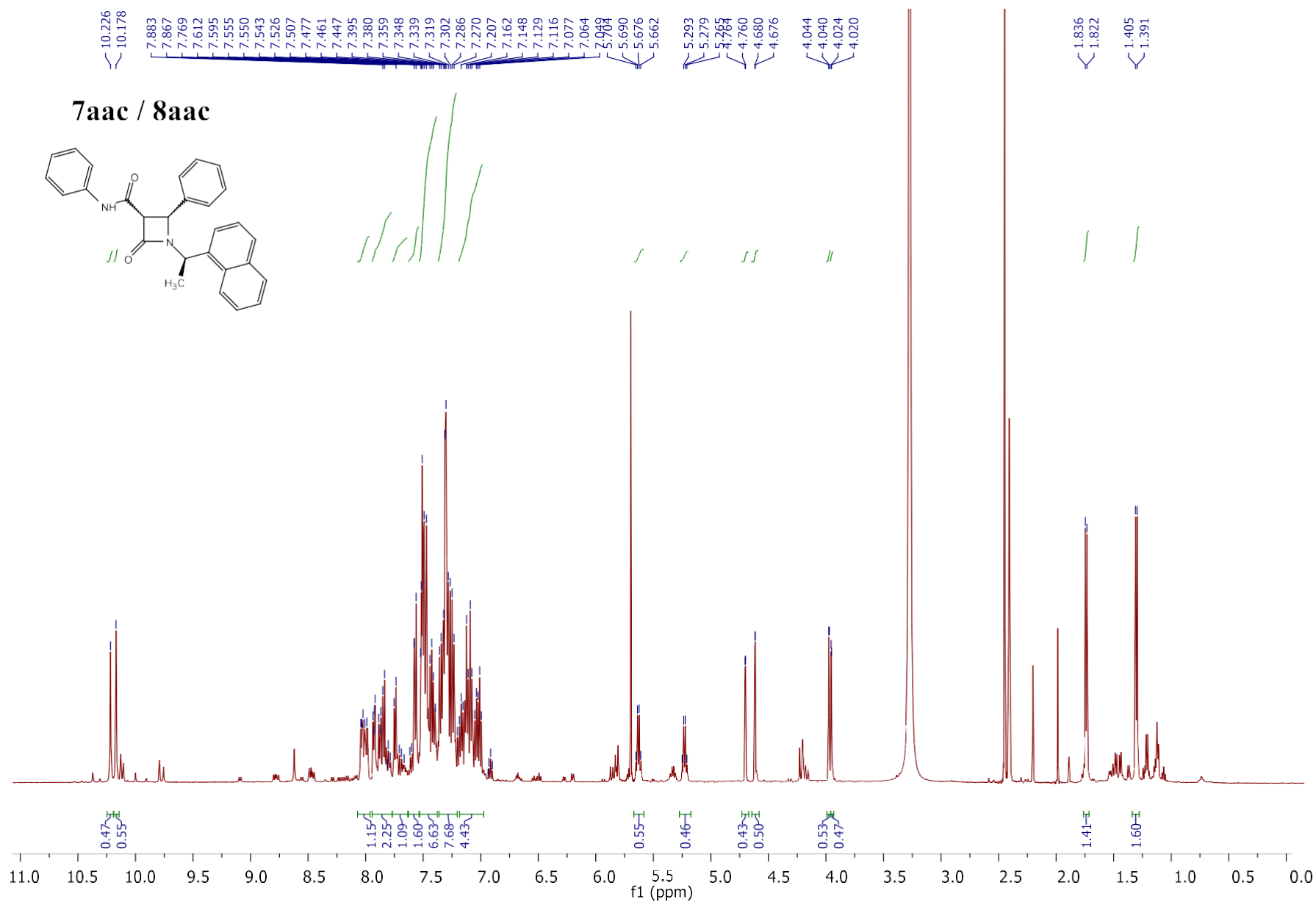
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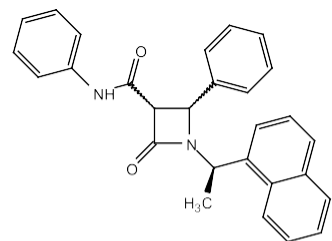
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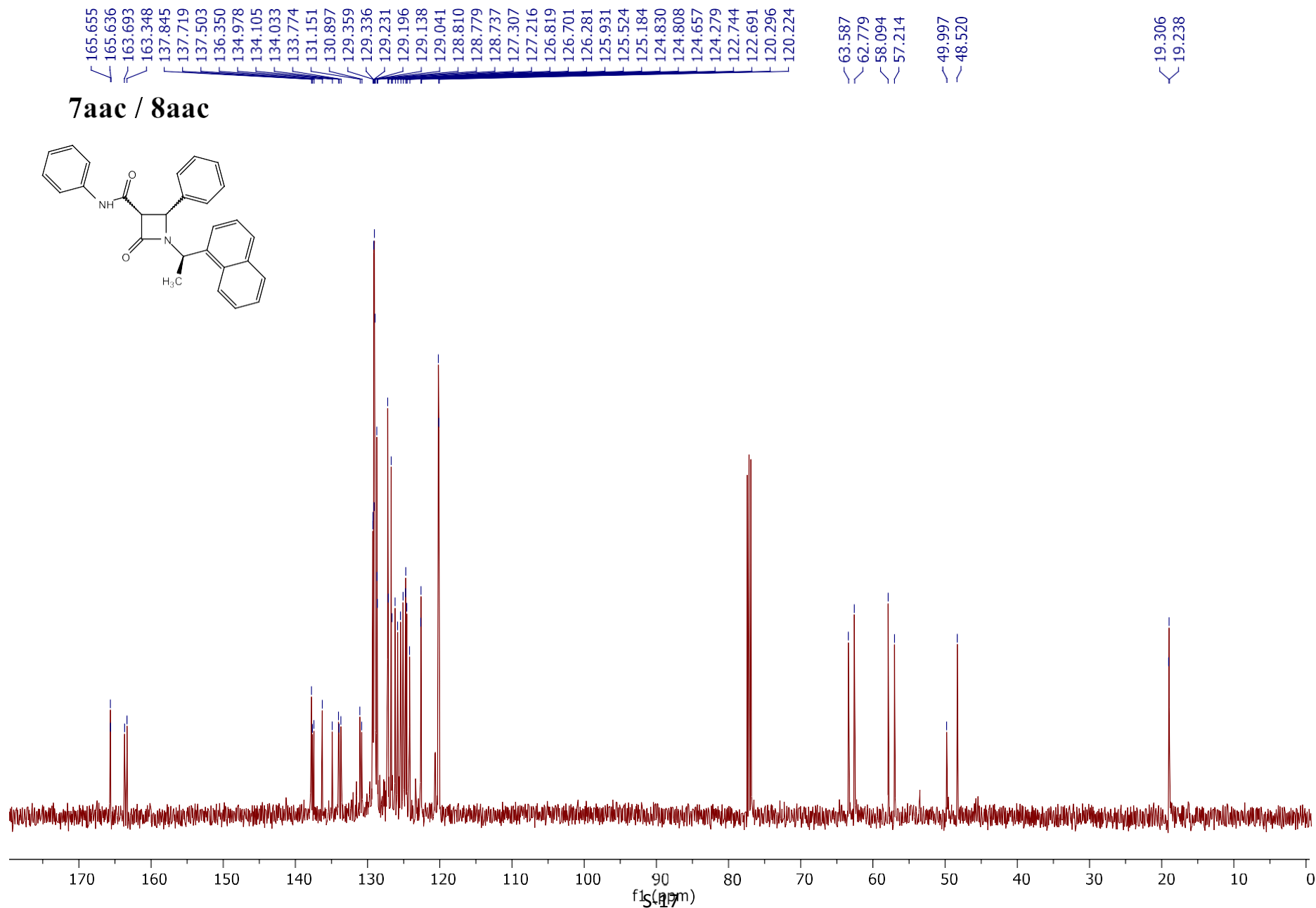
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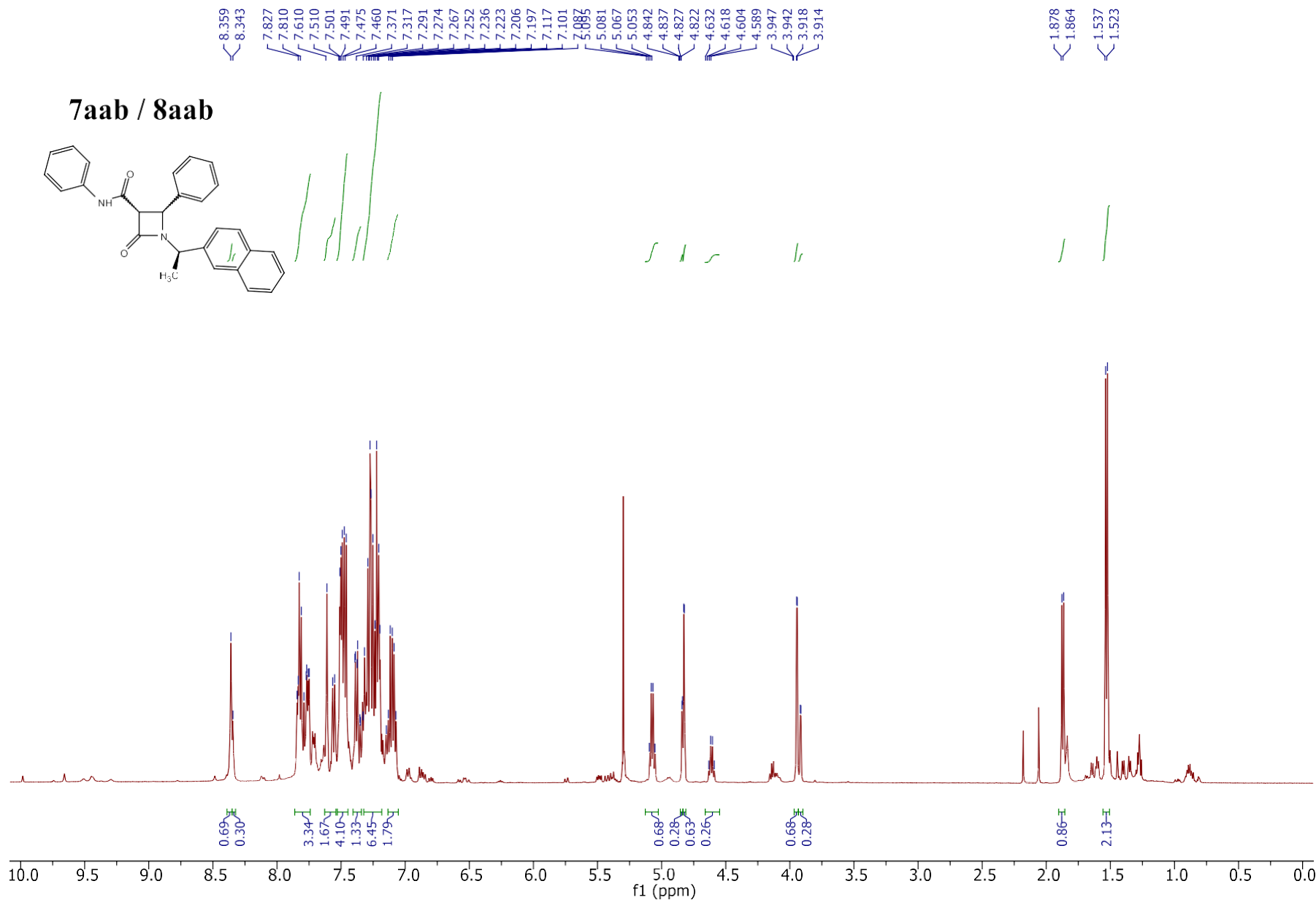
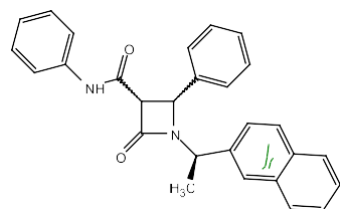


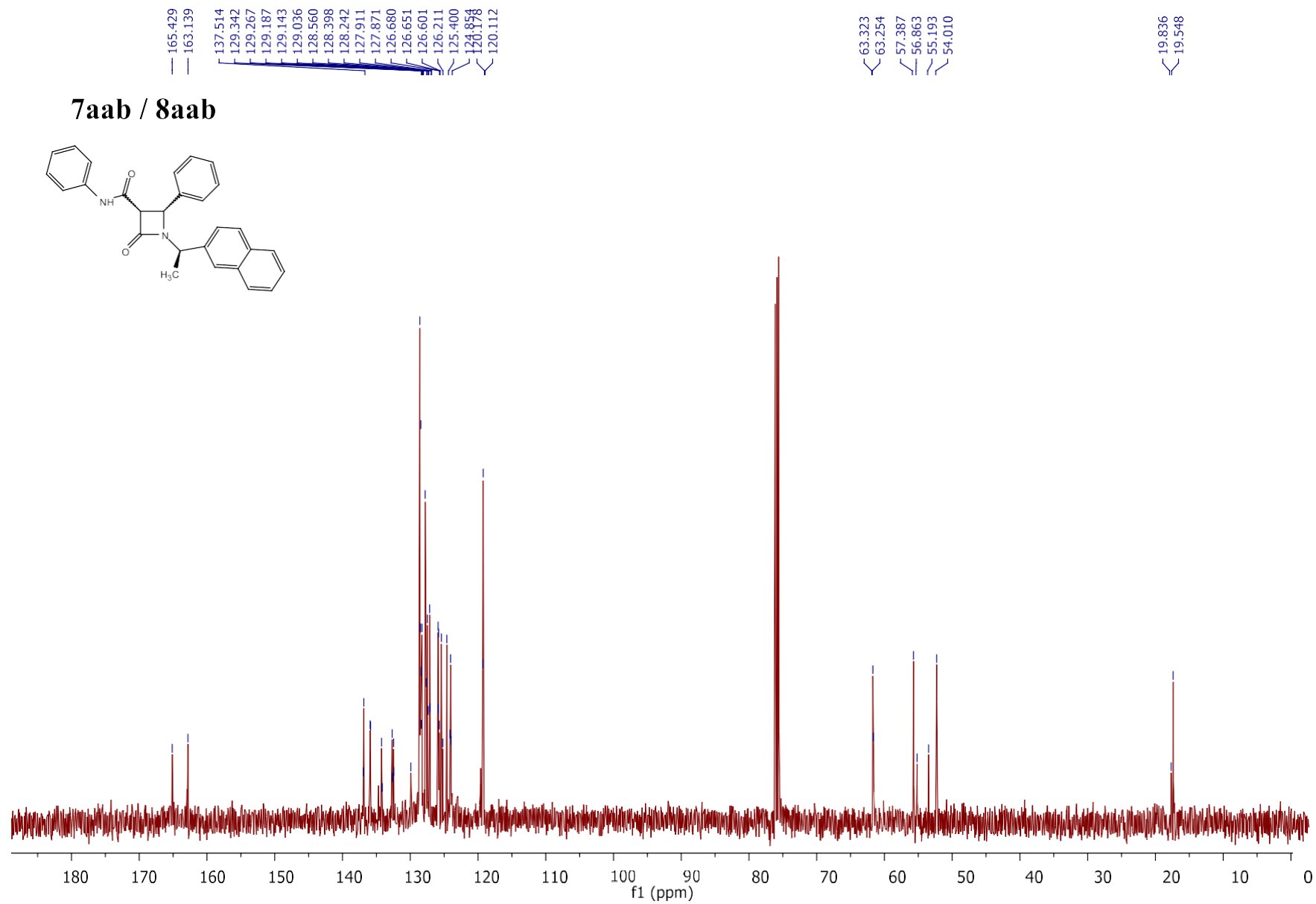


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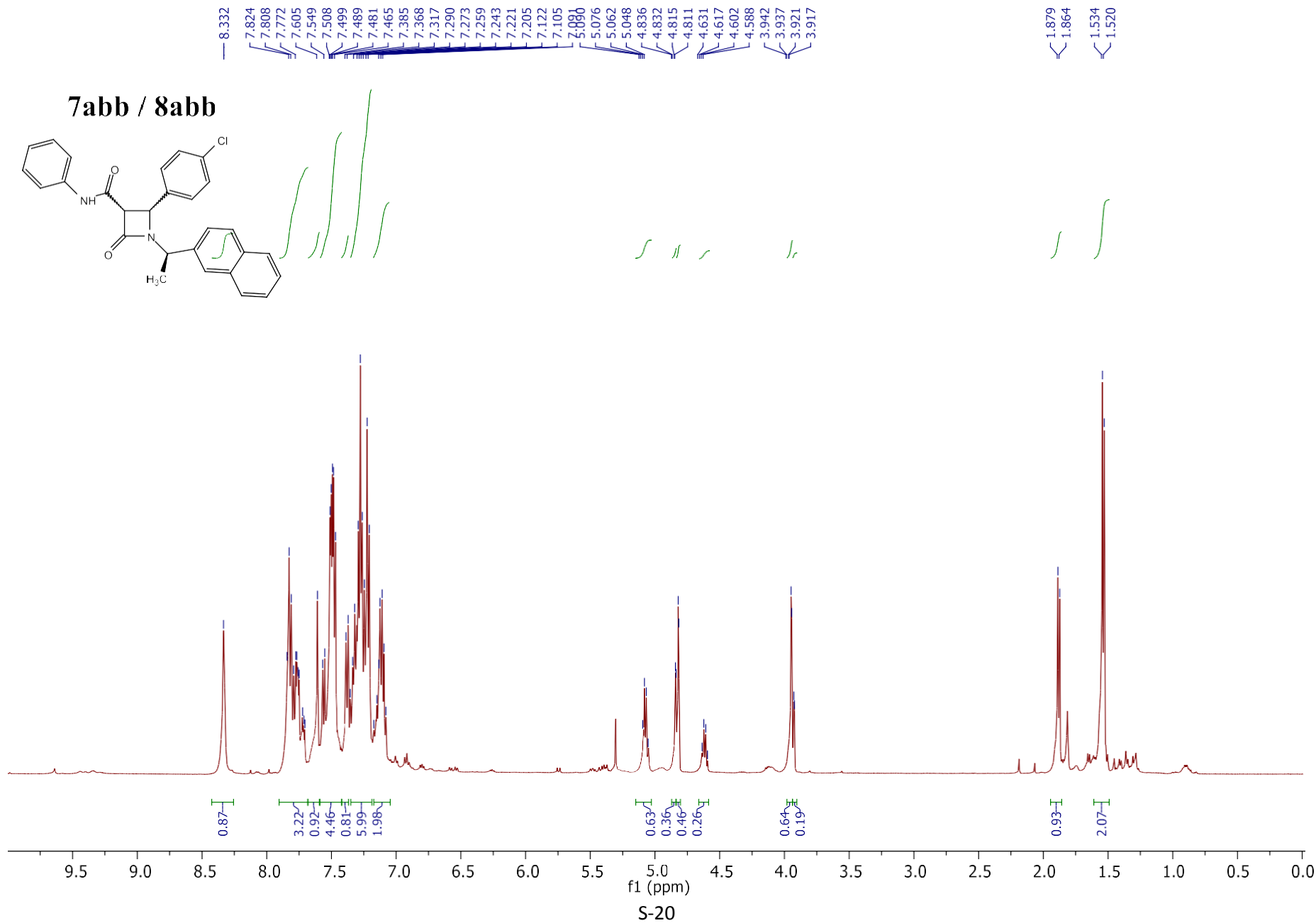
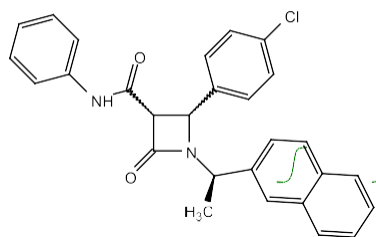


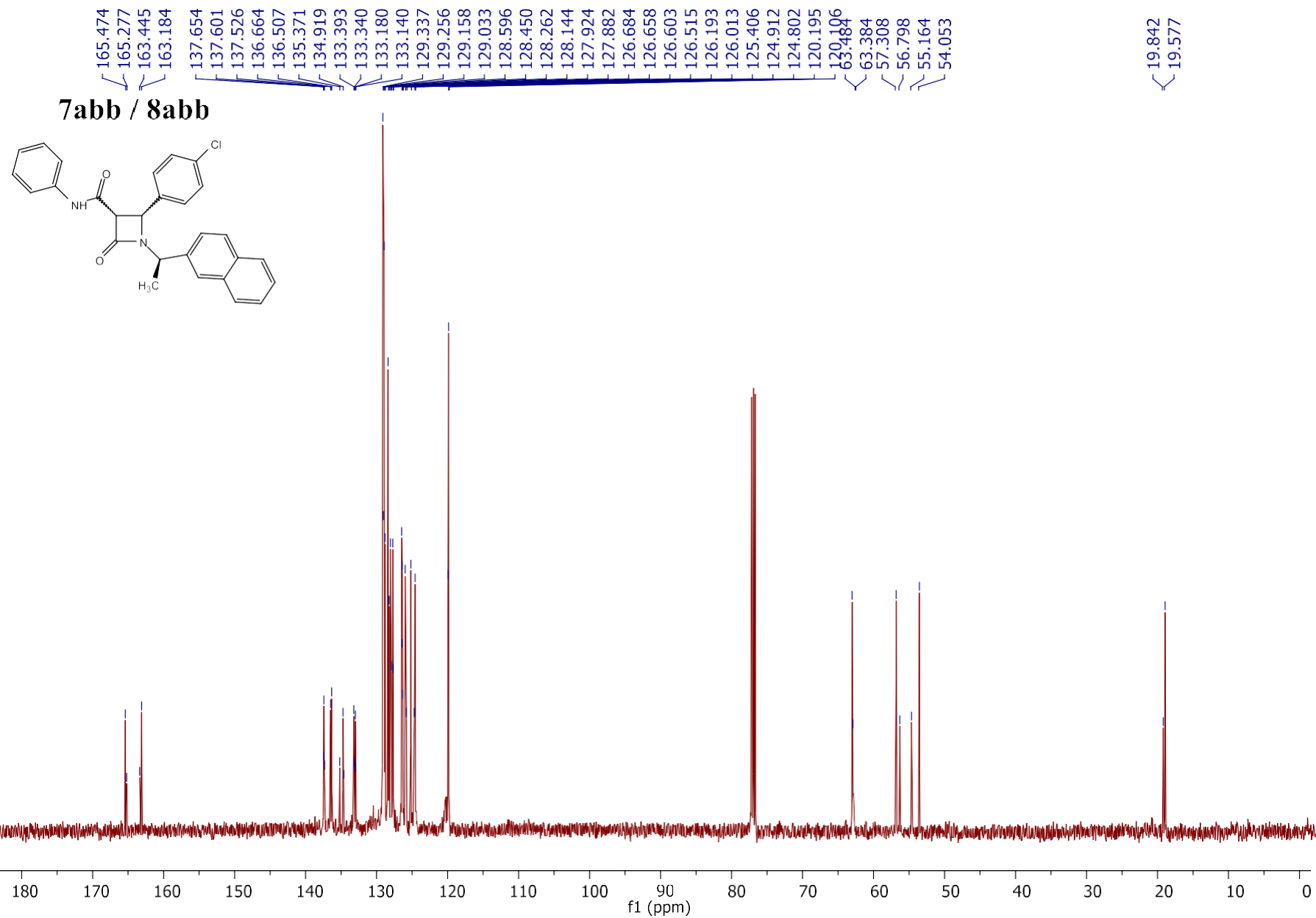
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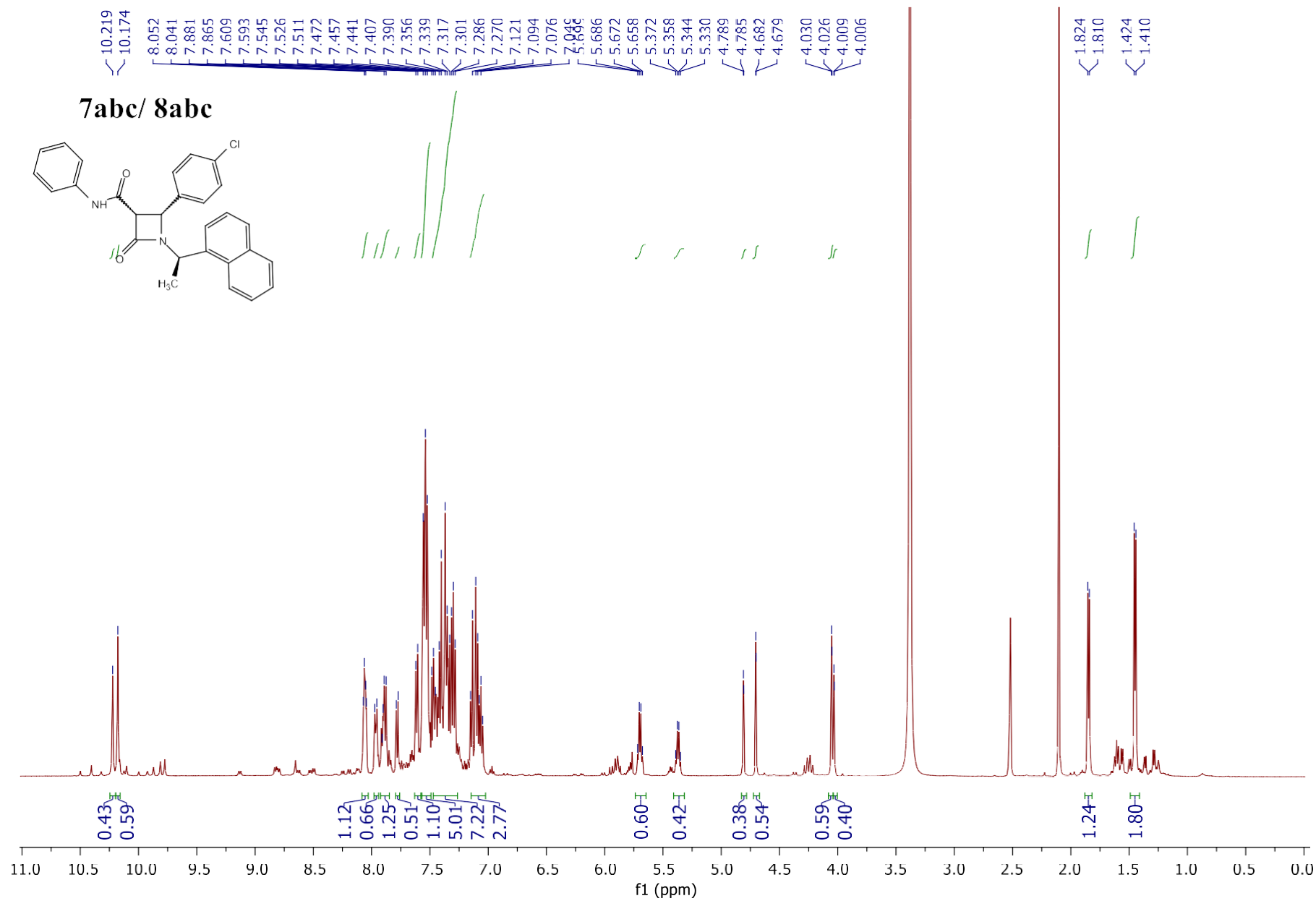


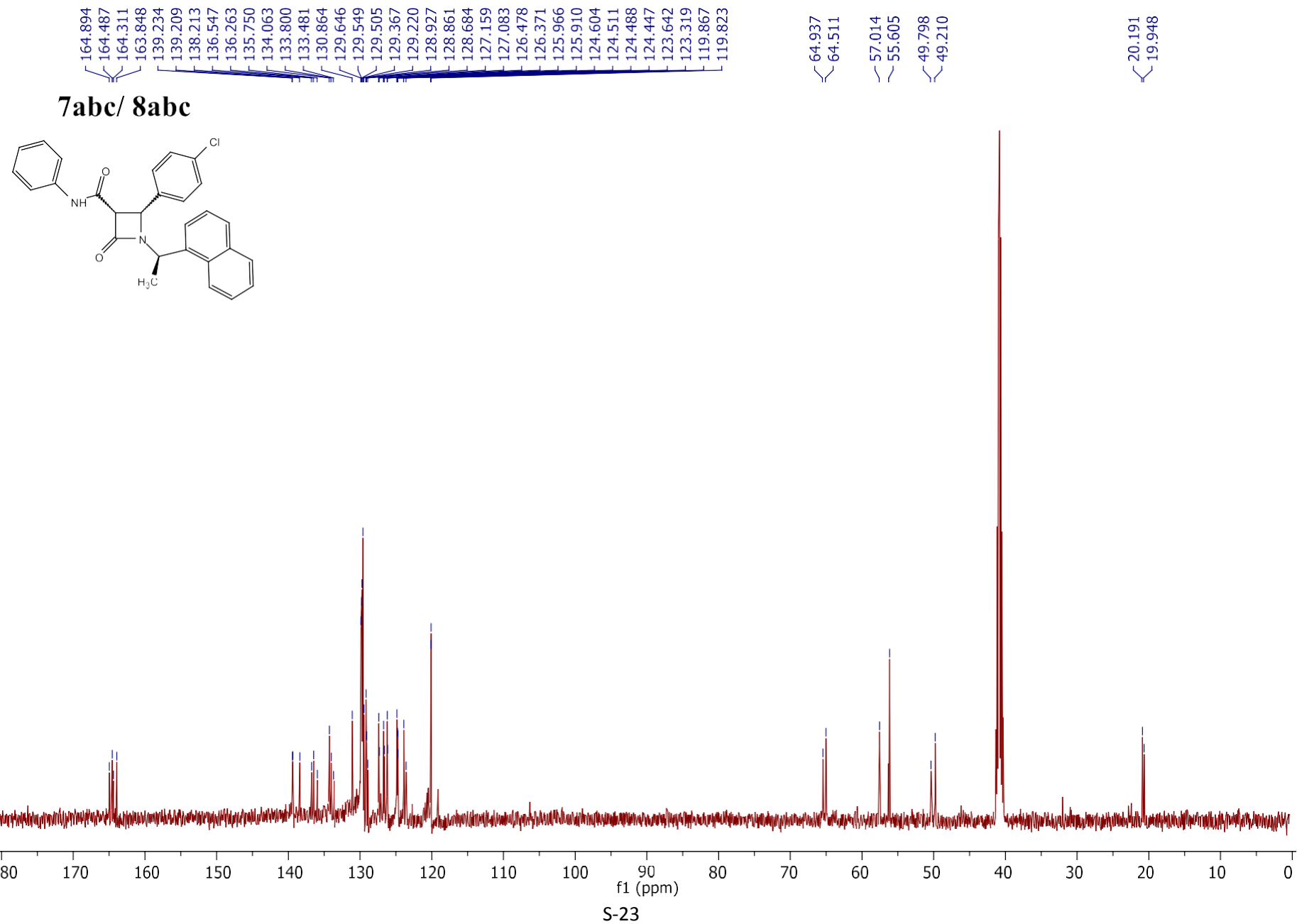


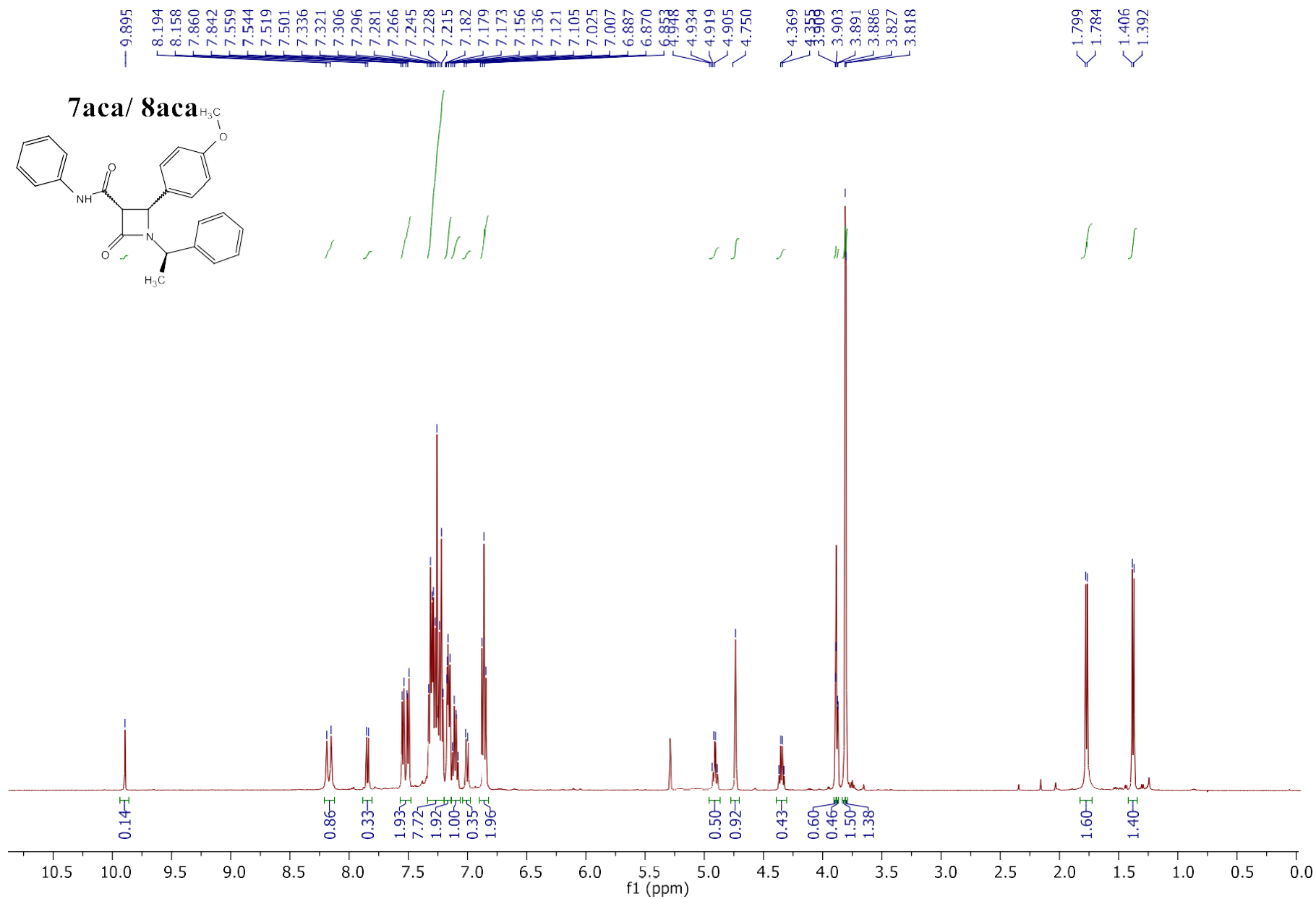
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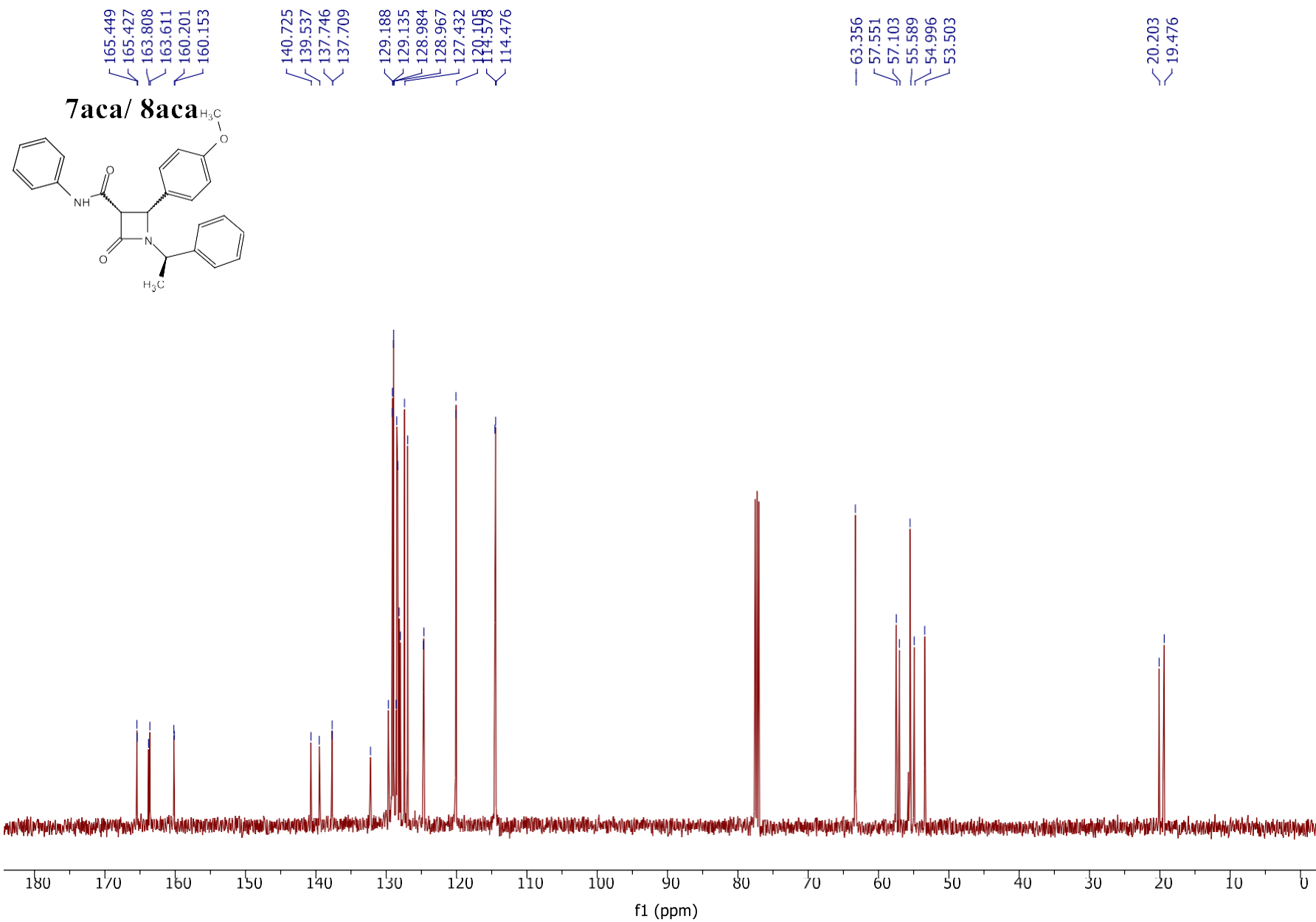




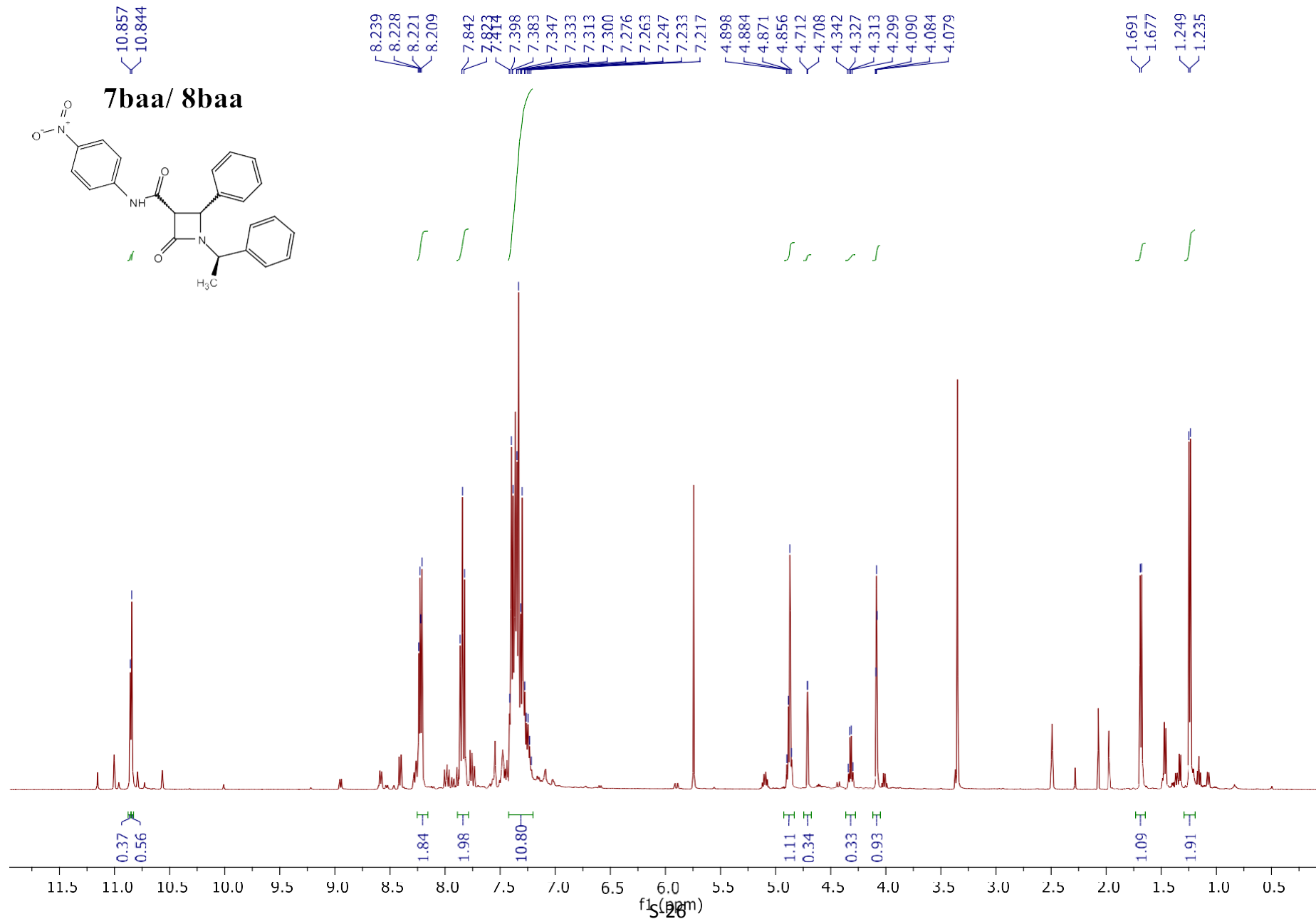
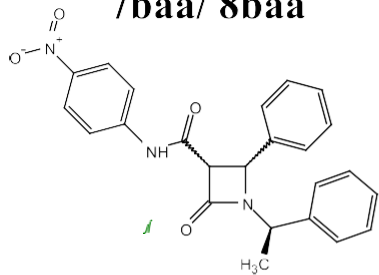


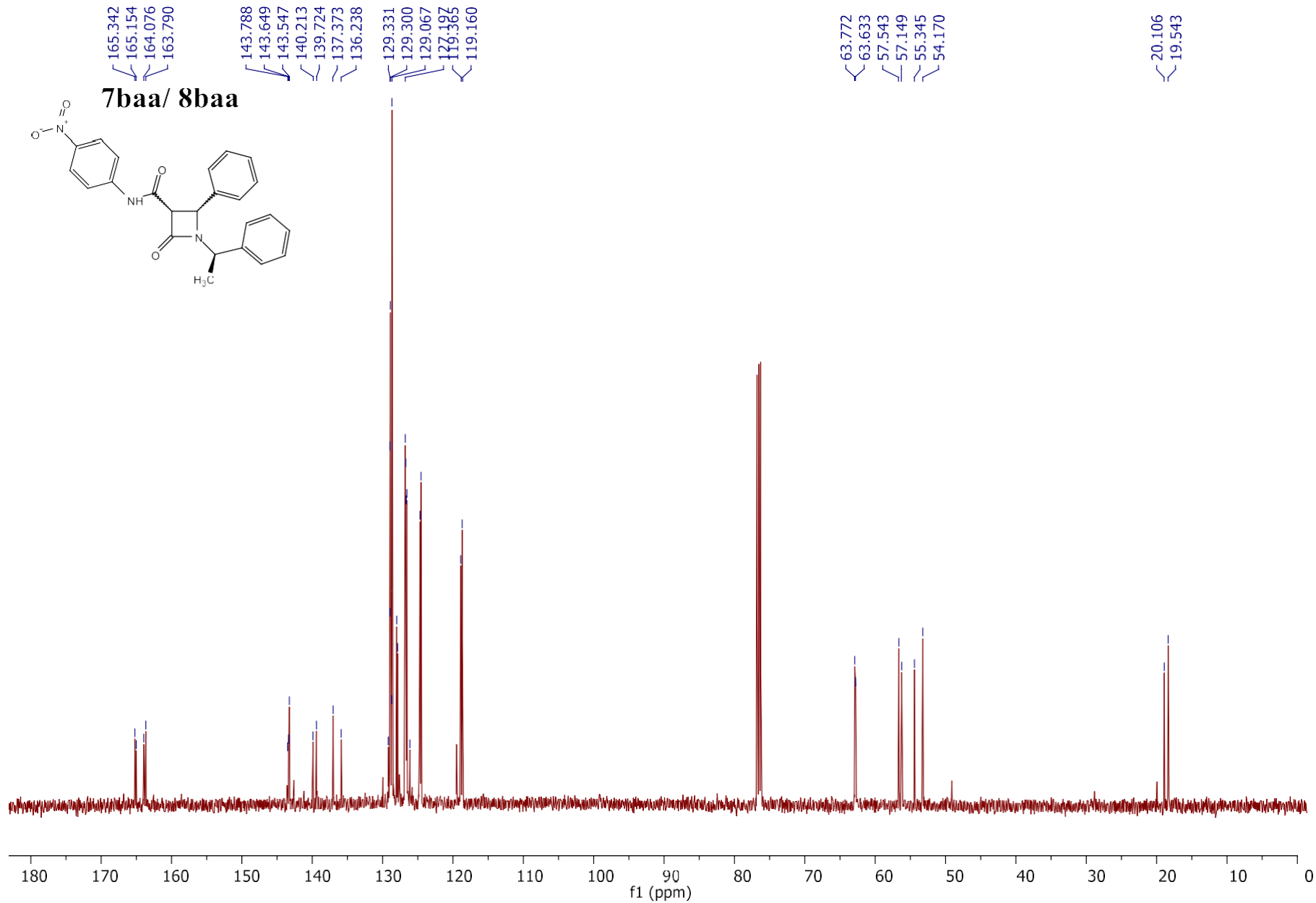
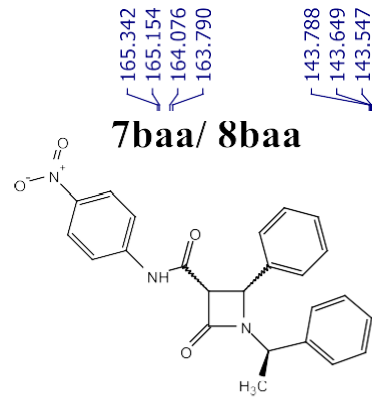


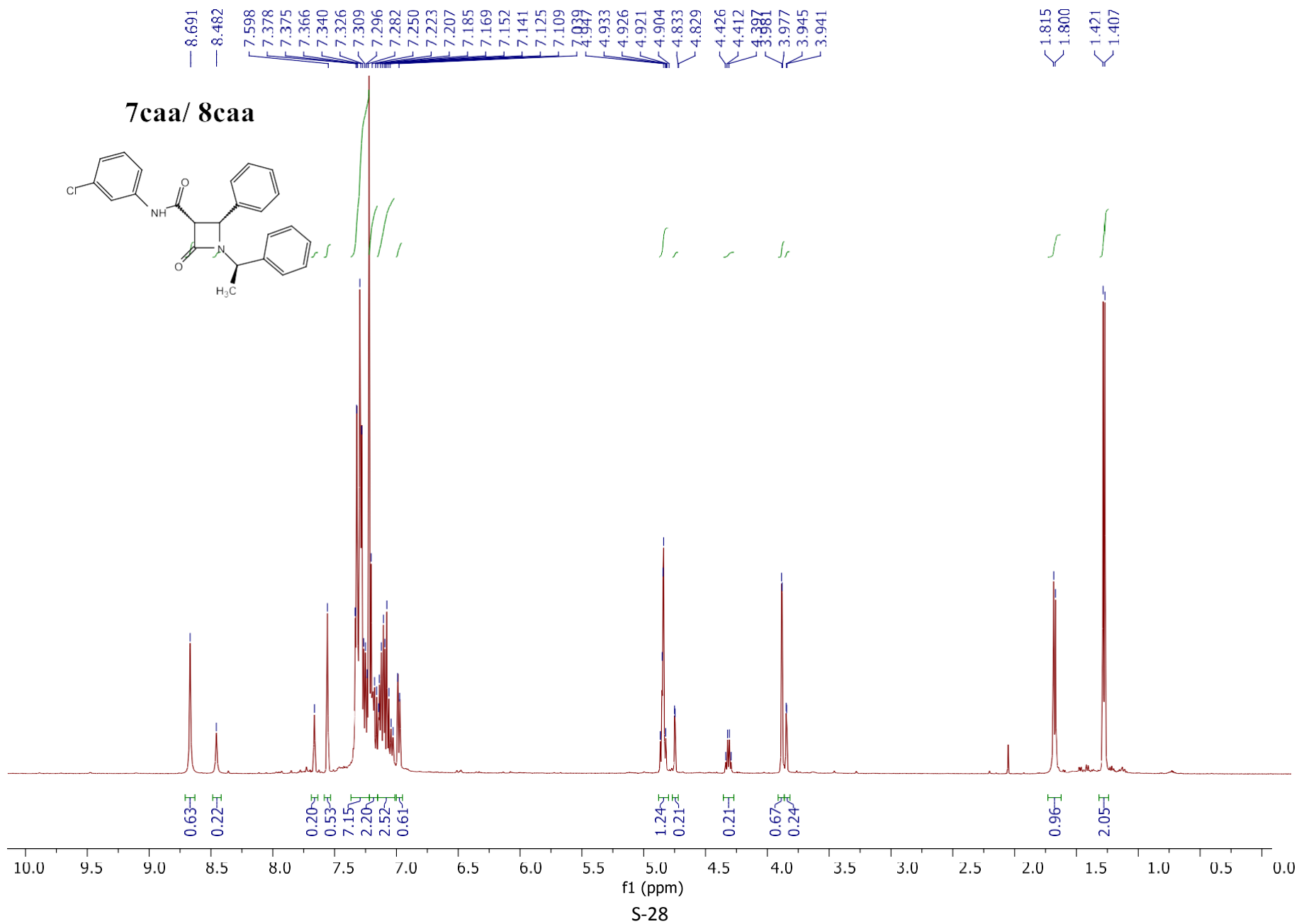


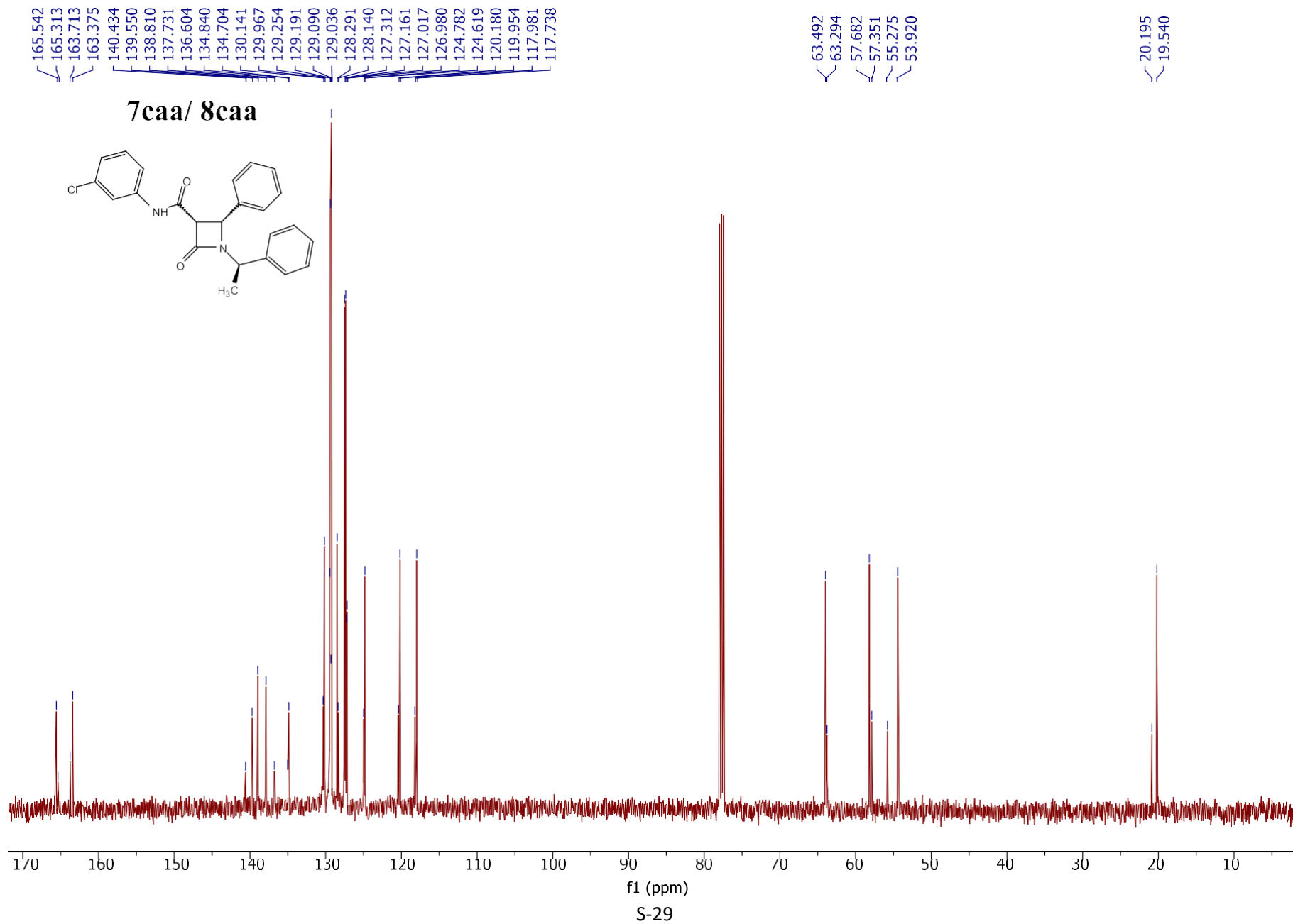
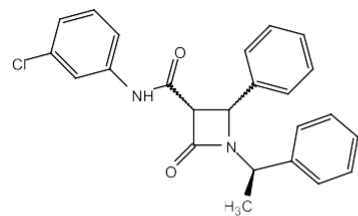


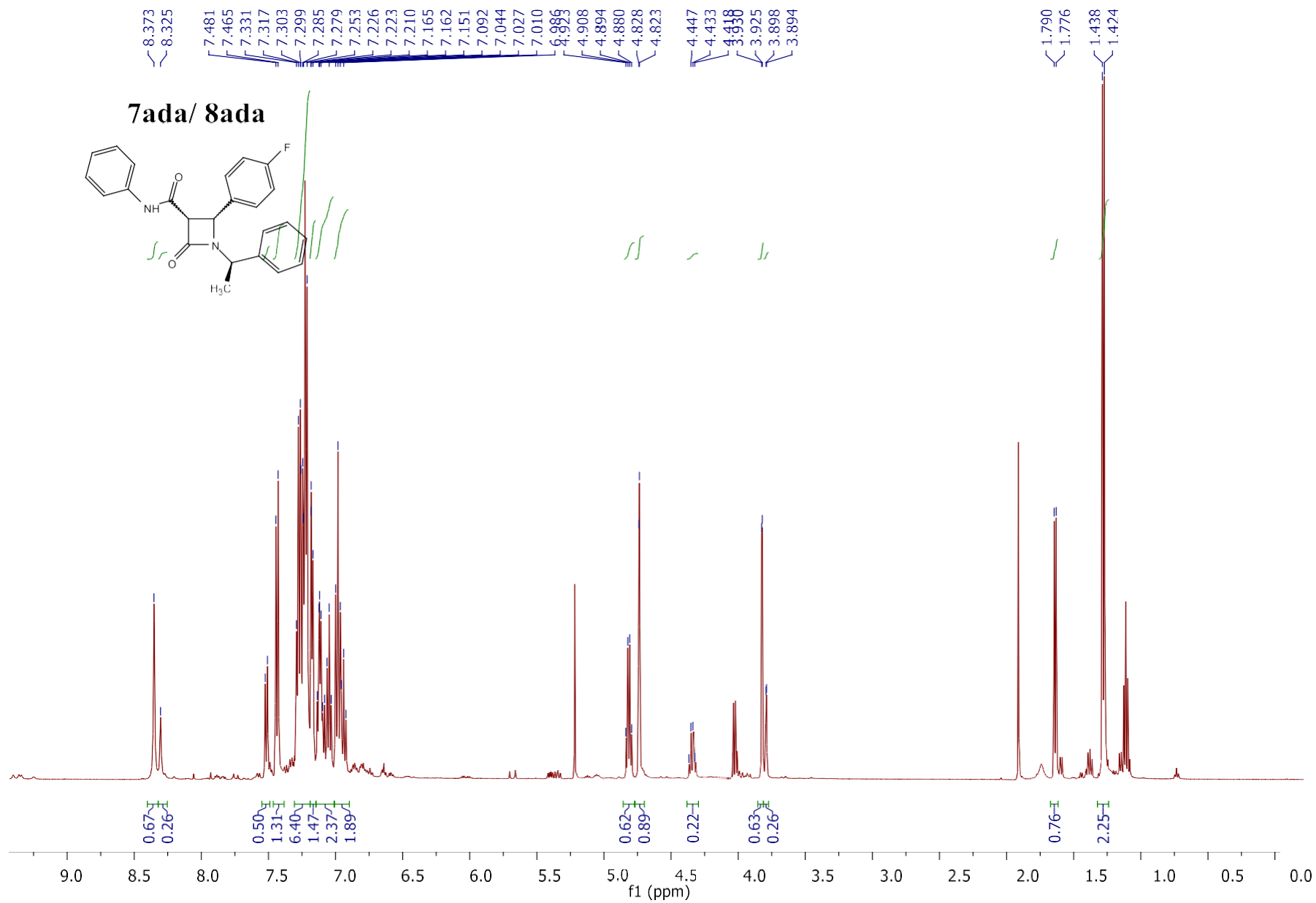
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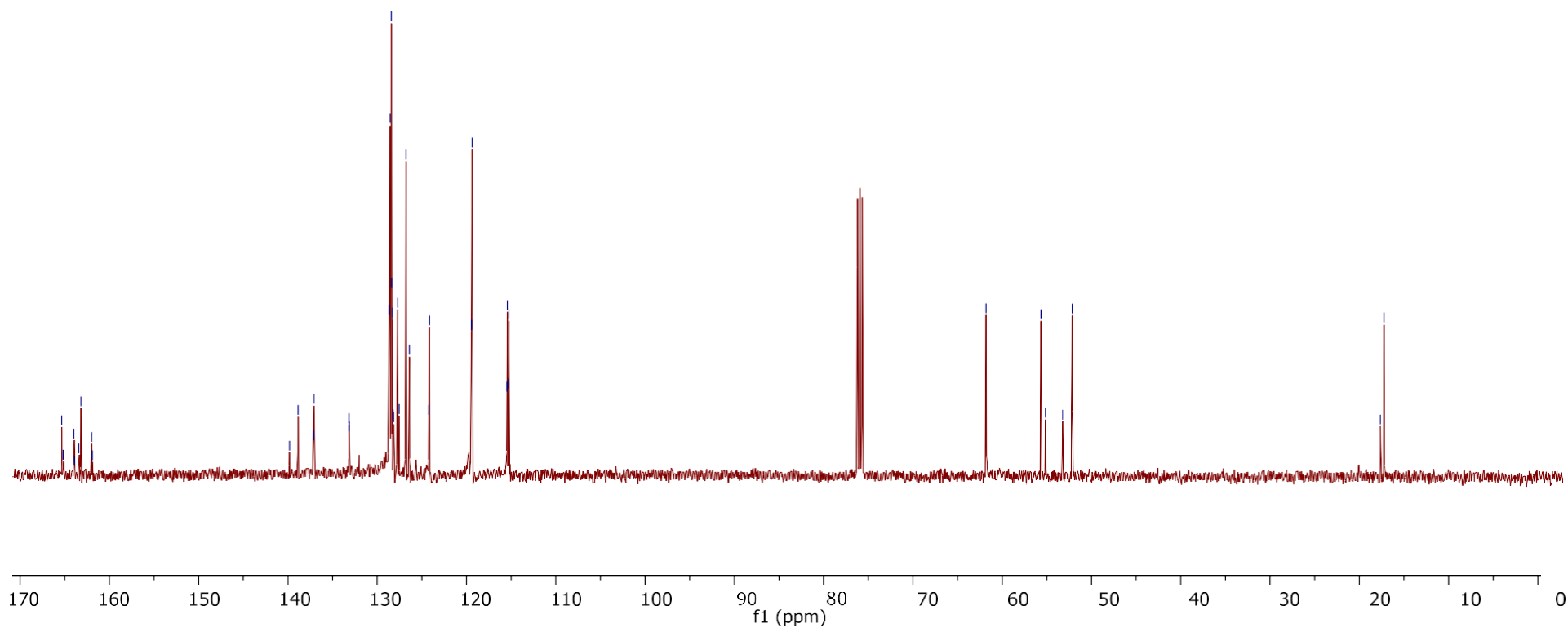
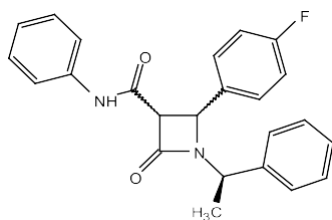


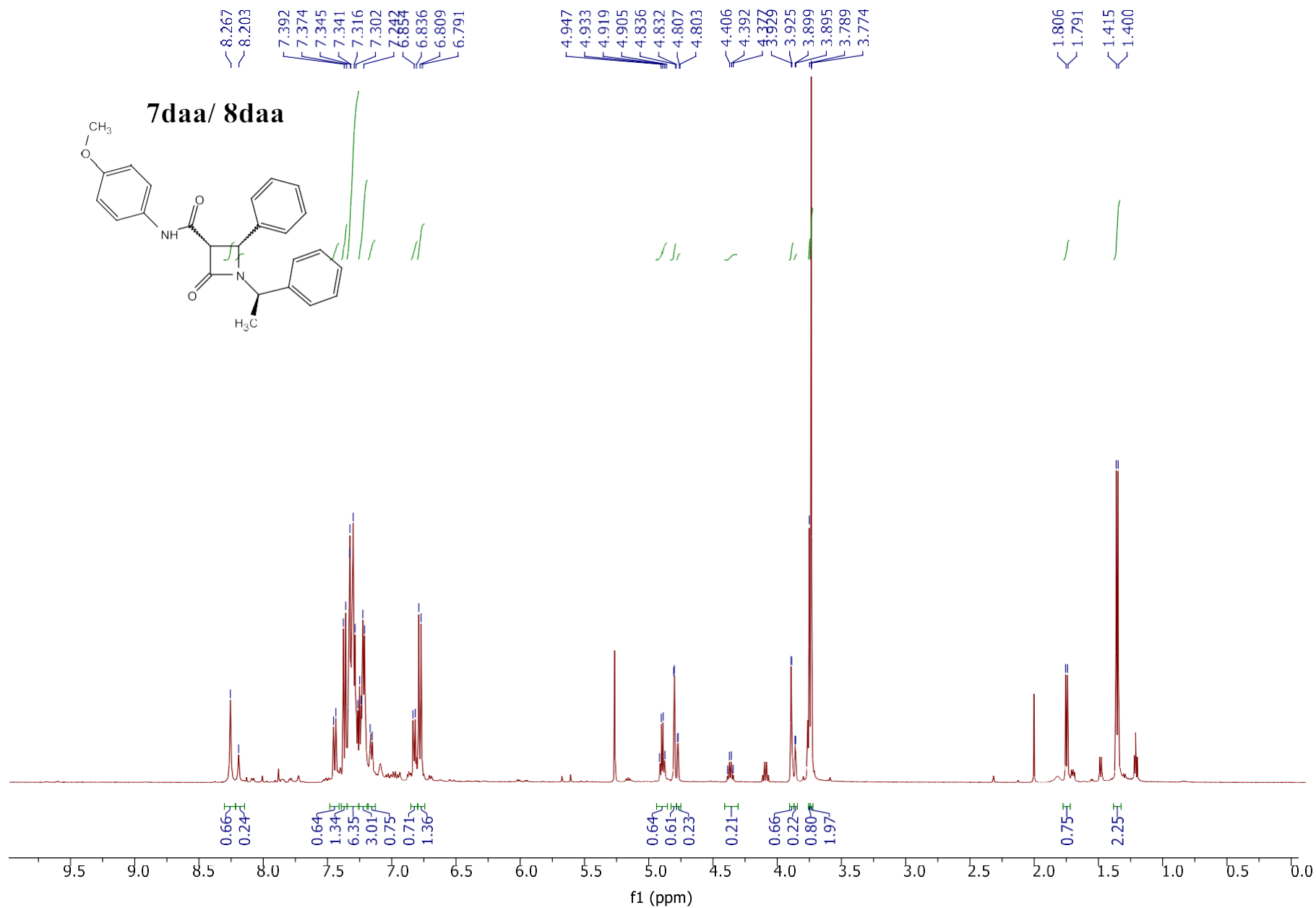
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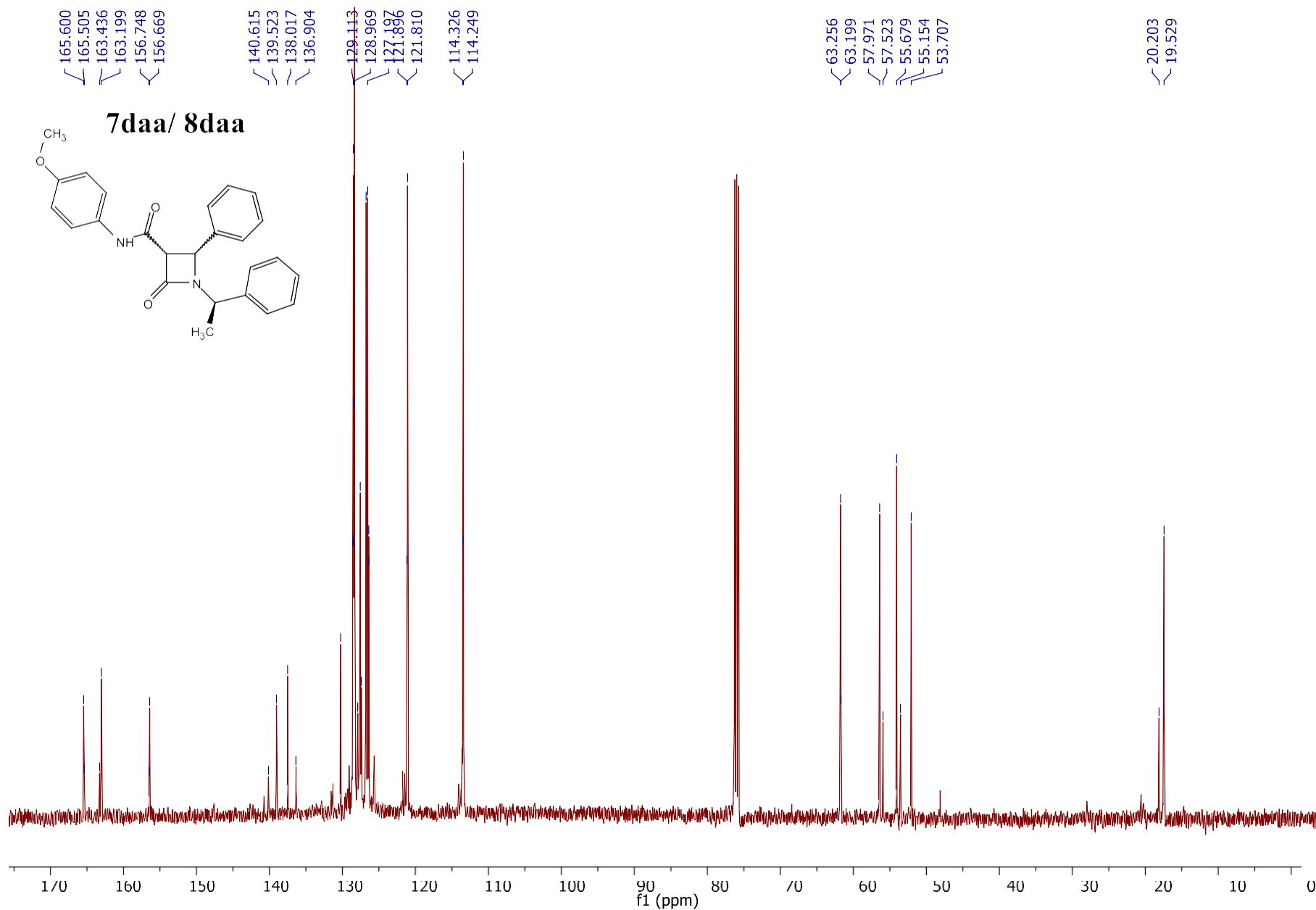
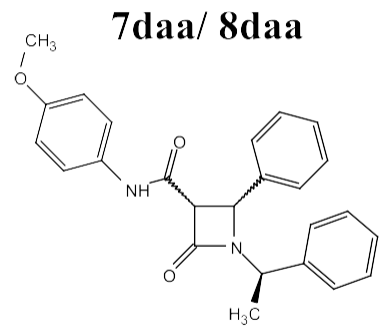
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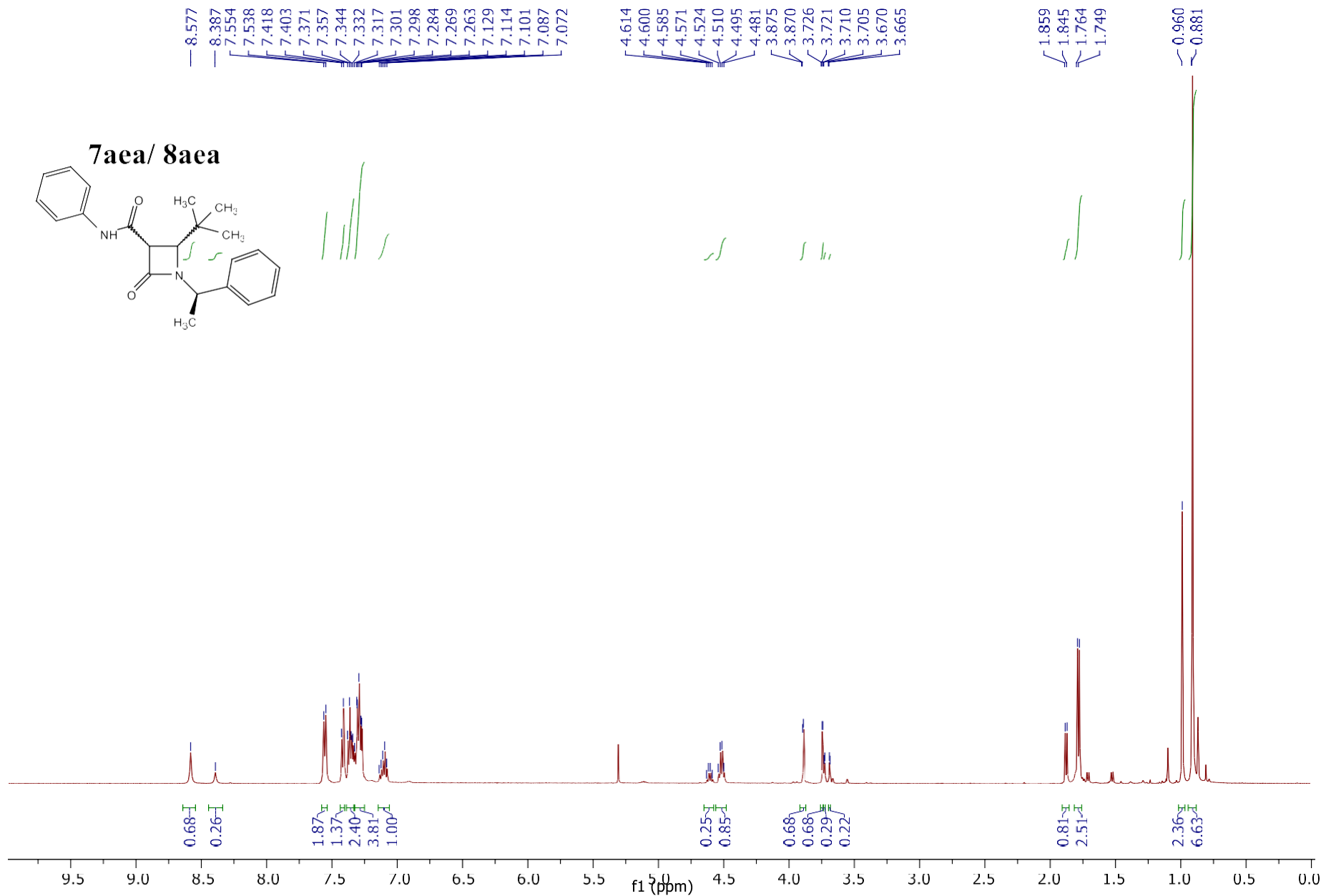
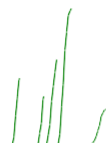
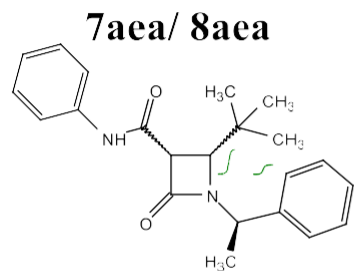
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7ada/ 8ada

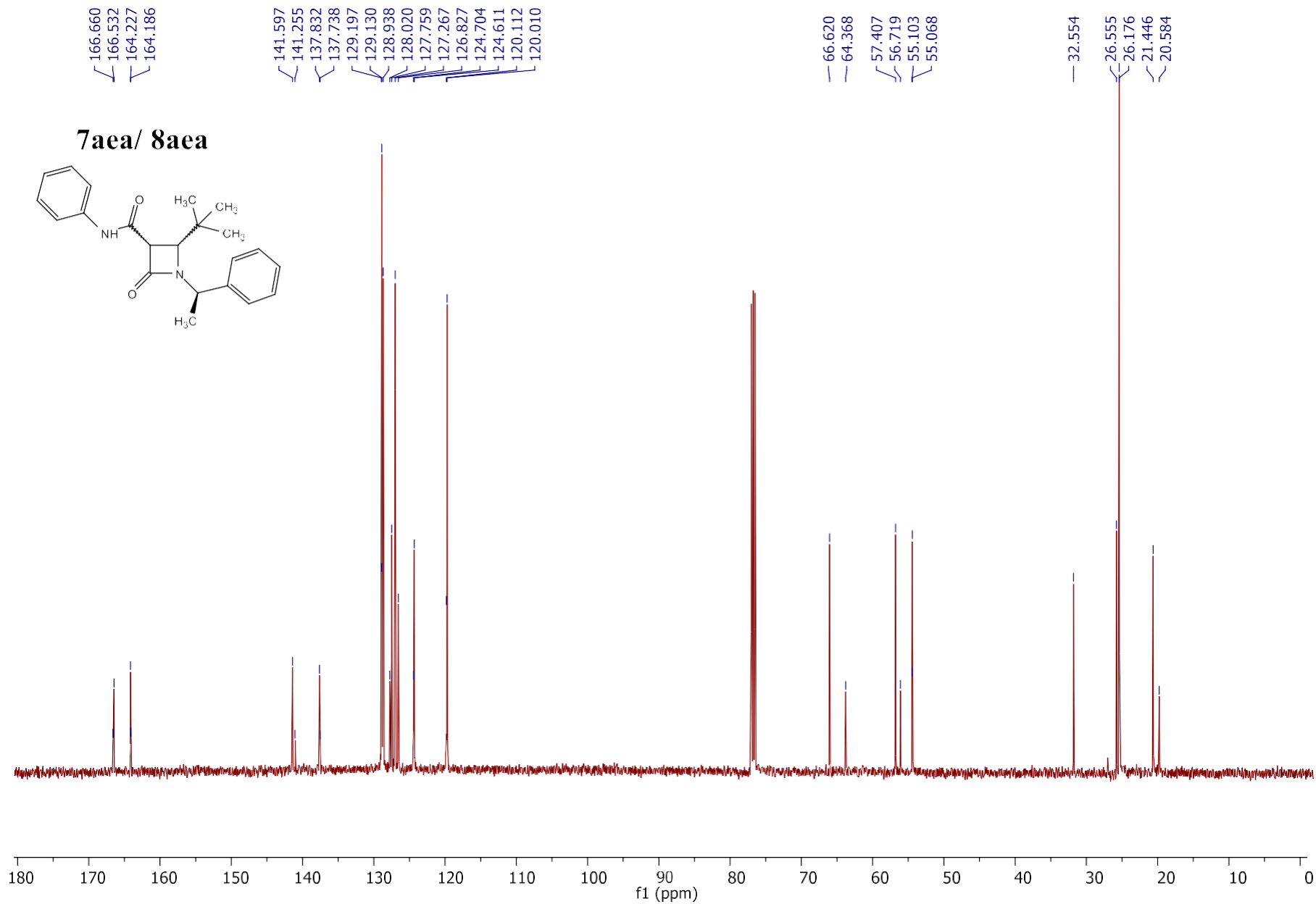
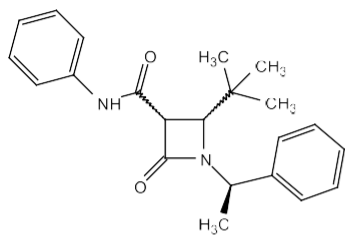


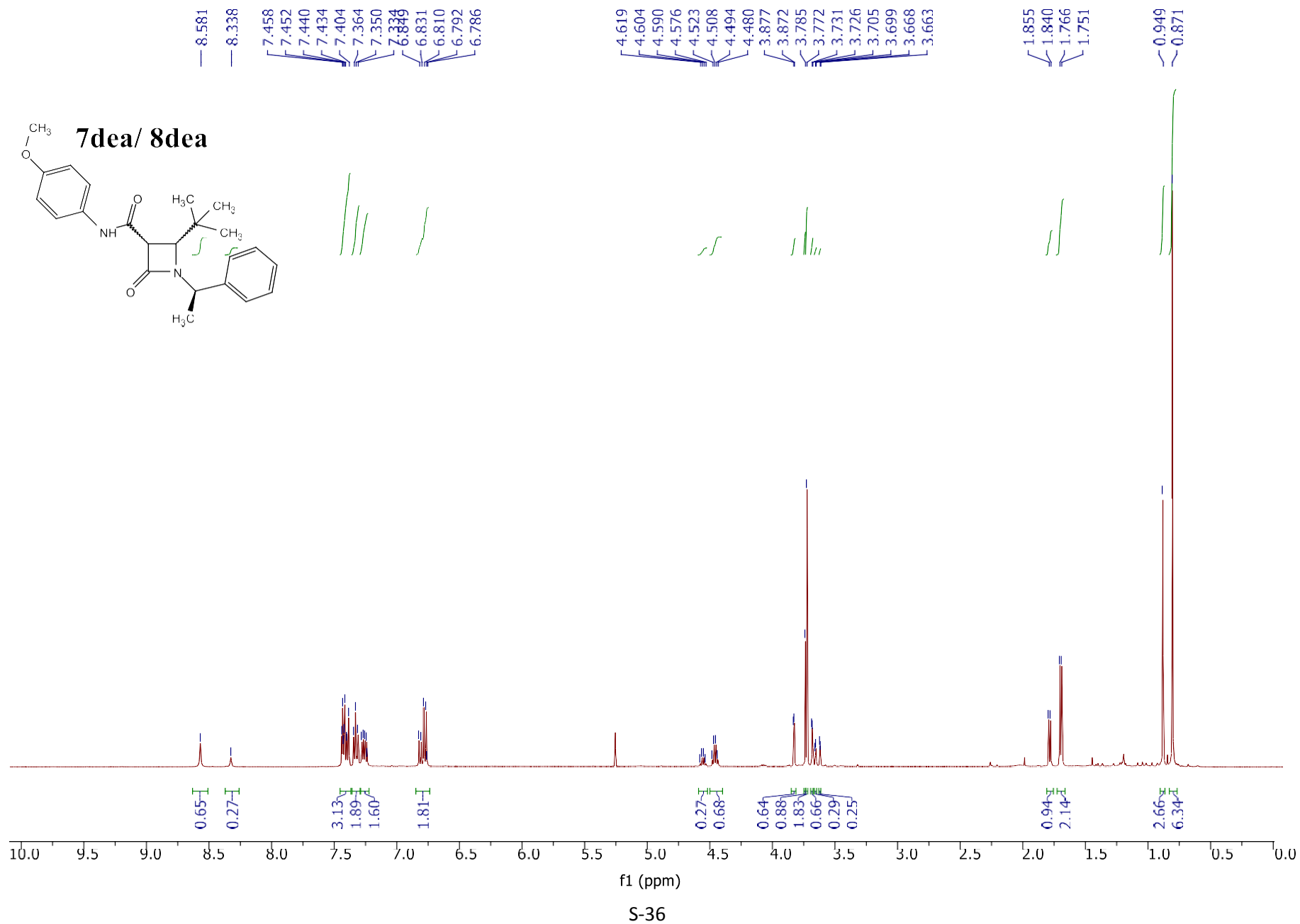


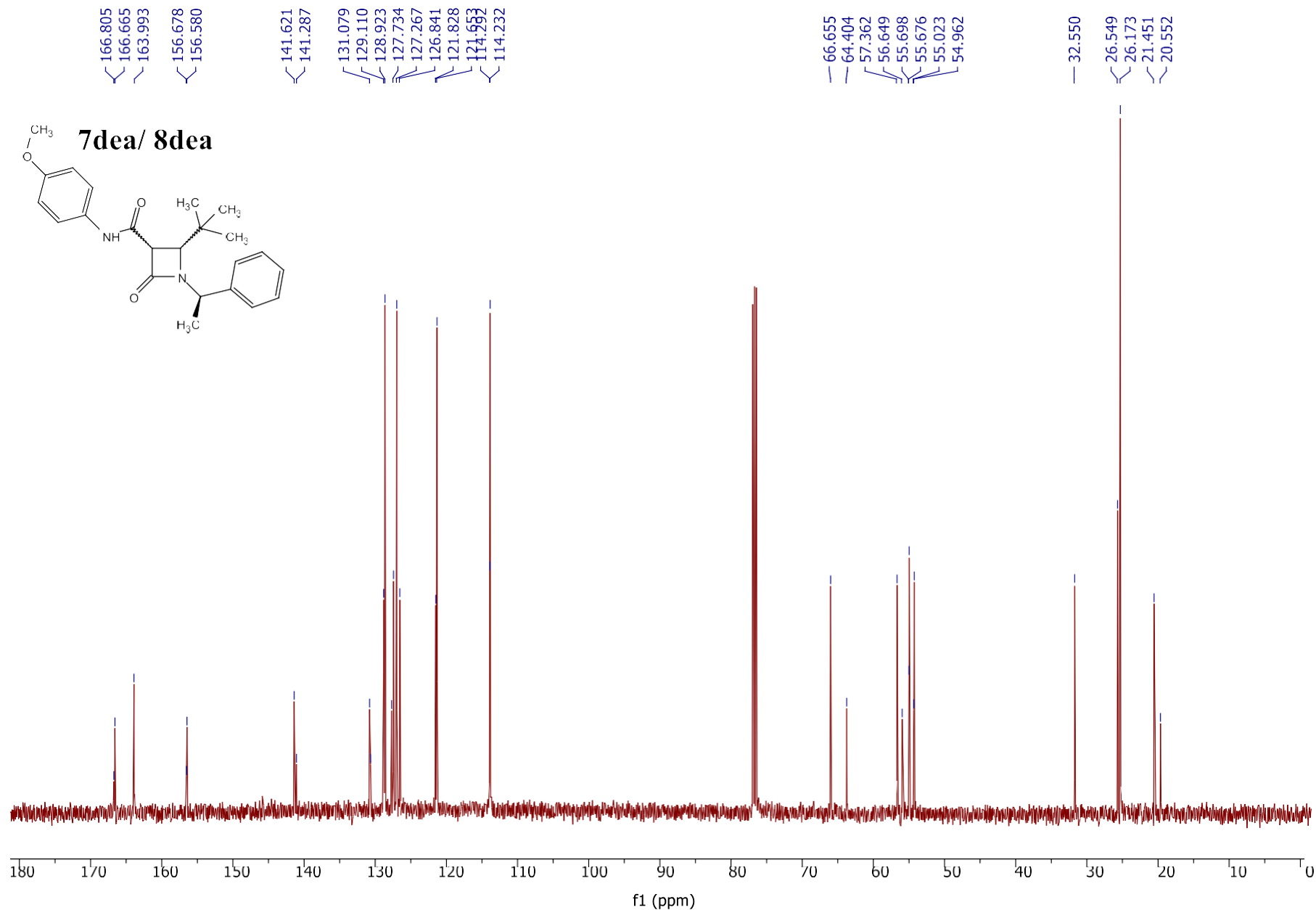
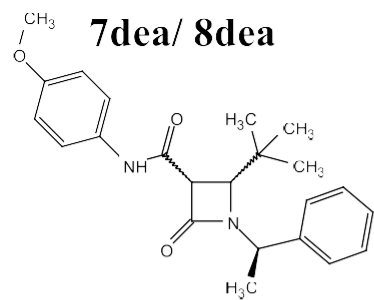


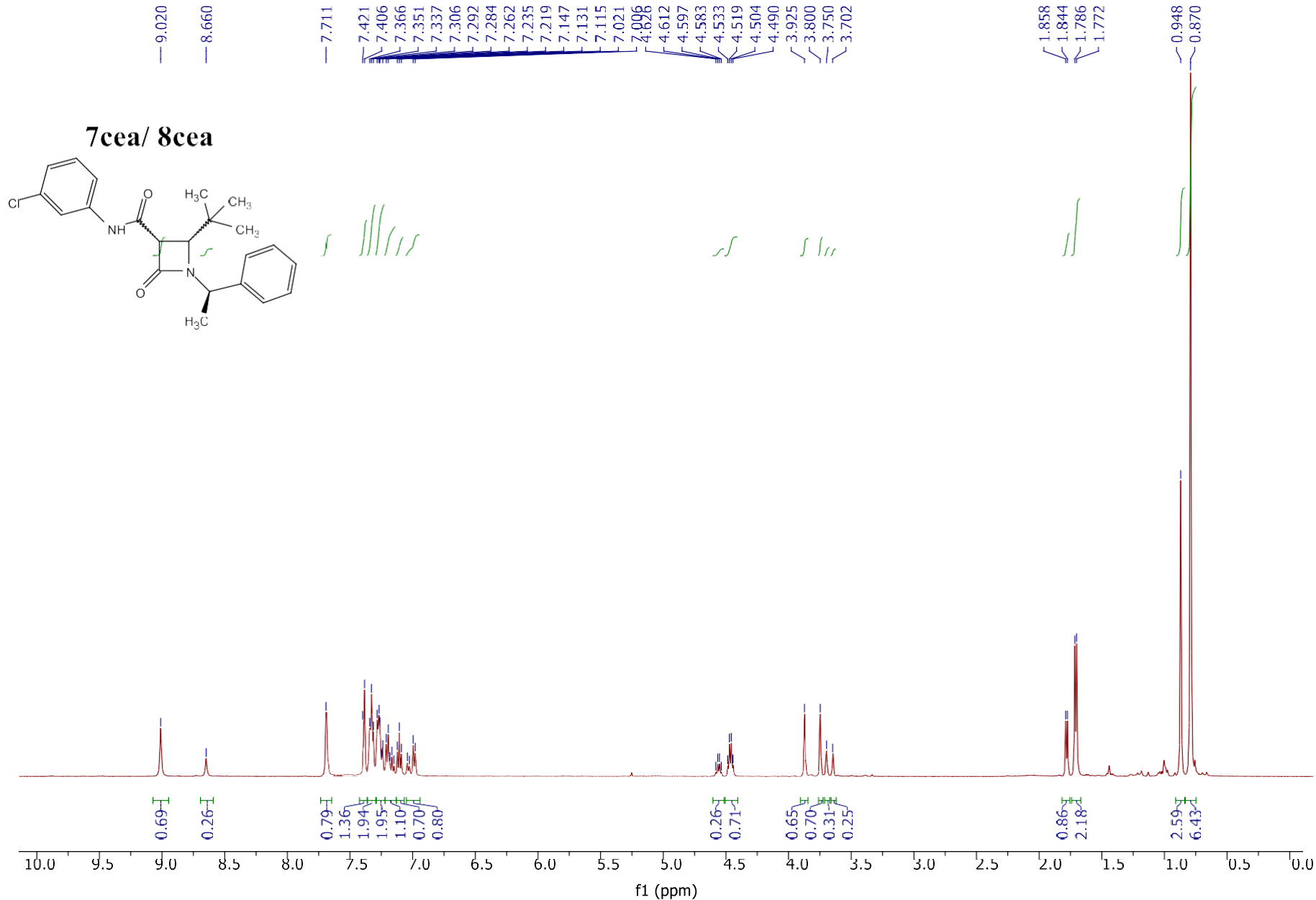


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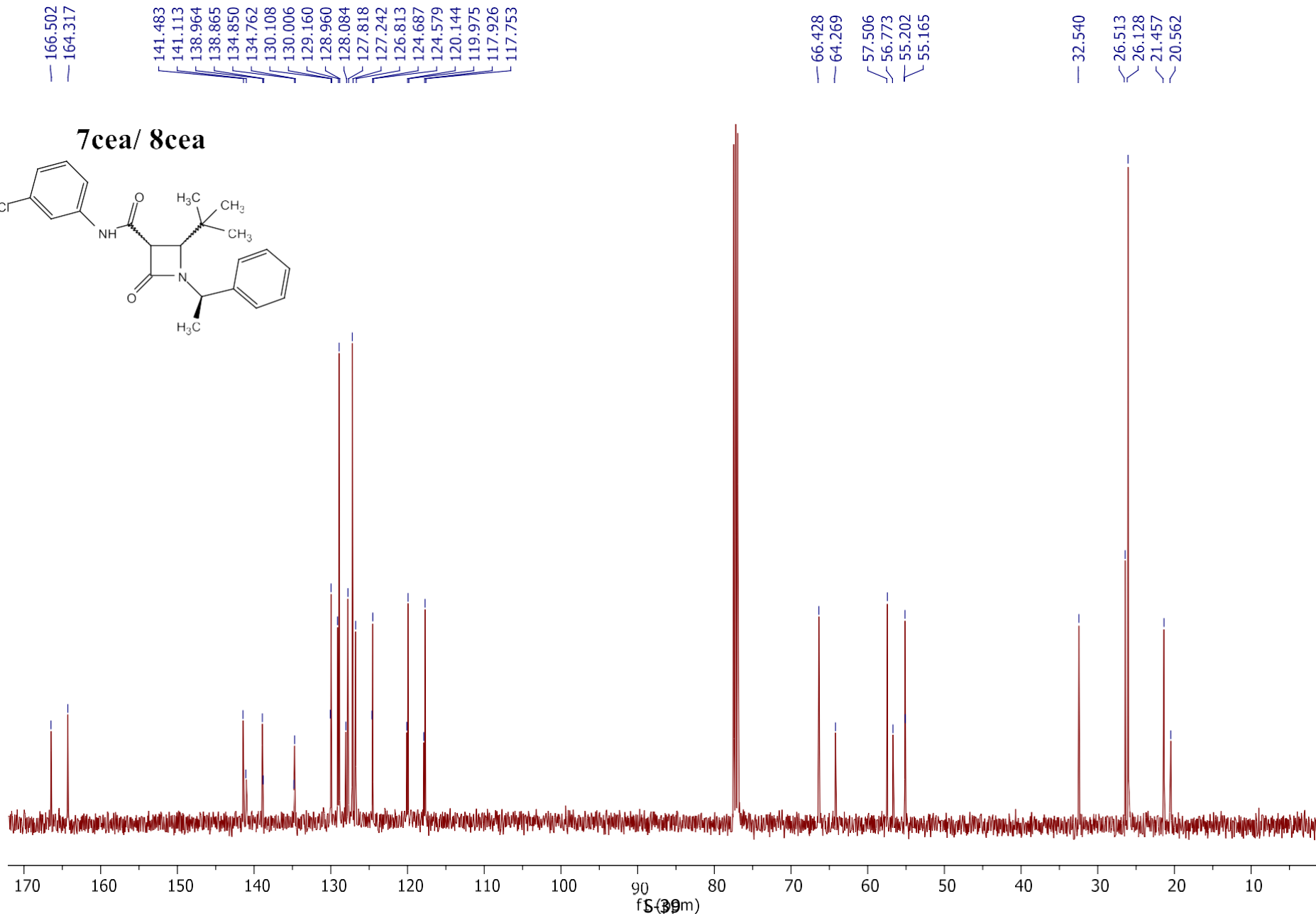
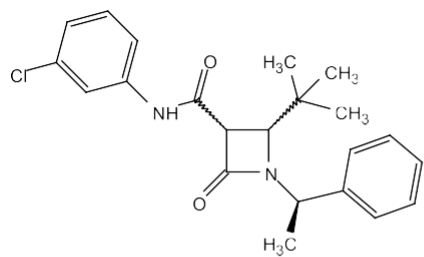


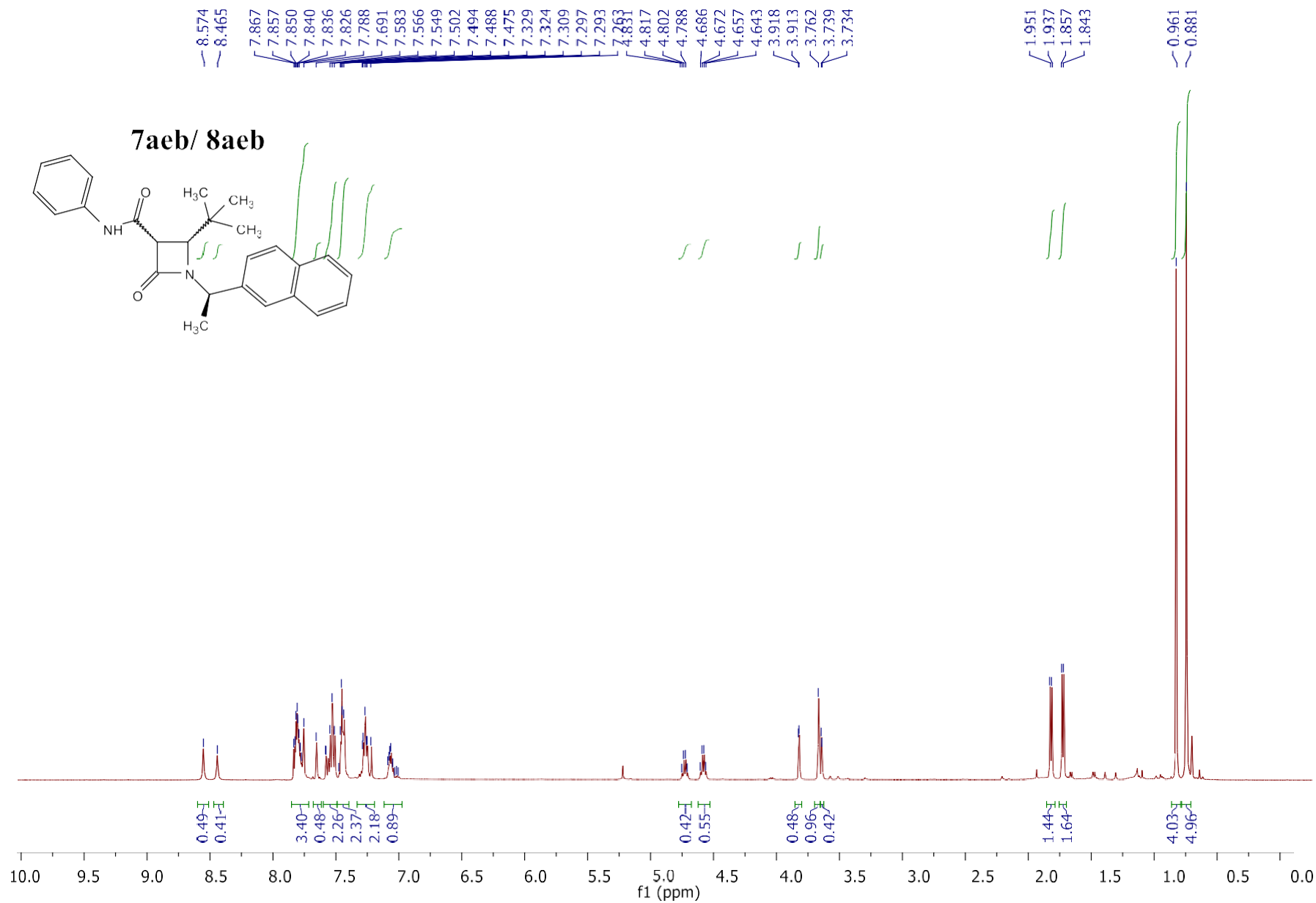


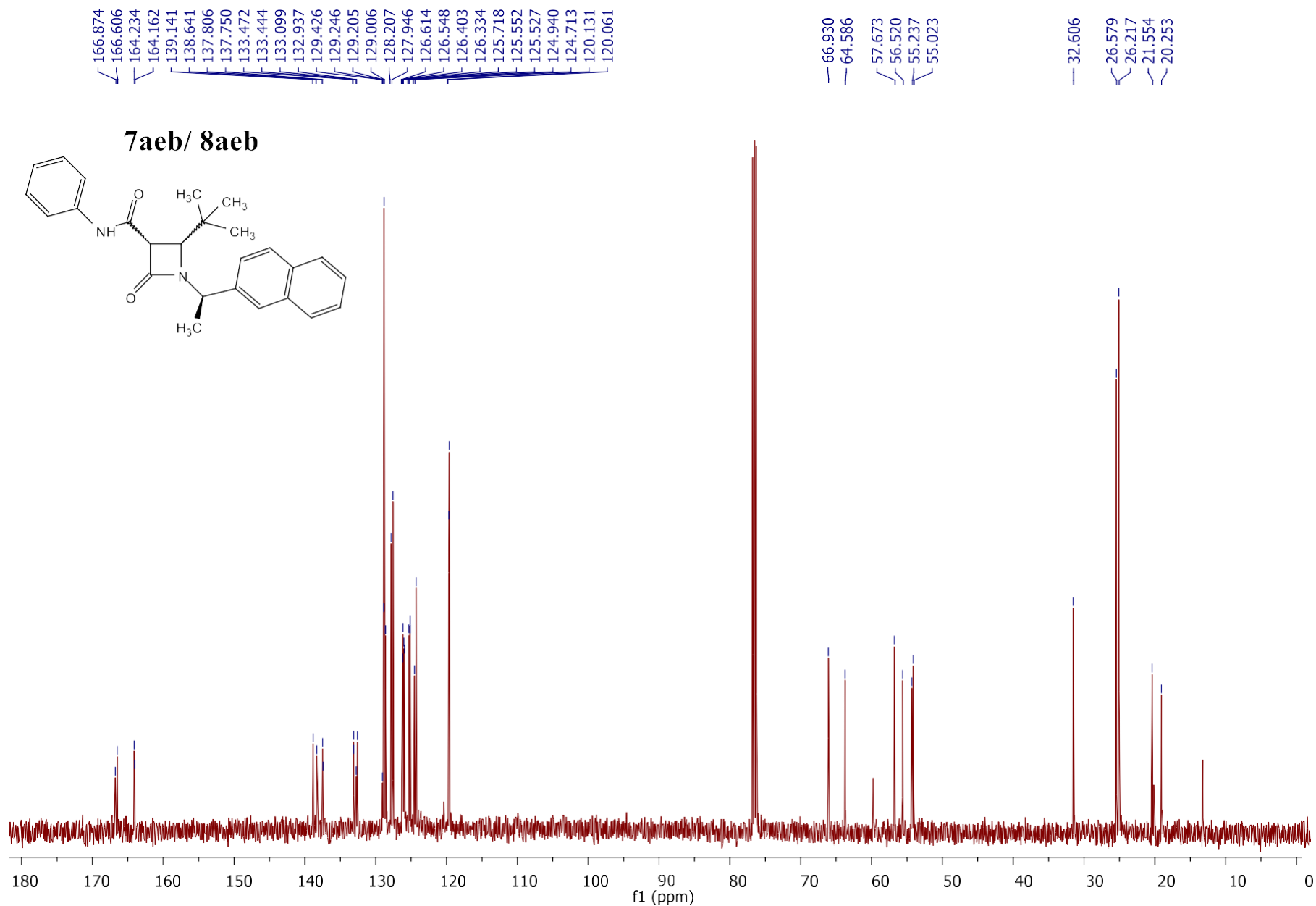


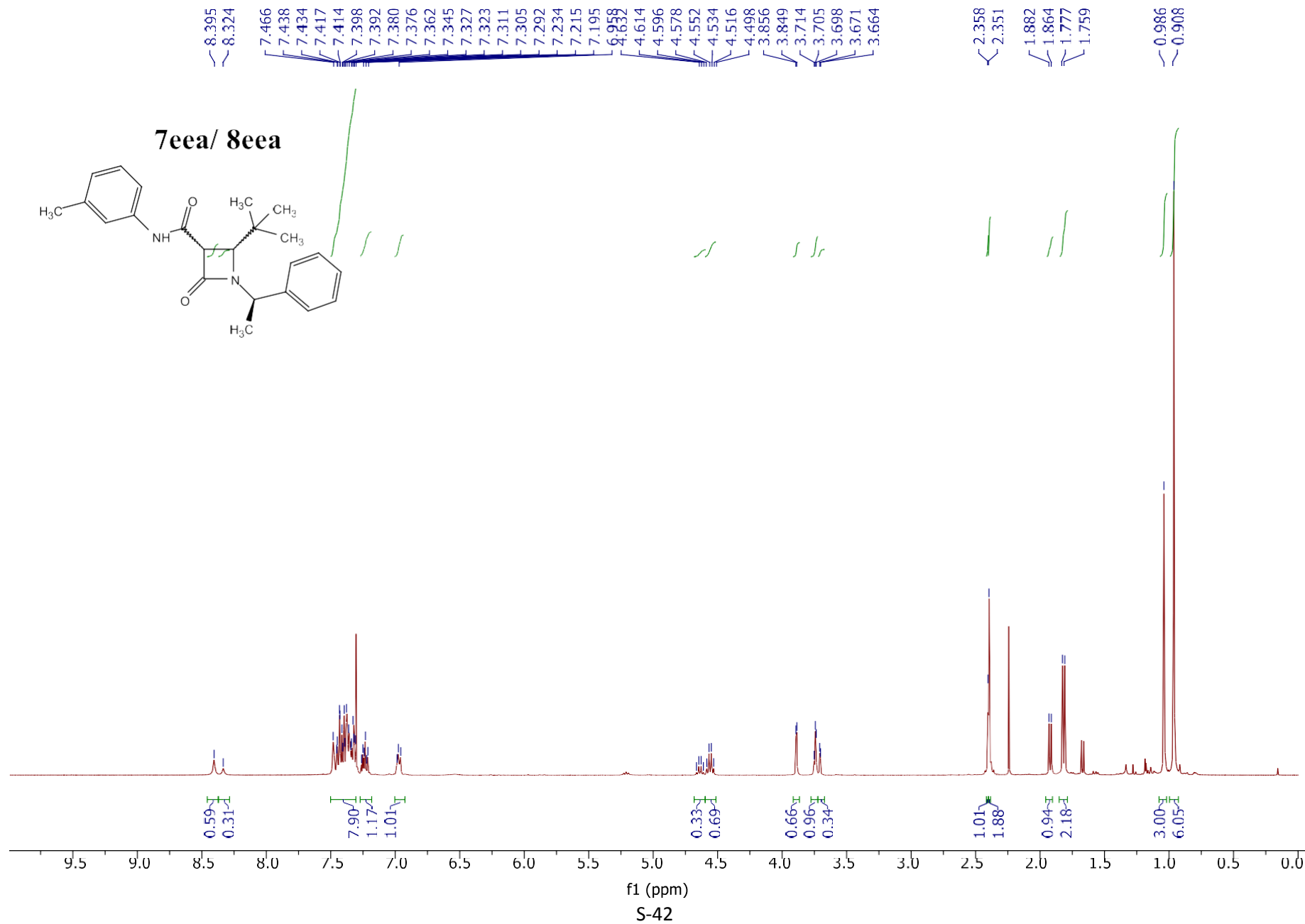
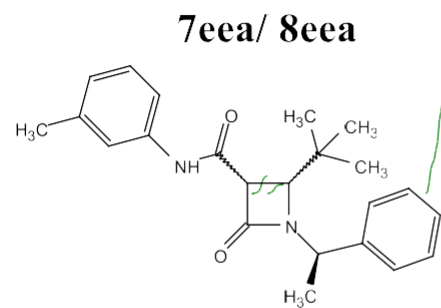


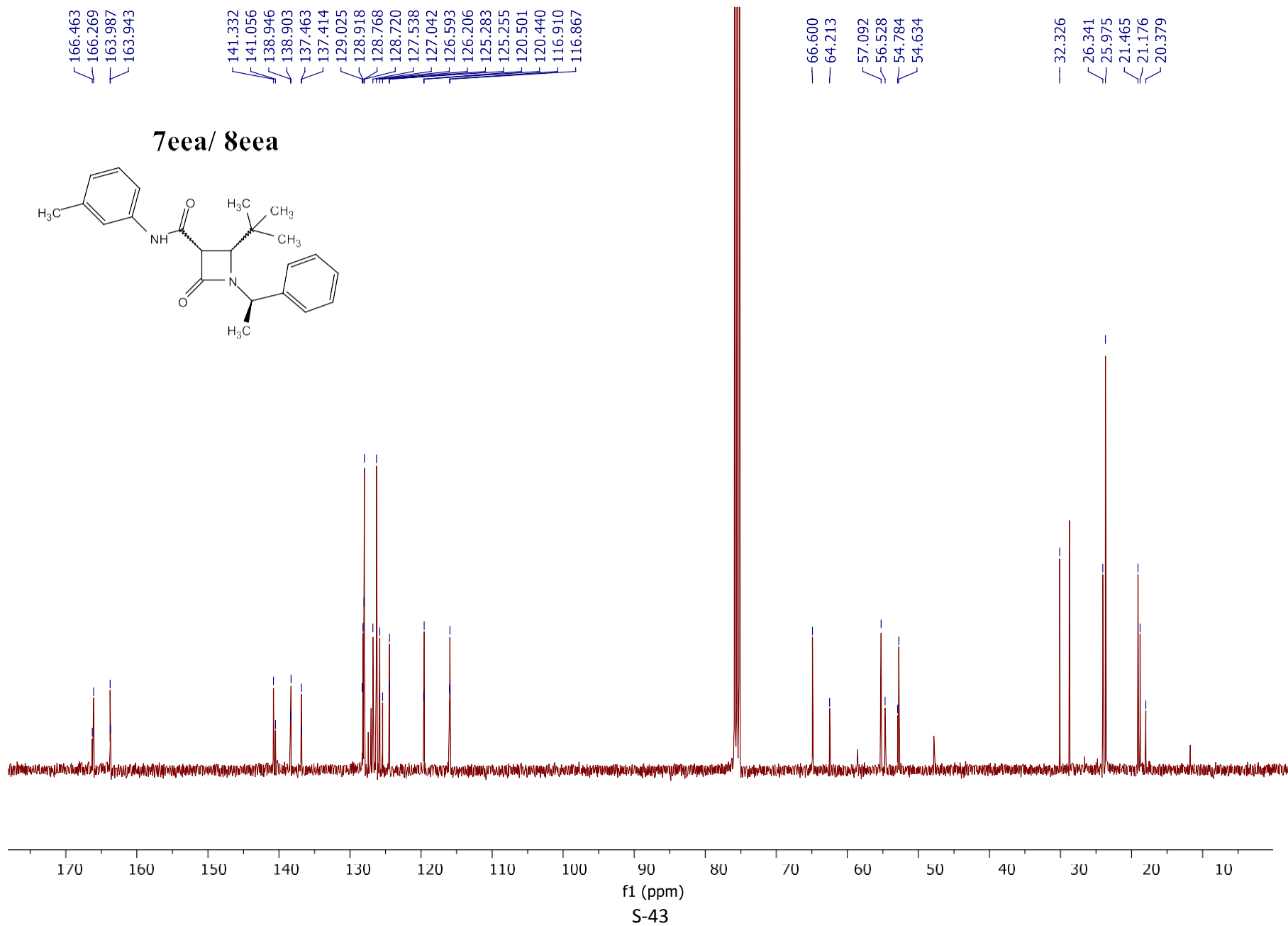
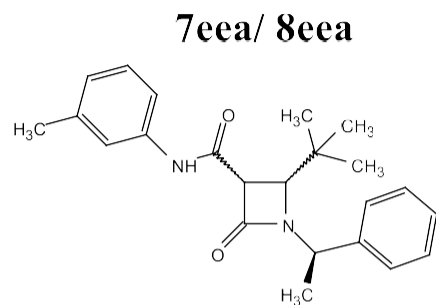
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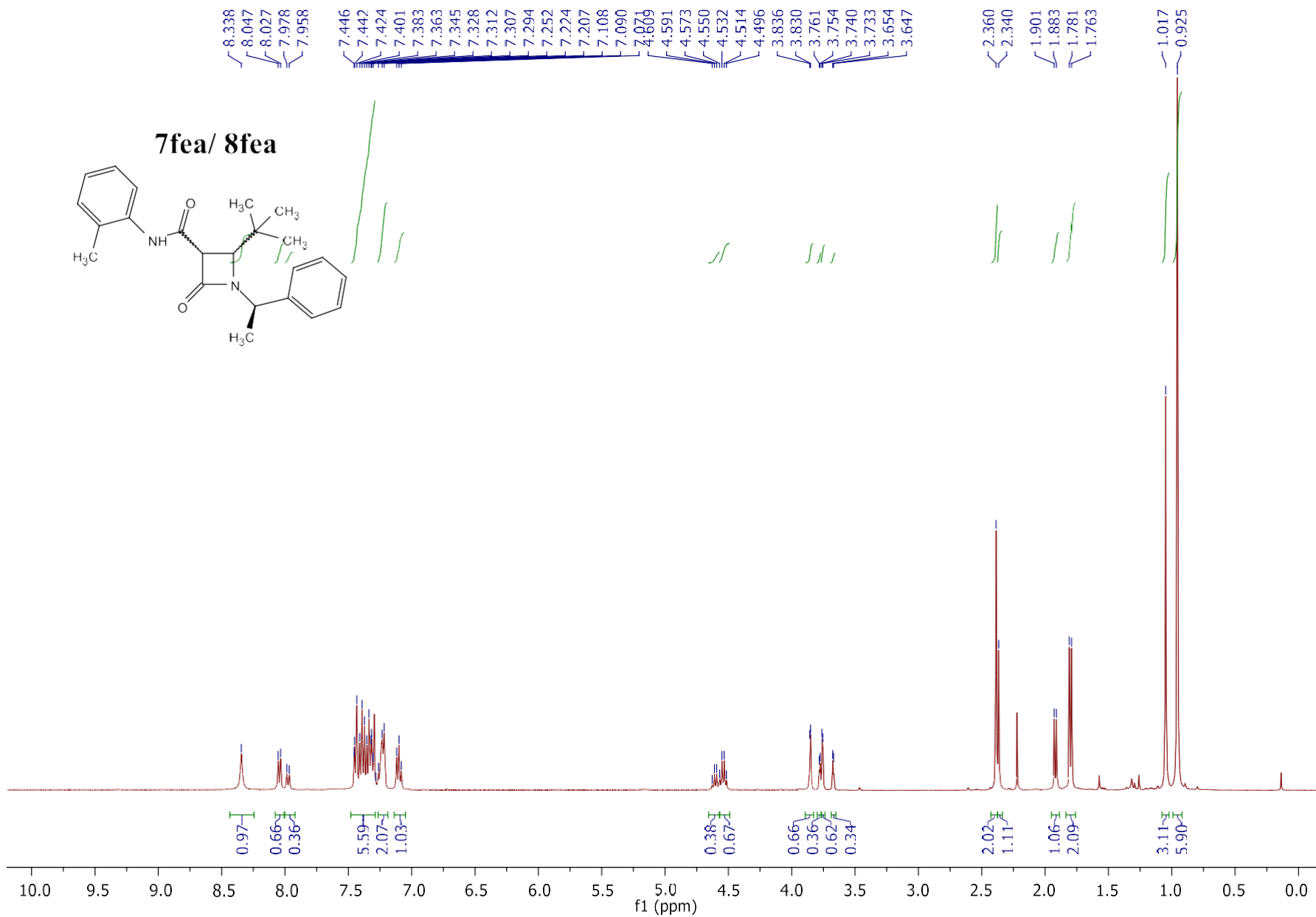












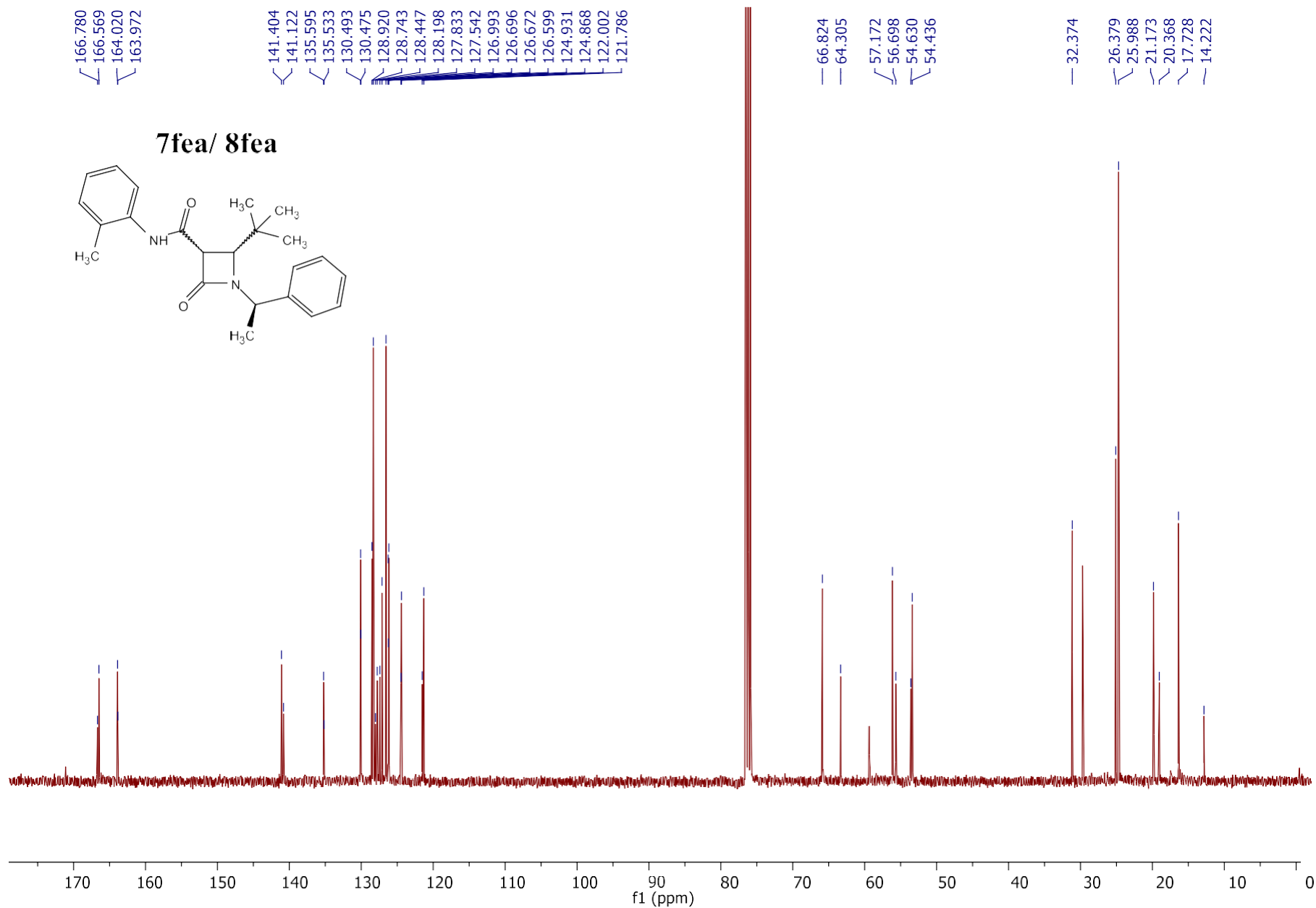
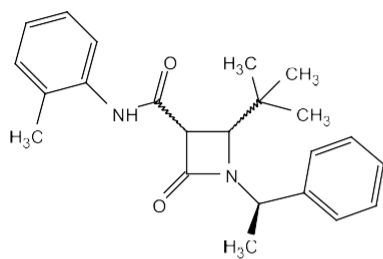
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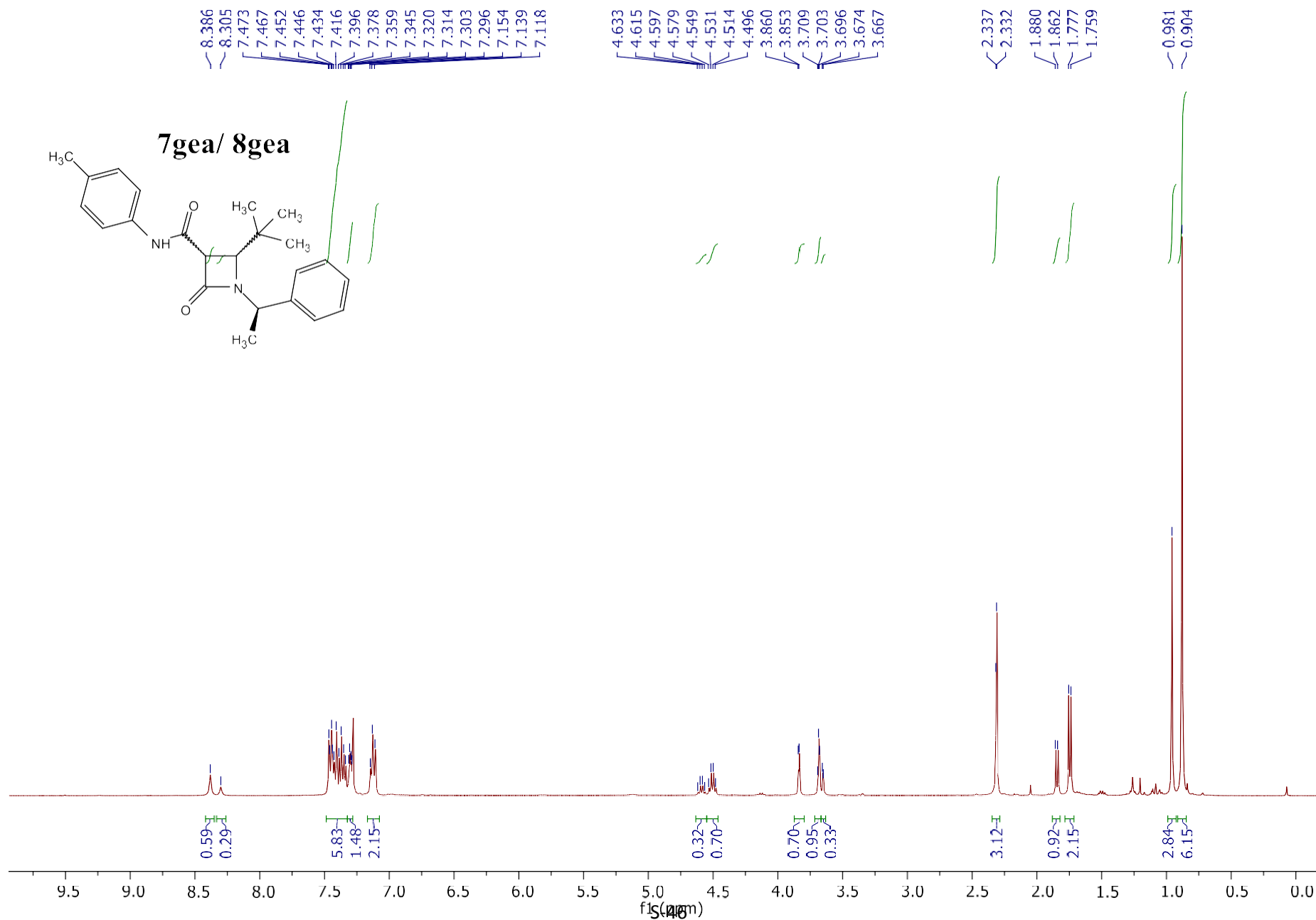
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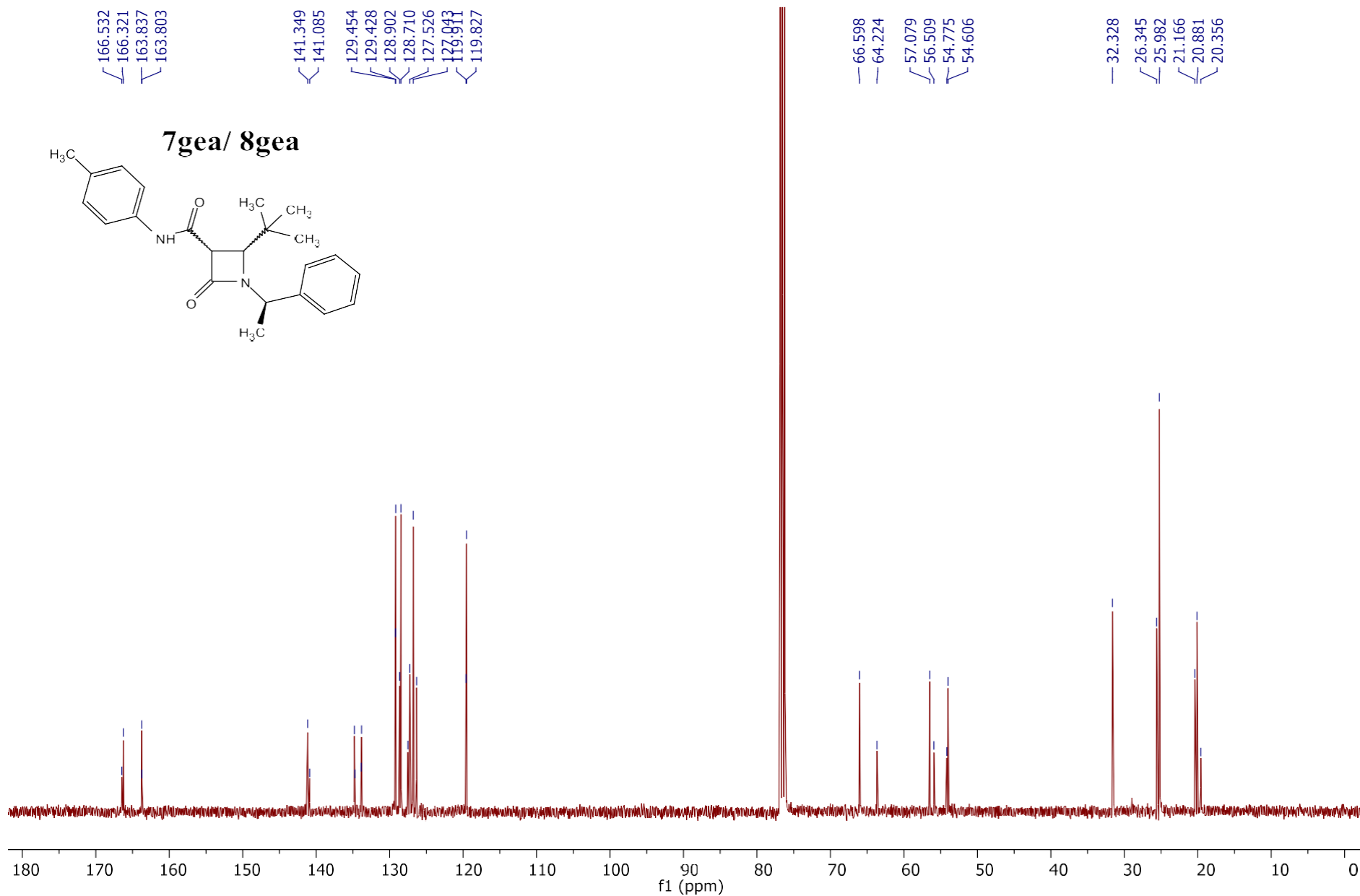
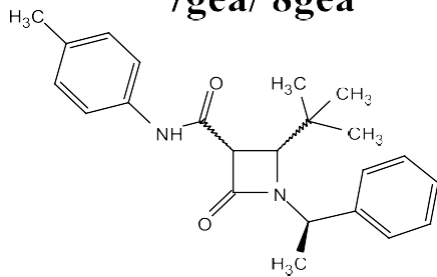
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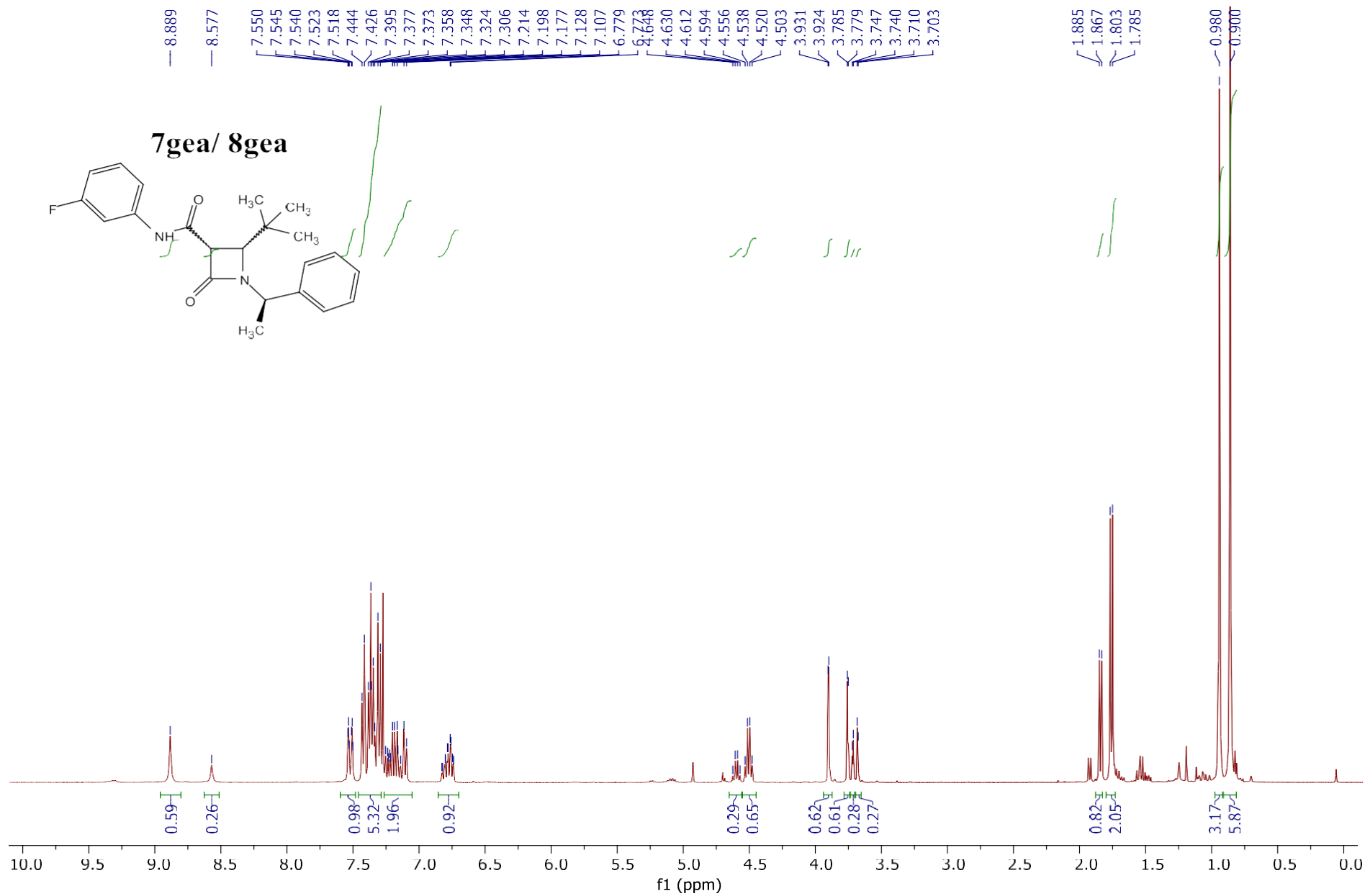


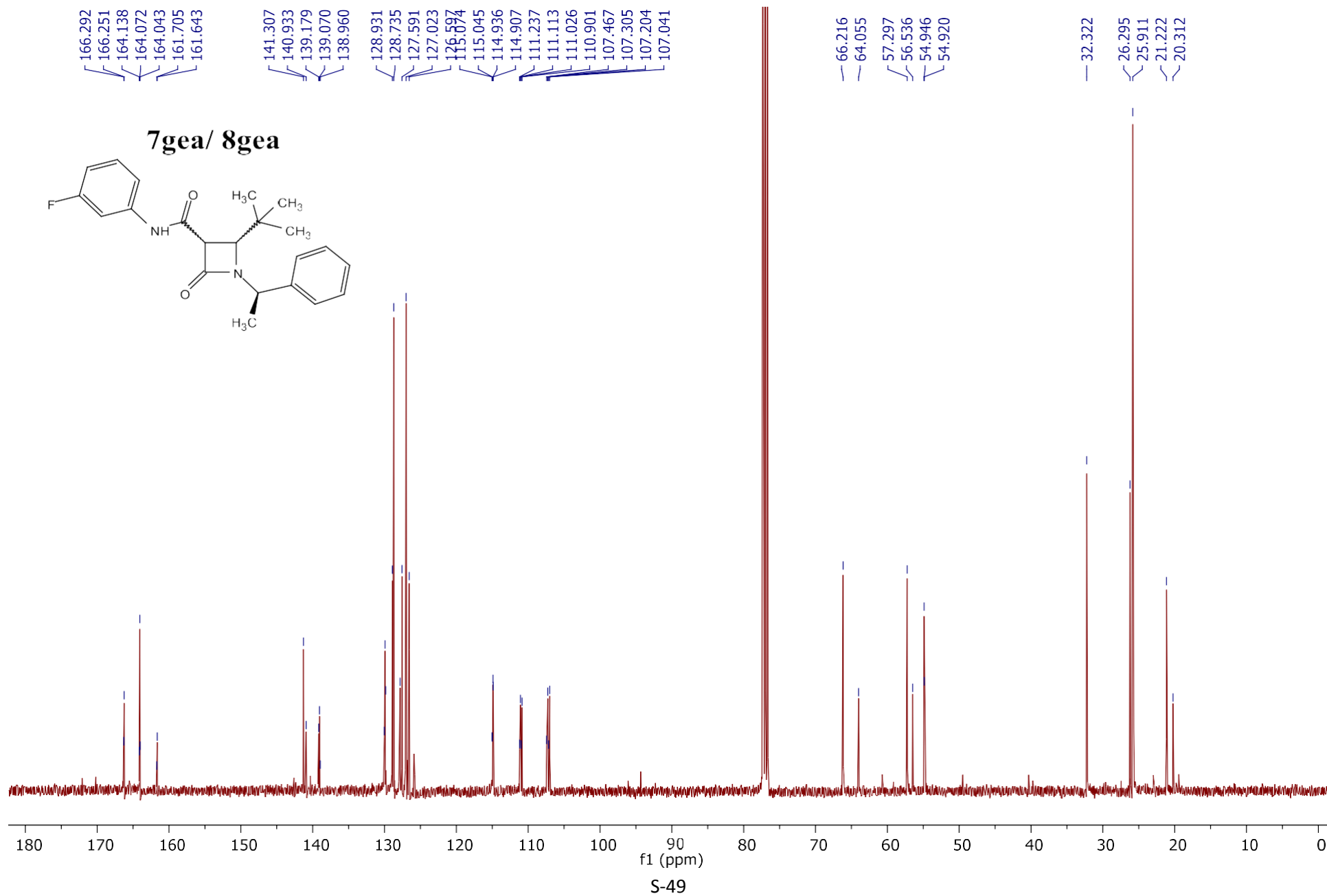
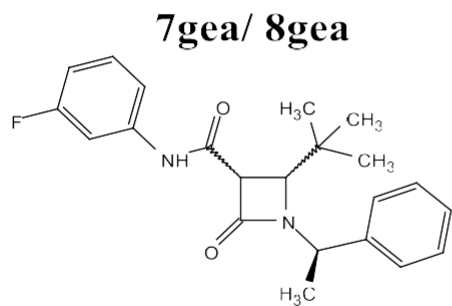
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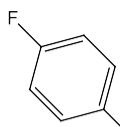


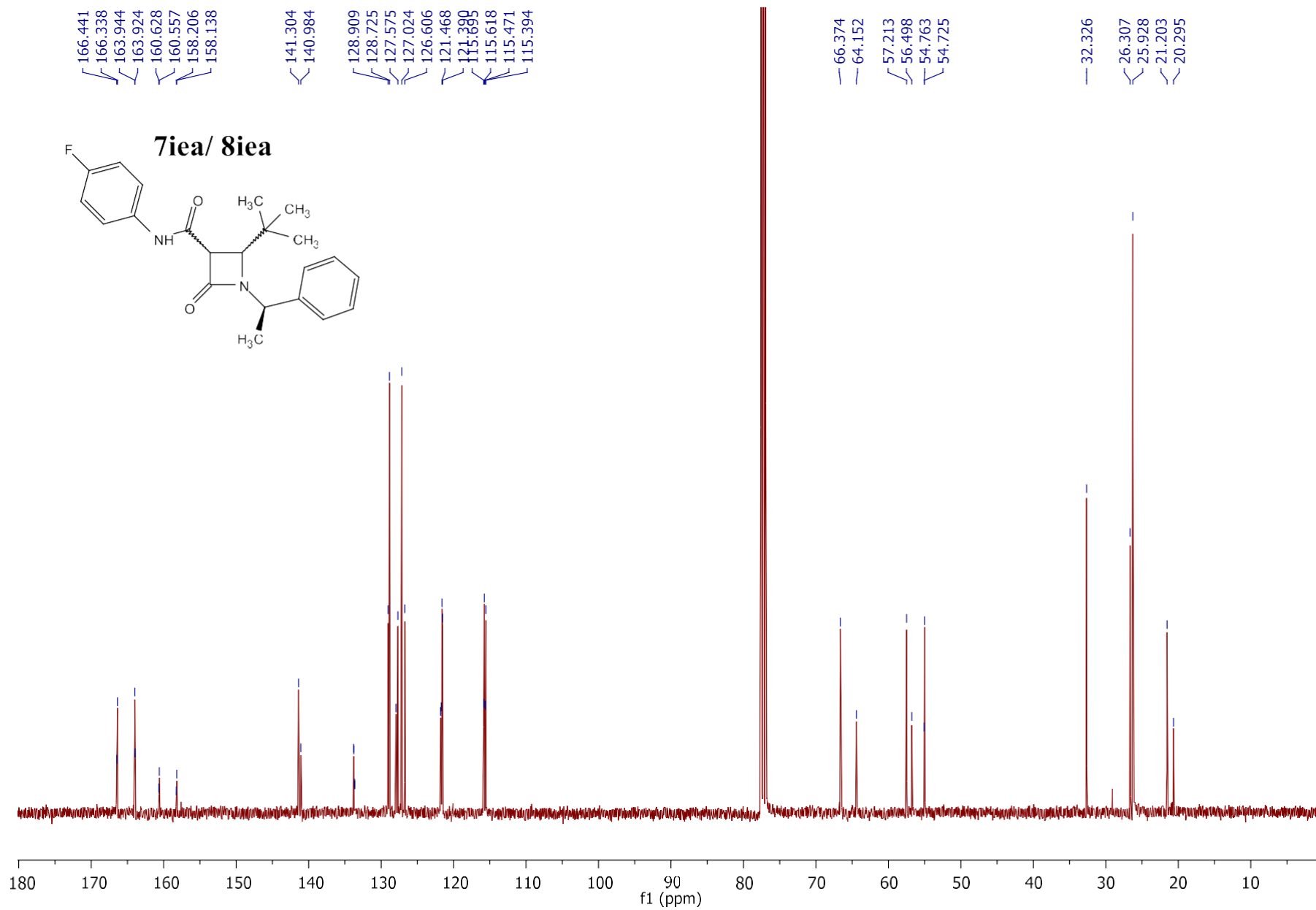
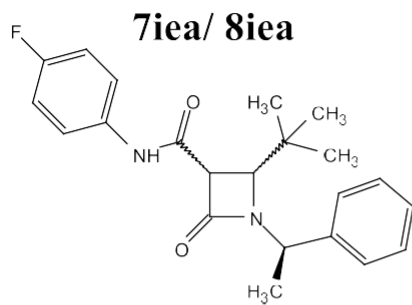
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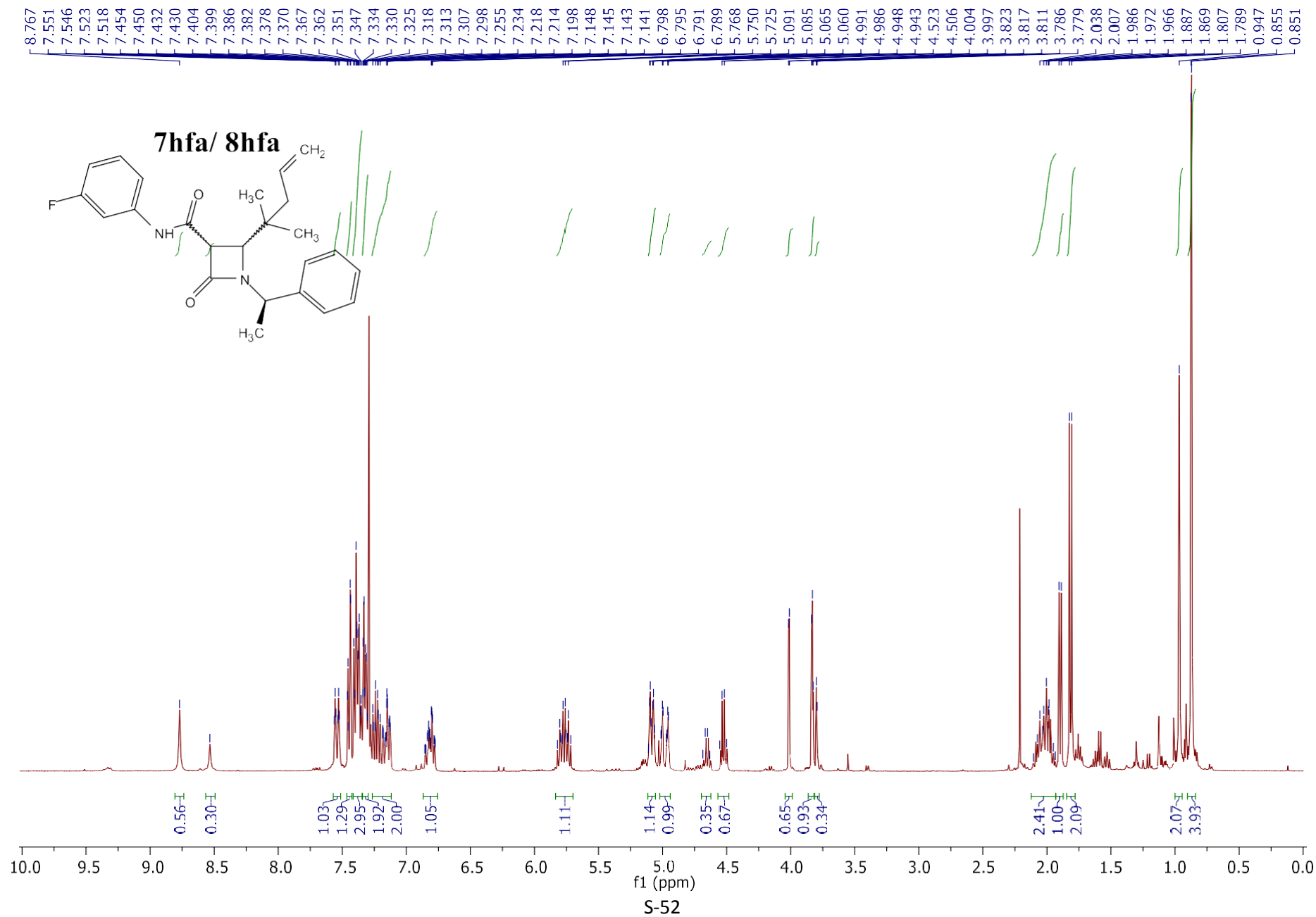


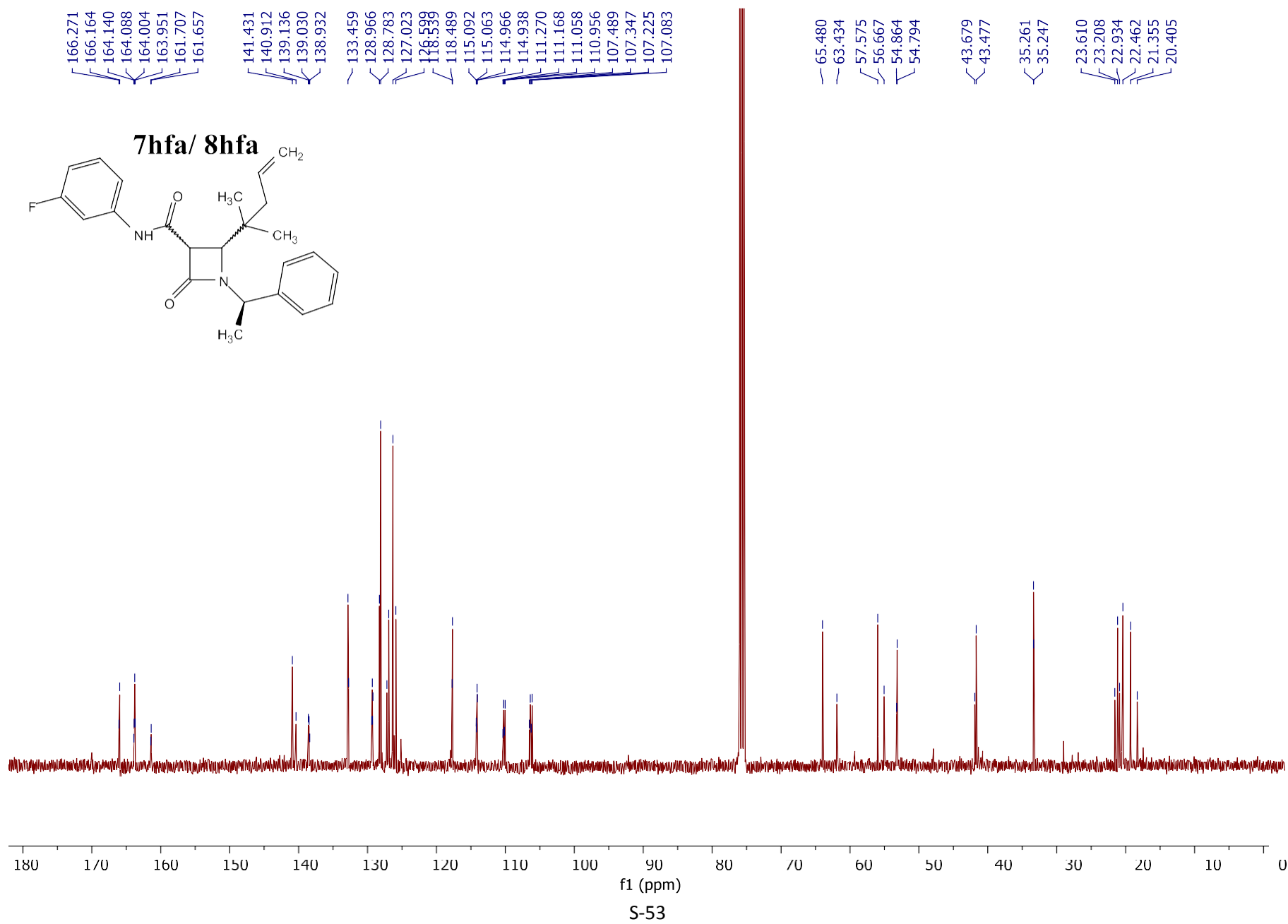


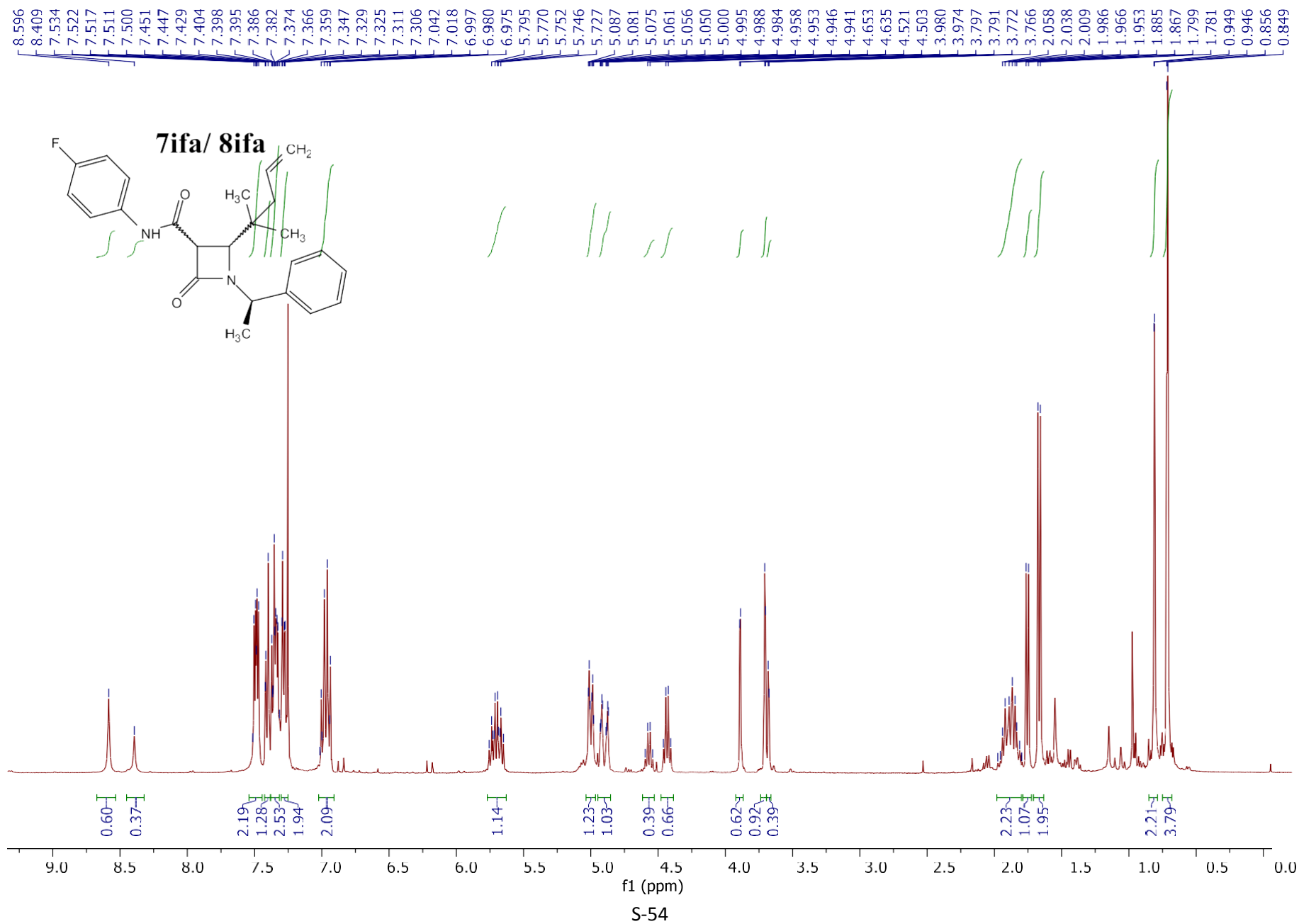


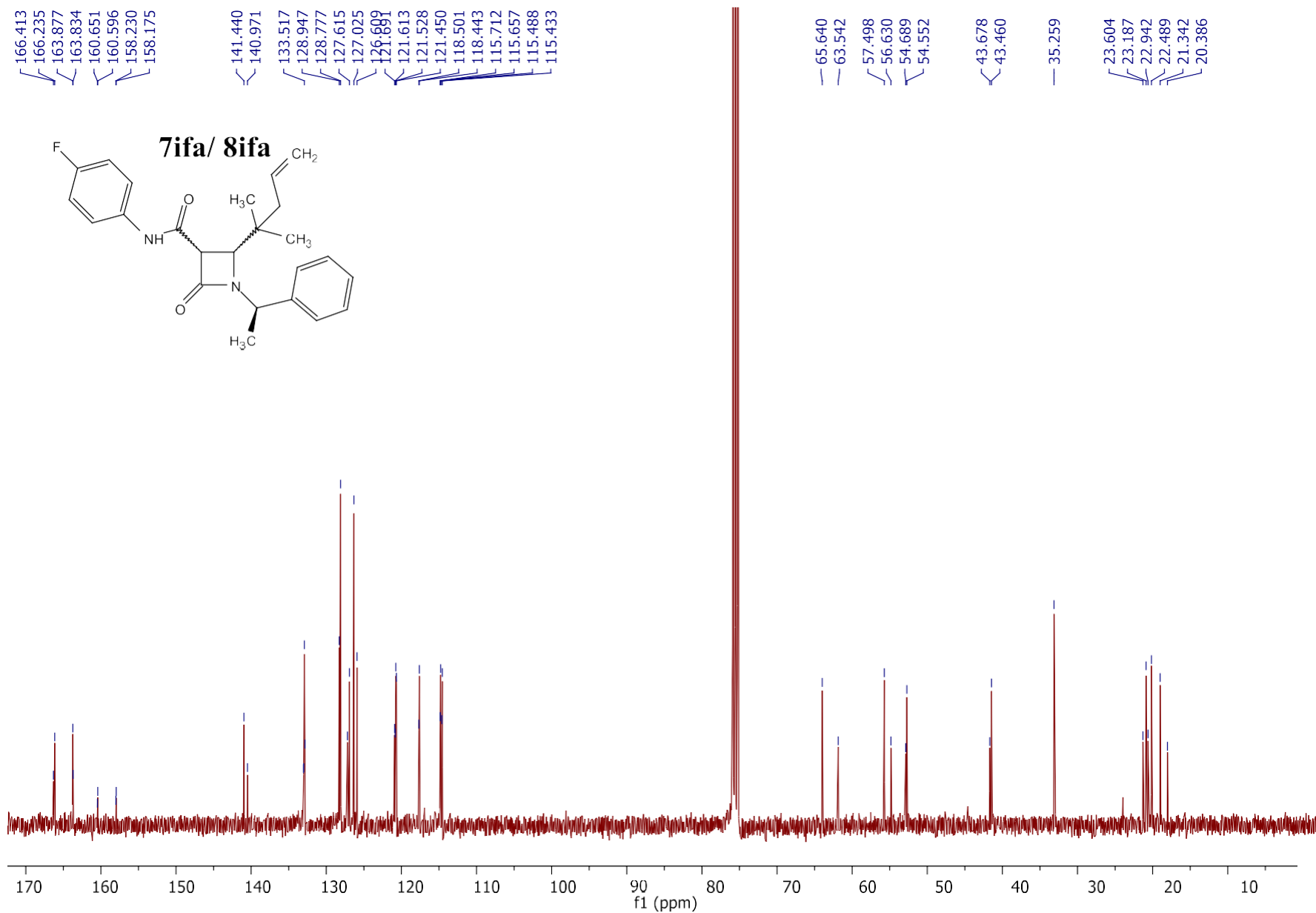


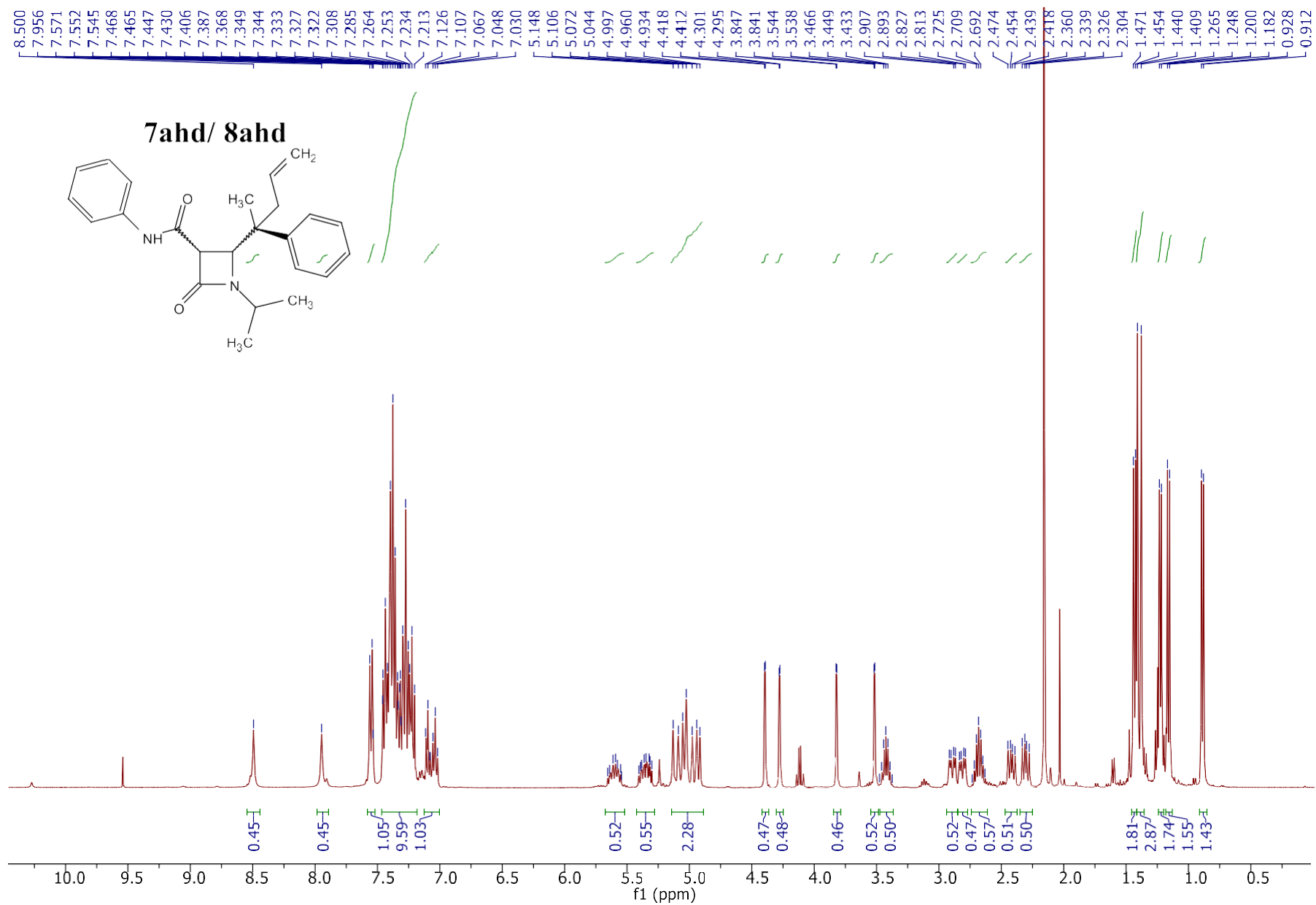












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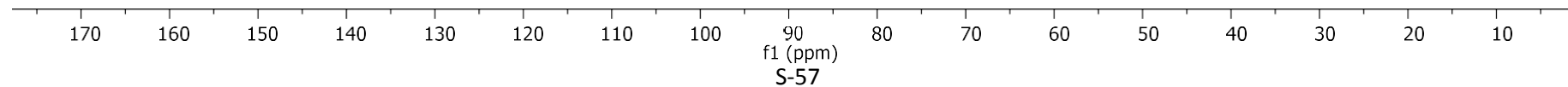
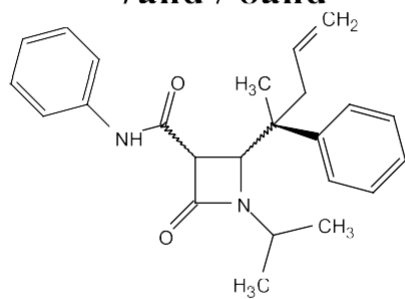
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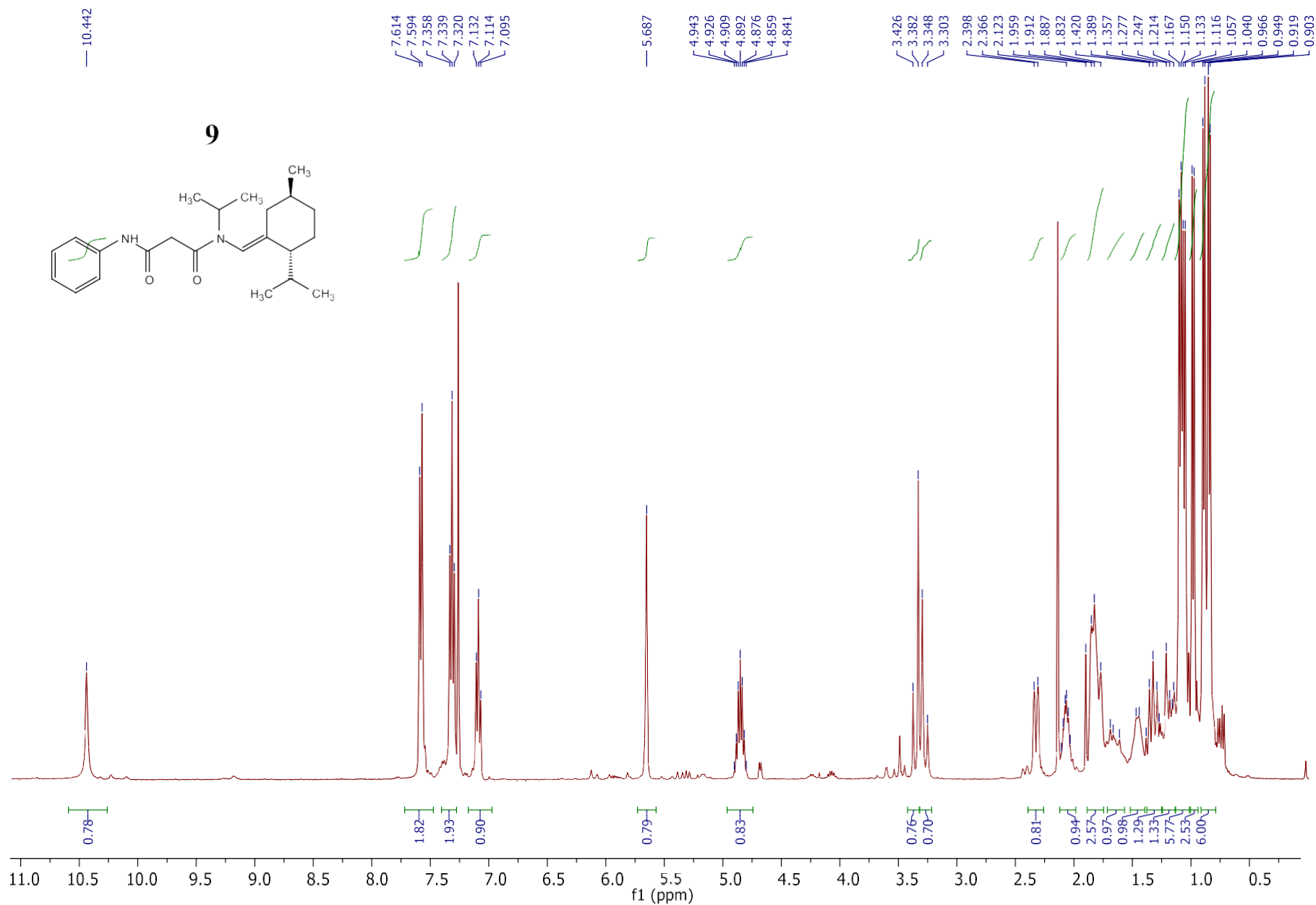
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32.330

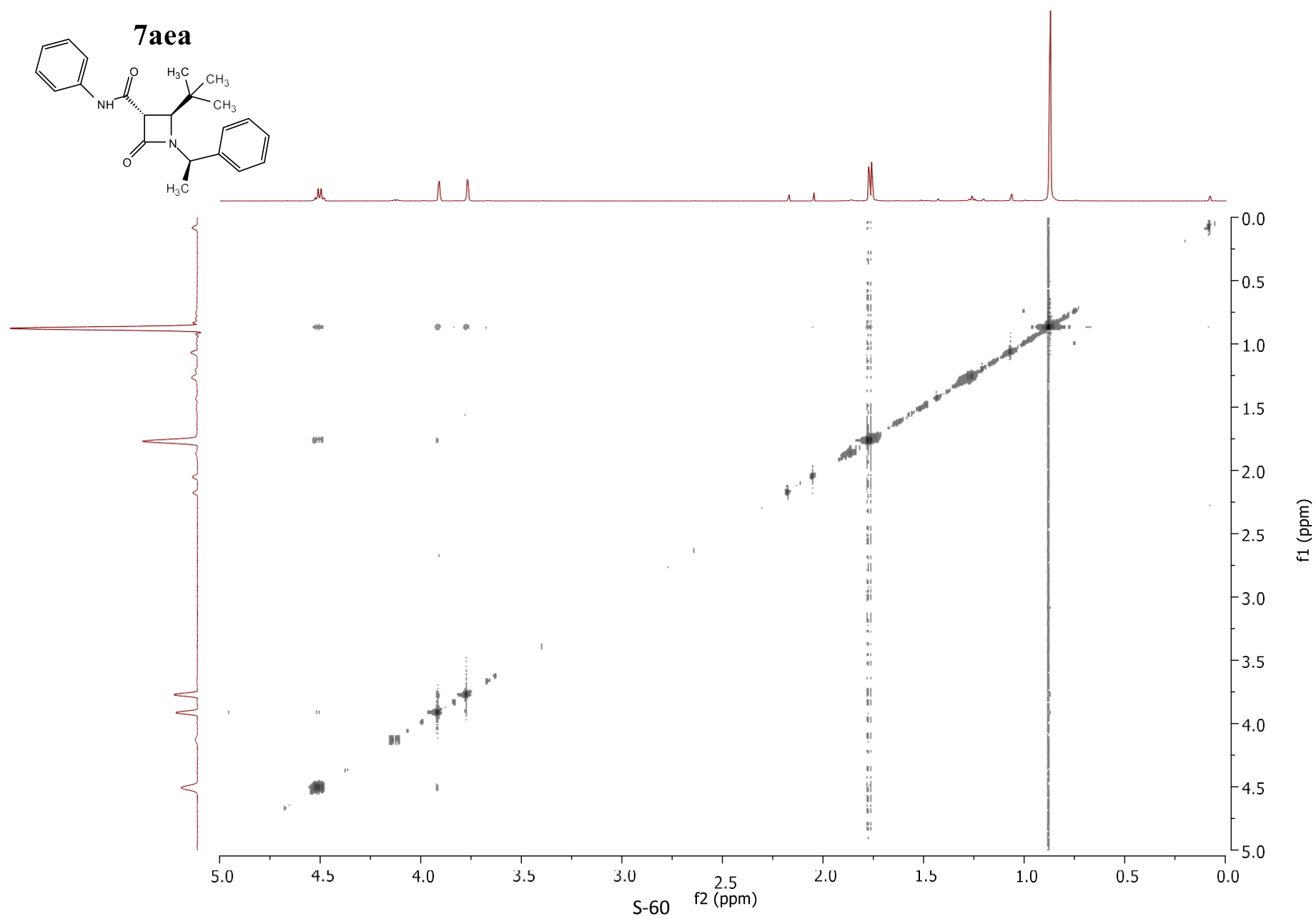
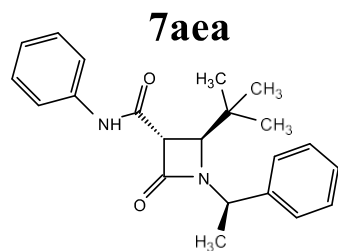
28.035
26.333
25.973
20.371

7ahd / 8ahd

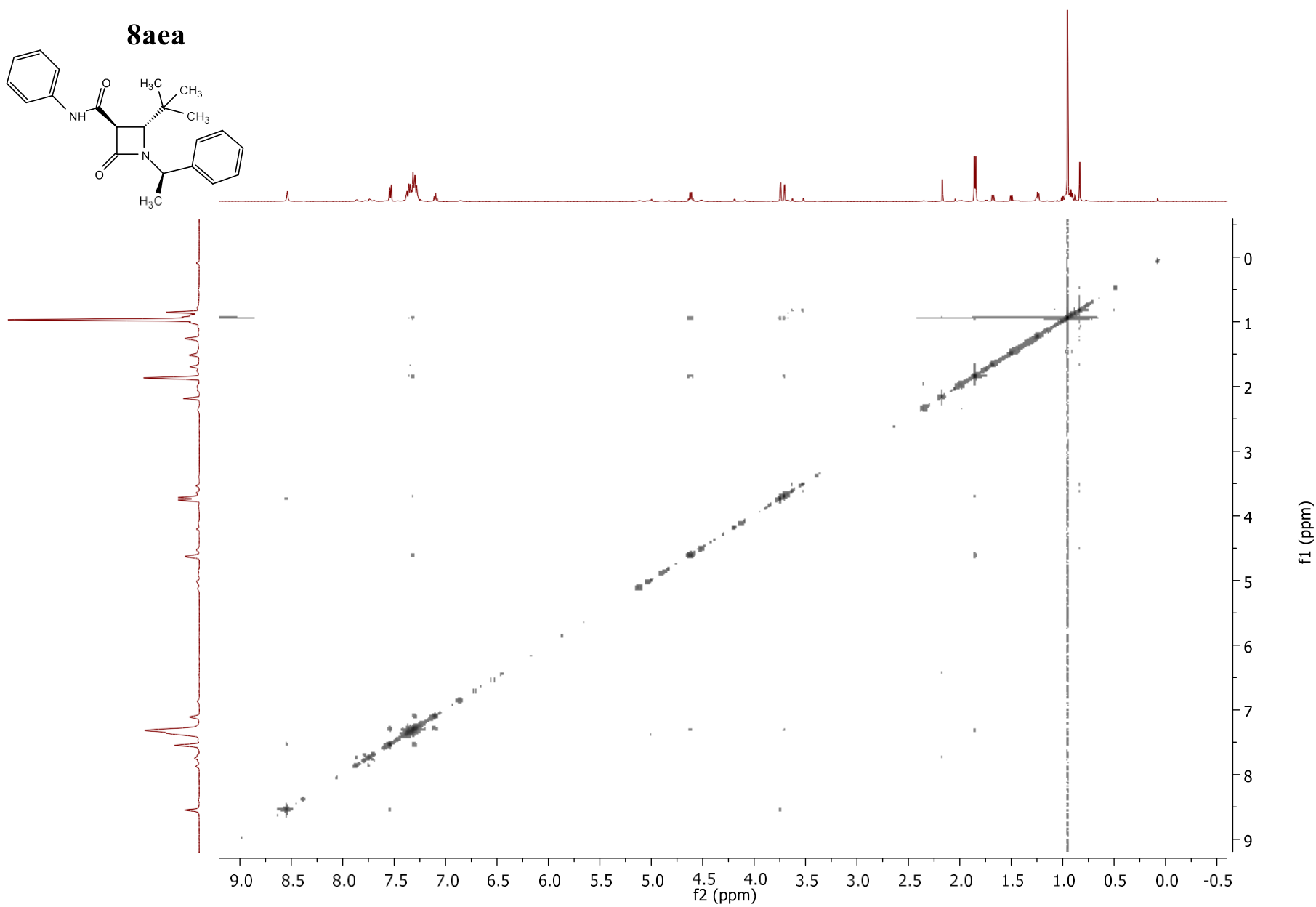
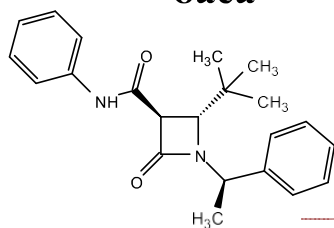




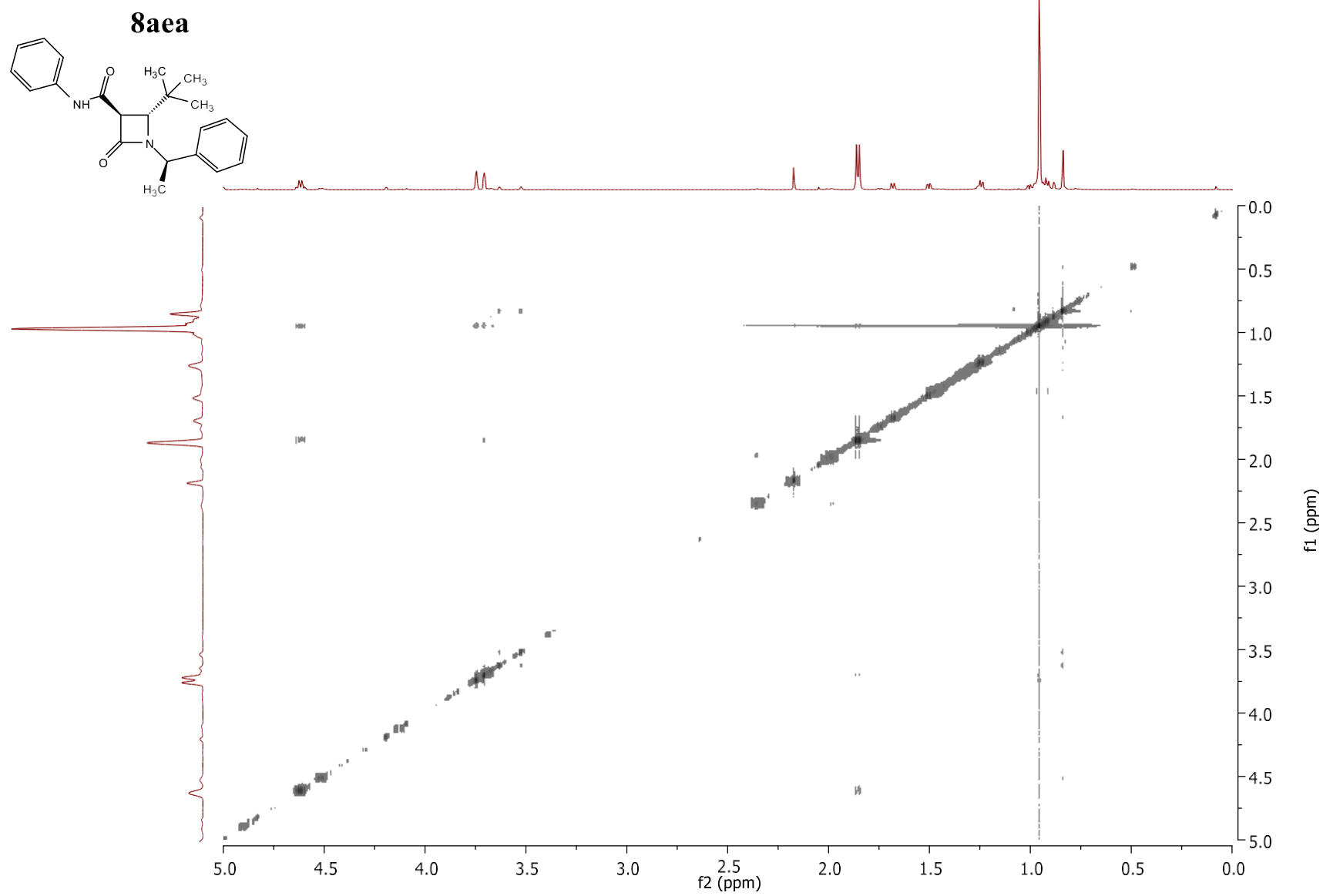


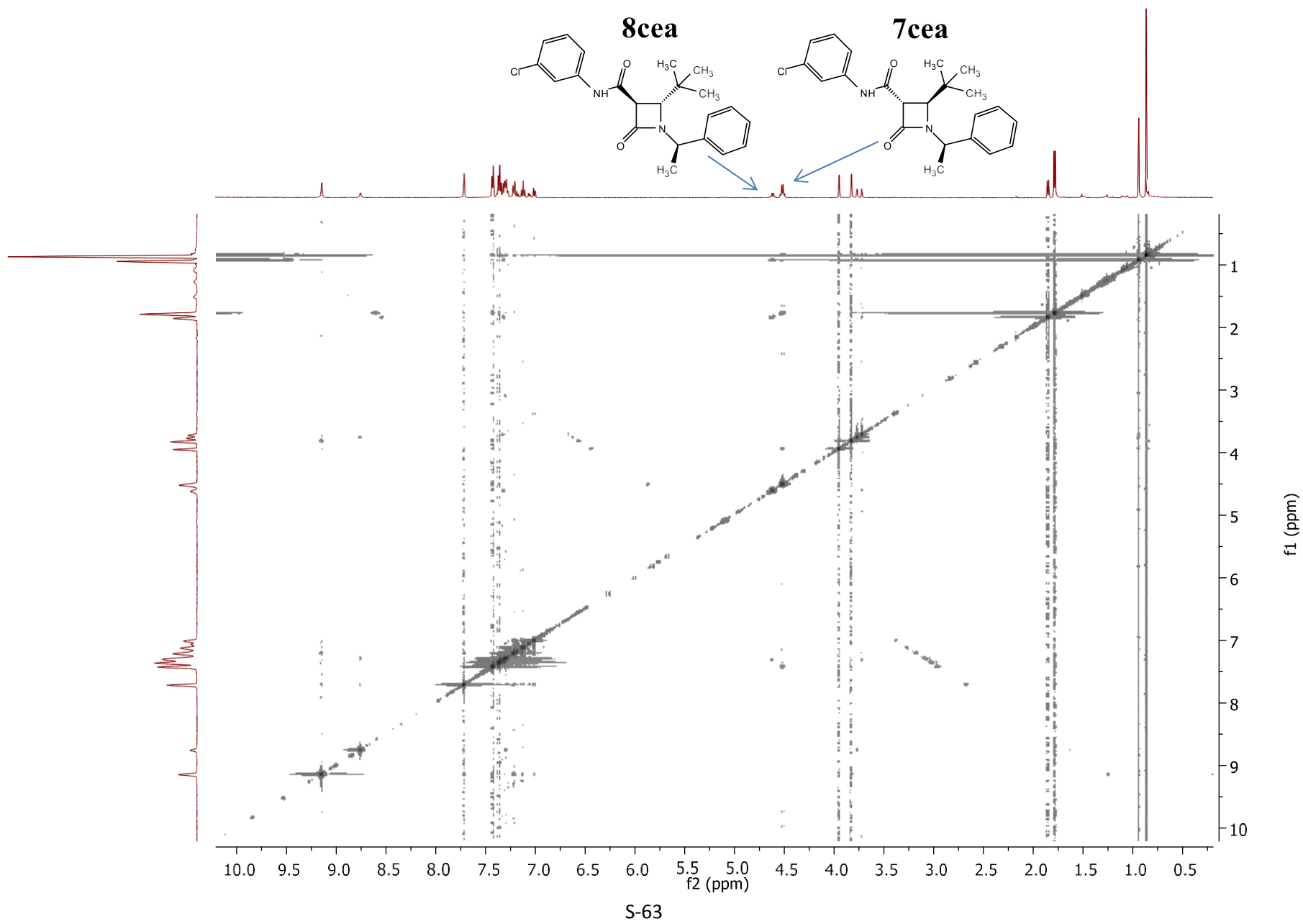


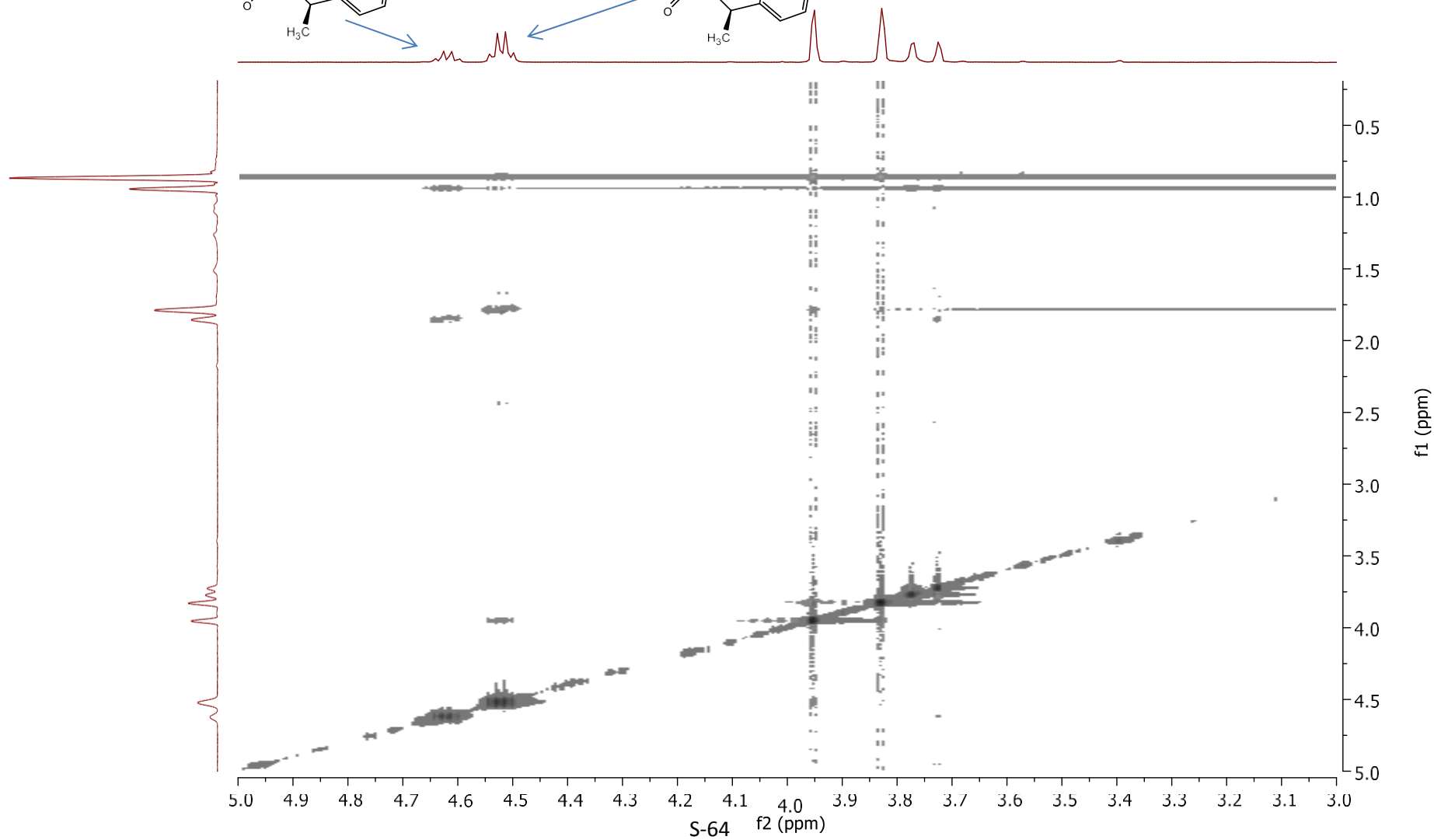
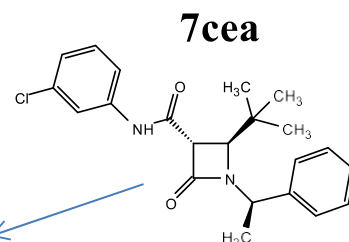
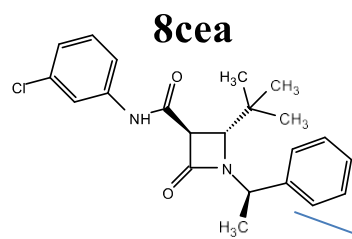
8aea

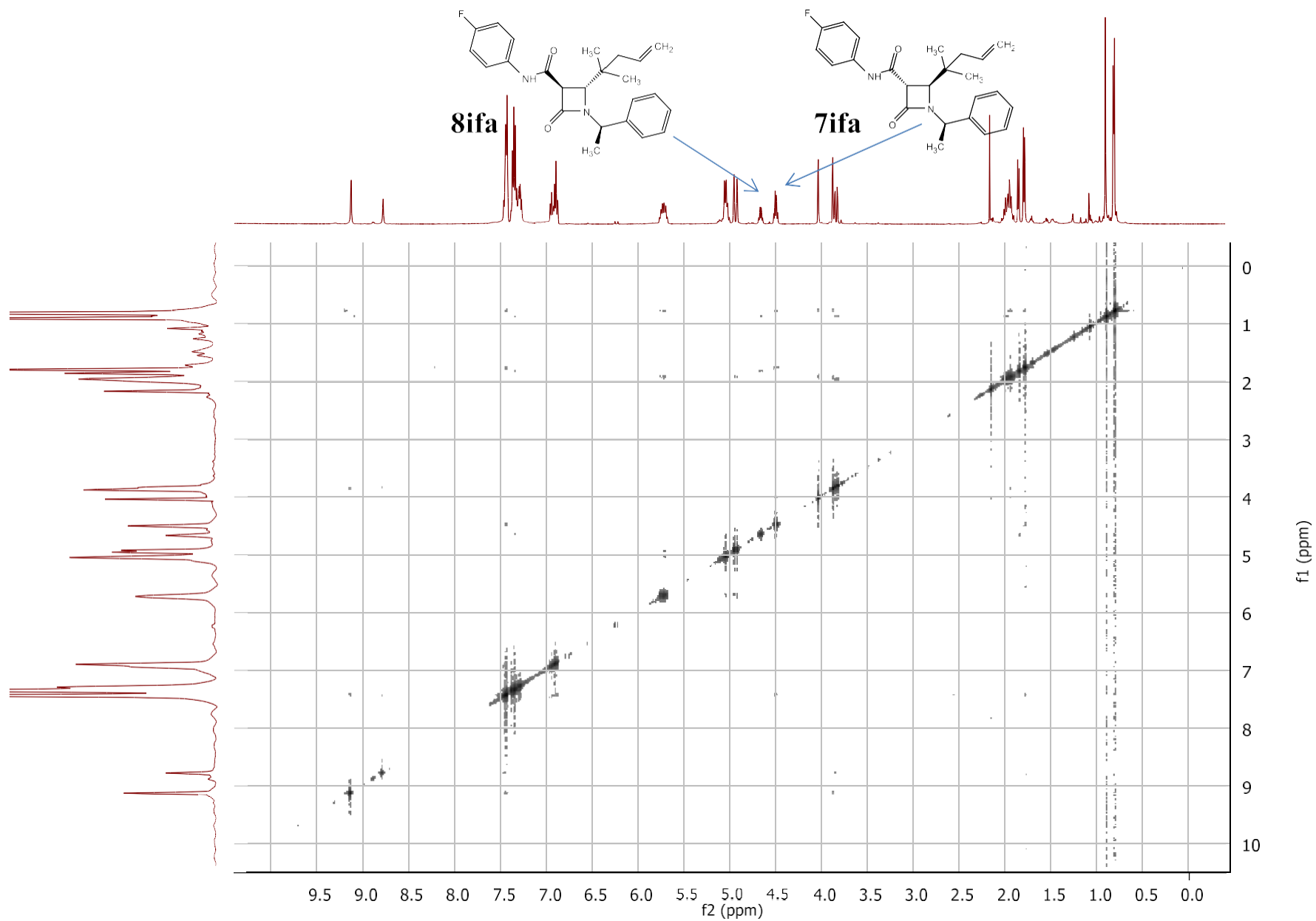


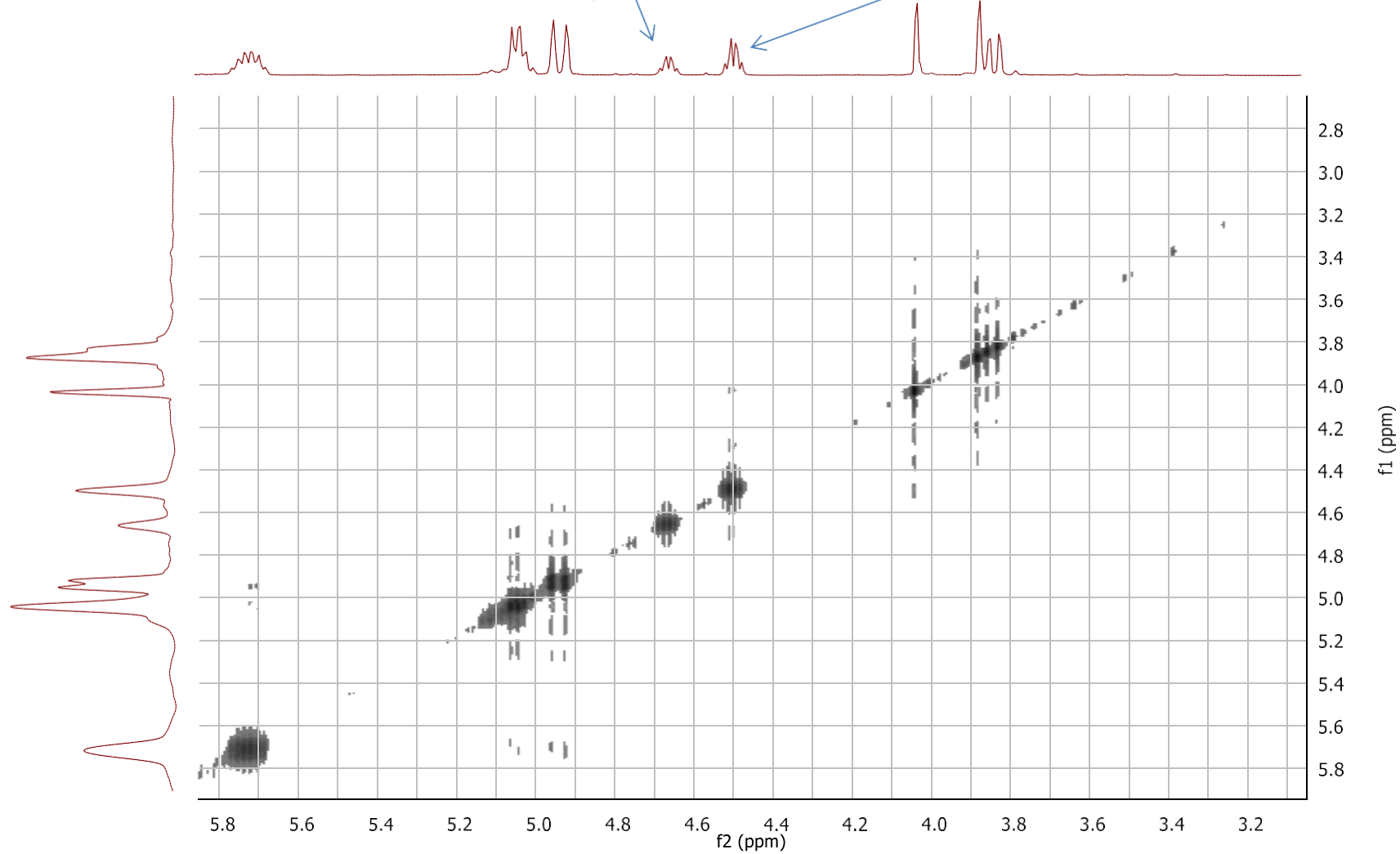
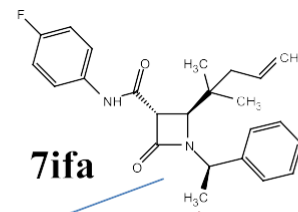
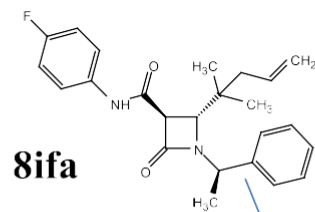
S-61











General procedure for conformational analysis.

Hyper Chem 8.0.8 software was used. Geometry optimization of each molecule was carried out with Molecular Mechanic MM+ method, Polak-Ribiere algorithm, RMS gradient of 0.018 kcal/mol.

Conformational search was performed for six torsion angles ,RMS gradient of 0.018 kcal/mol and maximum cycles 1000. Torsion angles numbers was assigned as depicted on Figure 1.

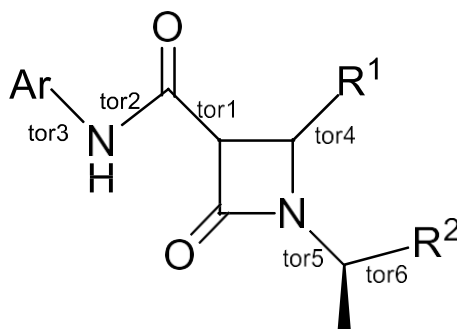


Figure 1. Torsion angles numbering in conformational analysis.

Conformational search results for **7aea**

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor4	tor5	tor6
1	26.6774	9.48157E-03	42	52	156.6508	172.3626	-7.2097	148.1588	-61.1545	179.185
2	26.74062	9.817086E-03	31	36	156.3806	172.4537	171.7998	-135.5095	65.56019	-60.2157
3	26.75458	9.906839E-03	7	36	159.4245	-179.6766	0.560353	147.9397	-61.19976	-63.51108
4	26.79822	9.794713E-03	7	37	158.7057	178.128	-1.691359	-132.9361	-53.46858	-60.22661
5	26.88153	9.999935E-03	1	4	160.1148	-174.5899	5.6526	-135.0393	65.39281	61.06177
6	27.18455	9.997828E-03	2	5	155.6382	170.3581	-8.928063	-168.3579	65.17762	57.17505
7	27.41239	9.992455E-03	34	39	157.6019	172.7519	172.2029	20.48248	178.5599	178.7669
8	27.47007	9.999797E-03	8	23	159.6974	178.9266	-0.7301308	20.95338	178.4937	-64.1447
9	27.52279	9.998096E-03	3	7	159.5786	-176.1258	-175.3407	21.78852	178.9033	56.22713
10	28.20886	9.776277E-03	2	12	92.96881	171.1231	171.46	148.6499	-61.23859	-64.00205
11	28.32037	9.927281E-03	7	38	76.78335	177.6452	177.7441	-136.0027	-172.3964	61.04264
12	28.34472	8.776924E-03	16	38	77.5271	176.5019	176.3071	148.9407	-61.26017	178.6422
13	28.38355	9.991606E-03	9	44	74.57779	175.2577	174.3142	-131.9243	66.07875	-178.3492
14	28.39677	9.990401E-03	10	27	74.16315	174.992	174.1265	148.0929	177.7572	57.09462
15	28.44878	9.984082E-03	3	14	72.40412	174.6177	173.3112	148.6979	-61.32403	178.7138
16	28.46011	9.984234E-03	3	23	69.94359	174.7989	-6.11855	-134.3482	65.71863	-177.793
17	28.95102	9.988599E-03	4	14	97.5357	171.7327	172.3633	20.75629	178.5785	178.4246
18	29.02431	9.251391E-03	1	35	74.69635	175.6749	-4.481948	164.6104	-57.78164	-61.11464
19	29.14756	9.994902E-03	5	27	72.30705	175.0341	173.9477	22.24369	56.80833	-64.99423
20	29.35271	9.637861E-03	17	32	-76.82364	171.6415	173.0087	147.513	57.78163	178.3344
21	29.46578	9.456058E-03	25	42	-76.59778	171.3002	-6.38053	-137.3806	-172.4891	-59.93543
22	29.83521	9.617411E-03	33	47	-76.05836	171.4507	-6.134692	21.19304	178.5355	-64.61086
23	29.89901	9.16333E-03	2	21	-75.64195	178.7685	-178.3852	19.74634	178.6402	-63.99287
24	32.07793	9.719712E-03	3	2	-76.06666	169.7994	170.9737	-48.99151	-58.29214	-174.4473

Conformational search results for **8aea**

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor4	tor5	tor6
1	26.48157	1.474713E-02	74	43	-153.3343	-171.6522	-171.1082	123.3532	60.85748	-68.29374
2	26.5406	0.0148805	12	42	-157.6319	-177.6671	-177.6448	121.7857	61.17817	-67.68164
3	26.59499	1.237457E-02	18	38	-158.3242	177.9954	177.4538	122.5916	-179.2263	170.7057
4	26.64628	1.212035E-02	9	24	-158.9469	174.3386	-5.957538	121.2172	61.20856	-67.82074
5	26.75553	1.479925E-02	1	32	-161.6516	172.1984	-8.40484	122.0973	-57.87043	-67.4554
6	27.21689	1.491416E-02	4	42	-152.108	15.03432	18.48869	119.8506	-178.7224	50.07702

7	27.47103	0.0135412	5	22	-103.2536	-169.7219	8.861263	126.1155	180	170.5504
8	27.547	1.118753E-02	5	25	-97.05622	-170.6185	-170.6469	124.8985	60.48125	-67.62372
9	27.61605	1.445397E-02	6	21	-92.00495	-171.853	7.498827	126.1711	-58.56585	170.718
10	27.728	1.334901E-02	5	33	-84.11771	-172.3955	7.624637	124.4991	-179.7227	50.40003
11	27.7892	1.358227E-02	5	32	-79.33428	-174.4434	-173.4137	126.9829	-58.96471	49.83916
12	27.8455	1.279488E-02	8	38	-75.40861	-174.0482	-172.7849	126.6389	179.7043	50.01344
13	27.90747	1.372305E-02	55	31	-154.5035	-171.9813	-171.3814	-8.78905	-59.98797	172.4385
14	27.91532	1.274758E-02	4	34	-73.00935	-173.1218	7.825695	125.0631	179.9591	171.313
15	27.97459	1.447899E-02	9	40	-158.6162	-177.7782	1.757233	-9.097468	-59.99435	-66.52556
16	27.98134	1.439594E-02	4	32	-68.49776	-176.1829	5.651716	125.3539	-58.75312	171.3086
17	28.02724	1.457512E-02	7	21	-158.7285	177.1572	-2.99618	-9.11042	-59.79961	-66.78105
18	28.04652	0.0141351	5	21	-63.19285	-174.8139	-172.2998	125.9481	-58.68045	50.50448
19	28.08983	1.498306E-02	1	2	-160.275	173.7231	172.7775	-9.526678	-178.9299	-66.86855
20	28.11046	1.362485E-02	11	28	-153.5284	-171.8535	7.532113	179.6949	-174.5975	49.75729
21	28.1173	1.494108E-02	7	14	-56.03618	-176.1366	-173.027	129.6307	-59.41257	49.52353
22	28.16408	1.474403E-02	1	7	-157.238	-176.0386	-175.8141	-171.1326	-55.1187	-64.68158
23	28.22537	1.470204E-02	3	23	-157.7277	179.2345	-1.270796	-169.3695	-55.25177	175.9161
24	28.29665	1.499827E-02	2	1	-158.3119	175.3179	174.3232	-173.7613	-55.48678	53.96129
25	28.62882	1.496043E-02	1	28	-160.7308	-22.60775	152.557	126.2596	-179.992	48.95842
26	28.77879	1.408348E-02	56	38	77.28489	-172.4471	-173.7269	122.7613	-179.3717	170.8832
27	28.83223	1.497874E-02	5	27	76.7383	-179.528	-1.924907	123.4176	-179.4972	49.6355
28	28.89348	1.413241E-02	2	20	75.15991	175.7275	-7.052131	122.5147	-57.99866	170.6284
29	29.02749	1.498646E-02	1	1	-91.29049	-172.797	6.480034	-168.7095	64.14549	175.4016
30	29.99666	1.483251E-02	3	23	-161.8289	-22.60562	152.6214	-8.335053	-60.04404	51.1393
31	30.22957	1.436092E-02	12	30	-161.0924	-22.26567	152.7258	180	63.55688	170.5731
32	30.25495	1.357437E-02	9	31	-163.9898	-23.01218	-23.91334	-165.544	-55.00305	54.89637
33	30.33349	1.413607E-02	39	39	75.43237	-172.1009	5.753701	-9.57385	-179.3644	-66.19666
34	30.37793	1.492365E-02	2	27	-162.5413	177.7748	-2.78247	60.37283	-52.17666	168.0687
35	30.45441	1.499801E-02	4	28	-155.1037	-170.2448	-169.8676	-51.6276	-58.46199	172.18
36	30.50331	1.489517E-02	27	38	76.59966	-171.7765	5.907812	-168.9316	-174.4782	-63.79157
37	30.51163	1.499498E-02	7	29	-155.187	-170.2191	-169.7935	-51.67284	-57.96837	53.23834
38	30.55365	1.369309E-02	3	15	80.98478	-169.3283	8.831336	-167.7958	-55.15173	176.038
39	31.37761	1.476055E-02	2	18	-104.4604	-168.3645	-169.0992	-61.10506	-179.7423	-69.75152
40	31.64972	1.499894E-02	1	1	-92.07926	-170.8424	8.392976	-58.43024	60.55834	170.6068
41	32.43597	1.499874E-02	5	29	-160.6656	-21.7439	152.8238	-50.20895	179.5578	172.0259

Conformational search results for 7cea

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor4	tor5	tor6
1	26.78937	8.374312E-03	15	28	-21.87927	171.9534	-7.647754	-52.08293	148.0379	169.4759
2	26.79094	9.410238E-03	5	18	-21.17158	172.1023	171.4228	65.47101	148.0518	-11.08657
3	26.85249	8.666243E-03	7	7	-21.46646	171.7781	171.0515	-169.2707	-137.1545	35.87733
4	26.85294	8.190913E-03	12	14	-21.70507	172.2395	-7.261101	-169.6895	-135.3487	-144.5825
5	26.88582	9.731682E-03	3	13	-17.78572	-177.7647	2.482826	65.55222	148.3347	170.0094
6	26.9135	8.898837E-03	3	6	-17.43926	-176.3755	-175.6943	-51.86757	148.6543	-10.90792
7	26.93217	9.754093E-03	2	12	-18.4579	-179.5041	0.833309	-48.4279	-134.8373	36.20475
8	26.97777	9.937761E-03	2	14	-17.43277	-176.351	-175.6071	-169.4547	-135.4022	-145.3091
9	27.31529	9.978345E-03	1	4	-20.69099	171.2709	170.6427	-174.0638	-176.9044	-149.8239
10	27.3195	9.996598E-03	1	3	-20.42586	171.8019	-7.541806	65.16623	-177.5013	29.86683
11	27.5198	9.728155E-03	10	18	-21.24407	171.7284	170.9403	63.47579	21.19163	-123.1132
12	27.52485	9.473916E-03	15	19	-21.40505	171.7594	-7.790575	63.49596	20.7447	56.15838
13	27.60749	9.289565E-03	5	12	-17.51866	-179.091	1.153795	63.63382	20.83882	-123.5582
14	27.63402	9.997459E-03	2	8	-17.56797	-176.79	-176.096	63.75278	20.42889	55.63446
15	28.35601	9.998711E-03	3	13	-99.22061	173.606	-5.612742	69.02169	-136.2956	-141.6506
16	28.36868	9.998735E-03	2	1	-95.34752	172.7967	172.7825	-173.6686	149.247	170.322
17	28.40038	9.91234E-03	2	5	-100.2292	173.3435	173.2201	-169.7007	-137.5342	-140.686
18	28.43768	9.786257E-03	2	7	-104.4218	172.9514	-6.799595	-52.42193	148.9818	-11.08504
19	28.46691	9.994233E-03	3	6	-101.1435	-179.5124	-178.4657	-173.9804	148.133	-11.39878
20	28.49304	9.815214E-03	4	17	-111.9005	177.064	-3.468823	69.322	-138.0388	-145.6582
21	28.49684	9.396519E-03	2	4	-109.2412	175.7907	-4.719119	65.03493	149.0025	169.5044
22	28.51016	9.990752E-03	4	12	-109.4813	173.8447	172.6622	68.24955	-132.5201	-150.5483
23	28.53751	9.990449E-03	5	19	-110.0986	174.4977	173.3387	-174.1951	148.6867	169.2452
24	28.57226	9.995603E-03	1	1	-113.4023	174.1025	172.4587	-48.7786	-135.3222	-146.024
25	28.64528	9.998246E-03	1	12	-111.7141	175.3457	-5.685637	-173.3064	-118.0393	-169.5646
26	29.14645	9.869272E-03	1	6	-96.03749	171.9967	171.9669	-176.9378	22.89164	-122.3137
27	29.42511	9.878852E-03	9	20	100.5764	171.3727	-6.280231	-52.25488	147.6629	168.998
28	29.53605	9.772183E-03	15	19	100.5364	170.954	-6.634001	69.62345	-136.0462	-146.1996
29	29.56152	9.87826E-03	2	9	-21.12	170.8994	170.1753	68.4261	-42.50963	9.545157
30	29.56237	9.998986E-03	3	12	-19.94346	172.8119	-6.774982	-48.27028	-45.89364	-171.6316
31	29.57317	9.992905E-03	11	17	100.8743	171.1772	172.4705	-47.81164	-137.5445	-144.8654

32	29.89874	9.241235E-03	16	20	101.6934	172.1043	-5.494503	63.51292	21.14617	-122.6191
33	29.94187	9.996982E-03	10	23	101.7872	170.904	172.16	63.84039	20.40111	-122.8455
34	29.96379	9.955432E-03	4	19	102.6468	179.5239	2.260754	-174.8595	19.37678	-123.4981
35	29.9971	9.998439E-03	3	15	98.76045	170.619	-7.358525	-173.5006	-166.5959	34.12803
36	30.05569	9.973273E-03	1	4	102.8234	-177.2278	-173.7925	-175.1394	20.29379	-122.956
37	32.13937	9.994736E-03	2	10	100.9341	169.3647	-8.205412	-47.7393	-46.0214	-172.2988
38	32.16852	9.974893E-03	1	6	103.6652	178.5592	1.521658	-47.29591	-46.30306	-172.8141

Conformational search results for **8cea**

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor5	tor6
1	27.5415	1.453499E-02	13	16	-152.3587	-169.7459	9.537635	52.30764	52.95576
2	27.55991	1.231766E-02	7	12	-153.106	-171.0471	-170.3883	52.1718	-127.2555
3	27.68413	1.375094E-02	1	1	-157.1163	-179.7414	-0.1368893	50.5628	-127.9767
4	27.69981	1.387016E-02	2	11	-158.2835	174.5553	173.5528	51.1746	-127.5921
5	27.73862	0.0138477	4	5	-158.1362	176.7944	-3.605372	50.82193	-126.8459
6	28.47531	1.439782E-02	1	4	-105.6576	-168.7426	-169.1405	53.00276	-127.0105
7	28.47538	1.499424E-02	1	13	-152.3543	15.21234	-158.4974	49.1336	-127.8533
8	28.47773	1.497691E-02	1	16	-151.66	14.65848	18.35937	49.32117	52.18017
9	28.74483	1.457752E-02	2	5	-85.68981	-174.1509	-173.5288	55.1685	53.44684
10	28.97528	1.178994E-02	6	9	-153.113	-169.8796	9.34324	-91.09013	120.9285
11	28.99408	1.358455E-02	5	15	-153.801	-171.2073	-170.4789	-90.87975	120.7986
12	29.03242	1.450988E-02	2	11	-59.60977	-173.8345	-170.7021	53.3388	-126.6951
13	29.12469	1.448856E-02	1	2	-157.7319	175.3085	174.3159	-91.732	-61.10615
14	29.15551	1.485377E-02	1	2	-57.28622	-175.828	6.888362	56.29745	-123.7137
15	29.17055	1.257122E-02	2	4	-154.0452	-171.0078	8.43088	104.7032	106.0454
16	29.17434	1.474384E-02	1	2	-158.2732	176.3179	-4.178306	-91.4254	-60.37132
17	29.20028	1.139274E-02	2	15	-155.6896	-173.052	-172.5916	106.4868	107.6387
18	29.27889	1.499866E-02	1	10	-160.892	170.9407	-9.133334	-91.72961	119.8393
19	29.30255	1.360304E-02	1	3	-157.6319	-177.9397	1.551654	105.6795	107.2084
20	29.33069	1.498953E-02	1	3	-156.3646	176.7638	176.1108	102.243	-74.33907
21	29.37053	0.013078	1	2	-157.7013	178.0674	-2.466933	100.4664	-74.07626
22	29.39942	1.483425E-02	1	1	-159.9435	172.6388	171.5986	104.0899	107.7002
23	29.84439	1.450747E-02	8	6	76.91482	-171.8975	-172.9385	52.36226	-128.3142
24	29.91407	1.260545E-02	3	9	76.71909	176.7163	173.533	51.81465	52.03427
25	30.0352	1.415651E-02	4	9	76.80889	-170.0771	7.779036	52.97561	52.4943
26	30.12903	1.356062E-02	2	12	76.77184	176.0031	-6.296088	51.81184	51.90255
27	30.89655	1.489329E-02	1	6	-160.1256	-22.69027	-24.24576	-90.24226	120.0925
28	31.14661	1.489772E-02	2	3	-169.4253	-23.13148	-23.28936	107.0371	105.9049
29	31.41956	1.375153E-02	2	6	76.11193	-169.8365	-170.7363	-90.10706	121.465
30	31.53571	1.436788E-02	1	1	-166.6818	-22.53279	153.1744	110.4261	107.962
31	31.57124	1.384722E-02	4	15	75.91656	-171.6953	-172.7798	99.46987	-76.32856
32	31.59942	1.250988E-02	6	9	75.41615	-171.1745	6.77748	-90.60388	120.7986
33	31.60075	1.312833E-02	2	6	79.60197	-170.0205	-170.7359	110.611	108.5165
34	31.67557	0.0145662	1	11	-152.0765	-168.7482	-168.4384	175.1612	49.77555
35	31.75165	1.354283E-02	5	10	77.20426	-169.8305	7.882415	96.37689	100.3363
36	32.75566	1.499932E-02	1	3	-87.95517	-170.3647	-169.7265	-174.7317	52.56241

Conformational search results for **8ifa**

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor4	tor5	tor6
1	28.40053	1.634177E-02	6	3	156.7833	5.790531	171.5553	56.19939	31.57976	-126.9957
2	28.40083	1.365991E-02	4	4	156.1102	6.280001	-7.920145	56.24681	31.65405	-126.9893
3	28.40323	1.762184E-02	5	6	157.019	5.823031	-6.954693	56.40785	32.12003	54.20952
4	28.40546	1.757457E-02	2	6	157.6036	5.236295	172.3022	56.19358	31.53534	53.80447
5	28.49239	1.531712E-02	1	1	158.659	0.7908115	1.487729	55.77293	32.37376	53.66838
6	28.50113	1.651094E-02	1	1	158.8408	0.4209228	-177.936	56.12407	31.402	54.09183
7	28.53376	1.673848E-02	1	6	159.1638	-0.9470868	4.837696	56.24484	32.19018	-126.9005
8	29.02428	1.799784E-02	3	3	152.8536	-177.1439	159.4156	56.40143	33.64444	53.68654
9	29.02433	0.0173687	1	4	152.0114	-178.0699	-17.36806	55.10759	34.11679	53.46039
10	29.0367	1.799451E-02	1	3	151.8078	-178.1268	160.2803	56.21541	33.30761	-127.1327
11	29.04269	1.799524E-02	3	5	152.845	-176.7893	-17.96522	56.5394	35.13819	-125.3015
12	29.04471	1.541619E-02	7	8	156.3377	6.154199	-7.655082	61.25326	107.7882	-81.60061
13	29.04508	1.264465E-02	5	6	156.1981	6.458678	171.0728	61.16474	107.9994	98.23128
14	29.04538	1.672328E-02	5	4	156.3408	5.559876	171.3304	61.32133	105.9909	-80.93315
15	29.04577	1.774061E-02	4	5	155.7946	6.685036	-8.112634	61.23678	106.9661	98.03264
16	29.1038	1.714838E-02	7	7	156.7752	6.00934	171.2222	-179.3435	30.87482	54.494
17	29.10386	1.571605E-02	4	6	156.1157	6.183698	-7.963732	-179.683	30.73583	54.28759

18	29.10445	1.587626E-02	3	8	156.1223	6.355135	-7.905728	-179.8834	30.61534	-126.8028
19	29.11161	1.645877E-02	2	4	158.1387	4.635824	172.4896	-179.3321	30.52621	-126.4595
20	29.1334	1.557007E-02	2	2	158.5635	1.286974	-179.4878	60.92095	109.0181	-83.23981
21	29.15056	1.657443E-02	1	6	158.3671	0.6380782	2.225692	61.05144	110.8092	-82.23176
22	29.18722	0.0177615	1	6	159.5192	1.787161	179.8076	-179.7372	31.05345	-126.2843
23	29.20269	1.713668E-02	2	3	159.2972	9.576151E-02	1.8304	180	30.76529	53.88693
24	29.20608	1.780775E-02	1	3	159.3929	-0.7500752	-175.1782	60.60953	112.7465	-86.85418
25	29.2136	0.01486	3	4	159.0372	4.347525E-02	2.757317	-179.7051	31.40005	-126.3626
26	29.23042	1.788596E-02	2	5	158.0694	4.792318	172.256	56.87192	66.19691	90.35054
27	29.24157	1.397938E-02	3	4	159.6843	-1.370538	-174.5251	-179.4875	31.71535	-126.1066
28	29.24951	1.785973E-02	1	3	158.8684	3.678482	-5.443117	56.14854	67.53471	-88.1788
29	29.25811	1.776498E-02	2	6	156.6248	5.967923	-7.48866	-64.03429	31.31902	53.54475
30	29.26006	1.488761E-02	2	8	155.2033	6.080882	170.3549	-64.61476	30.6591	-128.249
31	29.26237	1.754716E-02	5	3	155.8363	6.438819	-8.394142	-63.69559	31.35805	-126.9361
32	29.26239	1.547877E-02	1	1	157.4269	5.210632	172.1716	-64.07931	31.25794	53.32757
33	29.26406	1.636459E-02	1	2	159.8873	-1.825697	5.730252	179.9218	30.87093	53.88559
34	29.30347	0.0149994	12	5	156.7724	5.756012	-7.641913	-176.2765	107.7406	98.45902
35	29.30449	1.502601E-02	4	4	156.414	6.387666	171.241	-176.4419	108.3017	99.21975
36	29.30494	0.0179584	3	4	156.3985	6.259266	-7.742253	-176.5738	108.2278	-80.82405
37	29.3063	1.622433E-02	6	2	157.4901	5.418521	171.8158	-176.2398	107.2623	-80.08201
38	29.35781	1.518553E-02	1	2	159.1788	0.3465699	1.447658	-63.95212	31.73281	-127.2597
39	29.35968	1.757637E-02	2	3	158.9374	1.039555	-178.4423	-63.26973	31.89583	-127.0049
40	29.36466	1.795262E-02	1	1	158.6911	0.3521572	-175.2155	55.28359	69.16814	94.41625
41	29.38267	1.349922E-02	1	3	160.1407	-2.166228	5.104953	55.97499	67.47606	91.44704
42	29.38676	0.0140019	5	2	156.2597	6.368314	171.3924	-60.16483	108.6663	-80.89215
43	29.38783	1.417211E-02	8	7	156.9774	5.458119	171.9588	-60.11382	108.1147	99.194
44	29.38825	1.616396E-02	1	2	156.8497	5.806881	-7.272994	-60.08005	108.6736	-80.08454
45	29.38896	1.683594E-02	3	7	156.6773	5.942432	-7.522513	-60.32632	109.2654	97.83883
46	29.39669	1.658097E-02	1	2	159.4963	-1.684721	4.77382	-63.99343	31.66748	53.76988
47	29.40965	1.714308E-02	1	1	160.0196	-1.699882	-173.6505	-64.01072	32.41508	54.34672
48	29.41904	1.617167E-02	1	3	159.6082	-2.543975	-173.2243	-63.91632	31.16959	-126.9895
49	29.46418	1.712181E-02	1	2	159.8237	-2.058811	-173.8119	-177.17	109.9603	-81.4228
50	29.47083	1.397984E-02	1	1	160.4743	-2.871635	6.541612	56.21365	76.72037	94.98053
51	29.47105	1.717047E-02	1	5	159.948	-2.791024	4.703169	-176.0529	108.4086	101.859
52	29.47258	1.611253E-02	1	4	160.0427	-2.577693	-173.5234	55.14421	79.0672	-82.6937
53	29.50506	1.650899E-02	2	2	159.264	8.431191E-02	2.971946	-60.41657	110.2377	97.08875
54	29.52046	1.735201E-02	1	4	158.6694	-1.69101	-174.5772	-60.38285	110.0403	-81.92641
55	29.53132	0.0176709	1	4	159.712	-0.8187115	4.689938	-60.50144	110.7965	-83.56069
56	29.56491	1.743068E-02	5	2	157.12	5.207167	171.6415	55.81497	-93.42071	-57.82902
57	29.56496	0.0158374	3	4	156.8658	6.027433	-7.845531	56.25406	-94.21622	-58.20797
58	29.56639	0.0137619	3	4	157.0308	6.087657	-7.411964	56.082	-93.63063	122.2541
59	29.56686	1.588811E-02	5	4	156.5109	6.168059	170.78	56.39389	-95.02752	121.7454
60	29.63185	1.424037E-02	2	3	159.2251	1.424859	-0.6480605	56.13141	-94.05295	121.9095
61	29.64363	1.796438E-02	1	3	136.3465	139.1669	17.43116	55.69211	32.25296	-127.2102
62	29.66729	1.487825E-02	2	5	159.4889	-0.4485746	2.761789	56.30859	-94.21626	-58.54529
63	29.66775	1.700823E-02	1	6	159.3275	0.1438496	-176.8233	56.00852	-92.7463	122.5118
64	29.68706	1.750566E-02	1	1	160.1368	-1.354442	-176.1485	55.99562	-93.11002	-58.09492
65	29.6925	1.799804E-02	2	5	153.7387	-176.4429	158.922	61.05698	108.5227	95.78657
66	29.71631	1.799223E-02	2	3	153.1357	-175.9622	-18.1006	60.20197	113.0807	94.40051
67	29.74935	1.747928E-02	1	2	160.2278	-3.307103	7.994422	56.37064	-93.68449	-57.95055
68	29.77902	1.696529E-02	3	2	153.3733	-176.4864	-18.26453	-179.6774	34.00404	-125.2164
69	29.79208	0.0177306	1	6	153.937	-175.9902	158.2173	-179.473	31.93045	55.02614
70	29.7972	1.550563E-02	1	4	156.7121	5.385058	170.3377	177.6585	73.86452	95.44005
71	29.80141	1.777757E-02	1	7	152.7117	-177.6553	159.7062	-179.5123	33.95754	-124.6489
72	29.84102	1.668335E-02	1	2	157.5694	4.461077	171.9784	178.5178	64.52217	-90.01425
73	29.84483	1.049251E-02	3	3	157.0158	5.90981	171.0821	178.9407	-94.67532	121.9724
74	29.84555	0.0111487	5	4	156.8504	5.985912	-8.162471	178.9211	-94.36163	122.3556
75	29.84582	1.203359E-02	3	5	156.9629	5.766761	-8.004572	178.3942	-93.4476	-57.84519
76	29.84711	1.547663E-02	5	6	156.7953	6.31181	170.9632	179.108	-94.926	-58.5598
77	29.86419	1.784476E-02	3	4	152.5264	-177.4873	159.6735	-64.04335	34.1913	54.48883
78	29.86683	1.792106E-02	1	4	152.9085	-177.5323	159.519	59.50542	121.3186	82.50075
79	29.87252	1.799938E-02	1	5	154.1843	-175.8596	-18.66054	-64.03313	34.29198	54.90136
80	29.88232	1.797845E-02	1	2	152.8187	-176.7423	-17.56565	-64.44838	33.18761	-128.0458
81	29.88805	1.798048E-02	1	3	152.0496	-177.8304	-16.60386	59.14795	121.5428	81.61184
82	29.88864	1.711556E-02	1	4	153.6767	-176.1575	159.1255	-64.10058	33.88466	-126.7011
83	29.89916	1.672763E-02	1	3	154.1974	-176.1754	158.797	58.97903	121.6793	-99.88619
84	29.915	9.547861E-03	2	16	87.67732	3.437638	-5.314116	55.65866	32.61871	53.91419
85	29.92665	1.482931E-02	2	8	158.7336	0.7315075	0.556861	178.1473	-92.38982	122.3319
86	29.94328	1.709812E-02	1	3	159.2047	-0.5588589	-178.0662	178.648	-93.88275	121.962
87	29.94676	1.587673E-02	1	2	153.3212	-176.6801	159.5071	58.34384	124.0881	77.04956
88	29.95191	1.713131E-02	2	3	158.8483	-0.6209495	-175.9815	178.8224	-93.97596	-57.48419
89	29.96854	1.740801E-02	2	4	159.3524	-0.852199	4.451366	178.5533	-93.46501	-58.16581

90	29.96949	1.798765E-02	1	2	82.19793	2.539605	175.5026	56.03334	33.12169	53.93934
91	29.97435	1.797636E-02	2	3	152.2071	-178.2883	159.6687	-60.26219	109.1948	-78.79882
92	29.98741	1.682123E-02	1	2	80.58904	3.554628	-5.104817	55.6931	32.52152	54.04659
93	29.99002	1.436609E-02	2	2	81.10613	3.596677	-5.69546	56.21244	33.62818	-126.3015
94	29.99422	1.799071E-02	1	1	153.6927	-175.9834	-18.38572	-175.9178	108.0767	-80.55052
95	29.99645	1.604407E-02	2	1	153.3207	-176.7495	159.2731	-176.9431	111.7108	95.87276
96	30.00732	1.461351E-02	6	4	157.335	5.492828	-7.146306	-64.72886	-94.16212	-57.68915
97	30.00748	1.766427E-02	3	2	156.9747	5.903614	170.8143	-64.77334	-93.87281	123.0247
98	30.00763	1.491667E-02	5	6	156.972	5.580804	170.8386	-64.74968	-93.90775	-57.41861
99	30.00833	1.309534E-02	7	7	157.2587	5.78486	-7.3663	-64.6308	-94.34716	122.6487
100	30.01129	0.017999	1	2	154.565	-175.4979	-18.92067	-60.54838	110.5967	-77.21045
101	30.01184	1.792681E-02	1	7	152.9711	-176.3201	-17.70668	-177.3321	112.72	96.03304
102	30.01362	1.704389E-02	1	3	160.1434	-2.740301	-173.1146	-66.38965	73.98841	99.004
103	30.05567	1.770298E-02	2	4	75.65349	3.479668	175.3046	56.29384	32.28478	53.9971

Conformational search results for 8ifa

Index	Energy	Gradient	Found	Used	tor1	tor2	tor3	tor4	tor5	tor6
1	28.95215	1.587759E-02	3	3	-153.3278	-6.943878	-156.6413	41.77769	-118.9241	51.79061
2	28.9574	0.0174445	2	3	-153.3068	-6.654859	23.08677	-77.62108	-118.6667	-127.7526
3	28.96118	1.476907E-02	1	2	-155.4893	-5.92438	-159.8895	41.47561	-117.308	-127.4504
4	28.98181	1.701482E-02	1	3	-153.34	-6.767879	-157.492	163.1256	-116.8604	-126.6692
5	28.98338	1.544486E-02	1	4	-153.2916	-6.997758	24.28284	163.2084	-116.4262	53.4147
6	29.04563	1.425786E-02	1	2	-157.1931	-2.257428	-173.0171	163.2624	-118.799	52.42677
7	29.05856	1.469751E-02	1	2	-157.4464	-1.187249	1.377488	-77.70427	-119.0623	52.72278
8	29.0726	1.648829E-02	2	3	-157.9764	-0.5375329	179.7478	-77.85095	-118.8893	52.47446
9	29.10807	1.579856E-02	1	2	-158.116	0.5881892	-8.421871	-77.96947	-119.1136	-127.7647
10	29.11387	1.416172E-02	1	1	-158.413	3.508385E-06	174.5043	163.1196	-118.4119	-127.1464
11	29.16994	1.774942E-02	1	1	-158.7351	2.843914	167.2015	162.4987	-116.0578	-124.905
12	29.84452	1.759773E-02	2	4	-155.8409	-5.34966	20.3272	42.98239	107.7681	-60.04861
13	29.84541	1.668951E-02	1	1	-153.5553	-6.786227	24.24913	43.19794	107.9803	121.0982
14	29.84694	1.380397E-02	3	2	-153.4613	-6.707059	-156.921	43.00068	107.284	-60.1962
15	29.84723	1.767858E-02	1	2	-152.8274	-7.088761	-156.2715	43.13248	107.7425	121.2011
16	29.87458	1.798496E-02	1	0	-150.6093	176.7587	36.87699	-76.26524	-121.9861	-128.0315
17	29.87676	1.732657E-02	1	1	-151.5509	175.5461	39.05629	163.8126	-120.486	52.64501
18	29.89025	1.799809E-02	2	1	-151.8109	176.257	-143.9017	41.96373	-120.5826	51.58174
19	29.8966	1.775367E-02	2	4	-151.566	175.9822	-144.0965	-76.6702	-121.1482	-128.3184
20	29.91335	1.490562E-02	1	1	-151.68	175.9436	-144.2969	42.15269	-121.8559	-129.4033
21	29.92488	1.753722E-02	1	4	-150.5602	177.2255	36.03113	-78.06673	-115.6608	-125.9589
22	29.92651	1.619347E-02	1	2	-151.3511	176.0974	37.92615	-77.64381	-117.5985	54.0441
23	29.94085	1.740345E-02	1	0	-152.2031	175.827	39.02193	41.05279	-117.0937	-126.918
24	29.94147	0.0174707	1	4	-151.6201	175.4601	38.43071	41.86499	-120.1123	51.69491
25	29.94415	1.282485E-02	1	1	-98.82121	-6.815213	24.74078	41.52062	-117.4499	51.59409
26	29.95482	1.306449E-02	1	1	-158.8385	-0.7505406	179.2109	43.00884	107.6708	121.0055
27	29.95756	1.648119E-02	1	5	-158.7602	-0.2466472	-2.006629	42.53598	108.1746	120.6221
28	29.96475	1.799792E-02	1	1	-152.7813	174.8946	-141.4545	43.09302	-125.7722	-130.2528
29	30.01927	1.414537E-02	1	1	-95.49584	-7.899864	-155.8026	41.07495	-115.292	-127.7682
30	30.08834	1.244269E-02	1	2	-89.65318	-6.754108	-158.8794	163.6297	-115.4863	-127.1503
31	30.1561	1.757136E-02	1	3	-133.2364	-144.5378	111.4209	164.0264	-119.9435	52.33815
32	30.16339	1.753861E-02	1	2	-133.2584	-143.5933	111.1812	163.8986	-120.5249	-128.8907
33	30.19521	1.794251E-02	1	3	-133.8905	-142.9419	111.6293	42.90807	-123.0719	-130.0774
34	30.28254	1.660021E-02	1	3	-154.8413	-6.336801	-158.3002	163.0454	105.1631	-62.01956
35	30.30855	1.799398E-02	1	2	-70.76062	-5.510014	13.52161	-78.61809	-112.9994	54.20962
36	30.40617	1.556894E-02	1	5	-158.9169	-0.1962875	176.5675	163.0529	105.5945	119.1044
37	30.41036	1.393143E-02	4	3	-153.6207	-6.392489	23.19963	-76.97739	105.8877	-60.13625
38	30.41293	1.769298E-02	1	3	-152.6919	-6.848044	24.92327	-76.75797	106.1593	121.1047
39	30.47089	1.799934E-02	1	2	-62.35533	-8.856627	21.33846	-80.20459	-106.3904	55.46529
40	30.49626	1.797663E-02	1	2	-59.63035	-9.558355	-157.5237	-79.10685	-111.5194	-124.6824
41	30.50289	0.0179586	1	4	-64.86684	-7.947409	-164.3139	40.67366	-112.0926	53.41252
42	30.50482	1.753844E-02	1	2	-58.83365	-8.365673	21.68937	-77.99308	-112.9297	-126.1349
43	30.51672	1.784991E-02	1	2	-59.79896	-8.722457	-159.6371	163.2211	-112.309	-125.4093
44	30.52602	1.708558E-02	1	2	-59.12565	-7.977942	21.10314	-77.98234	-114.942	52.6015
45	30.53394	1.783766E-02	1	1	-57.94368	-9.302152	20.97353	162.2299	-107.9261	57.62466
46	30.54875	1.641494E-02	2	3	-158.4502	0.2882708	174.5674	-77.41045	104.9384	-60.70008
47	30.59083	1.616158E-02	2	1	-59.04359	-8.760232	-158.6739	40.93353	-113.6683	-126.8348
48	30.60872	1.551349E-02	2	2	-58.20761	-8.784025	22.06594	40.51245	-112.7147	52.55179
49	30.61287	1.751903E-02	1	1	-159.7676	1.977187	-14.55518	-77.03038	105.0478	-60.13699
50	30.67858	1.492857E-02	1	3	-152.3917	-7.109617	-156.5376	167.0688	-56.25535	-74.3151
51	30.71387	1.708945E-02	1	4	-153.3326	-6.750988	23.81649	46.60115	-55.47836	-73.89602
52	30.71556	1.601751E-02	1	2	-157.2126	0.369201	173.8752	-73.06988	-54.37993	106.6538

53	30.71594	1.353156E-02	1	4	-152.2333	-7.267317	-156.403	46.85769	-55.08769	-73.23576
54	30.73488	1.634663E-02	2	1	-156.374	-0.5447795	-3.187651	-74.04244	-60.45871	-77.75611
55	31.13113	1.764883E-02	1	5	-151.8766	176.1193	-143.3867	163.9702	104.1332	119.5325
56	31.26998	1.721417E-02	1	3	-164.6815	-171.9369	125.9187	163.5086	-116.1503	53.84466
57	31.30727	1.730391E-02	1	2	-152.5679	175.1773	-141.9043	-76.76748	104.5924	-60.01505
58	31.33338	1.753563E-02	1	4	-62.51769	-7.775559	14.57144	168.0865	-53.45964	-71.80201
59	31.37915	1.791132E-02	1	1	-62.19179	-7.961637	19.80807	168.0256	-52.49342	106.4601
60	31.38303	1.582682E-02	1	2	76.38448	-0.4499925	16.57396	164.6345	-118.6669	-127.7296
61	31.38447	1.338816E-02	1	1	75.88735	-0.8665138	-166.6558	164.4935	-117.5618	-127.5507
62	31.38672	1.649087E-02	1	1	75.72287	-0.8999566	-164.4504	164.3644	-118.2711	51.43096
63	31.40921	1.249119E-02	3	4	76.72588	-1.102191	15.54974	42.42599	-118.1693	-128.3923
64	31.4129	1.688886E-02	4	4	76.90121	-0.3380916	13.17991	42.34563	-118.5027	51.72266
65	31.42089	0.0149767	1	4	78.25867	-2.800851	-160.4988	42.88581	-119.5121	-128.7366
66	31.4479	0.015846	3	4	74.27426	-1.109624	-164.8705	-77.50441	-118.3372	-128.689
67	31.45155	1.000185E-02	3	7	73.61614	-1.134319	14.68126	-77.40698	-117.7593	52.65171
68	31.4661	1.674402E-02	2	4	76.34337	-2.788239	-160.1978	-77.44345	-118.487	52.25378
69	31.48074	1.798202E-02	1	1	-102.118	-8.860269	-153.3507	48.84746	-48.18375	-66.96602
70	31.48276	1.793202E-02	1	3	76.78118	4.228702	-9.29021	42.58553	-120.1788	-129.3767
71	31.4942	1.798957E-02	1	1	-133.375	-143.6172	111.3948	162.753	105.4464	119.2732
72	31.51246	1.797318E-02	1	2	-57.86521	-5.323133	-0.1648273	46.27829	-56.00314	101.5314
73	31.56703	1.745909E-02	1	4	-151.2941	175.7583	-143.7477	-73.42772	-59.22284	-76.15999
74	31.79141	1.798229E-02	1	6	-133.8662	-140.3041	110.8325	48.03444	-50.13245	-70.02833
75	31.79357	1.799996E-02	1	1	-133.2281	-141.5619	-71.05767	47.60262	-54.22327	105.4747
76	31.89924	1.799869E-02	1	3	-161.0261	0.8426896	-3.395808	159.8759	151.9696	-71.28039
77	32.44002	1.764283E-02	2	4	75.36569	-1.330791	-167.3858	43.55048	108.4219	121.2907
78	32.77698	1.751485E-02	1	1	-162.504	3.950493	168.4839	154.4214	177.631	-104.6554
79	32.82455	1.590997E-02	2	2	75.70569	-2.577594	17.15463	164.4017	105.8337	119.5519
80	32.83173	1.628025E-02	3	3	75.09939	-2.319893	-166.1935	164.4819	106.4824	119.8129
81	32.83657	1.636983E-02	2	3	75.56035	-0.5475061	-164.7264	164.3521	106.2027	-61.09446
82	32.85105	1.751235E-02	1	2	77.81706	-4.559357	21.87372	165.3653	105.2147	-60.75892
83	32.92018	1.754016E-02	2	2	-156.8369	-4.173184	-159.4015	-78.40821	64.25287	49.42238
84	32.98724	1.785255E-02	1	2	-168.9386	-173.6113	128.3053	169.9766	-48.71561	-69.82931
85	33.02474	1.797227E-02	1	1	-154.5175	-6.757224	-156.354	-73.81248	68.16607	-131.2119
86	33.04598	1.718693E-02	1	2	-166.5696	-171.9806	127.2872	48.96888	-48.83743	-69.51322
87	33.06064	1.789582E-02	1	1	76.00526	-2.555621	-161.8048	-76.20776	105.0251	-59.8338
88	33.06513	1.786804E-02	1	3	-164.1282	-171.0667	-58.20743	47.31288	-56.05496	104.9022
89	33.08432	0.0174752	2	2	73.16831	0.14036	7.007145	-76.58545	106.3905	-60.16684
90	33.1377	0.0178606	1	3	-158.6605	0.1179367	175.333	-73.41549	69.25844	-131.3237
91	33.23018	0.0179968	1	1	-160.221	1.731182	-10.93455	-73.93602	68.08604	-129.4995
92	33.24153	0.0162923	1	2	76.8625	-1.148121	-164.2393	48.42097	-51.55584	108.9885
93	33.25958	1.652169E-02	1	1	78.9649	-3.025442	20.74261	48.42151	-50.76609	108.6159
94	34.73665	1.739458E-02	1	1	-71.84536	-7.639229	21.42521	161.0003	61.26572	52.36687