

Solid-State Silica Gel-Catalyzed Synthesis of Fluorescent Polysubstituted 1,4- and 1,2-Dihydropyridines

Jovana Aleksić,^{1*} Milovan Stojanović,¹ Jakša Bošković² and Marija Baranac-Stojanović^{2*}

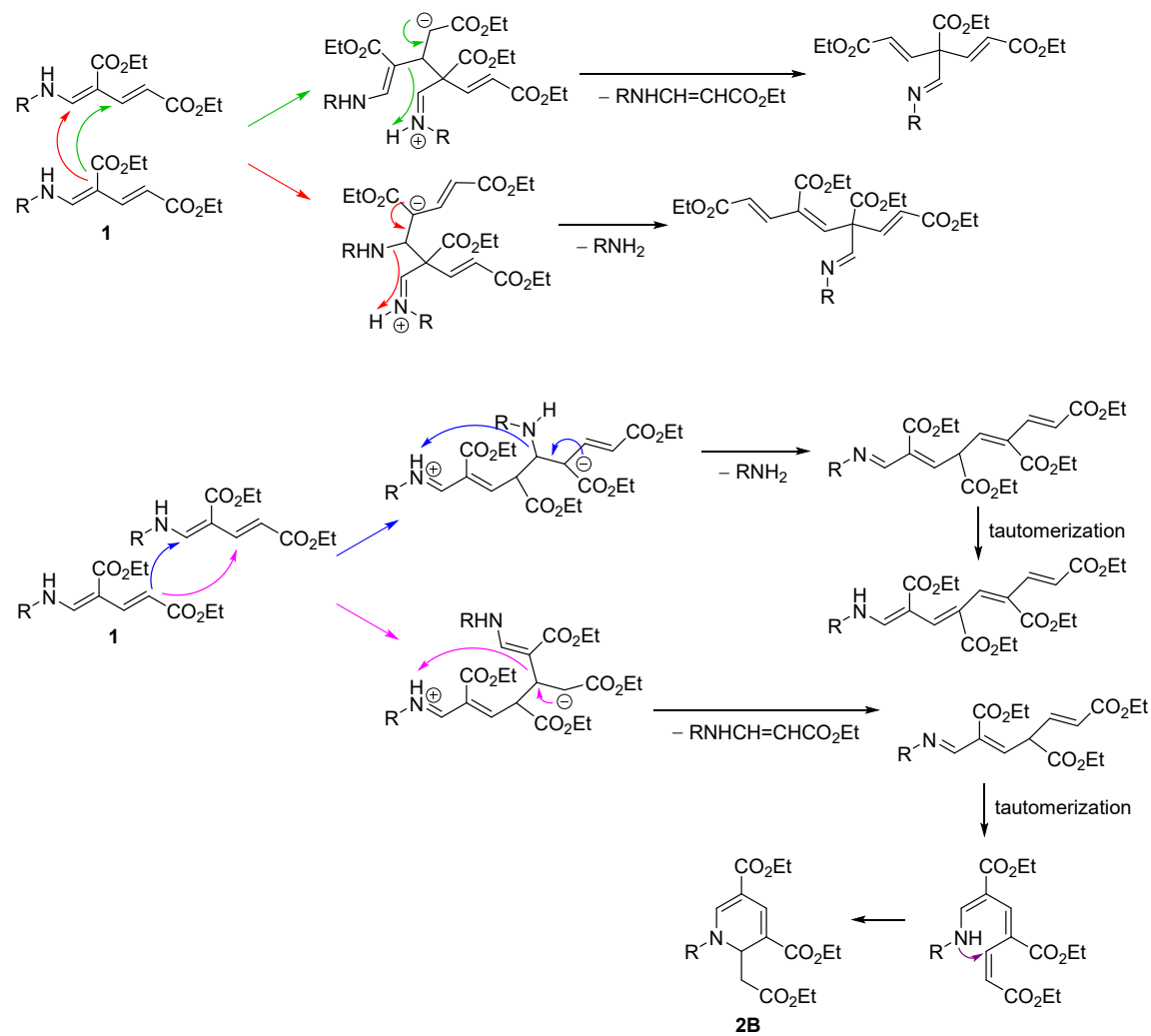
¹ *University of Belgrade - Institute of Chemistry, Technology and Metallurgy - Center for Chemistry, Njegoševa 12, P.O.Box 473, 11000 Belgrade, Serbia*

² *University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, P.O.Box 158, 11000 Belgrade, Serbia*

Supporting Information

Table of Contents

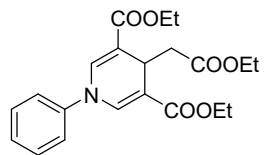
Scheme S1. Possible products that could be obtained by the reaction of two molecules of diene 1	S2
Copies of ¹ H NMR and ¹³ C NMR spectra of synthesized compounds.....	S3
Absolute energies and x, y, z coordinates of optimized structures at the M062X/6-311+G(d,p) level of theory at 373.15 K.....	S88



Scheme S1. Possible products that could be obtained by the reaction of two molecules of diene **1**.

Copies of ^1H NMR and ^{13}C NMR spectra of synthesized compounds

The signal at 155 ppm, which is visible in several ^{13}C NMR spectra, comes from electronic noise.



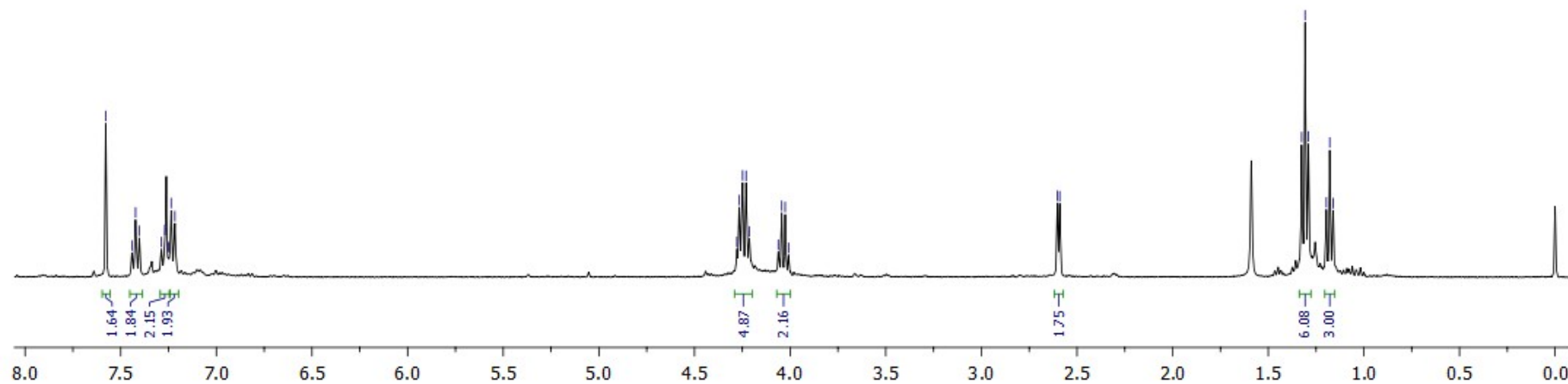
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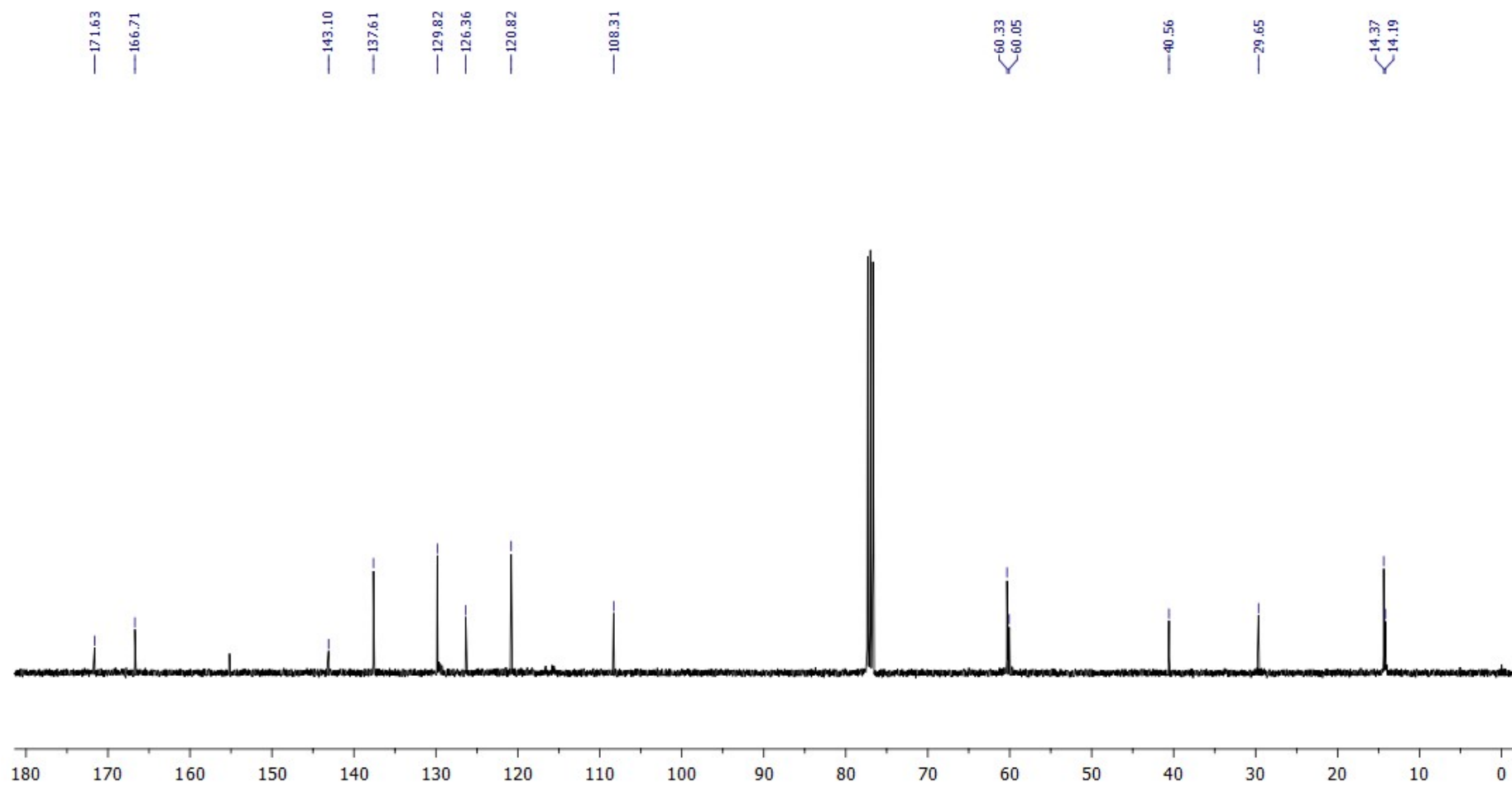
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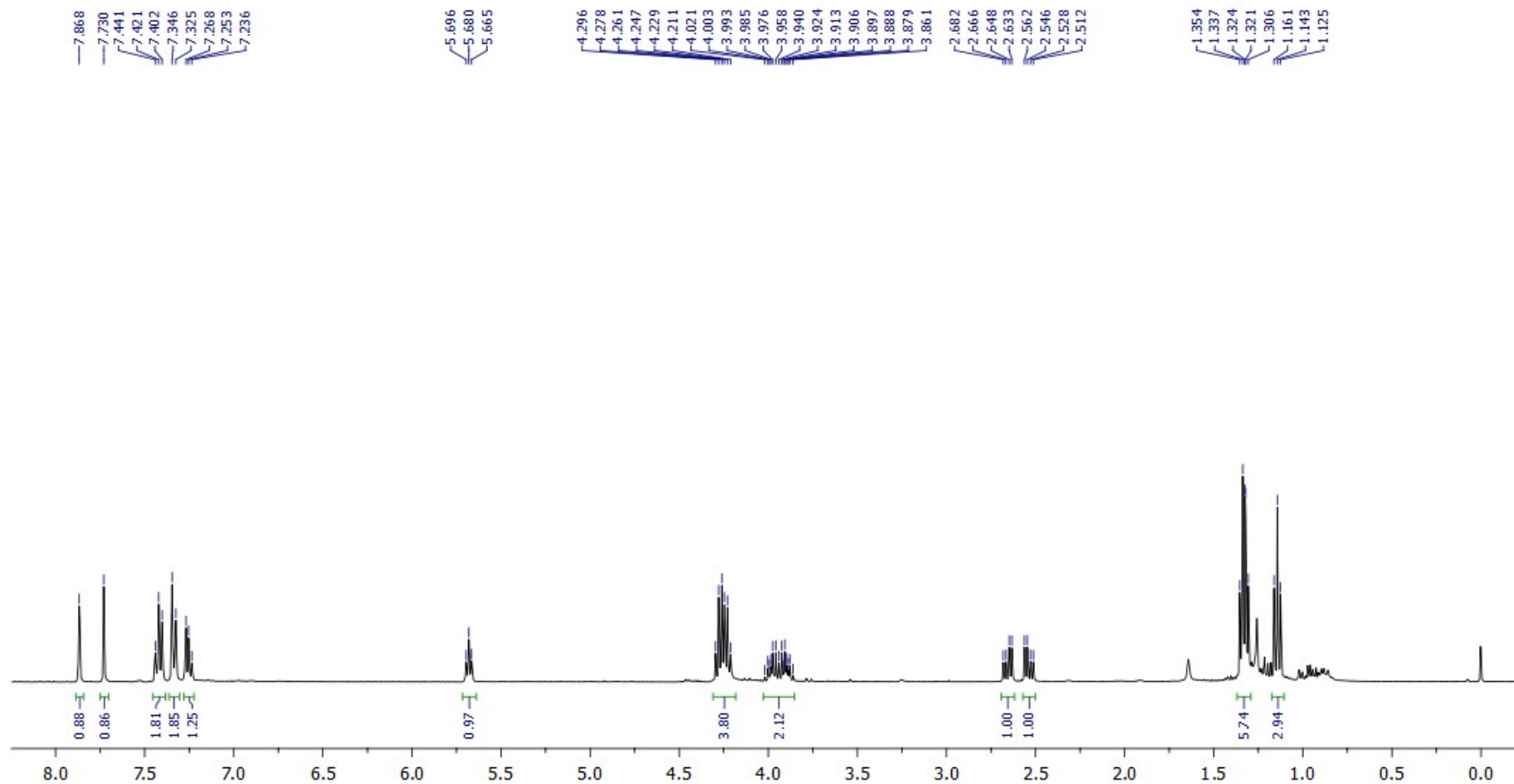
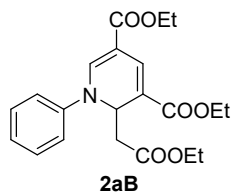
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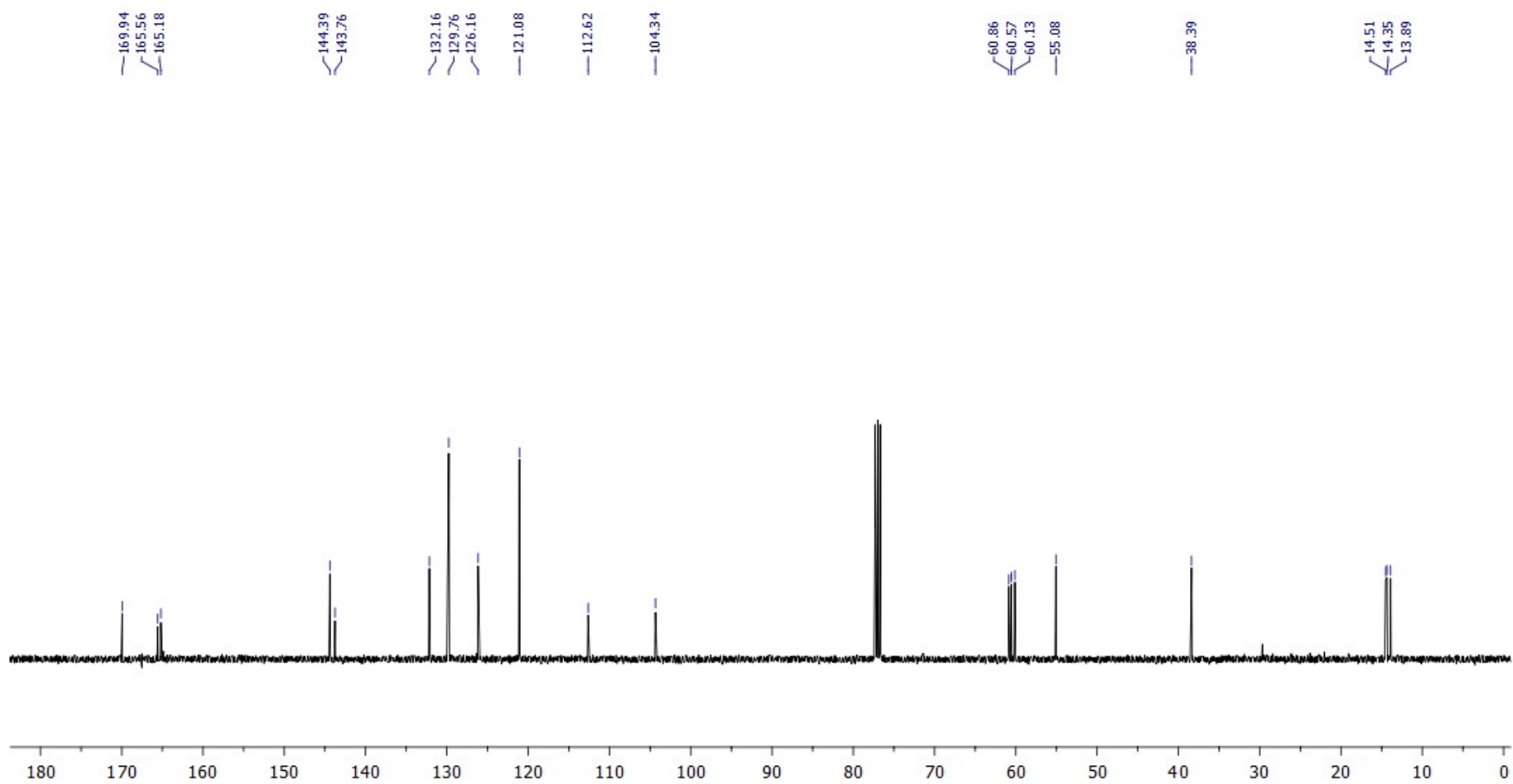
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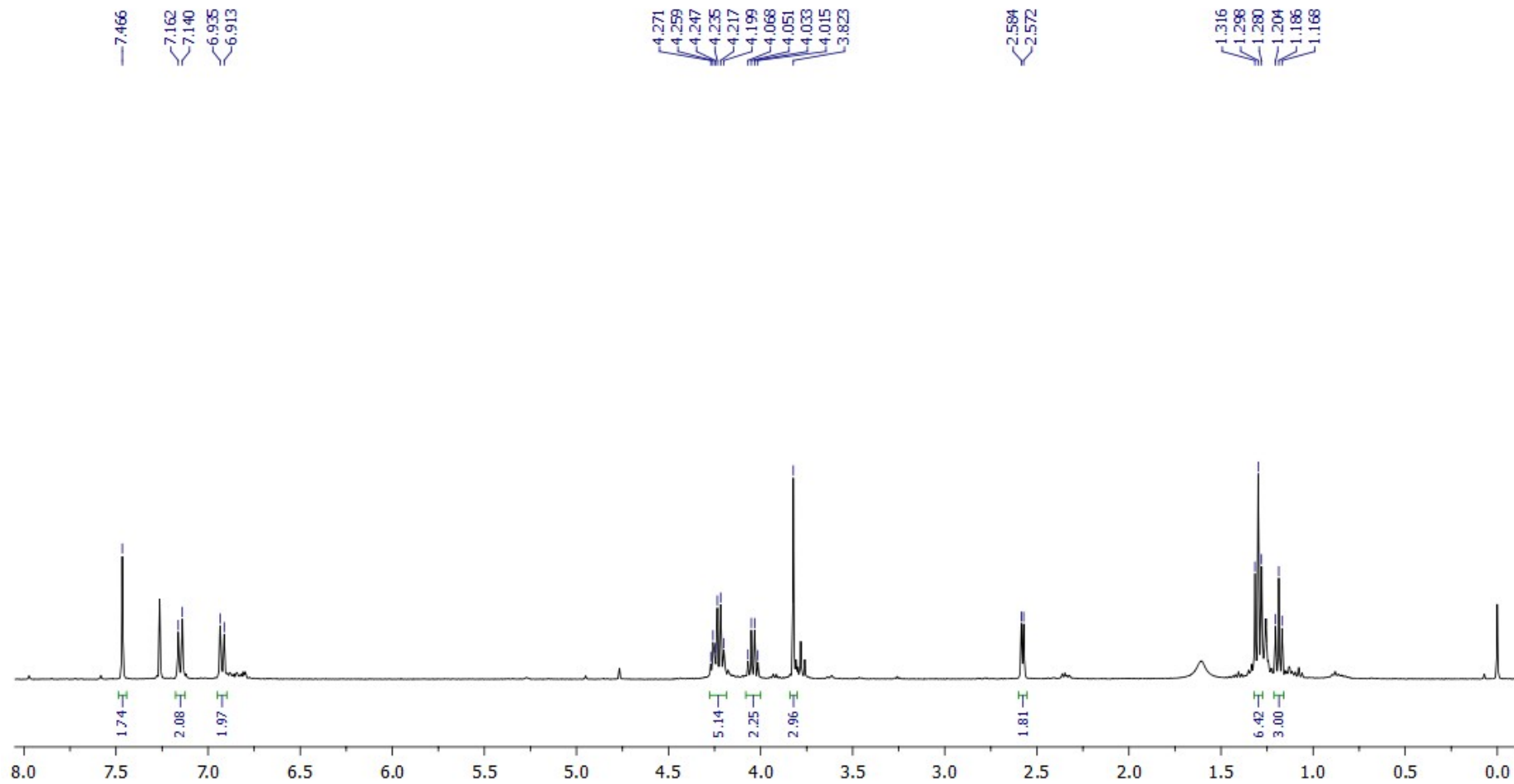
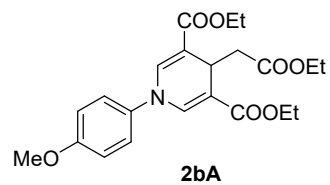
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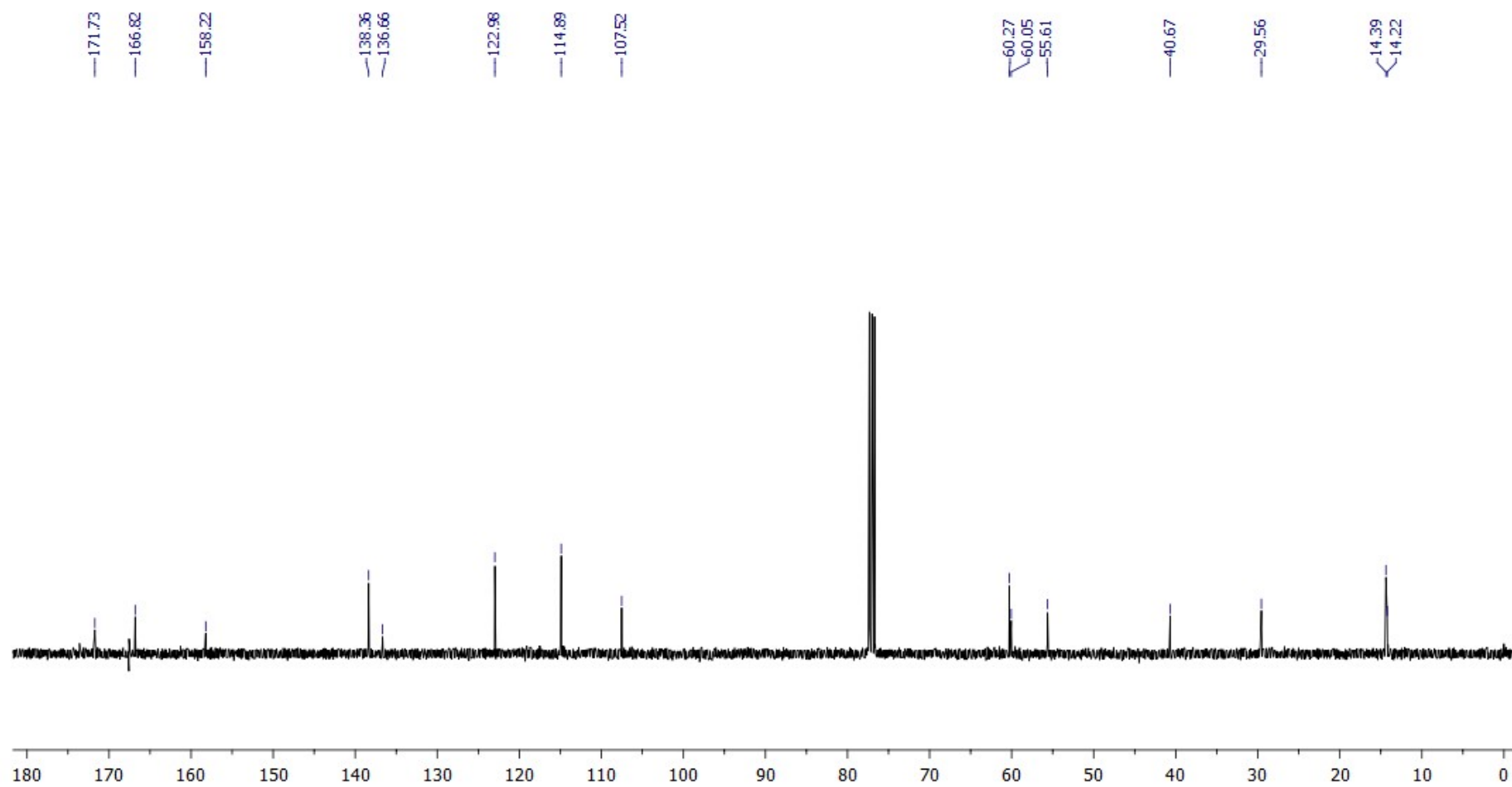
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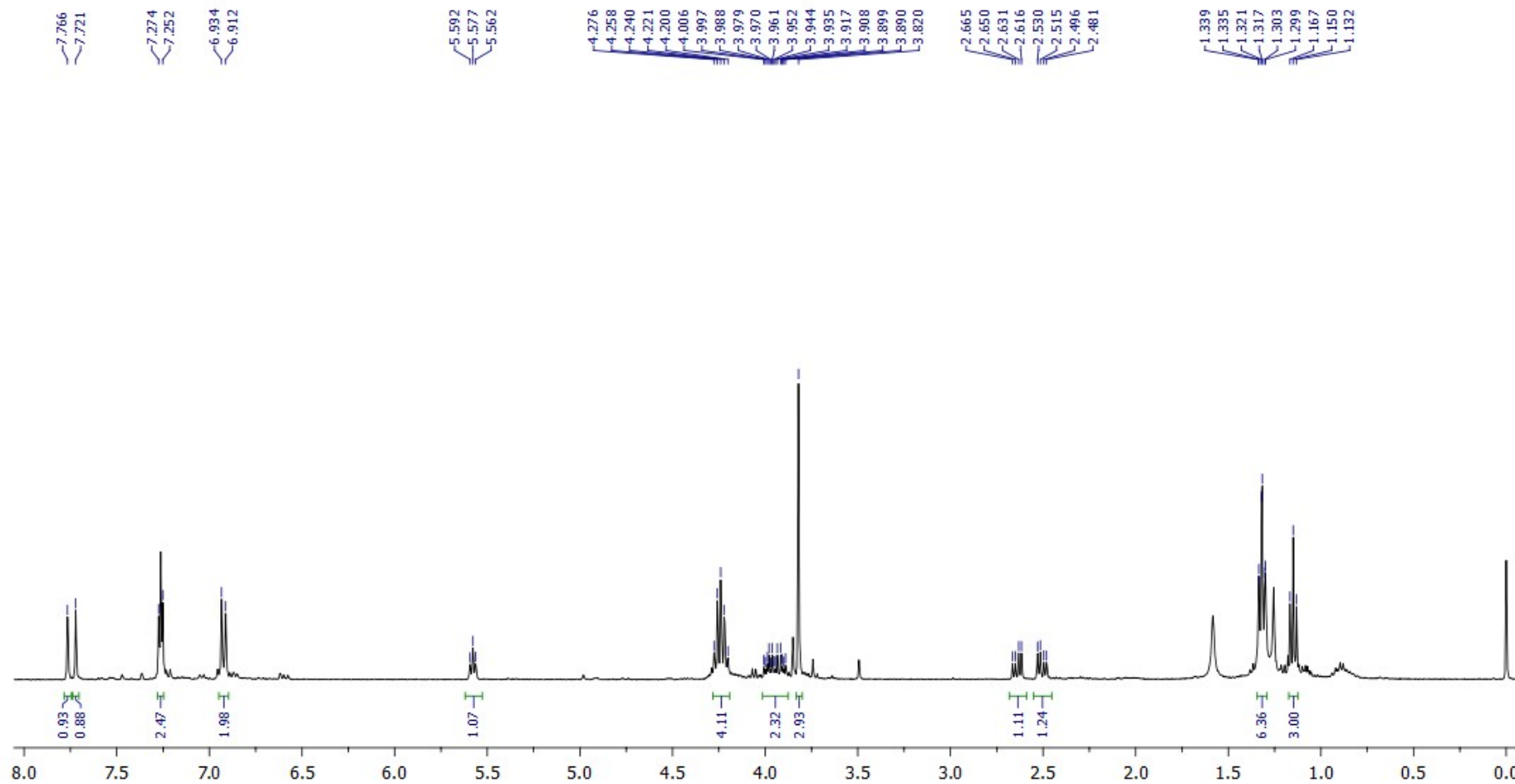
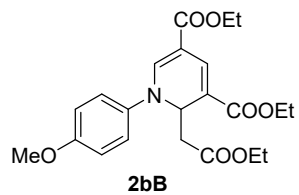
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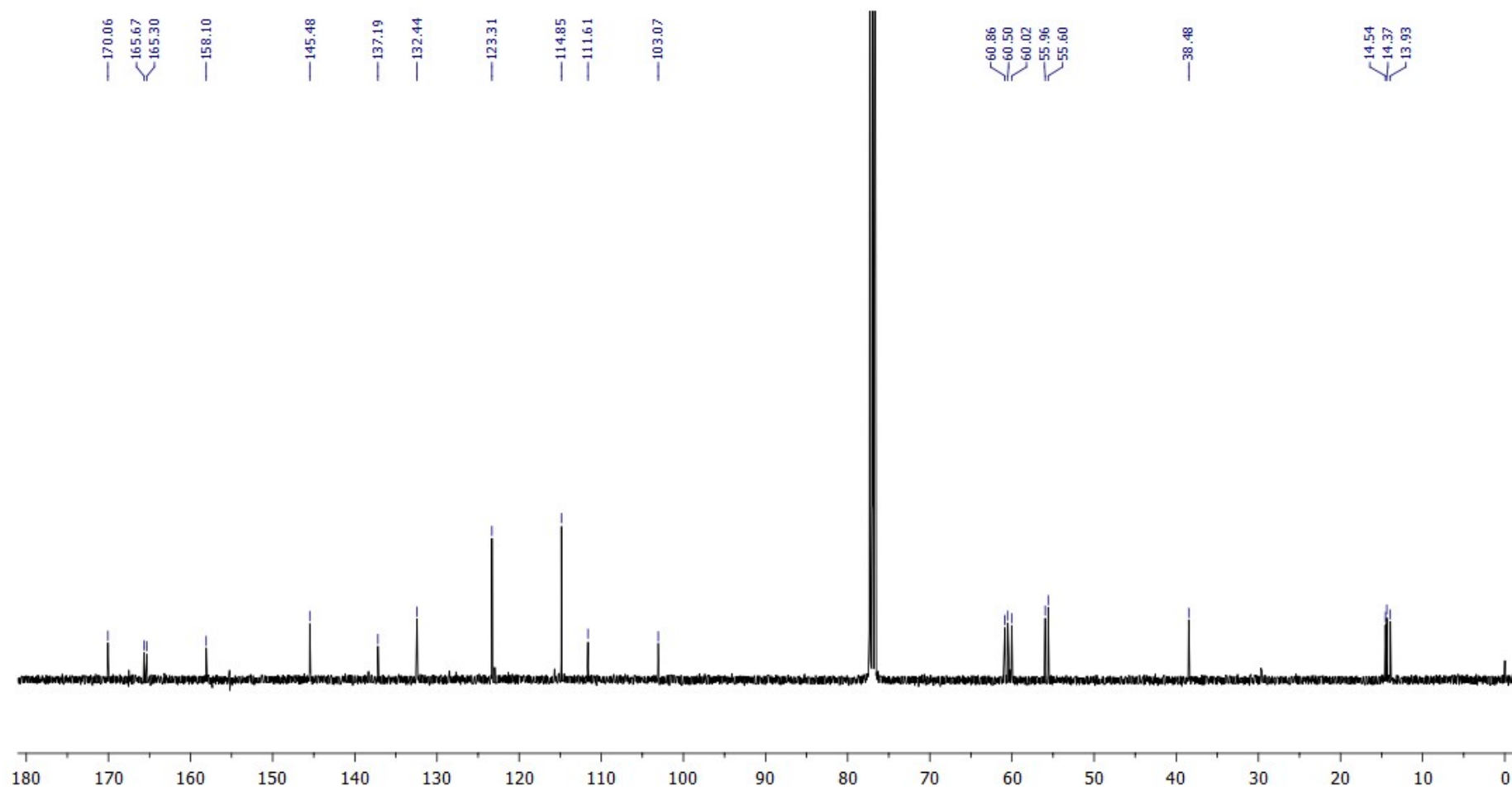
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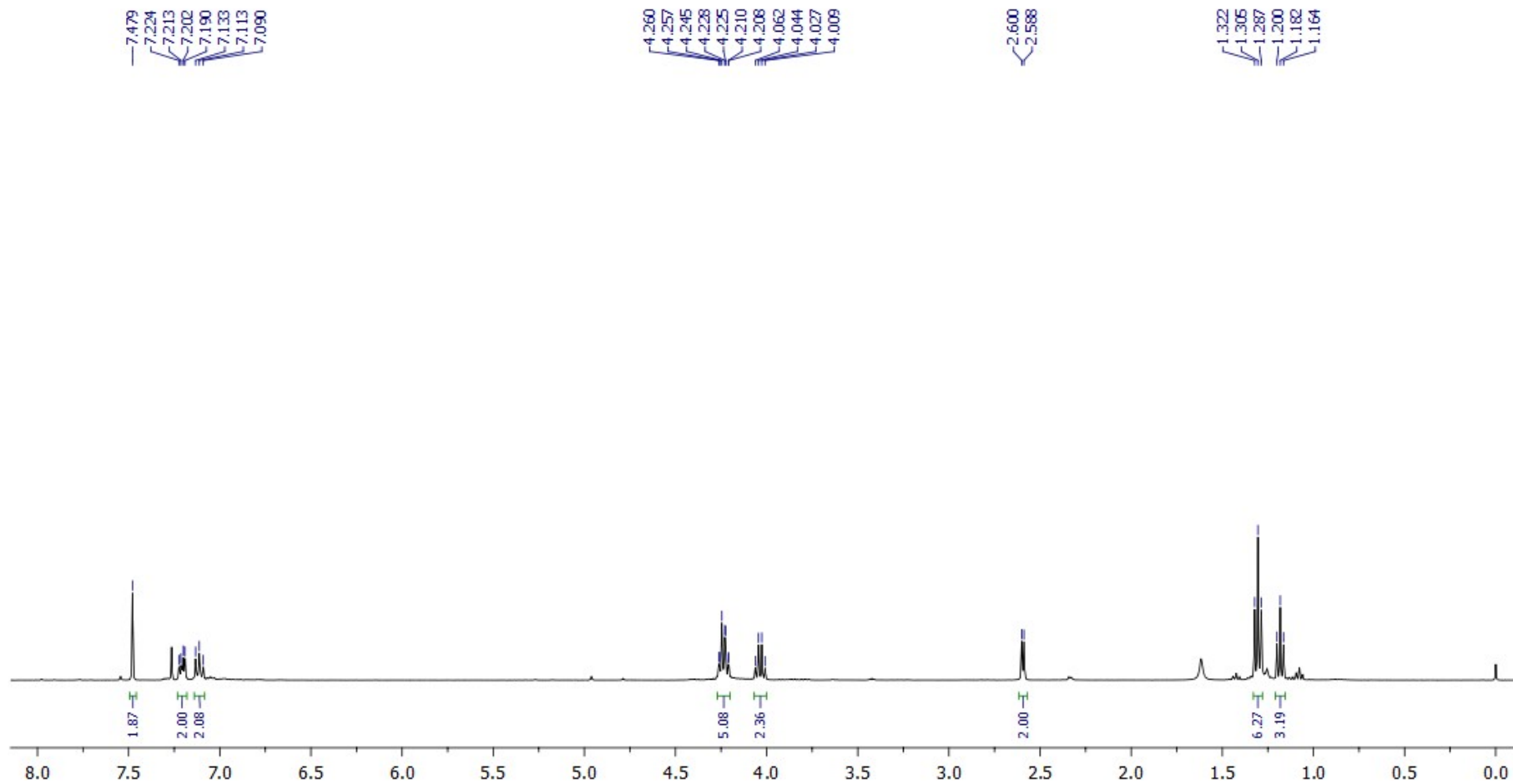
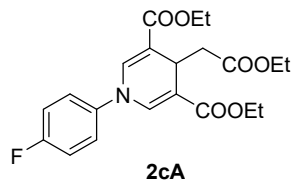
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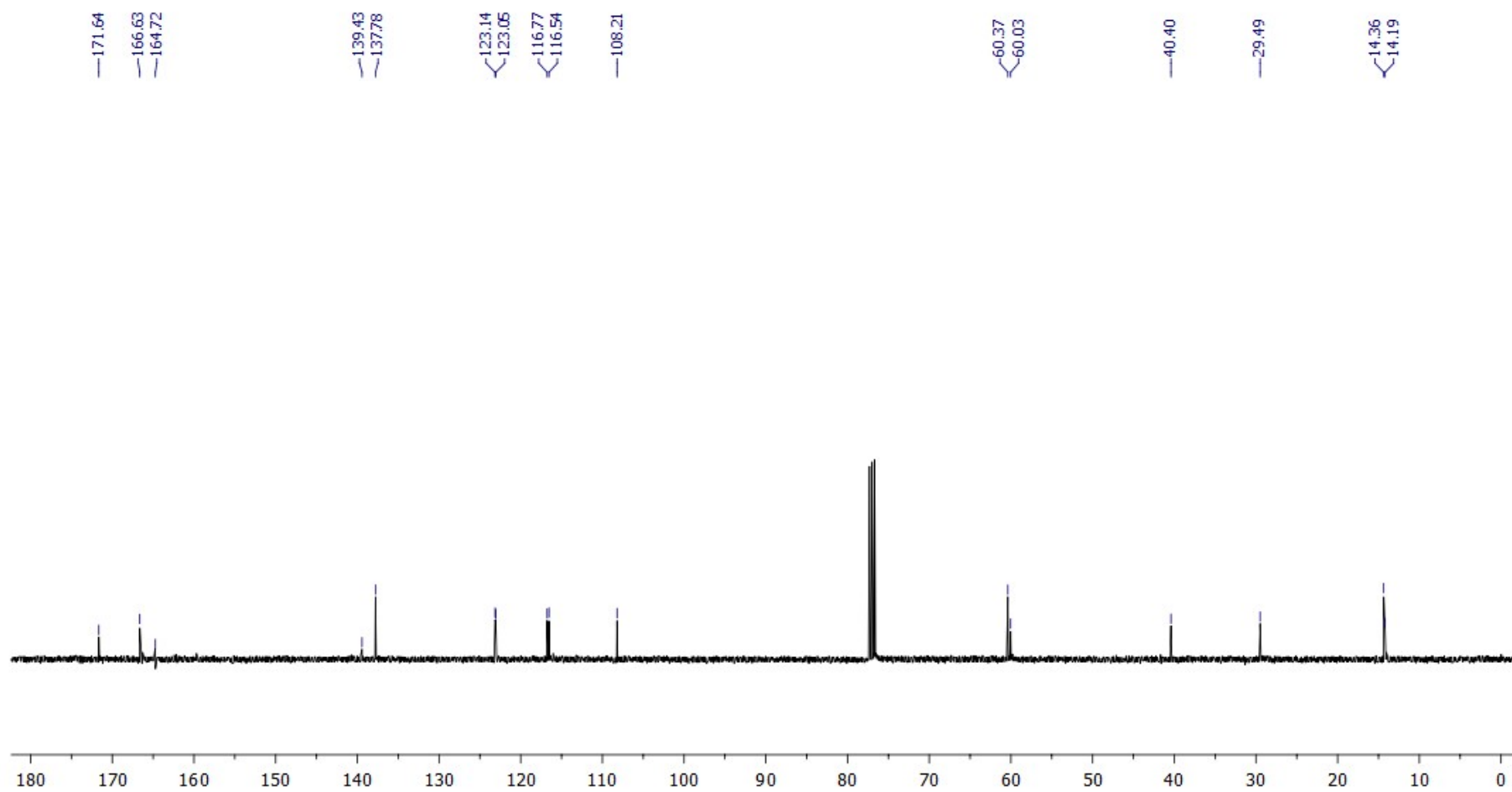
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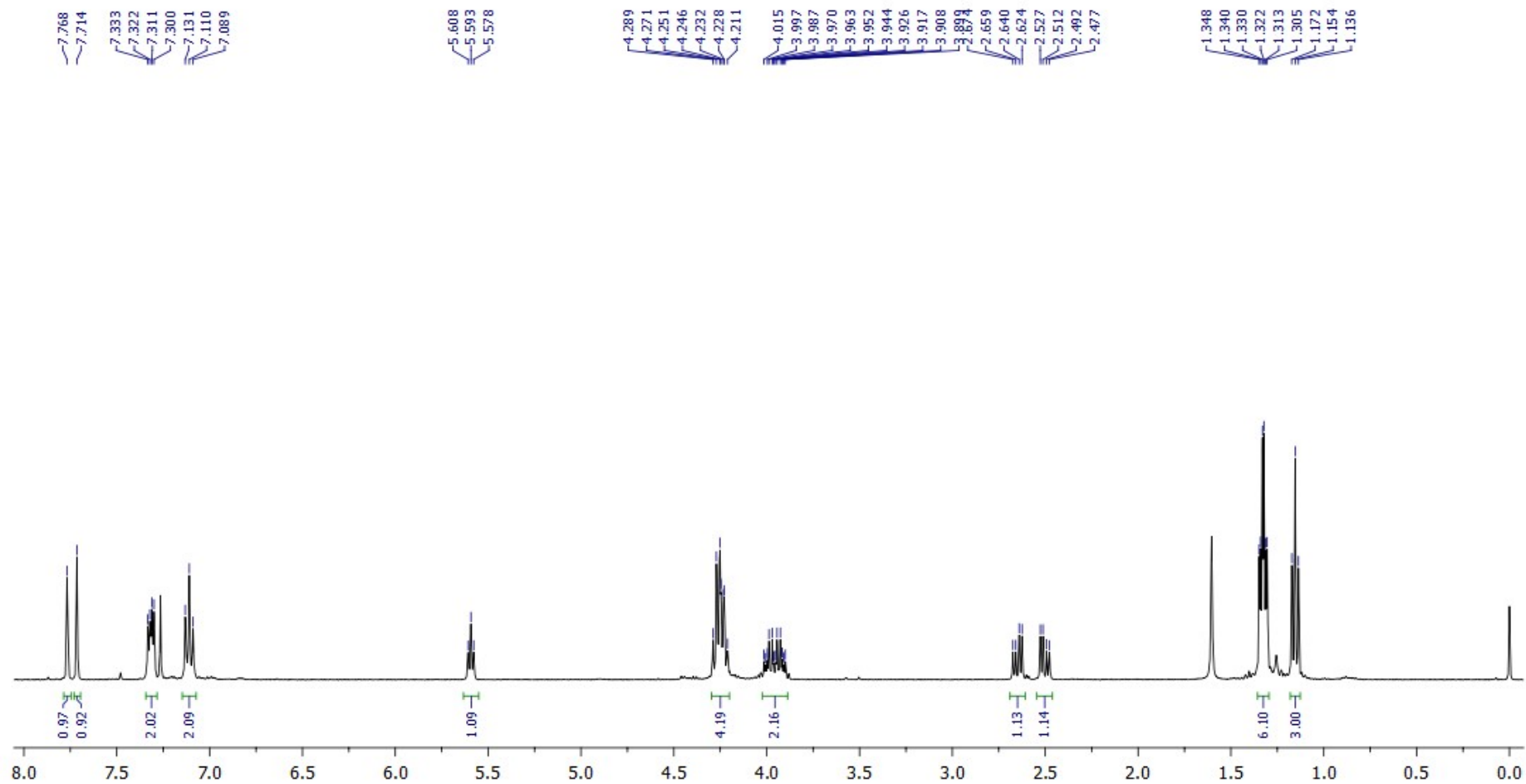
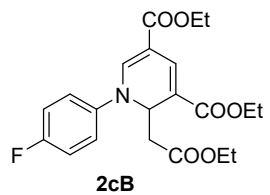
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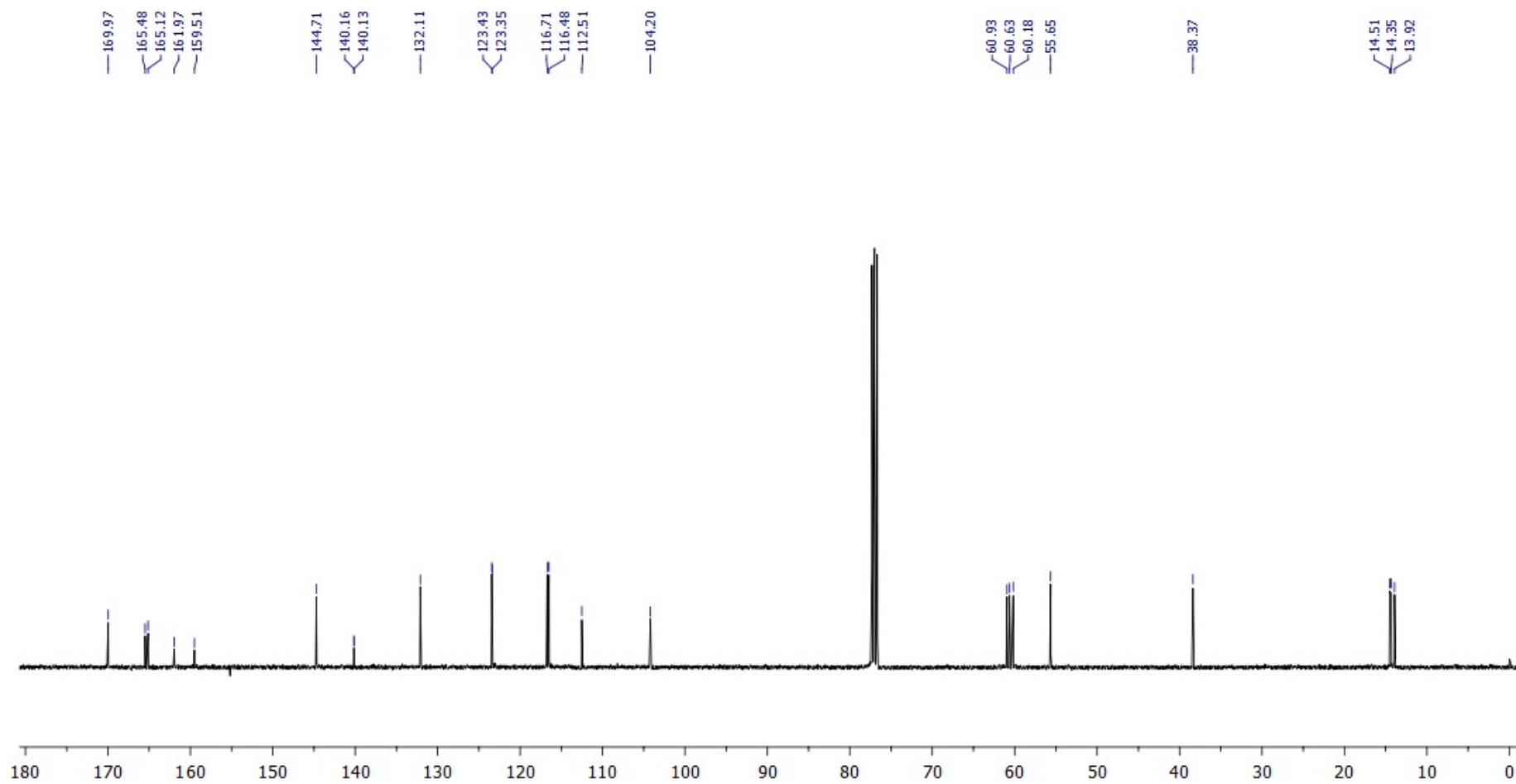
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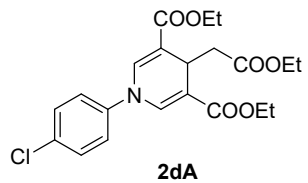
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$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)

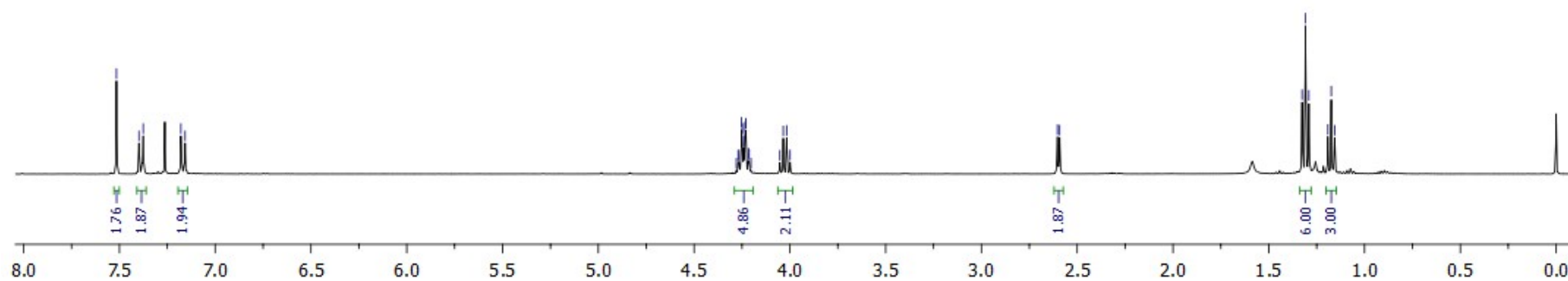


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7.157

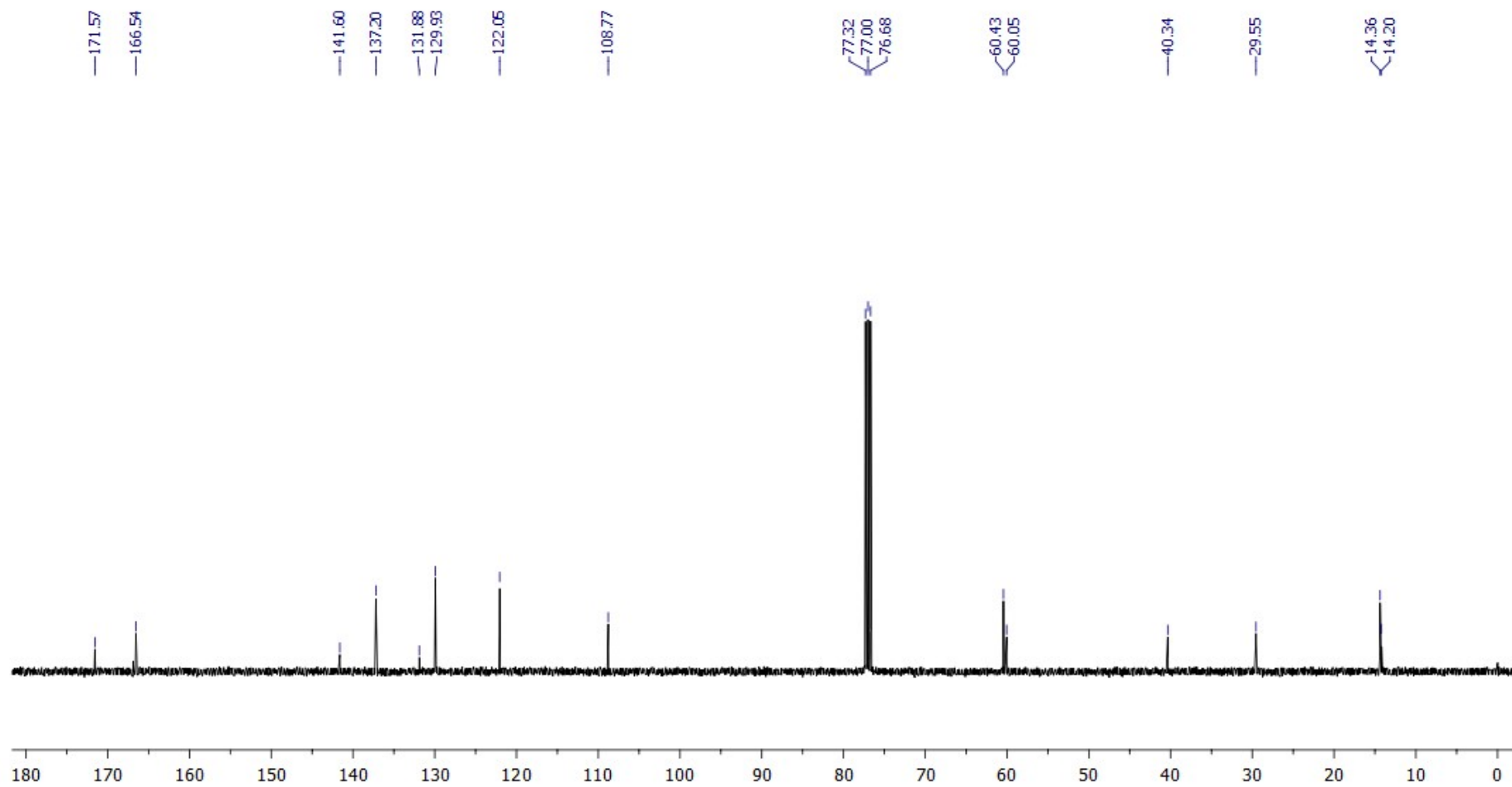
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3.999

2.604
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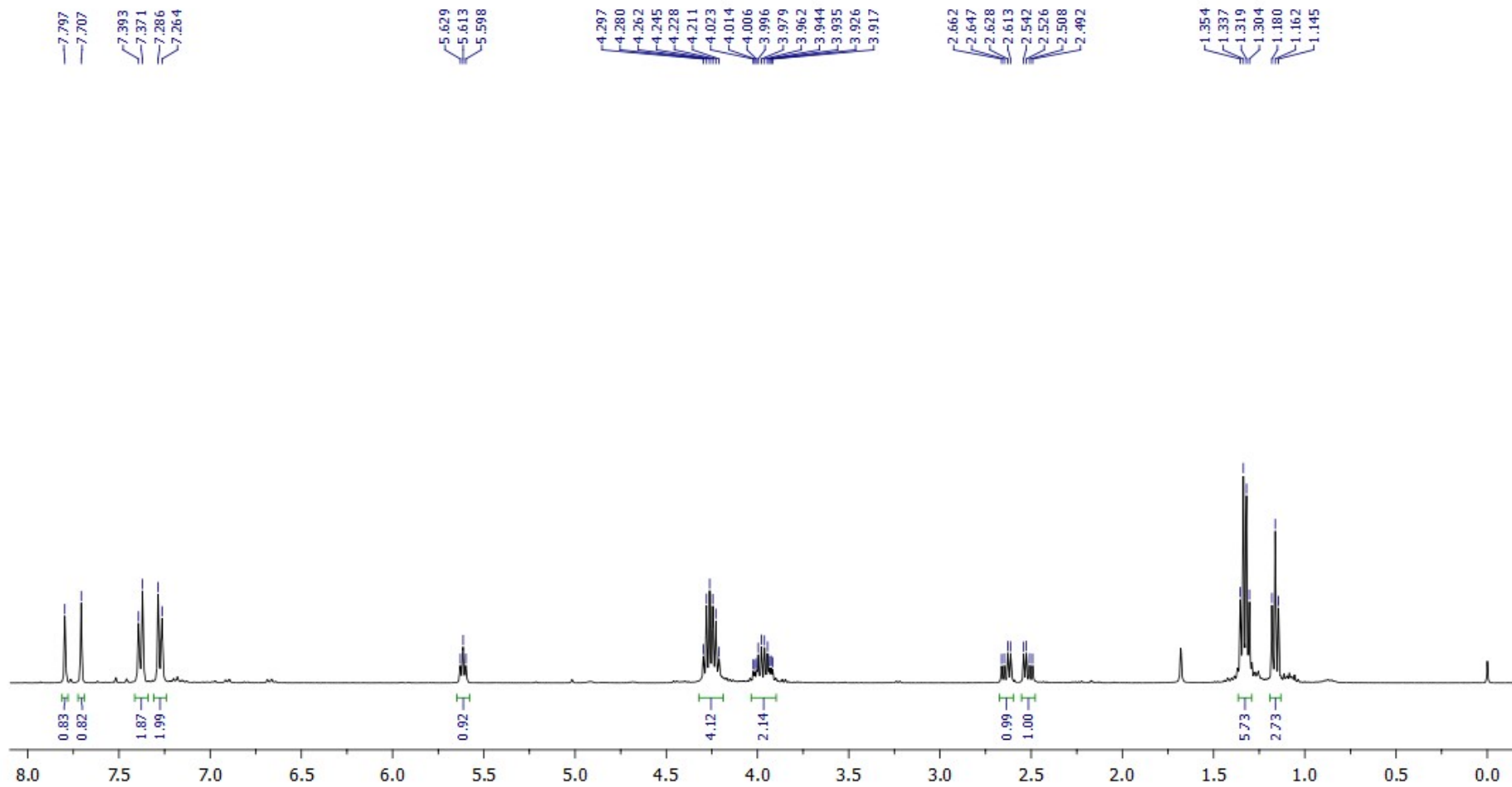
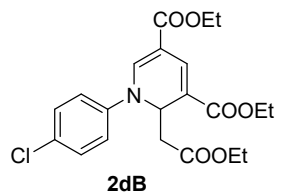
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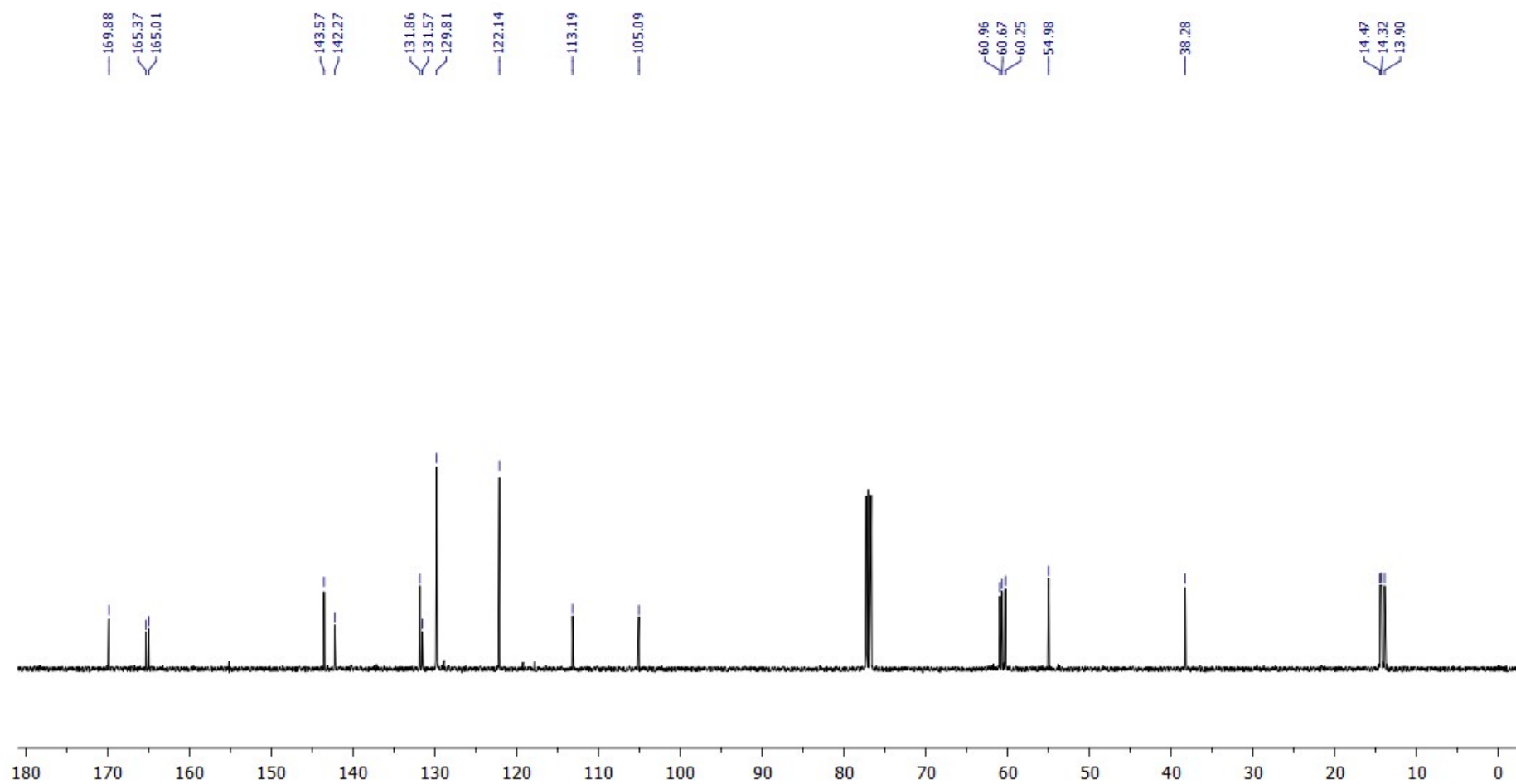
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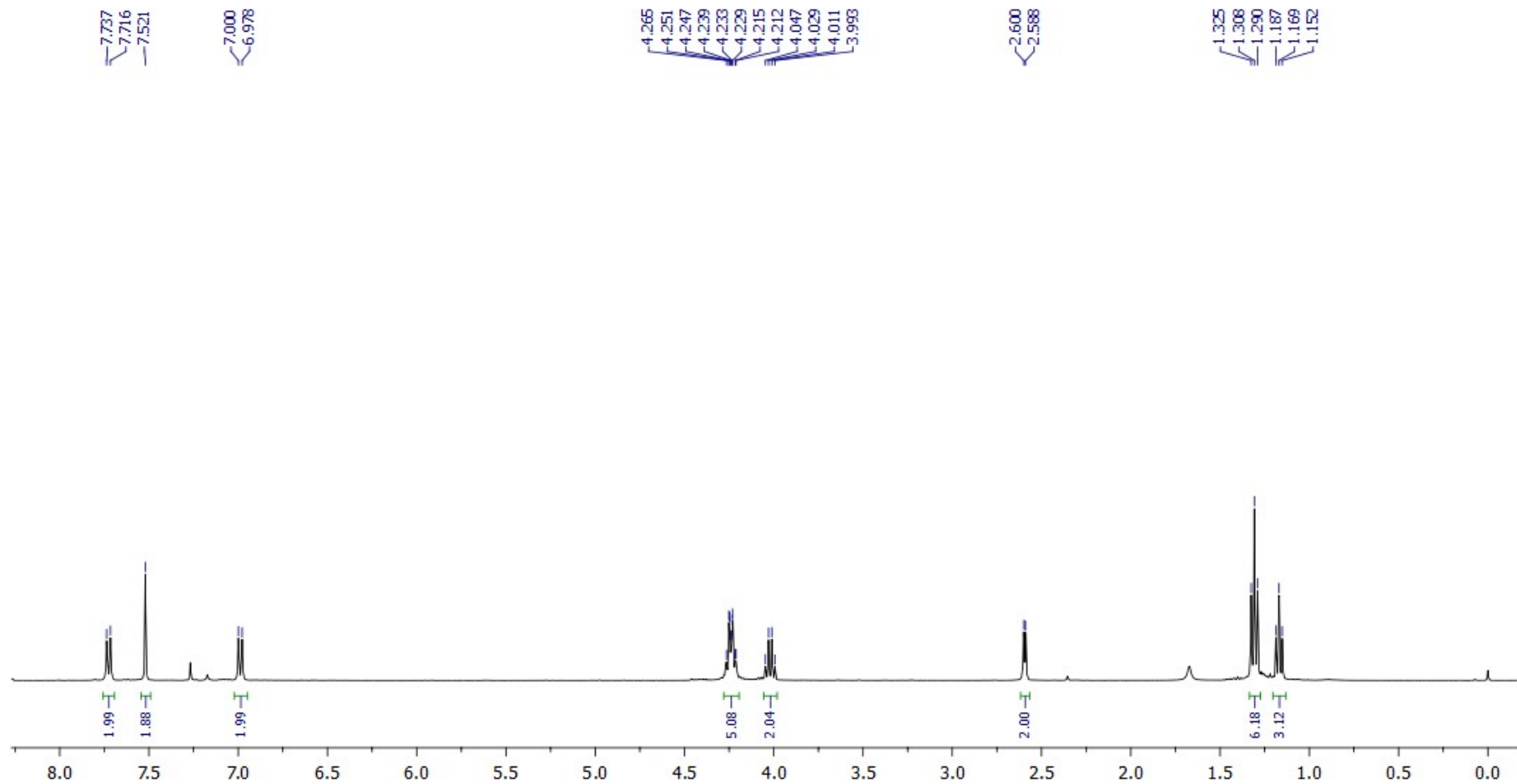
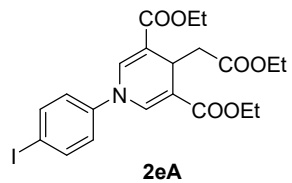
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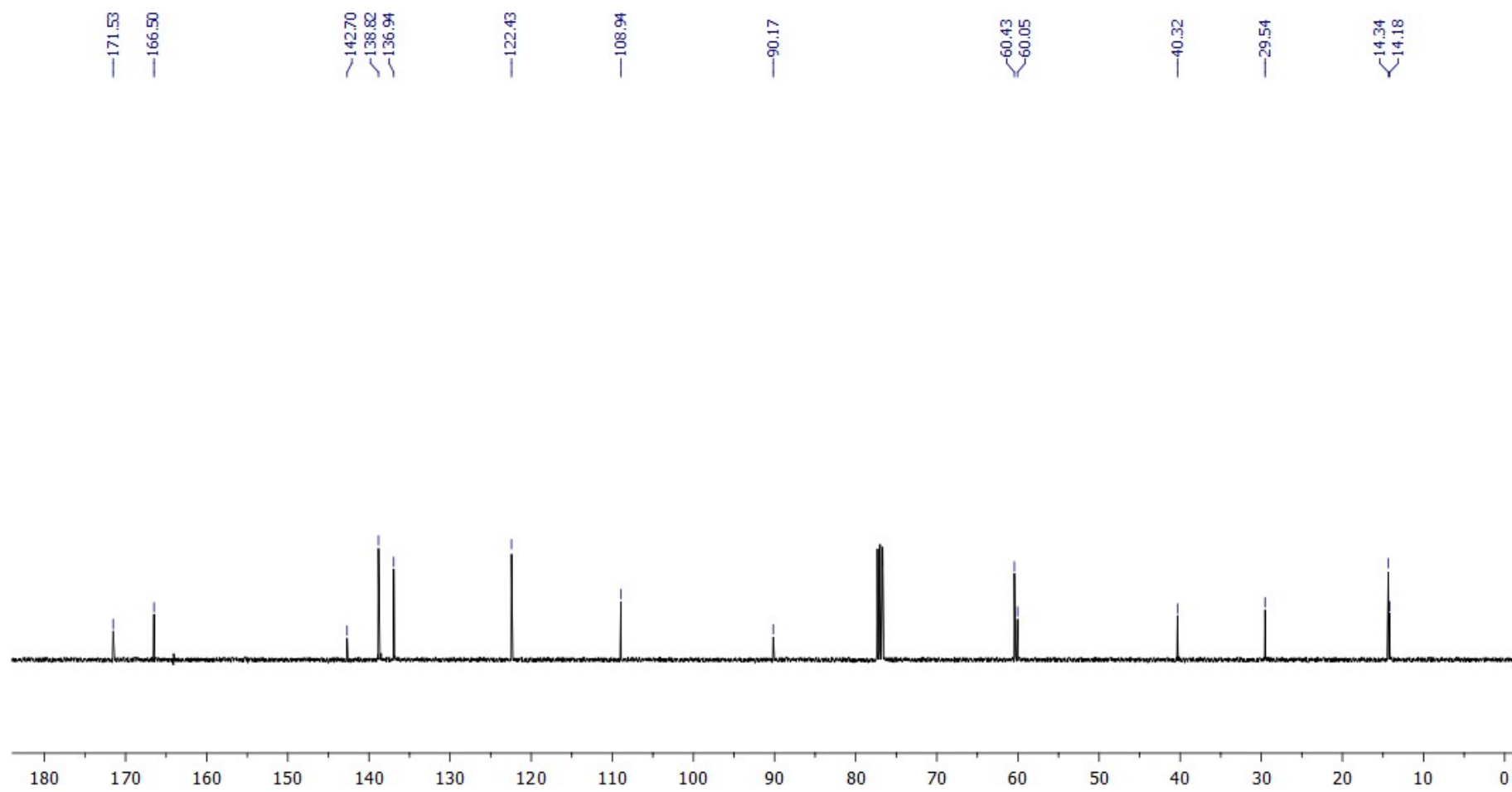
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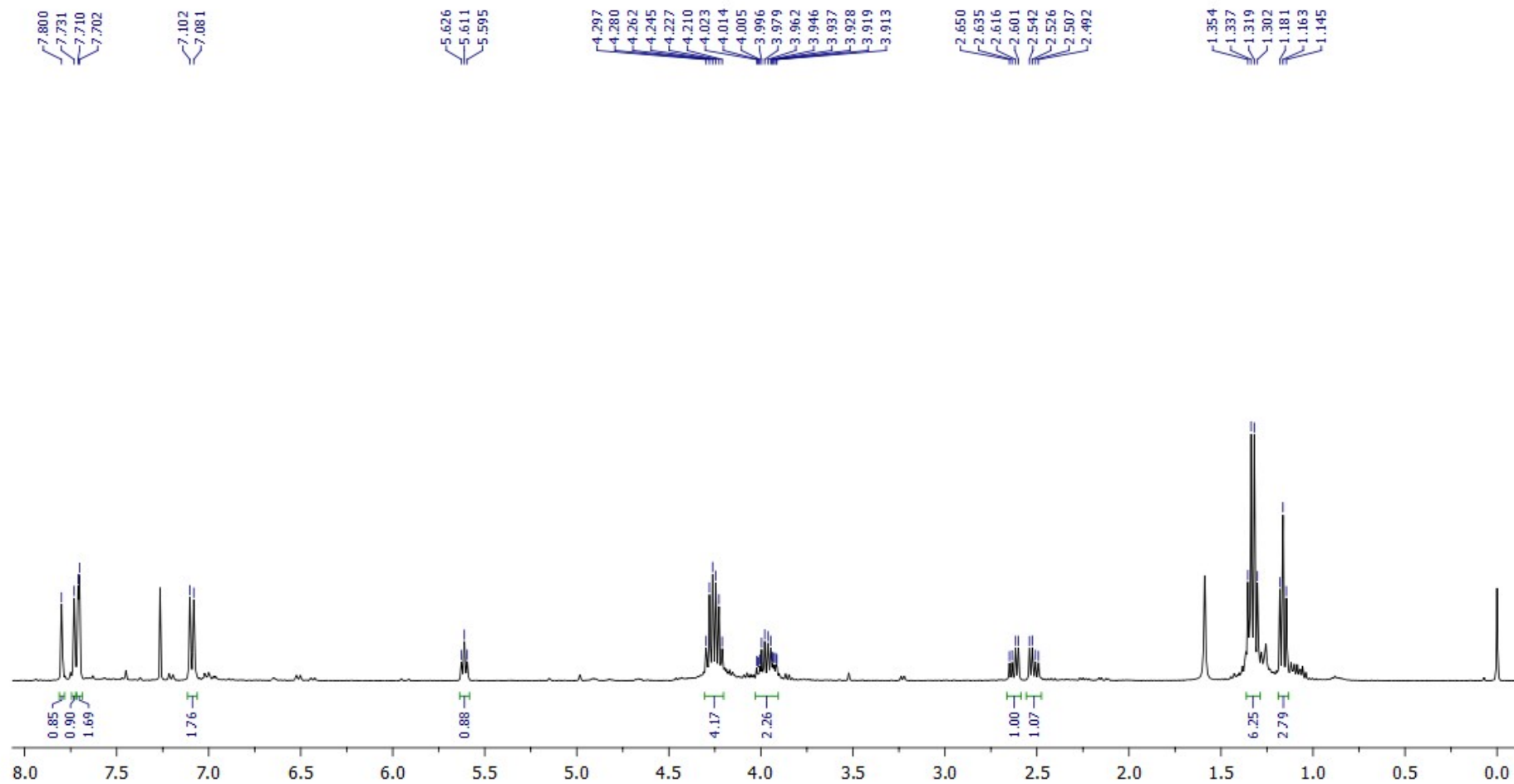
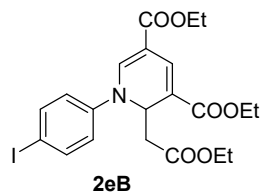
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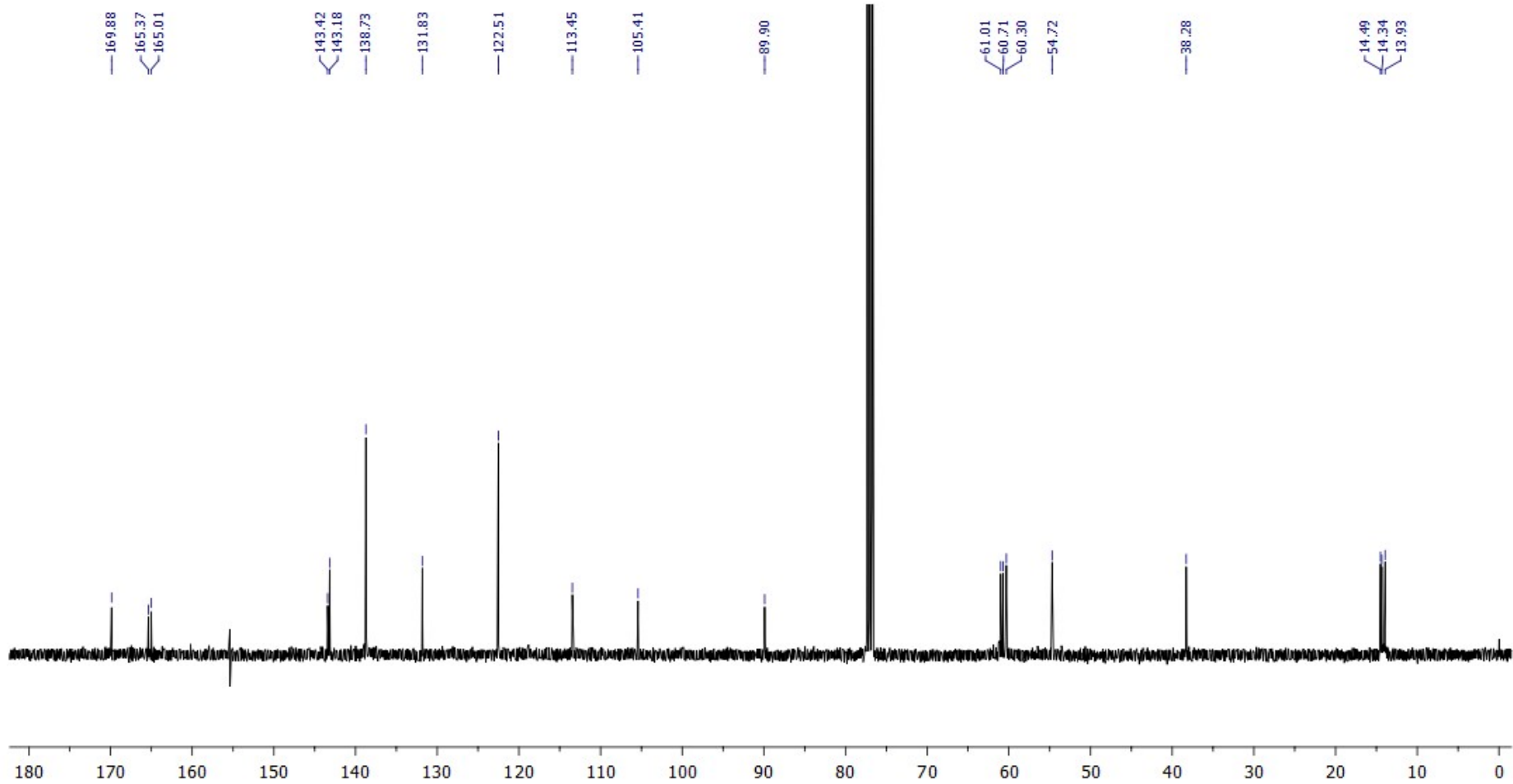
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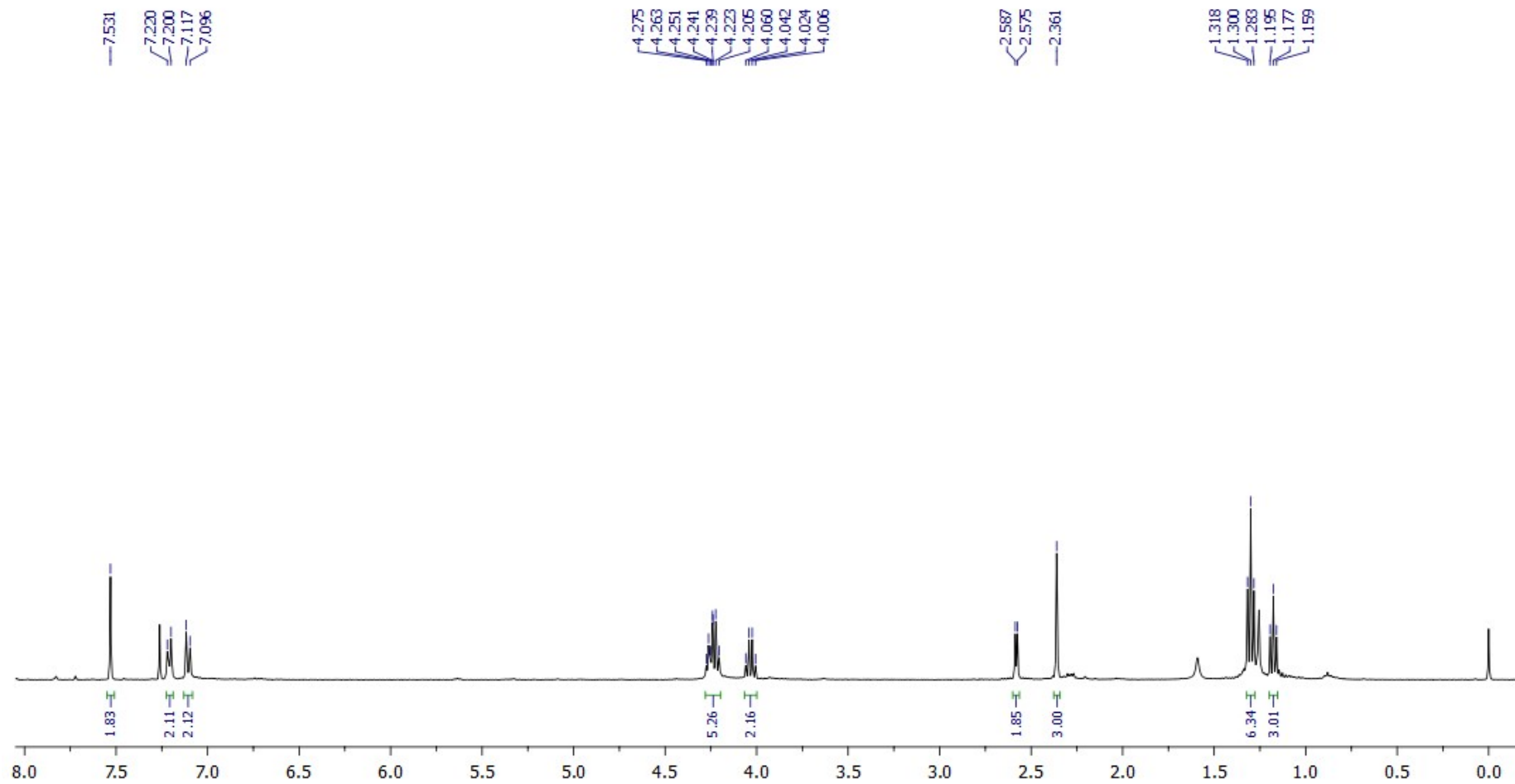
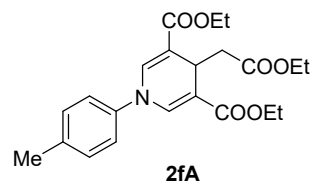
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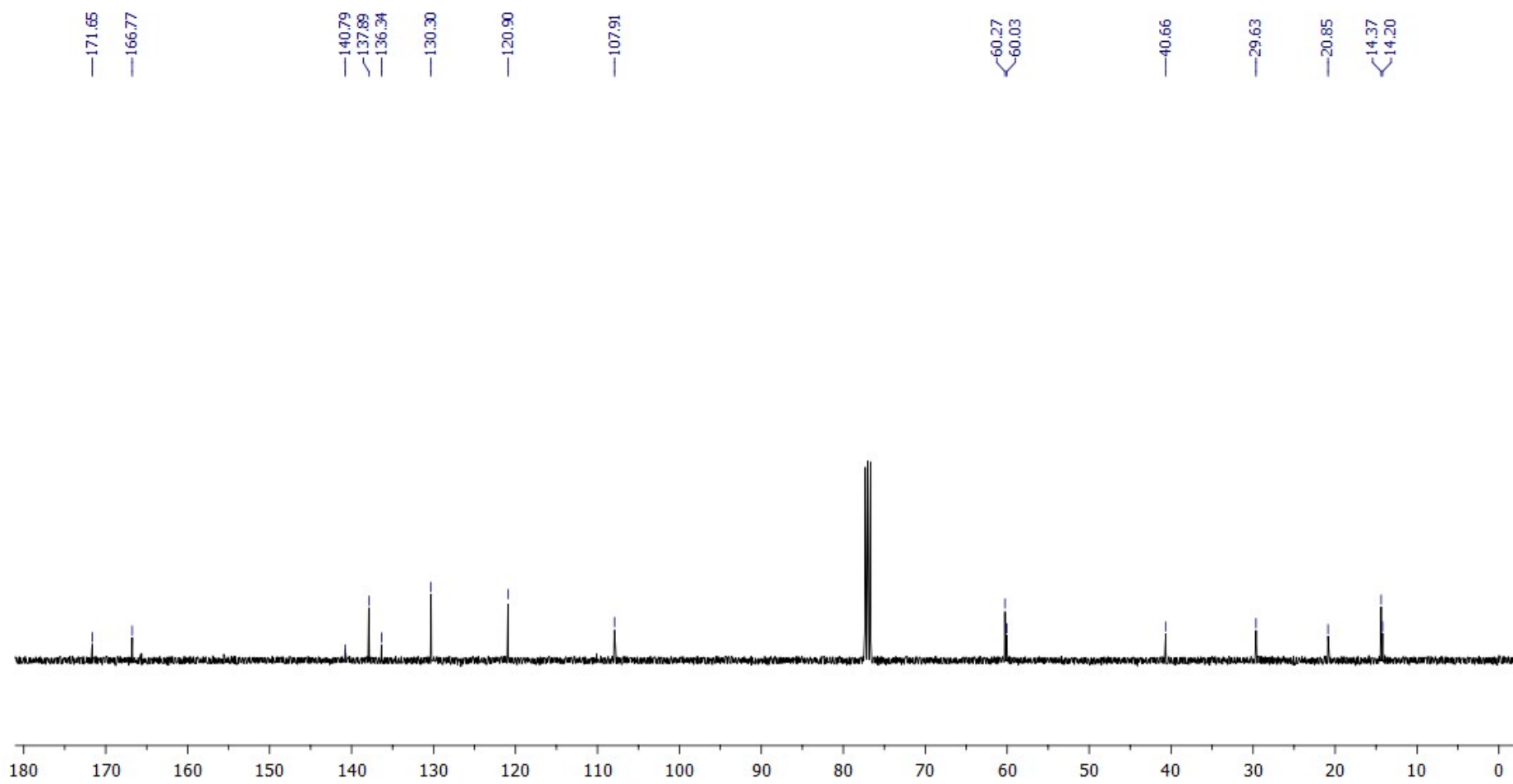
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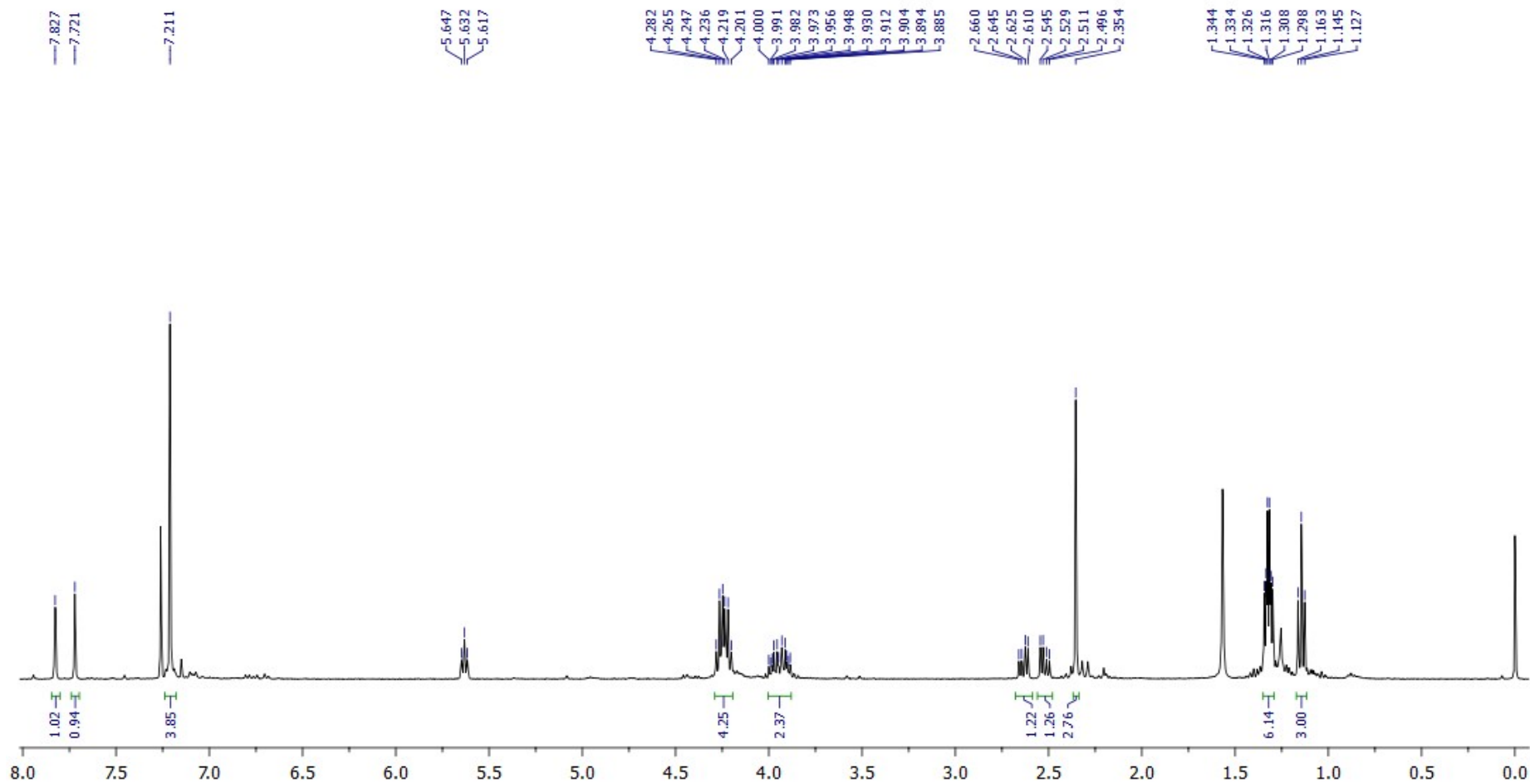
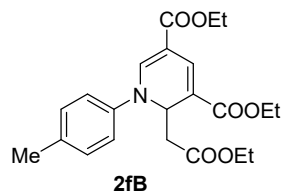
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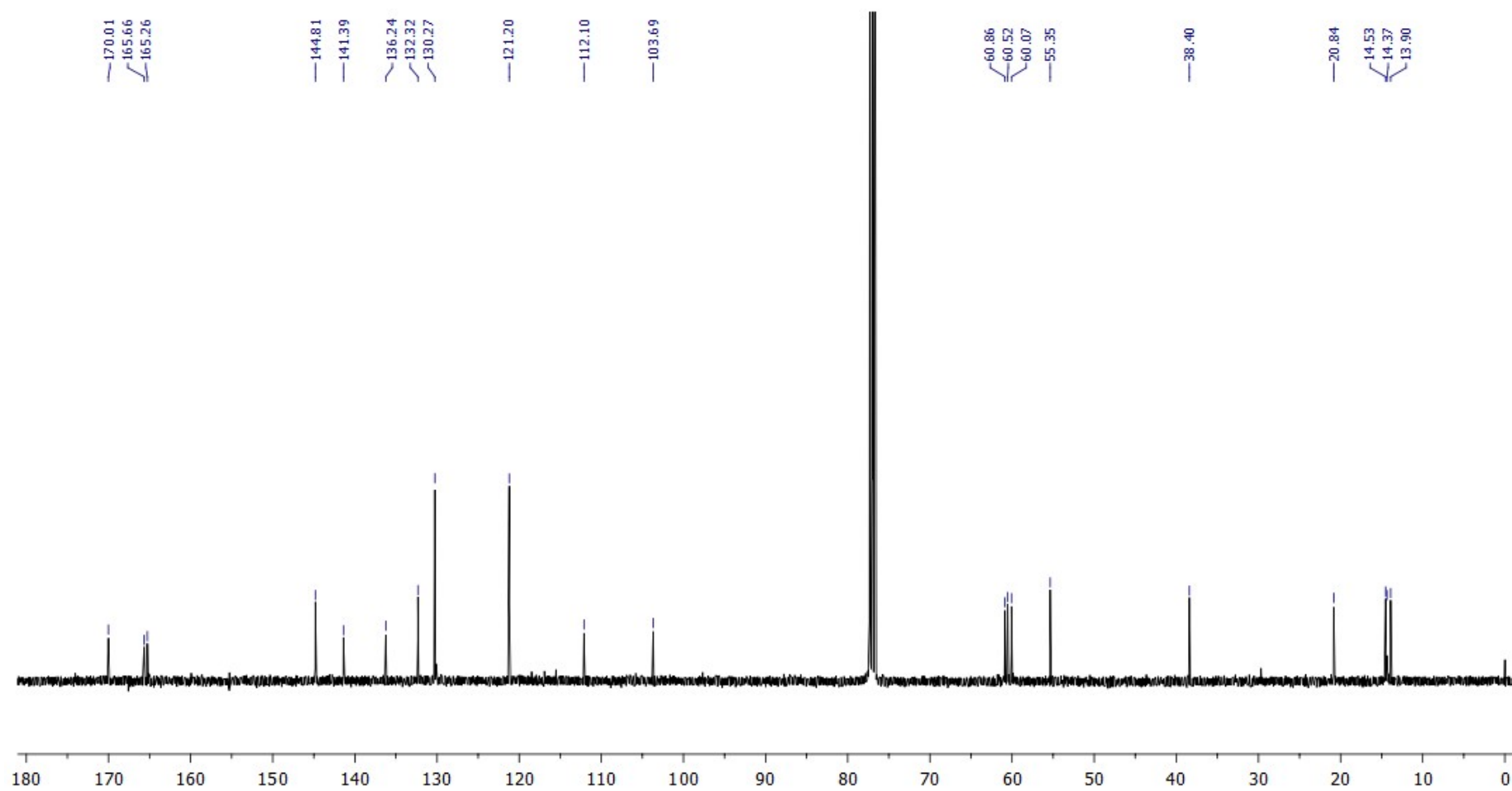
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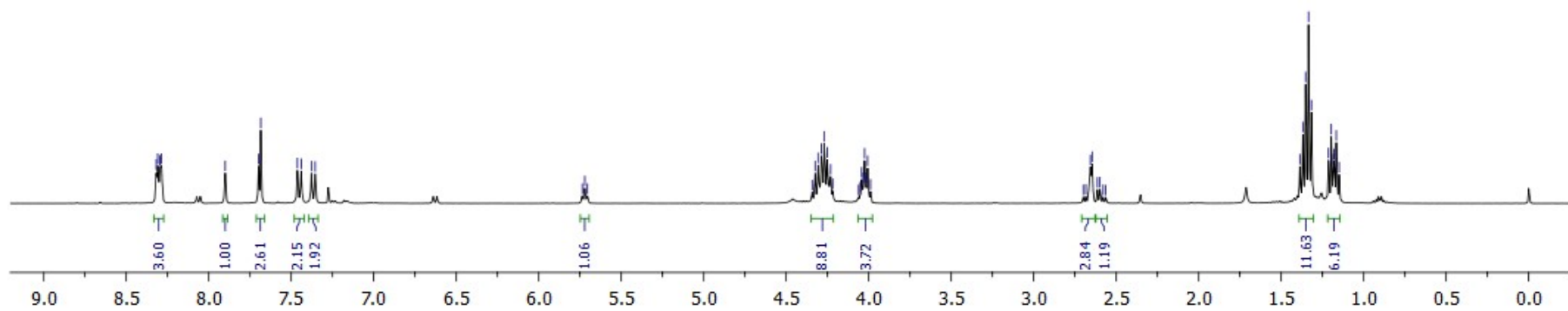
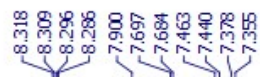
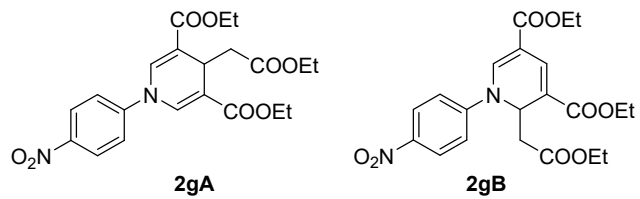
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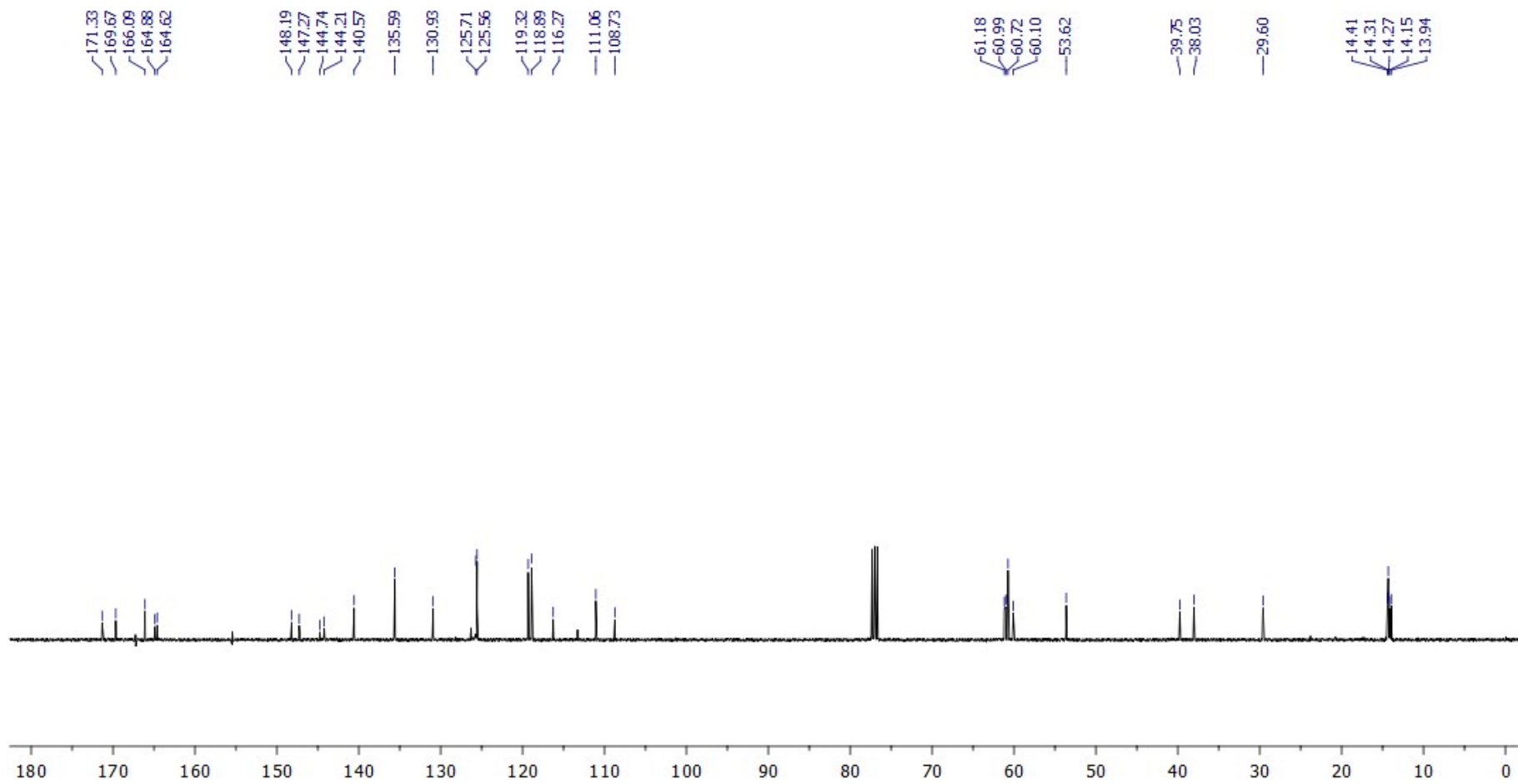
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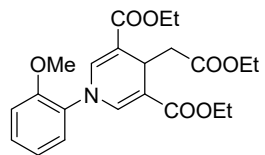
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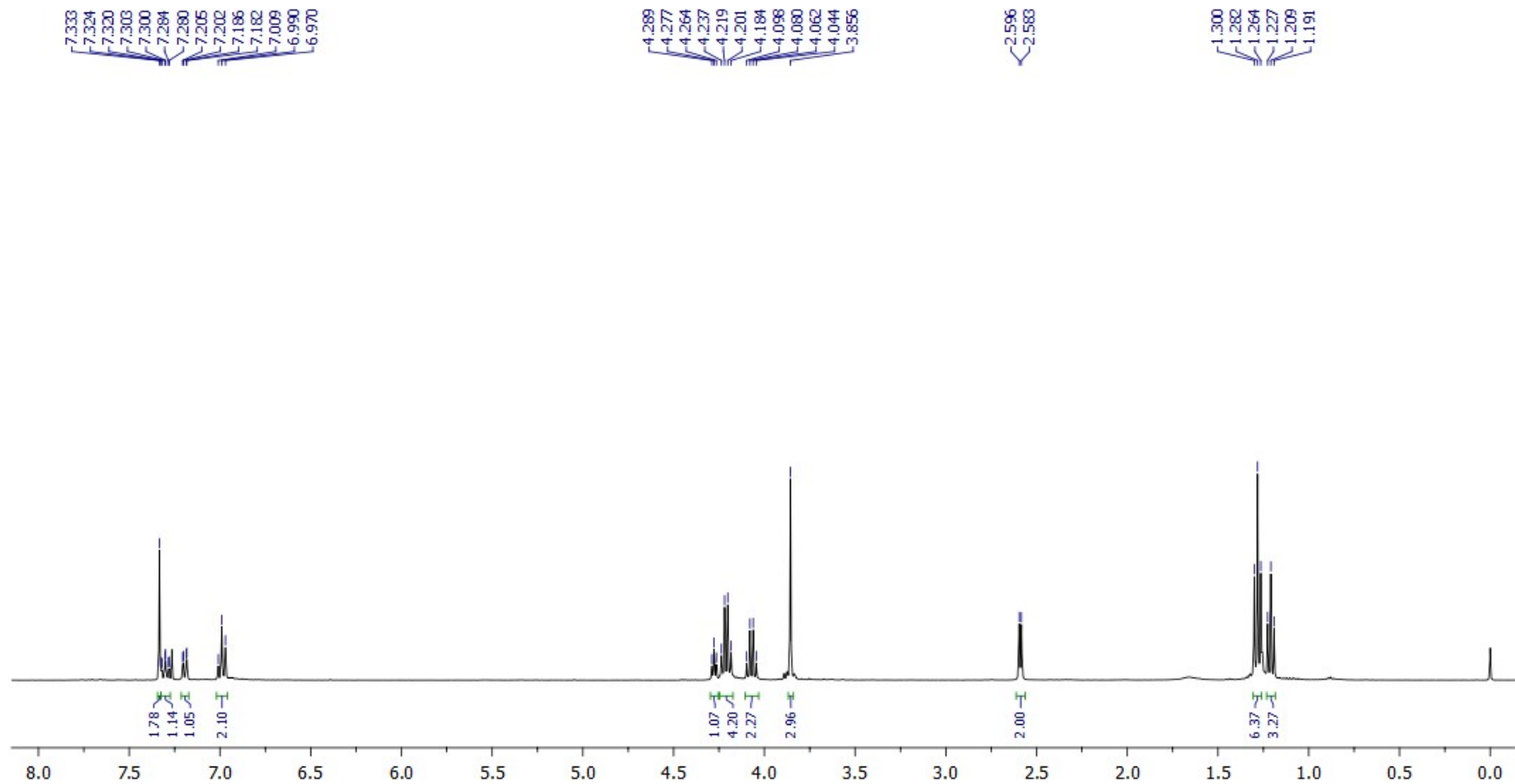
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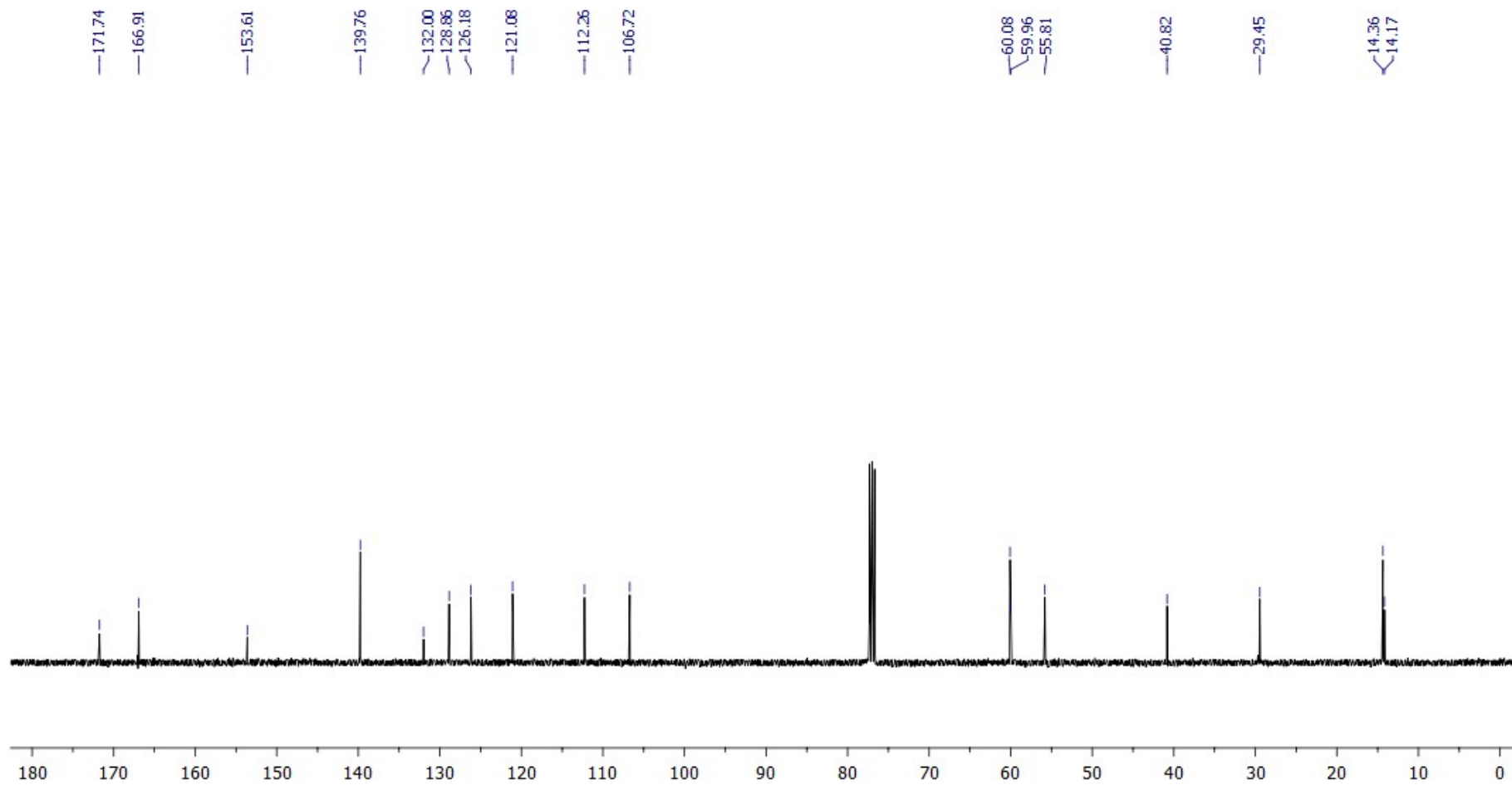
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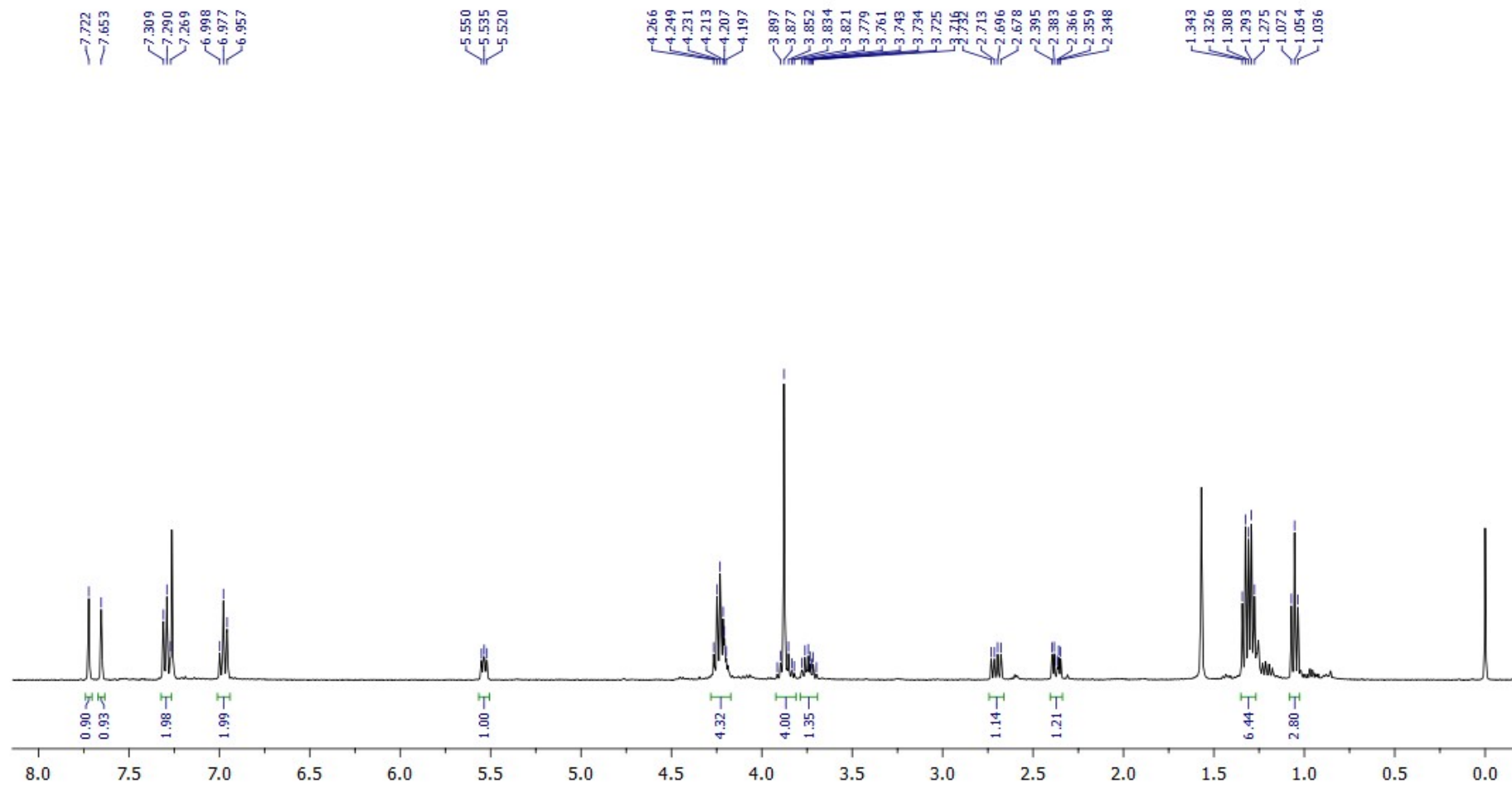
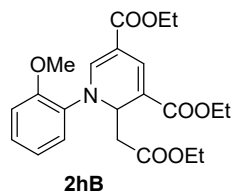
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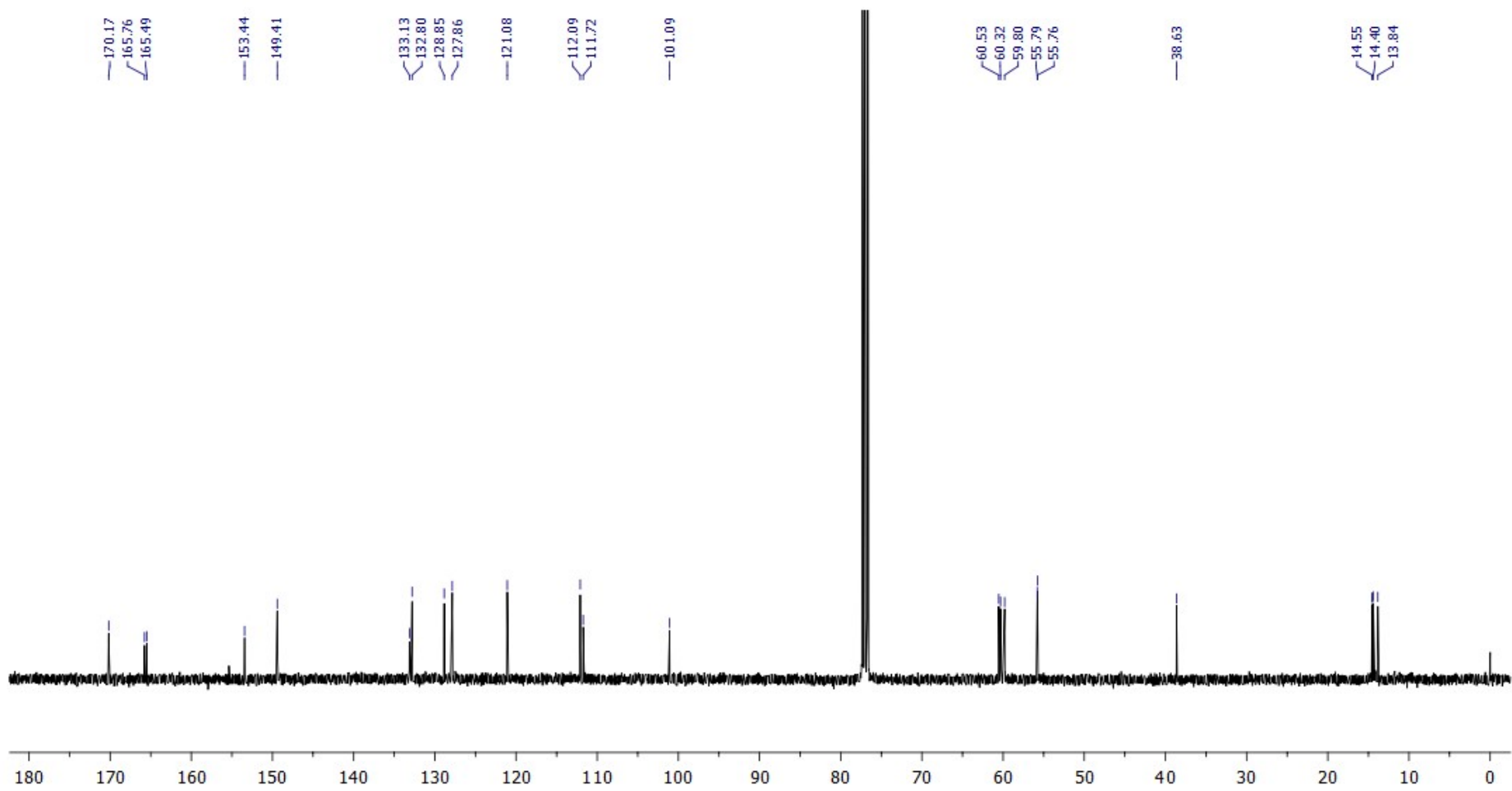
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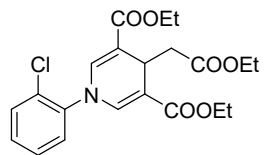
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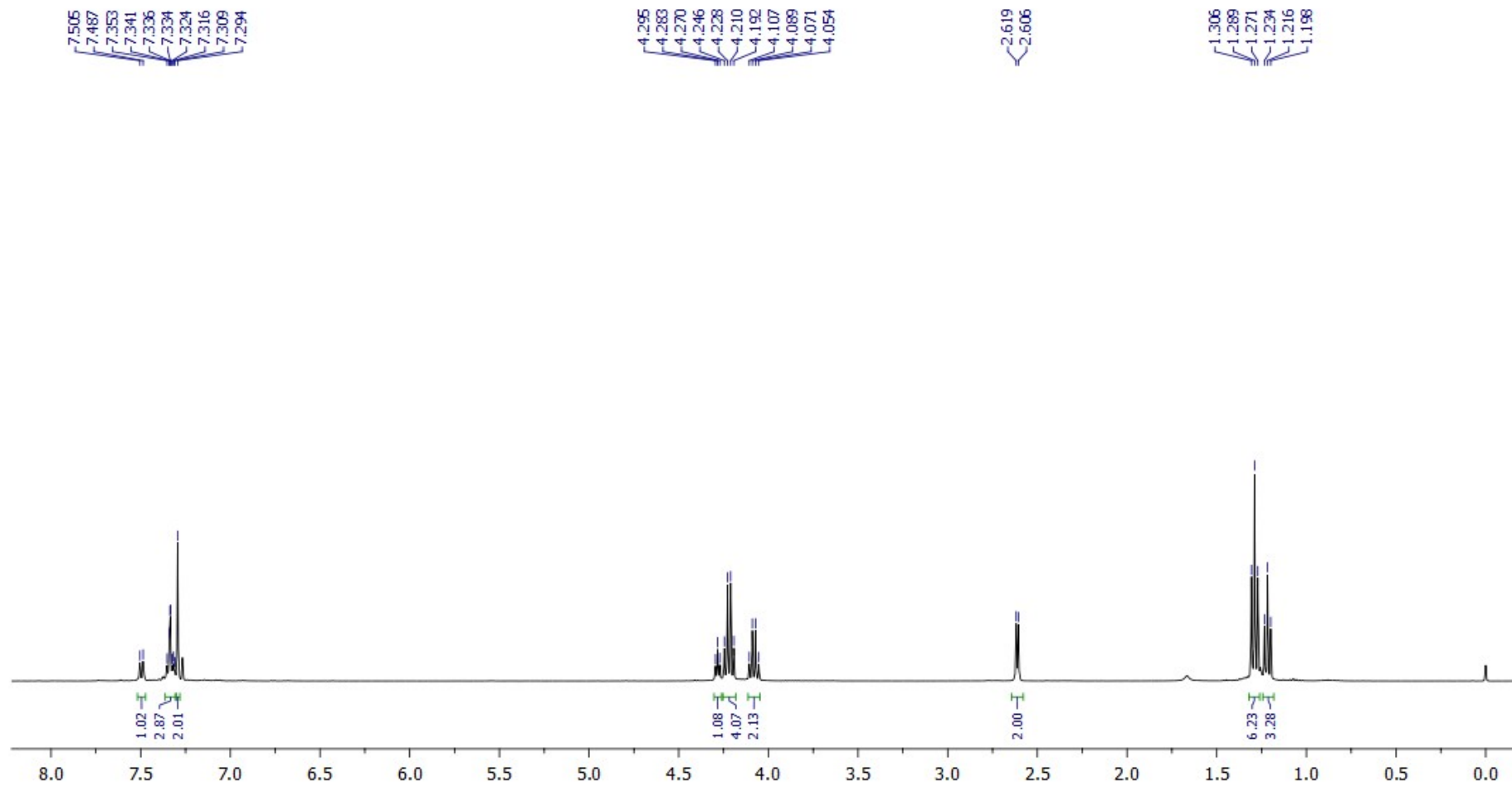
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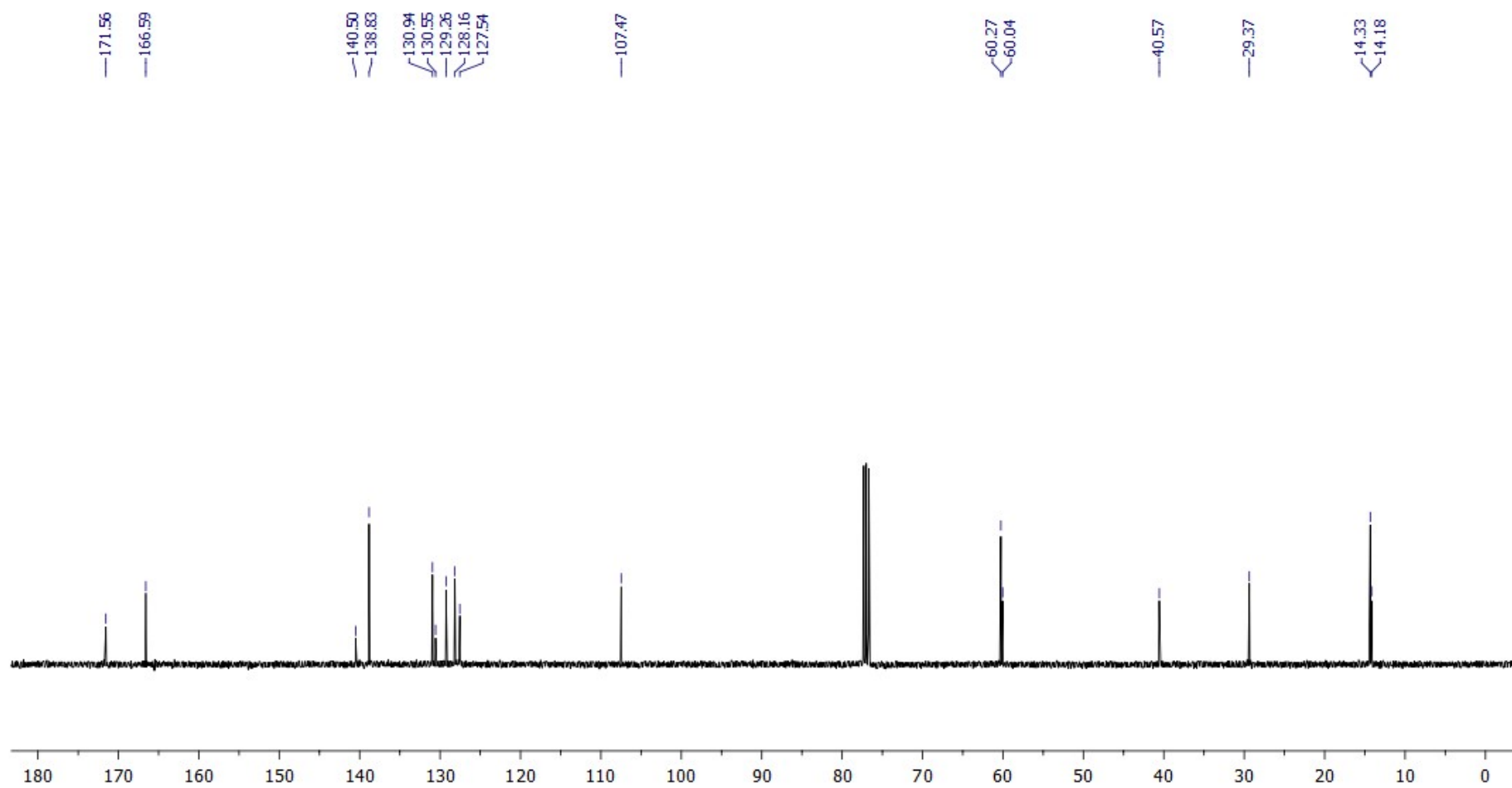
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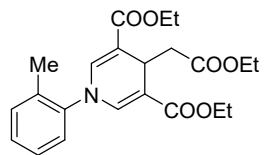
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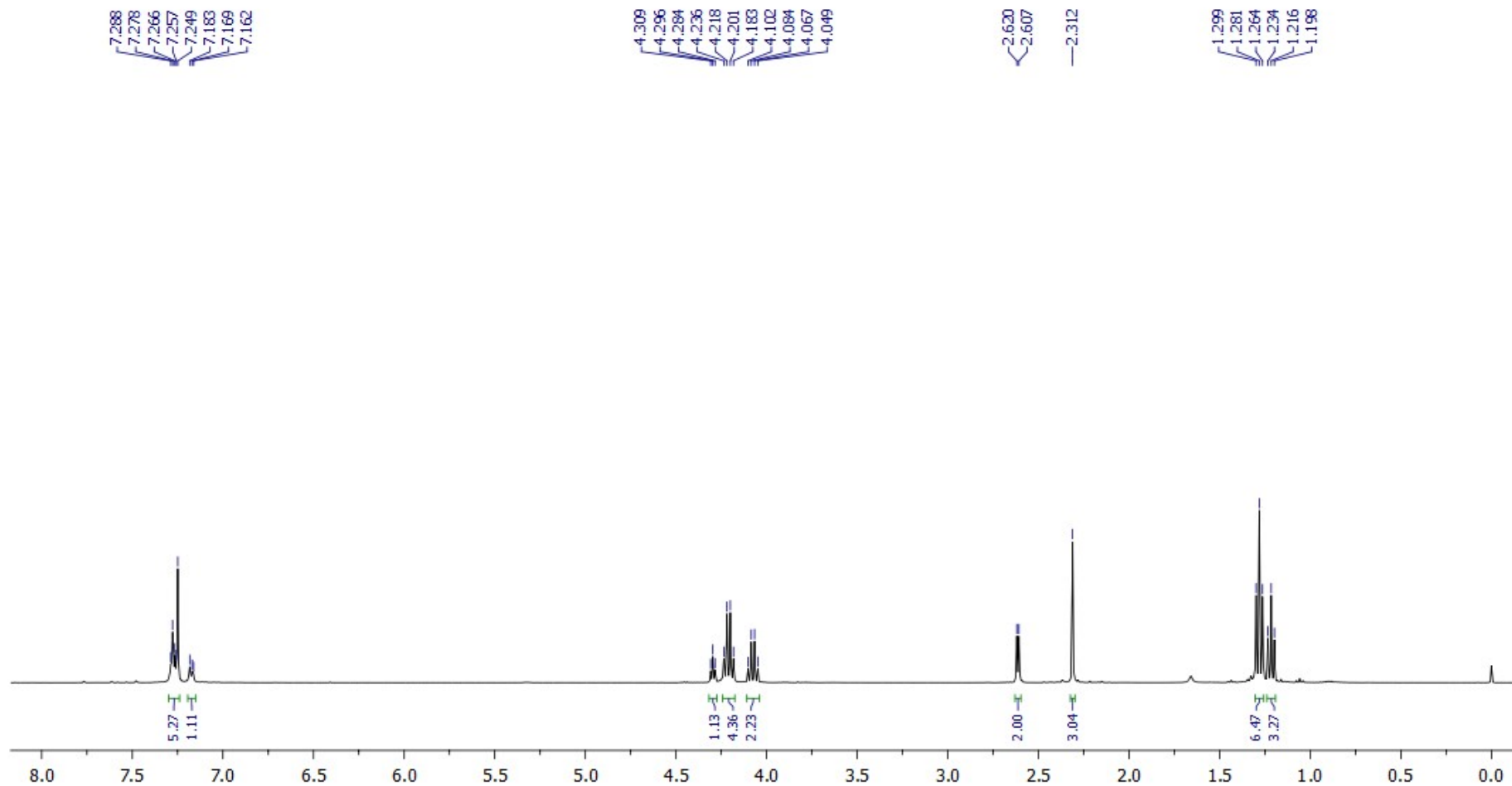
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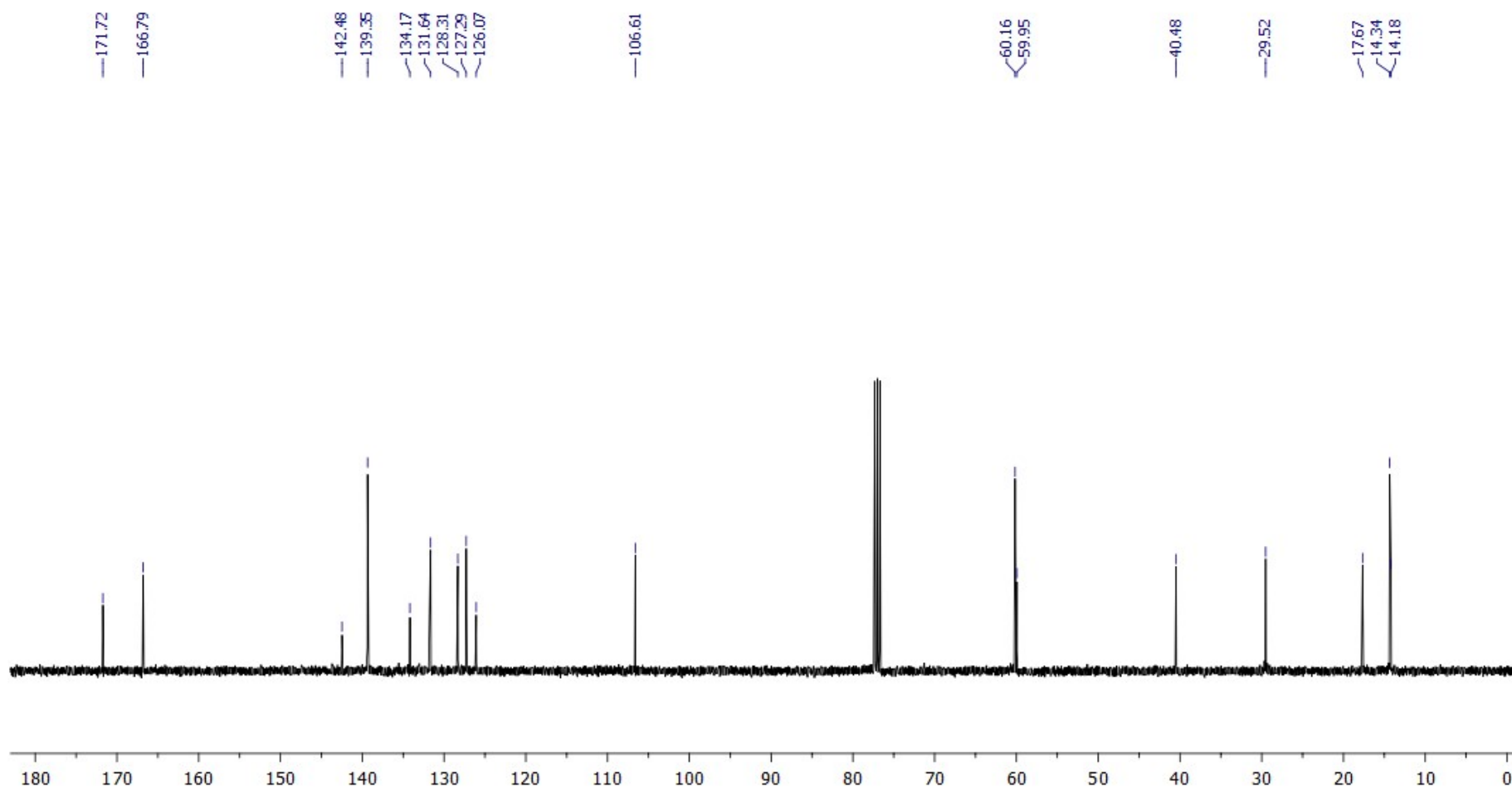
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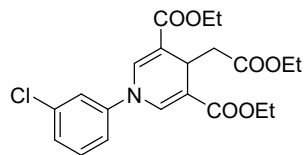
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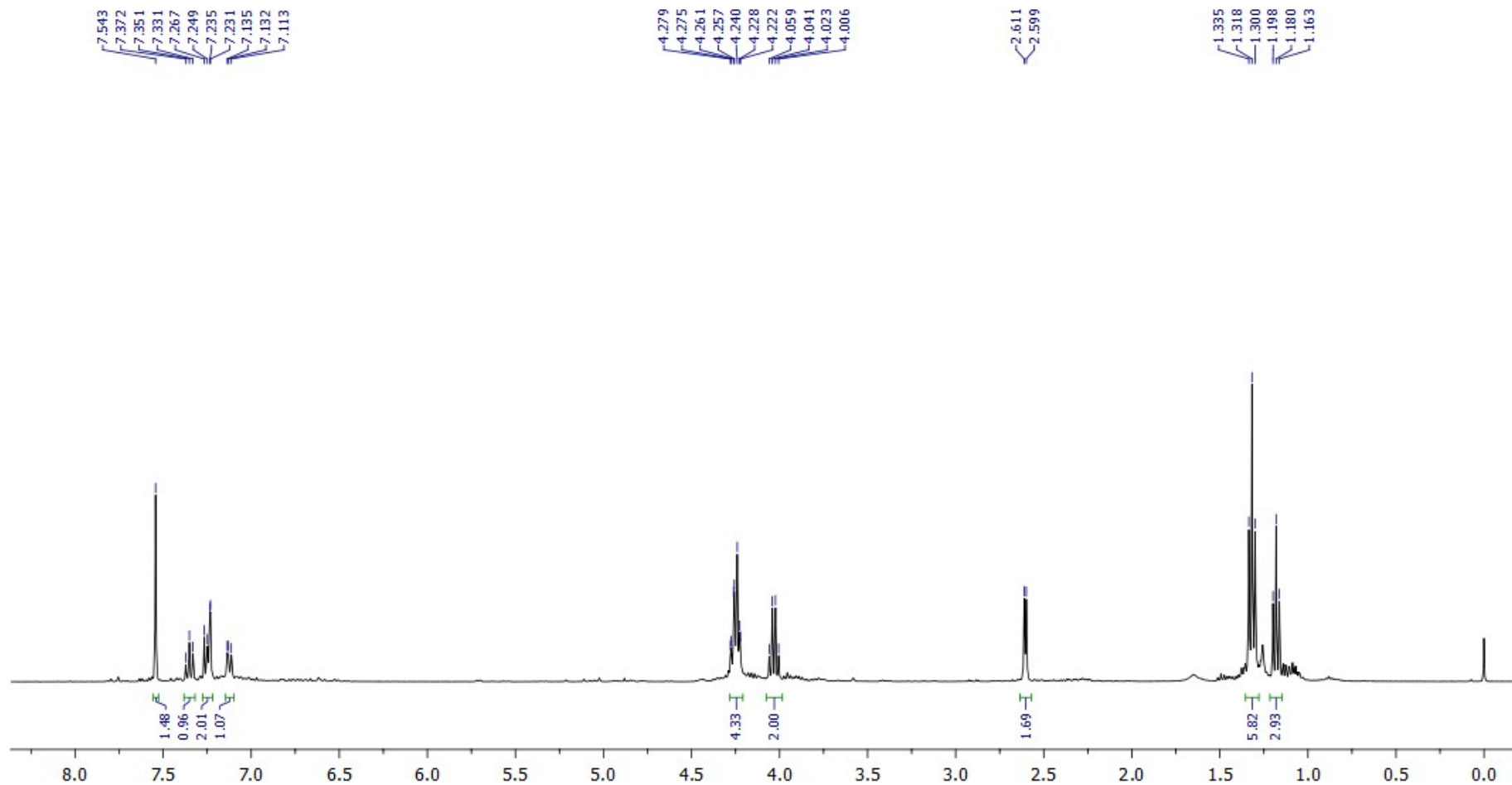
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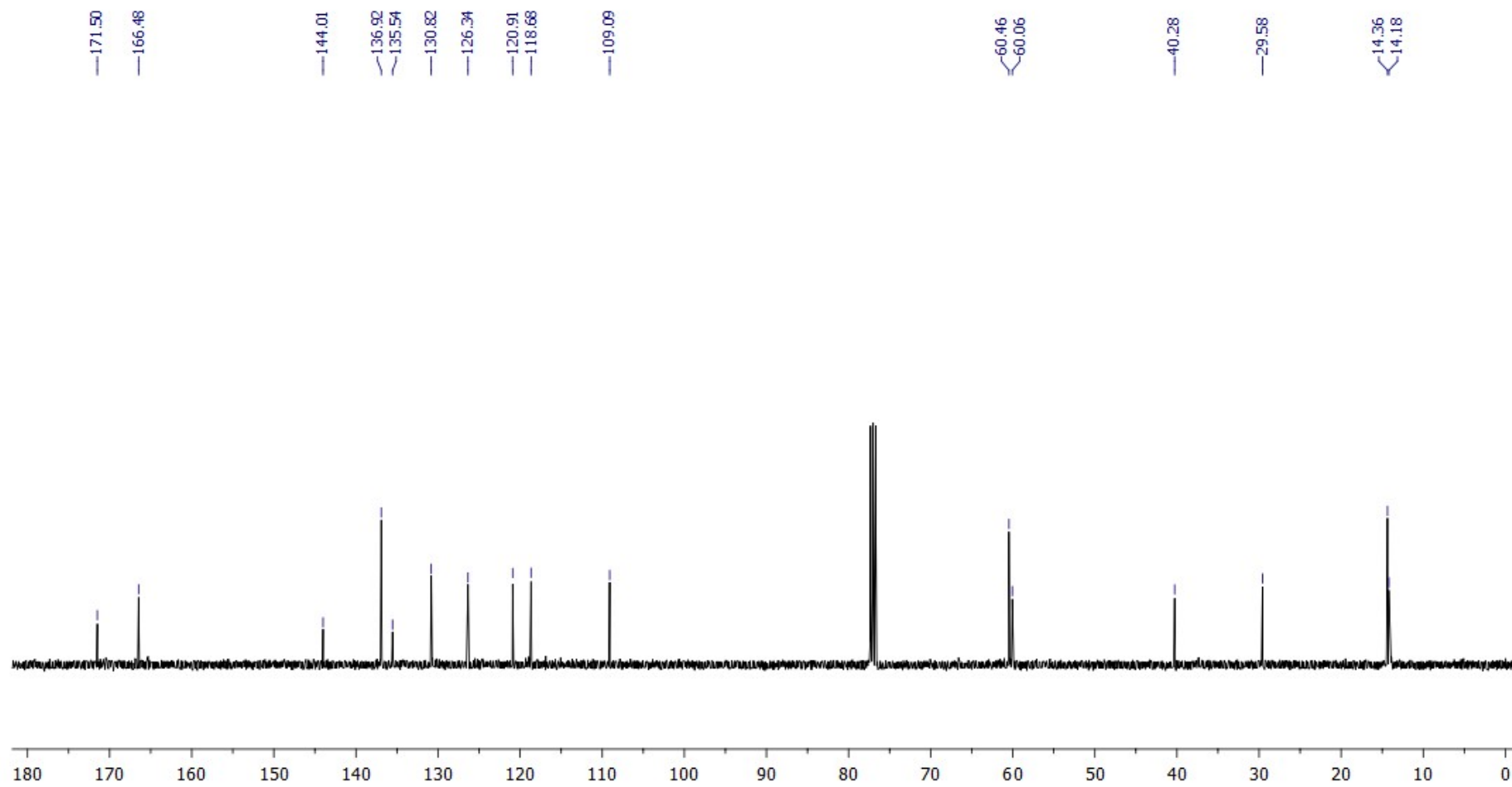
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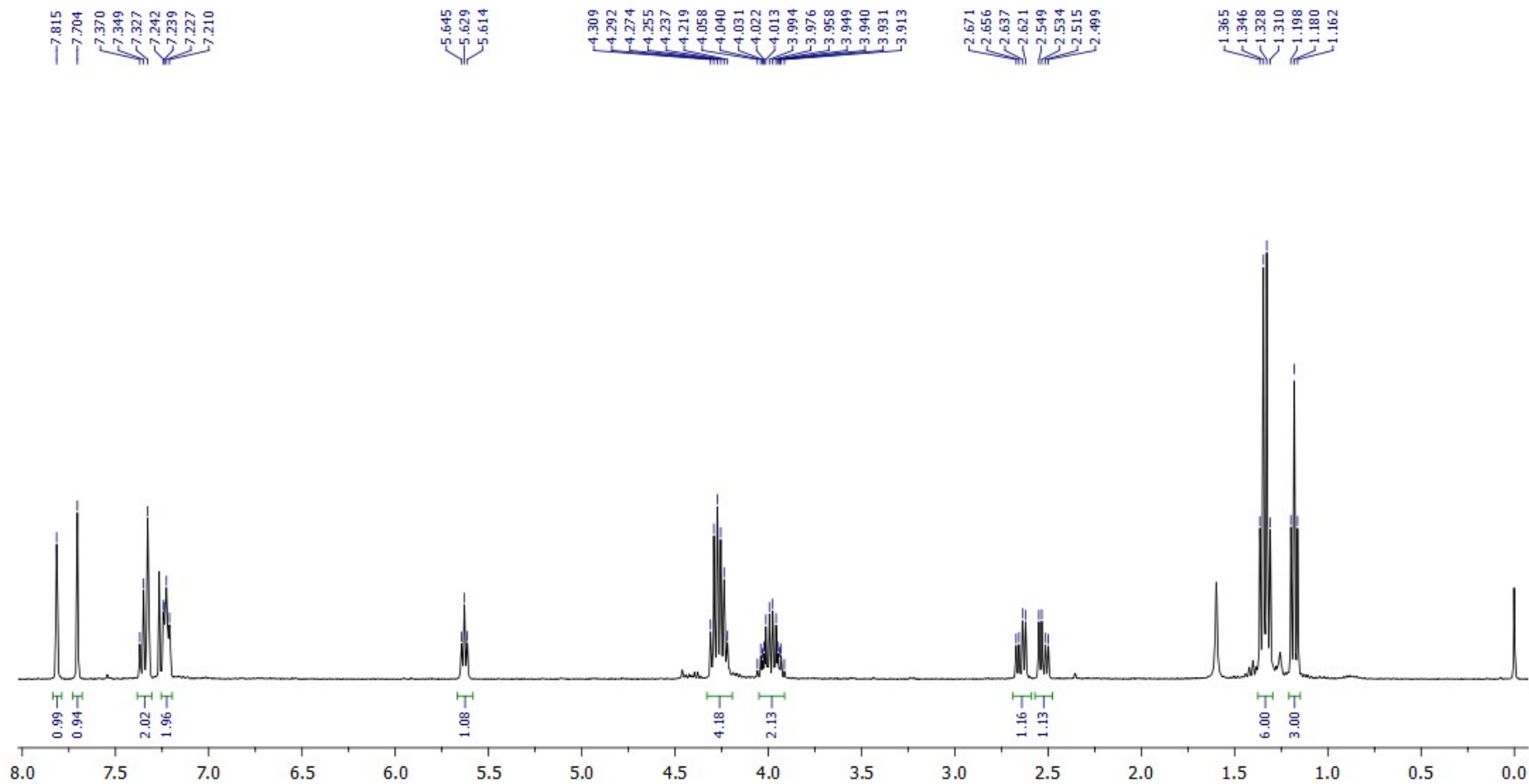
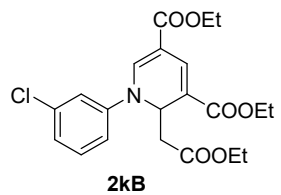
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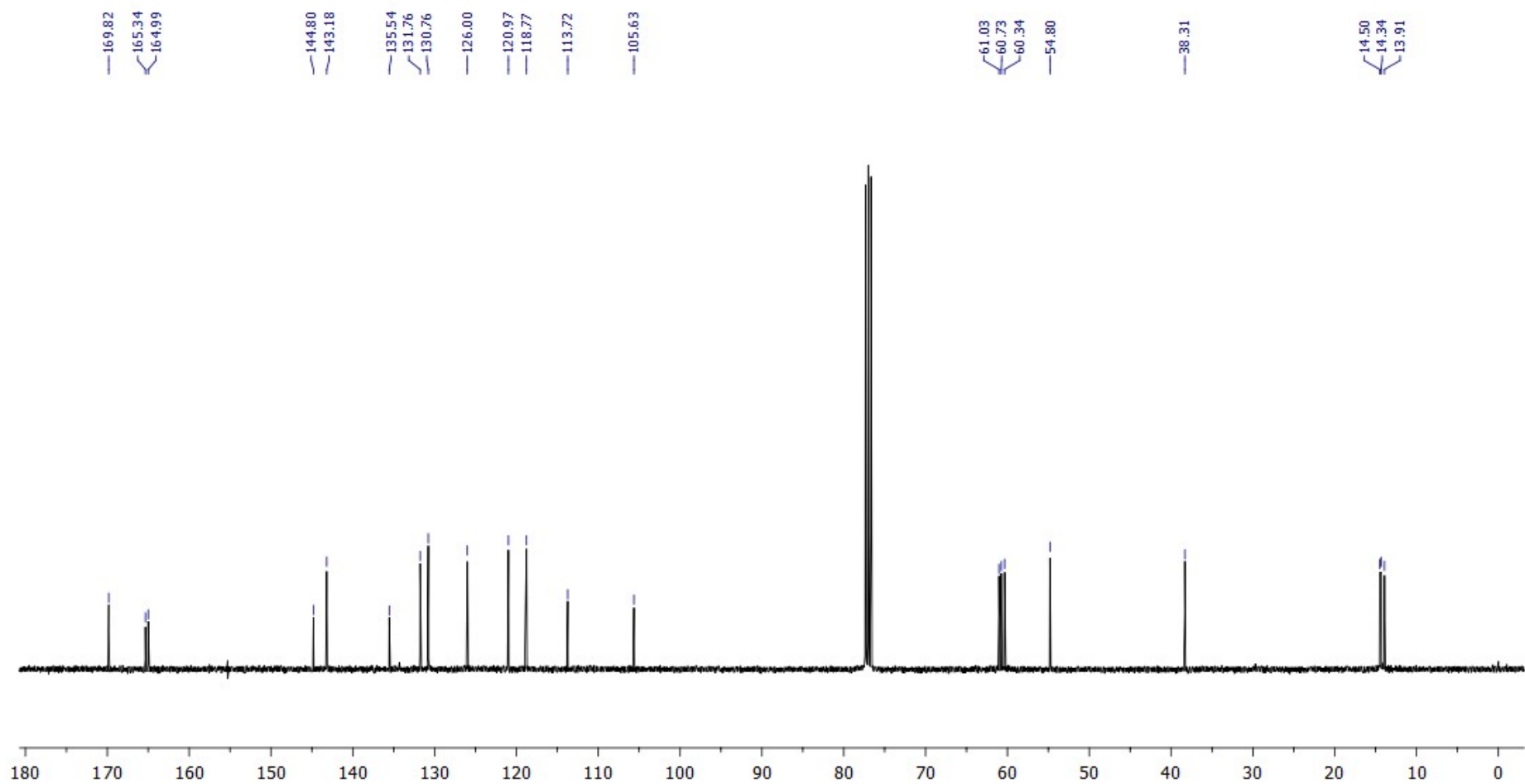
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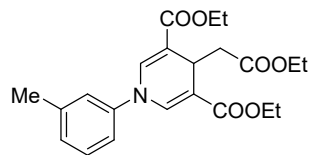
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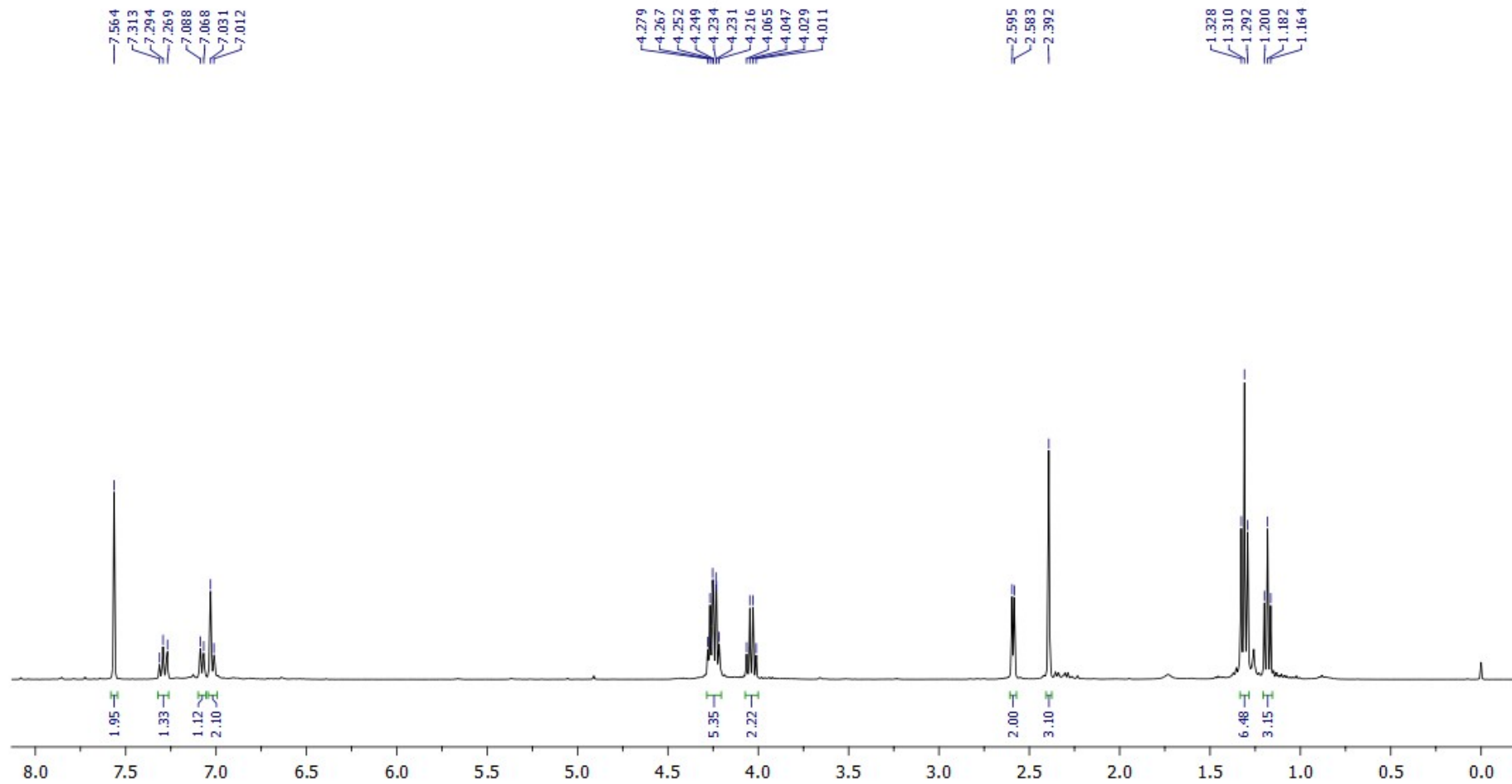
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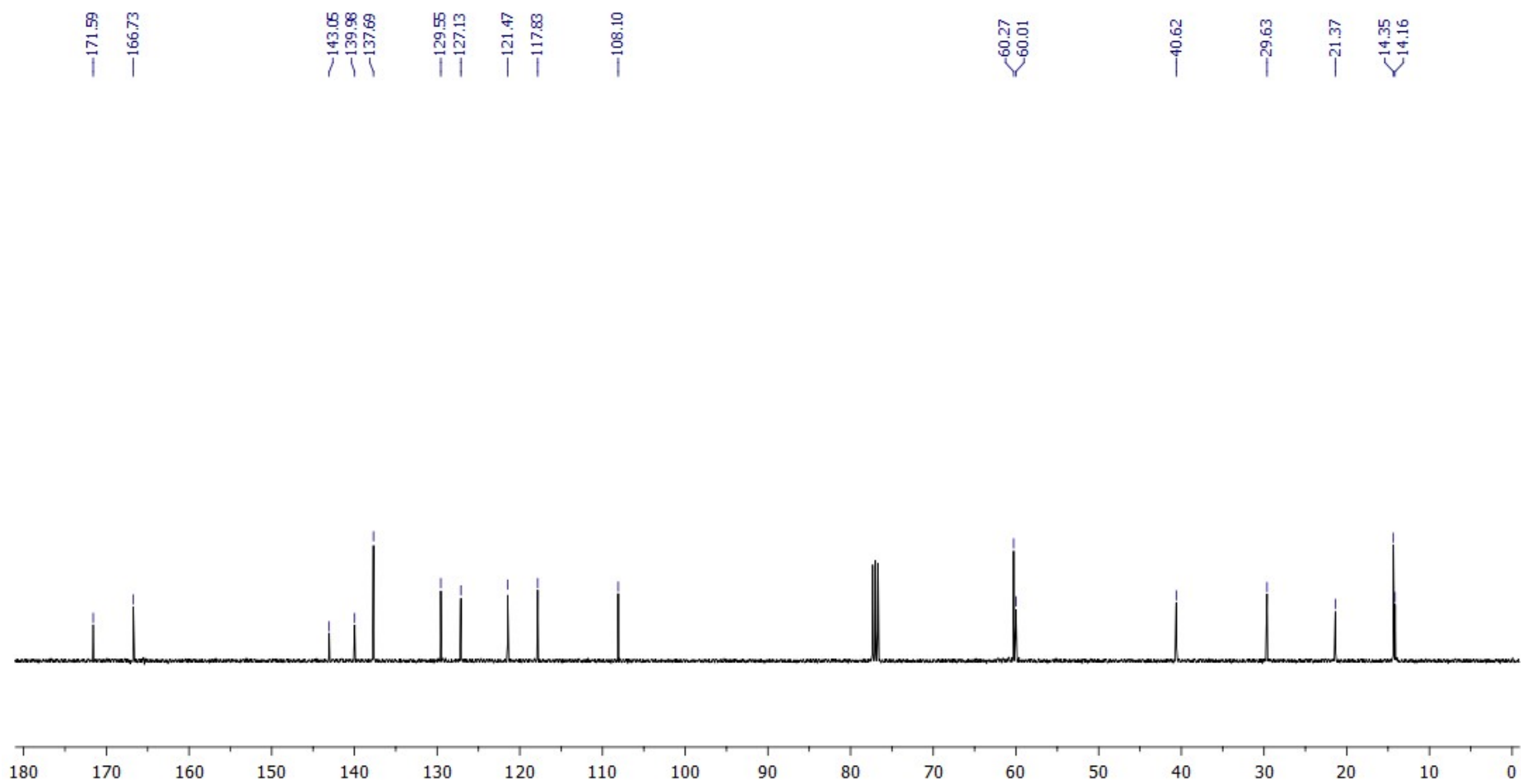
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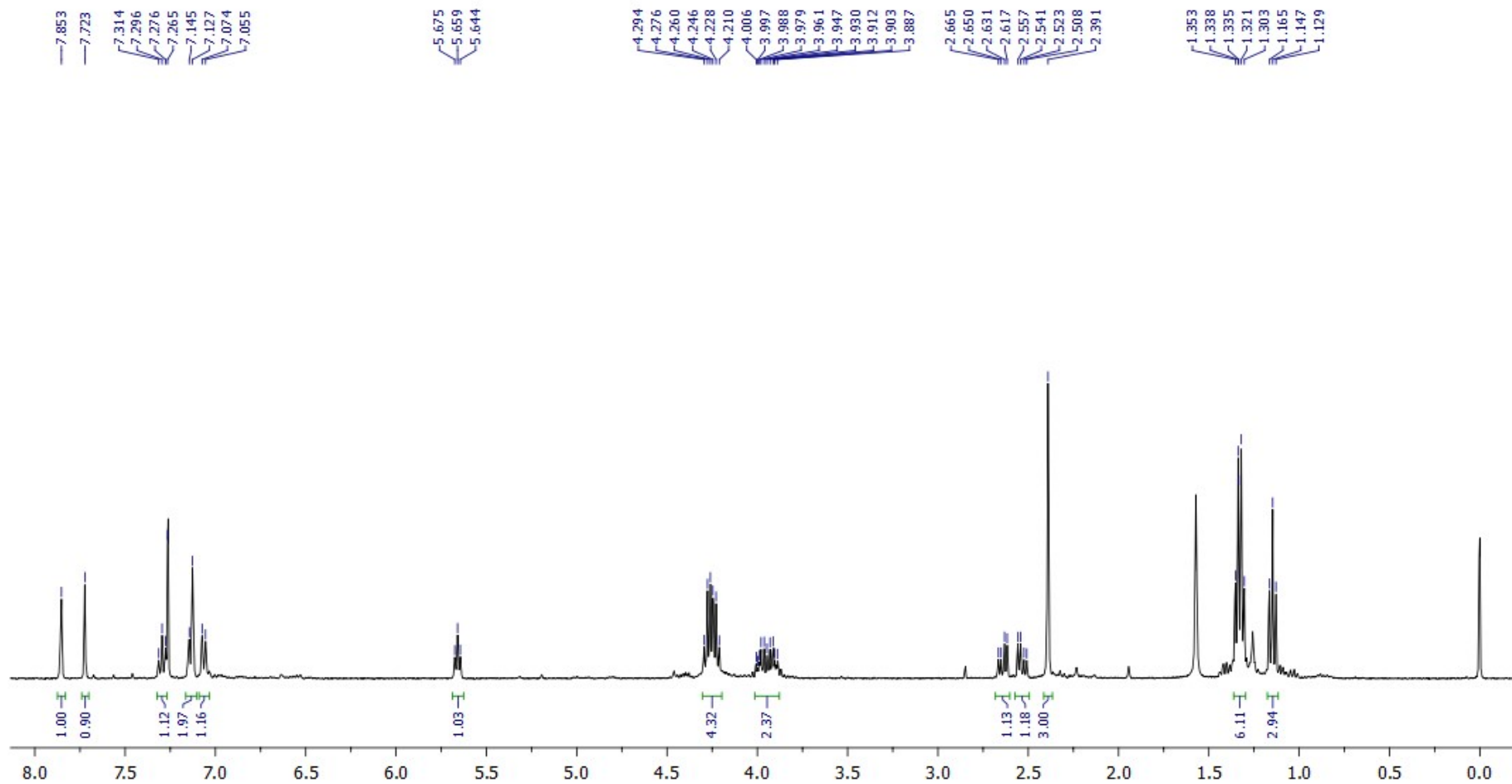
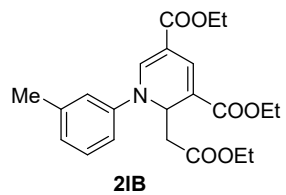
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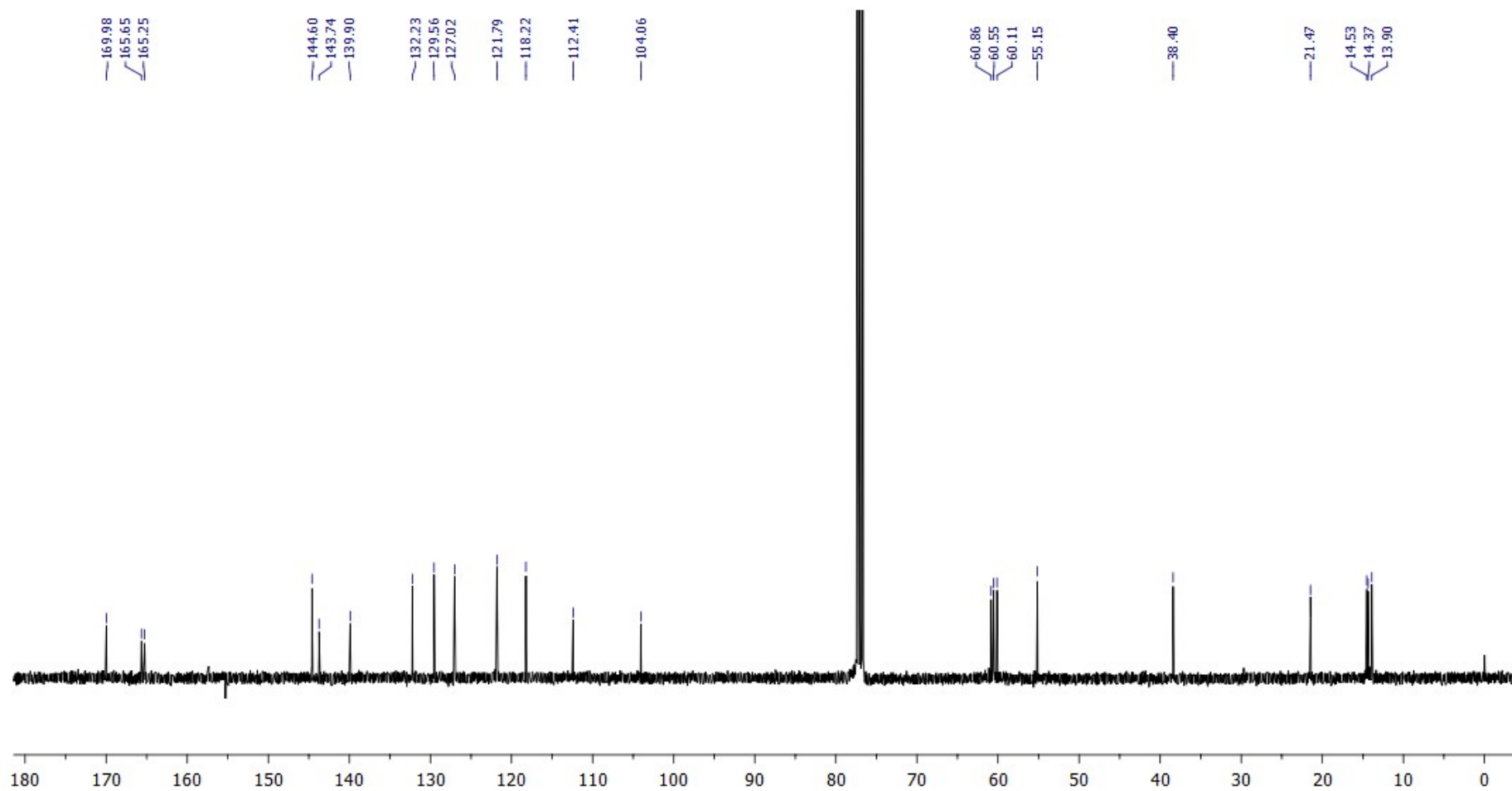
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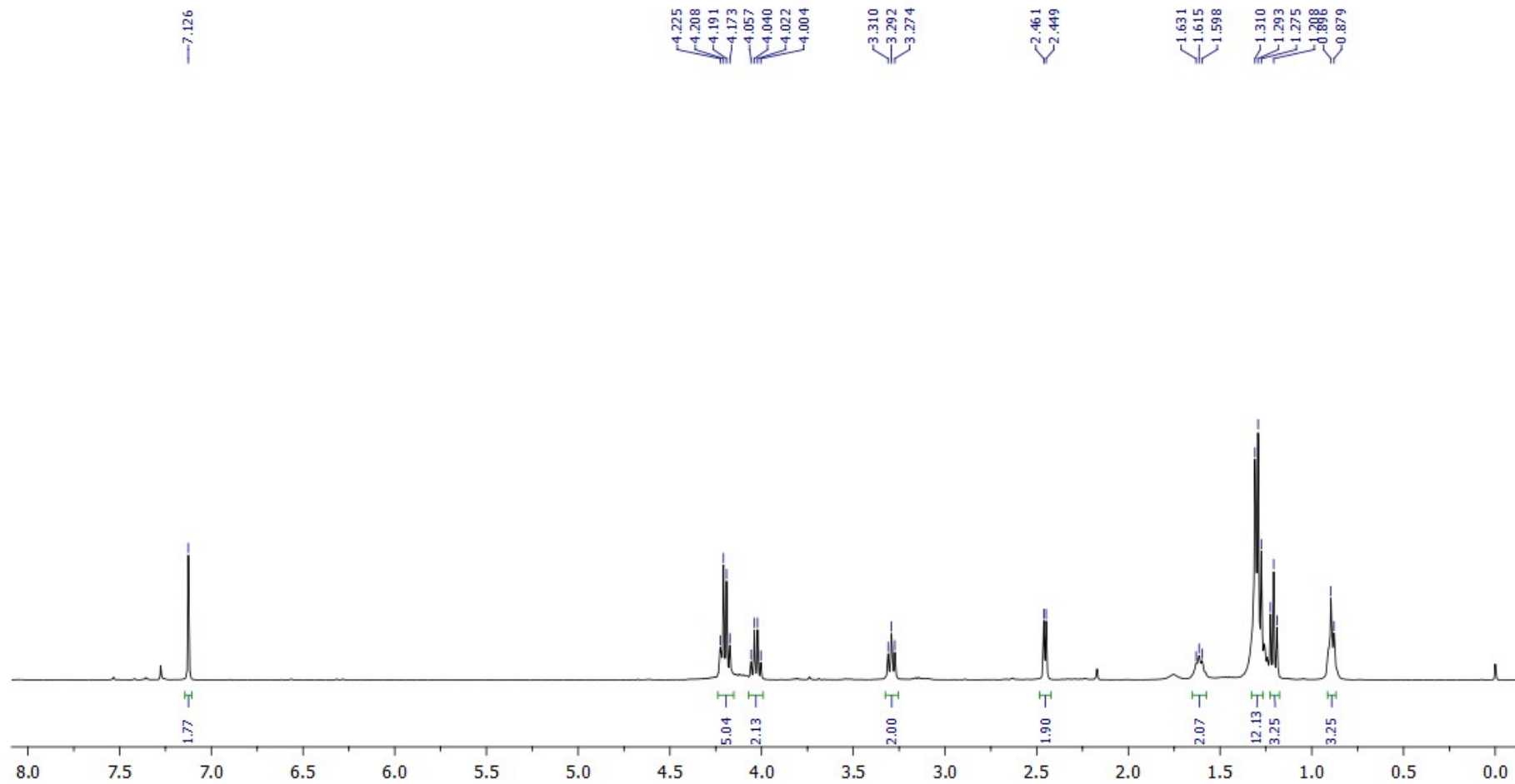
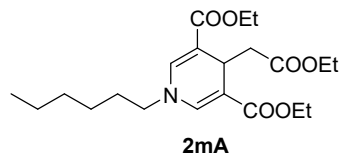
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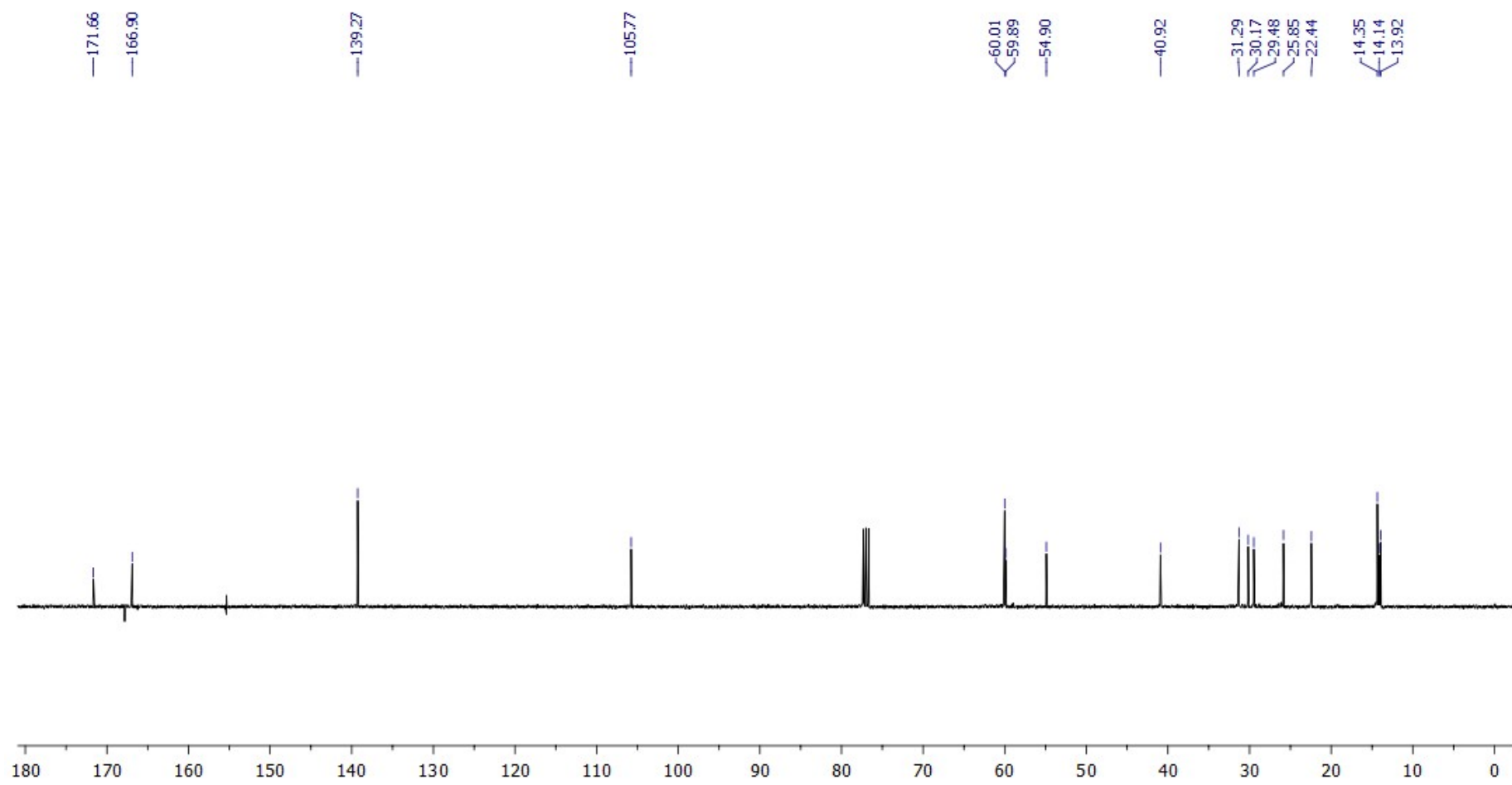
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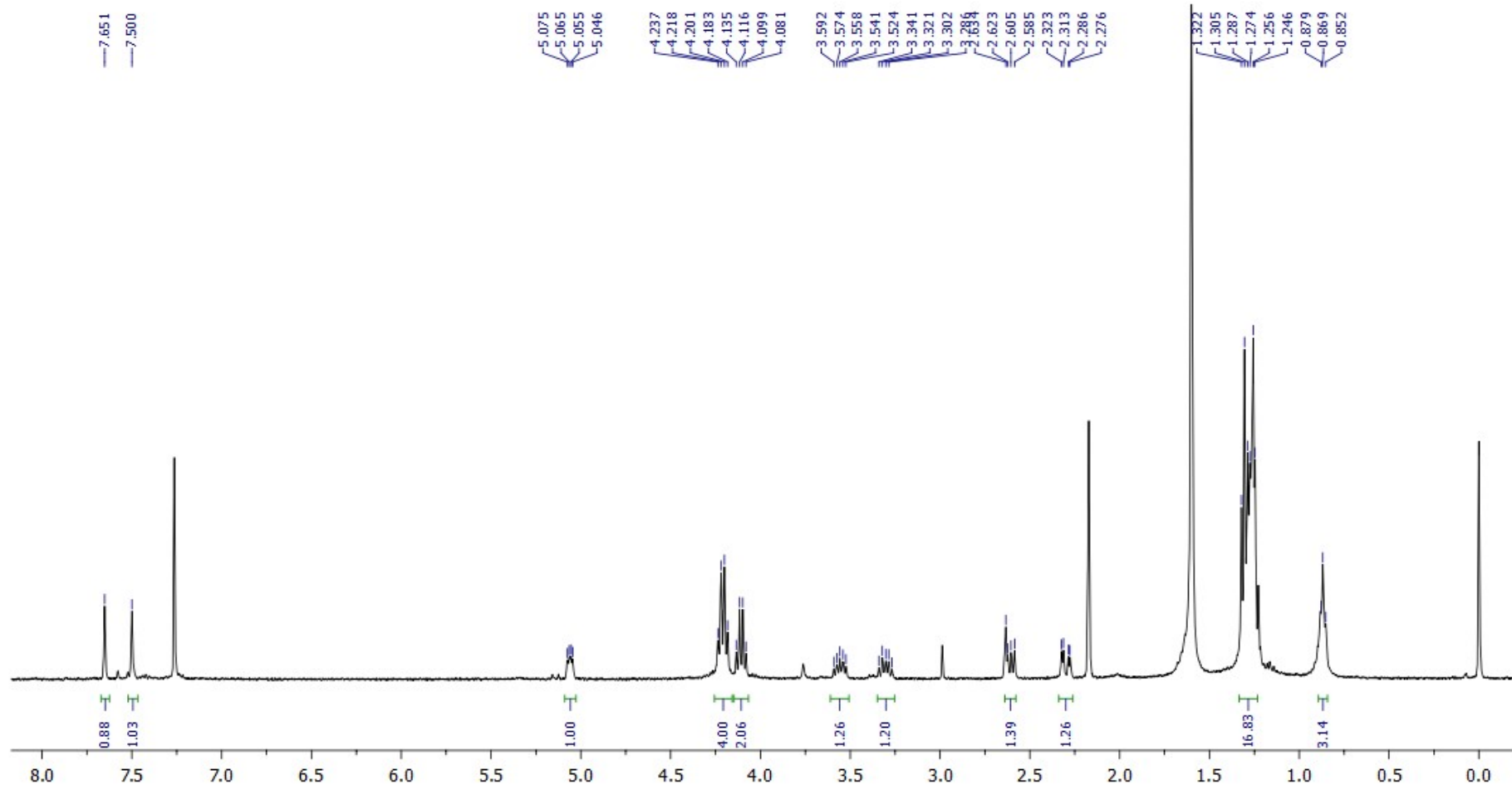
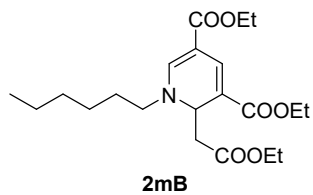
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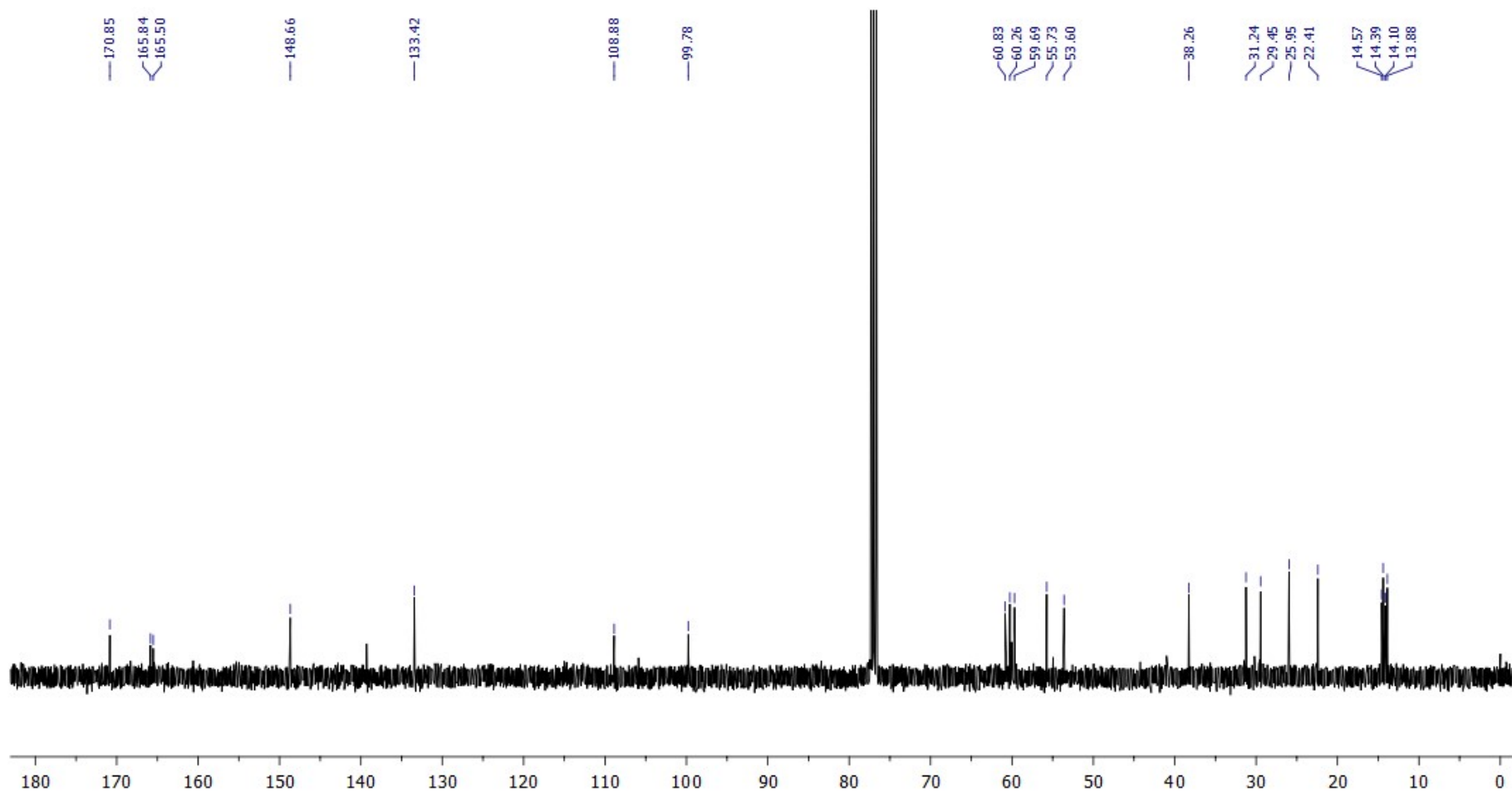
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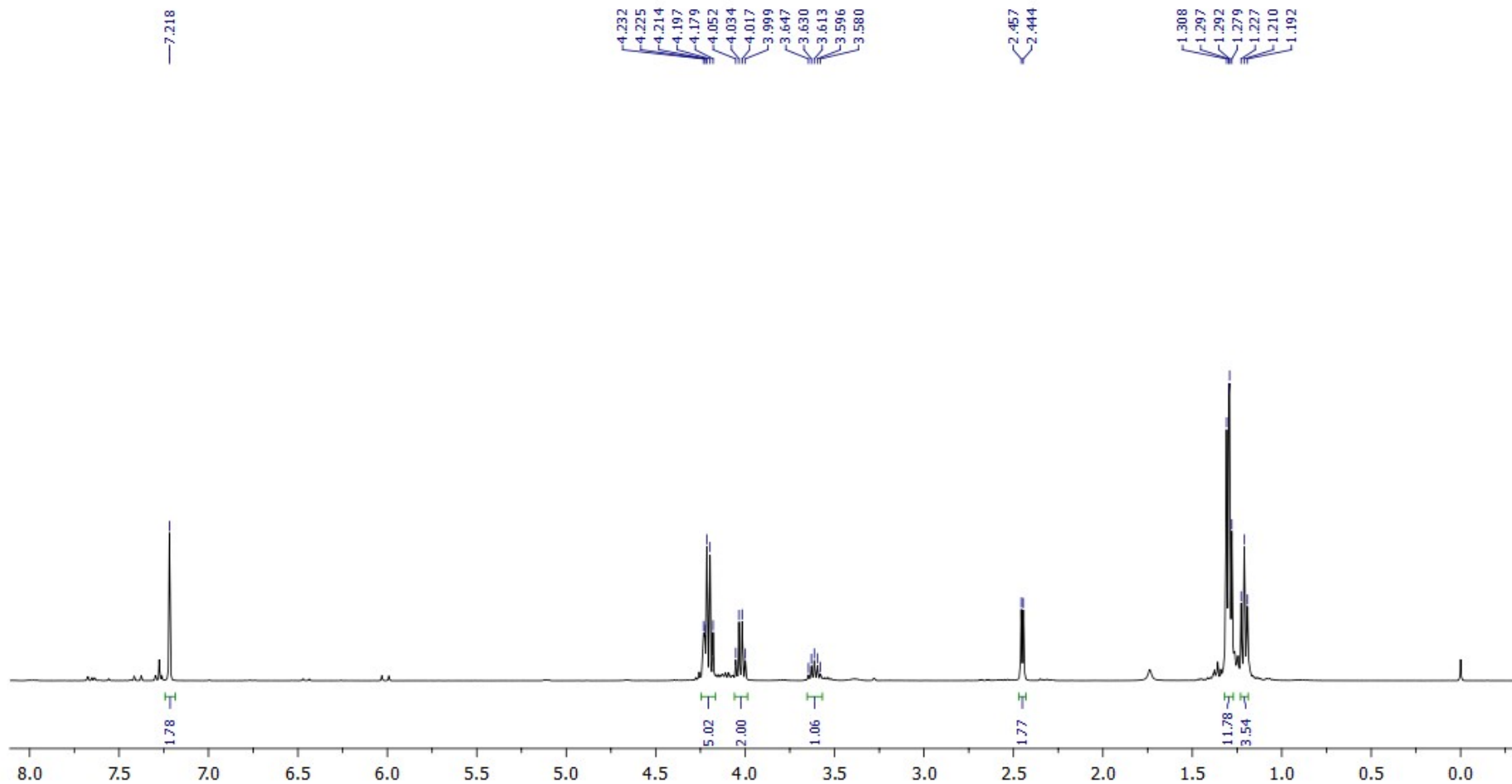
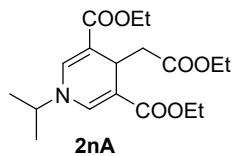
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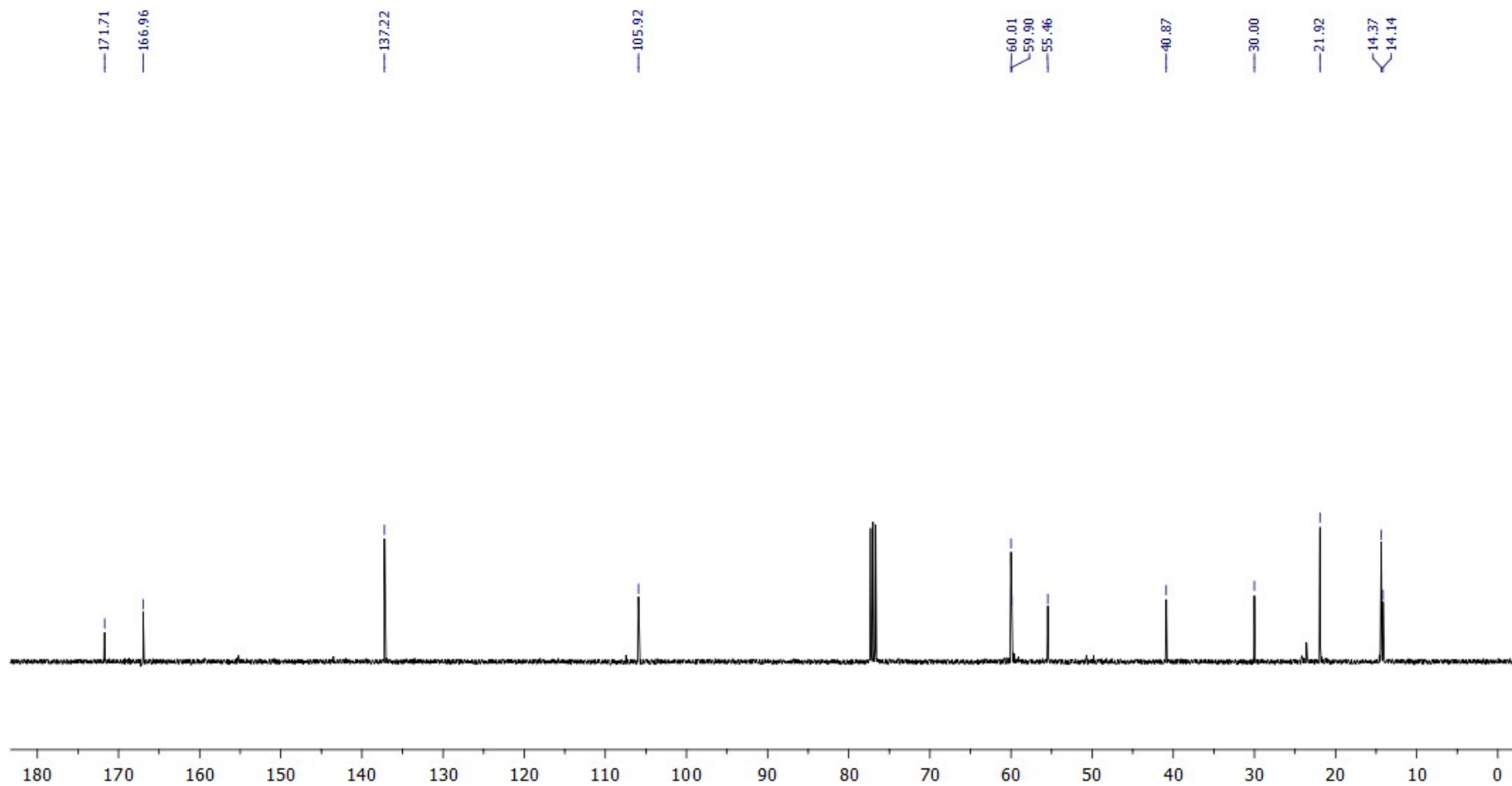
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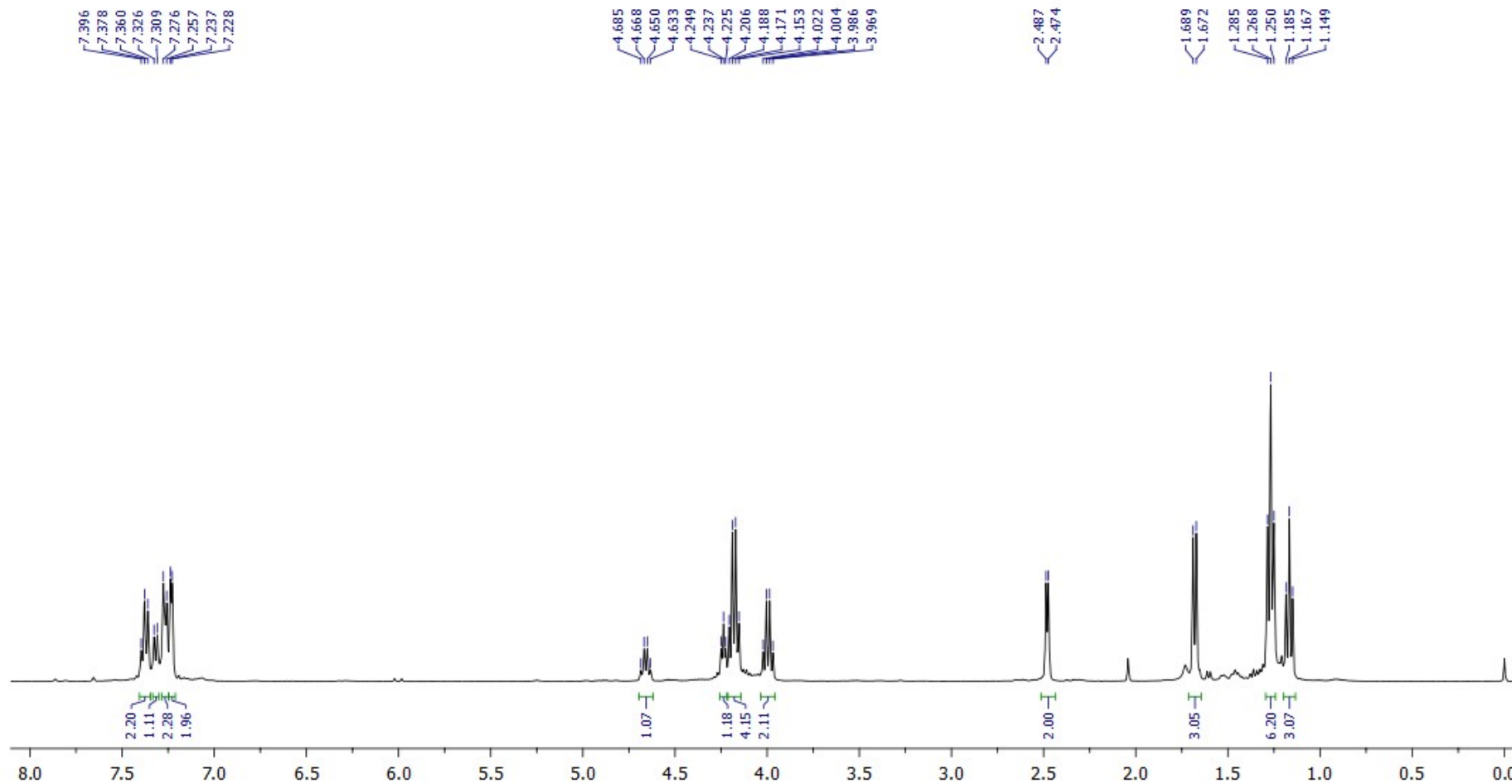
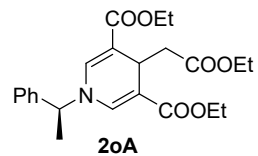
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



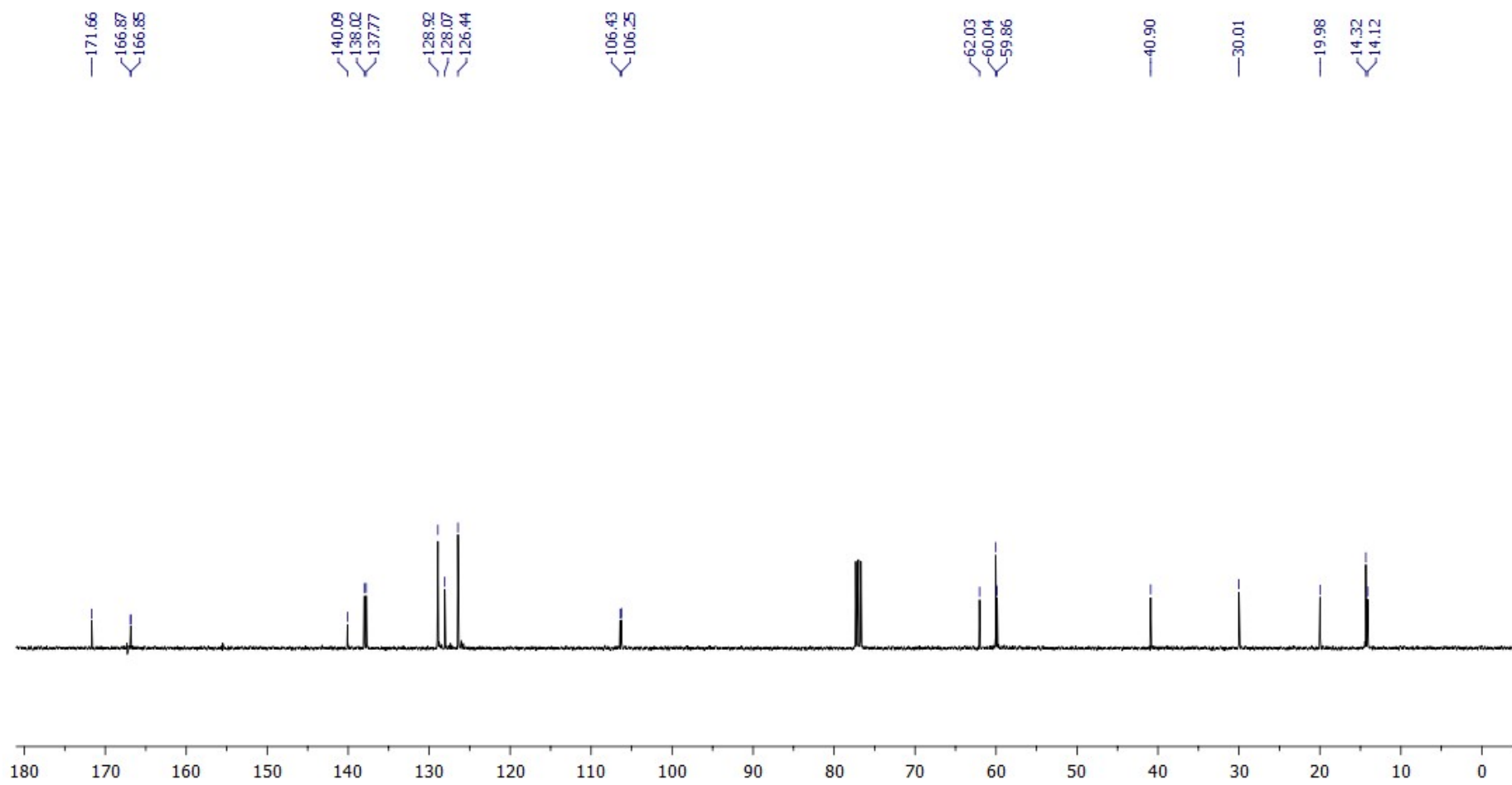
¹H NMR (400.1 MHz, CDCl₃)



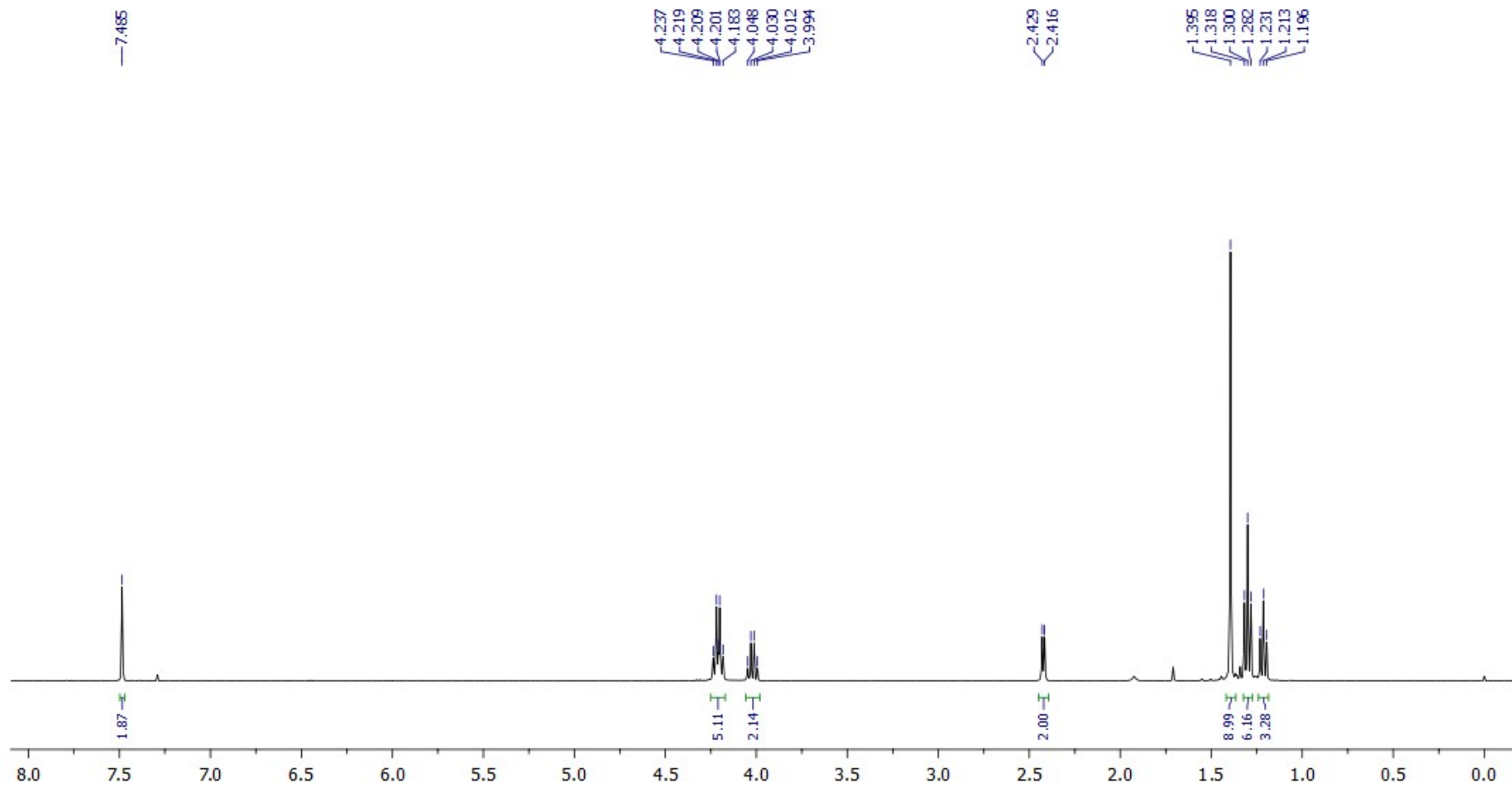
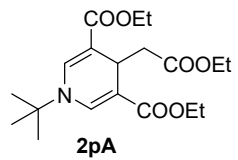
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



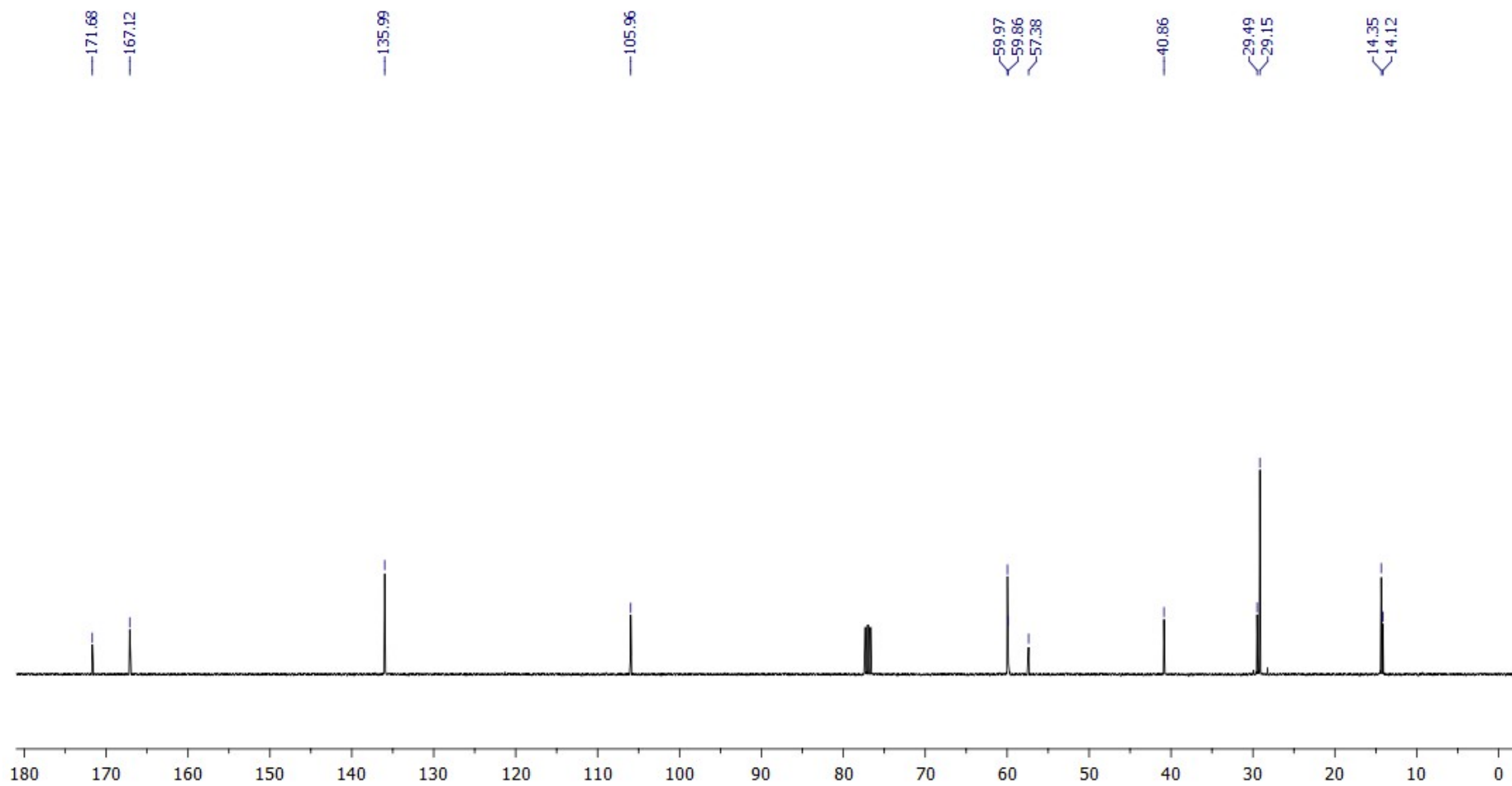
¹H NMR (400.1 MHz, CDCl₃)



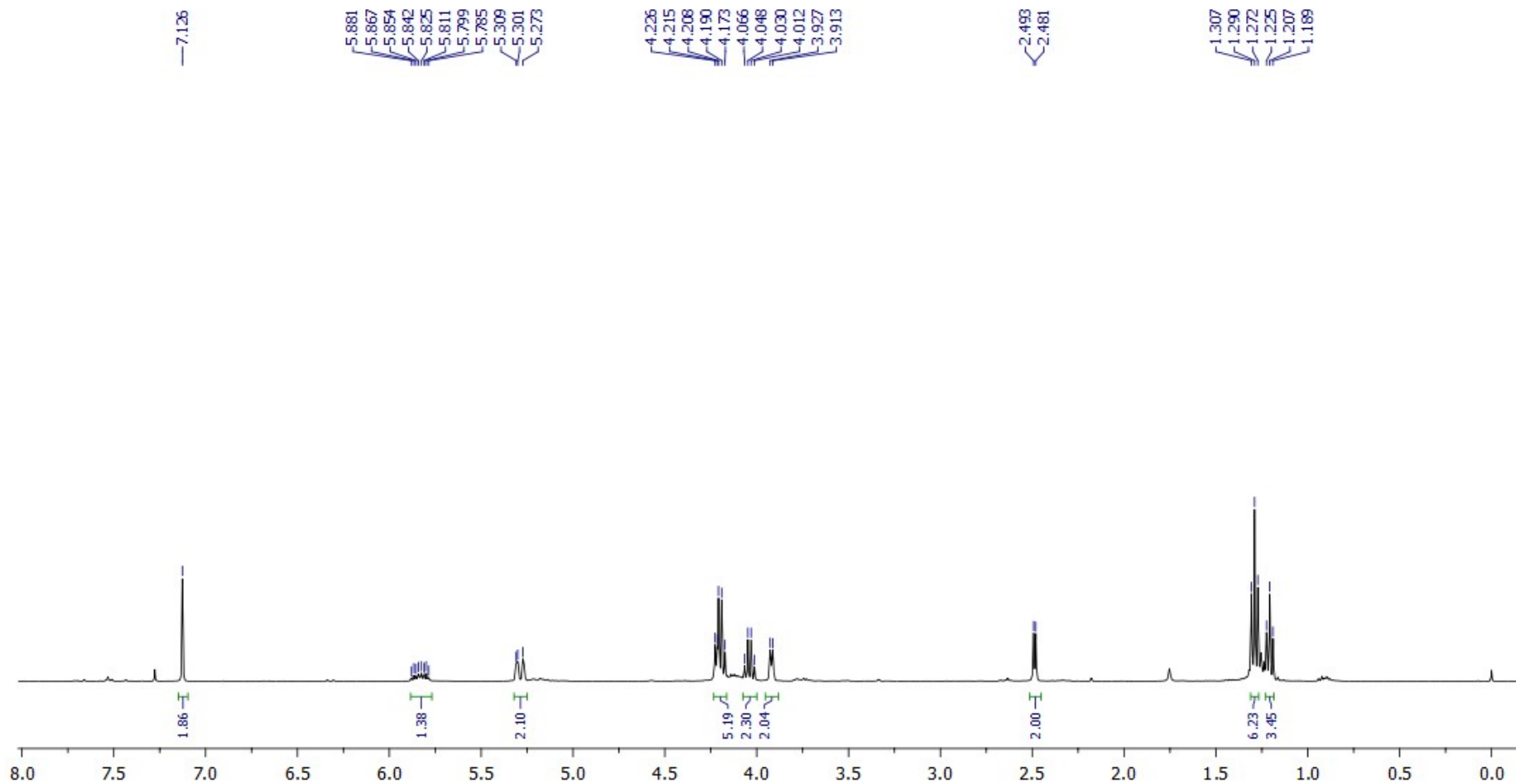
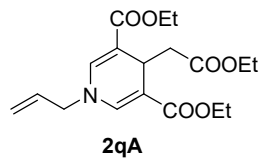
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



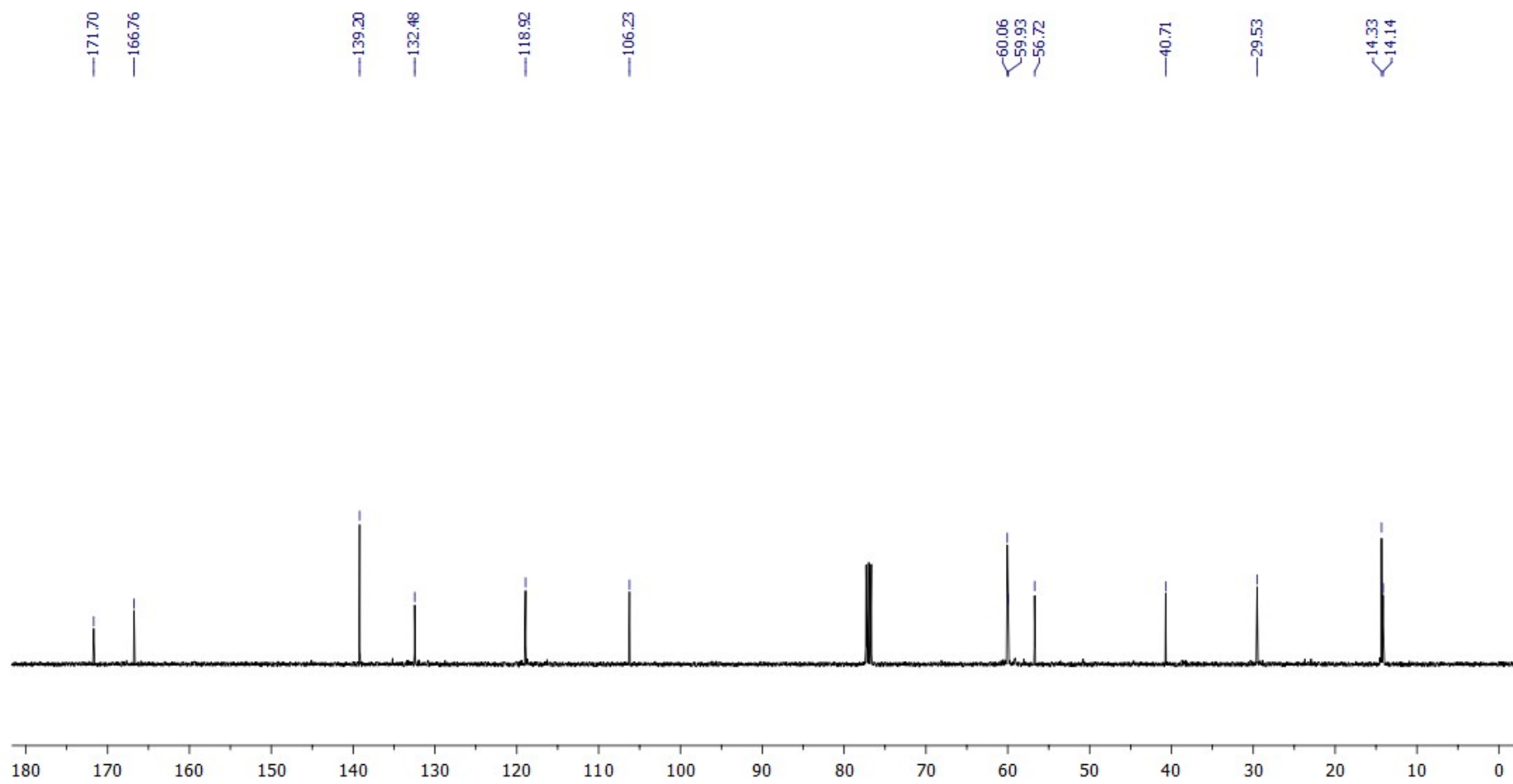
¹H NMR (400.1 MHz, CDCl₃)



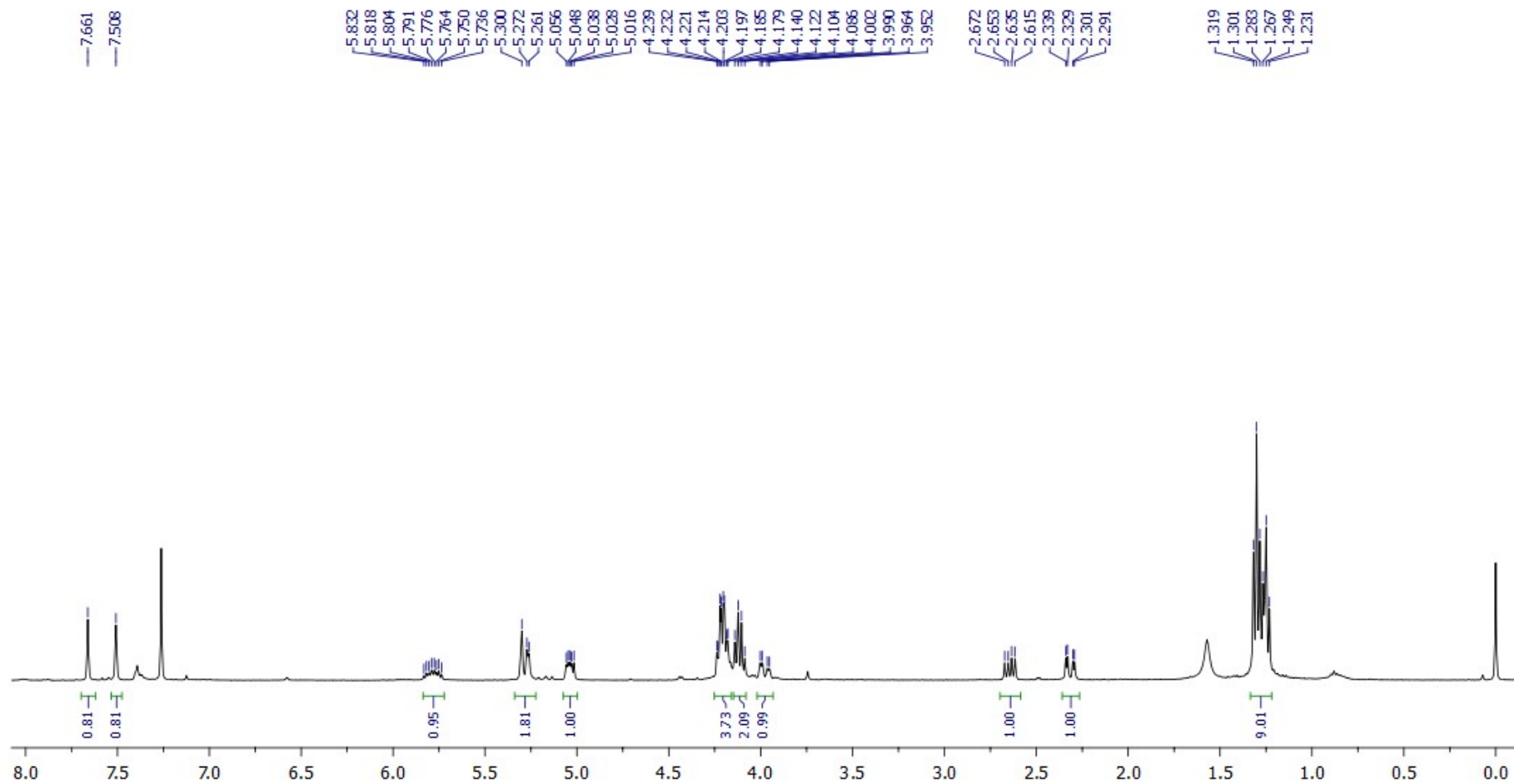
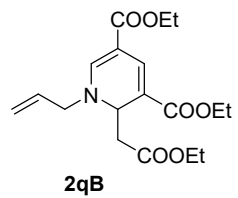
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



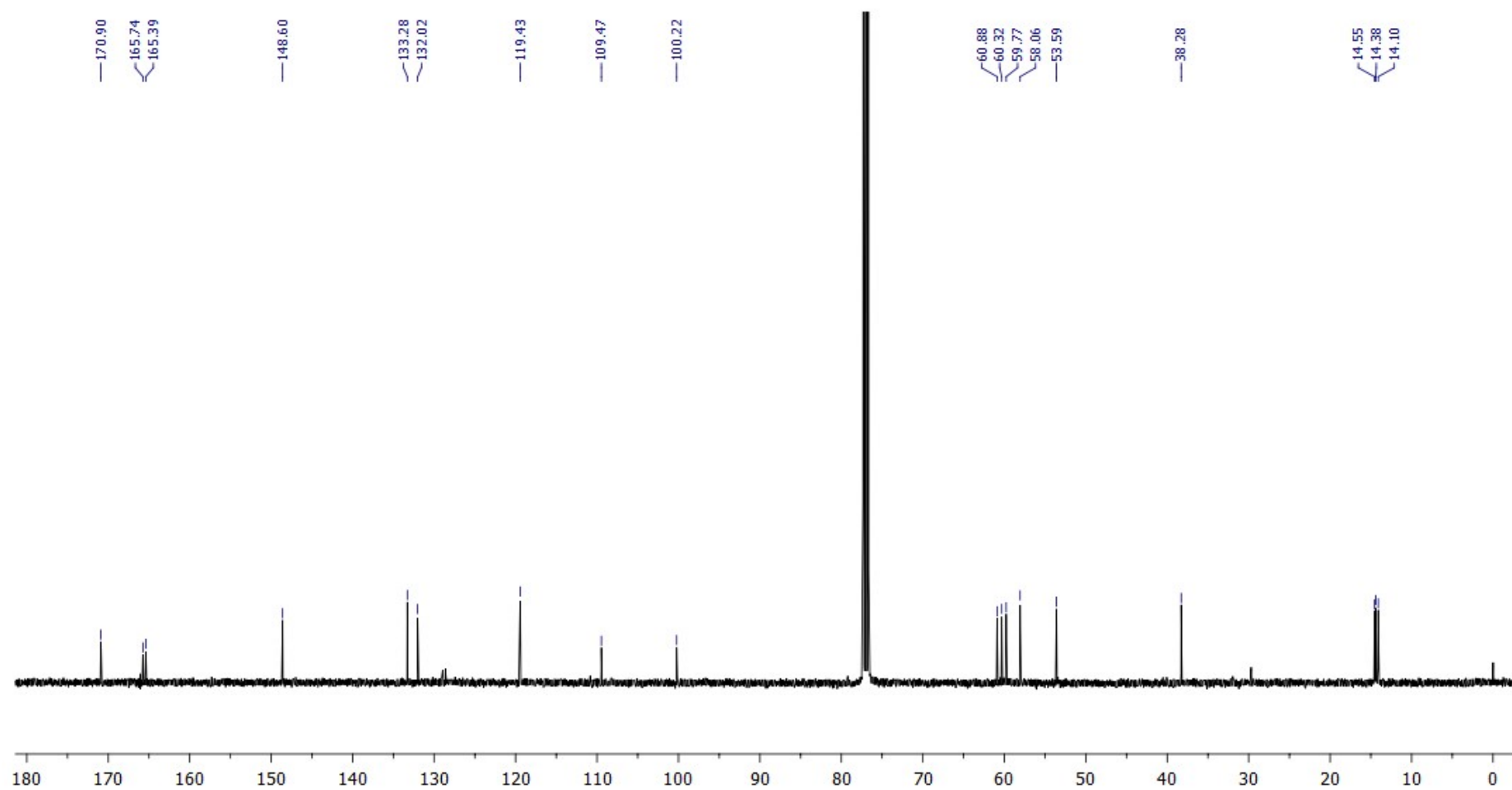
¹H NMR (400.1 MHz, CDCl₃)



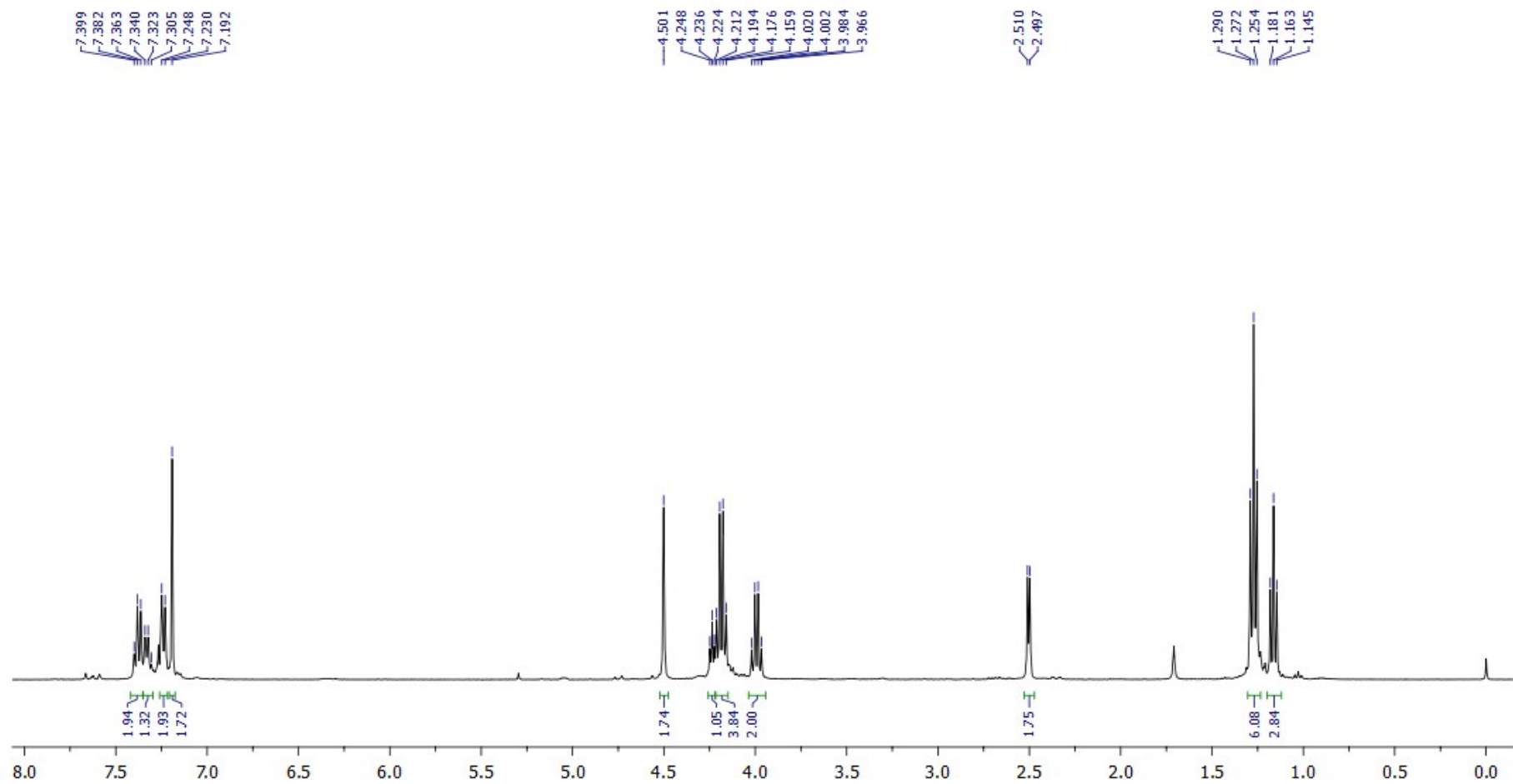
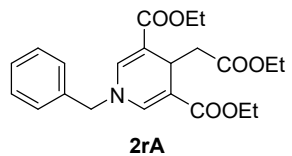
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



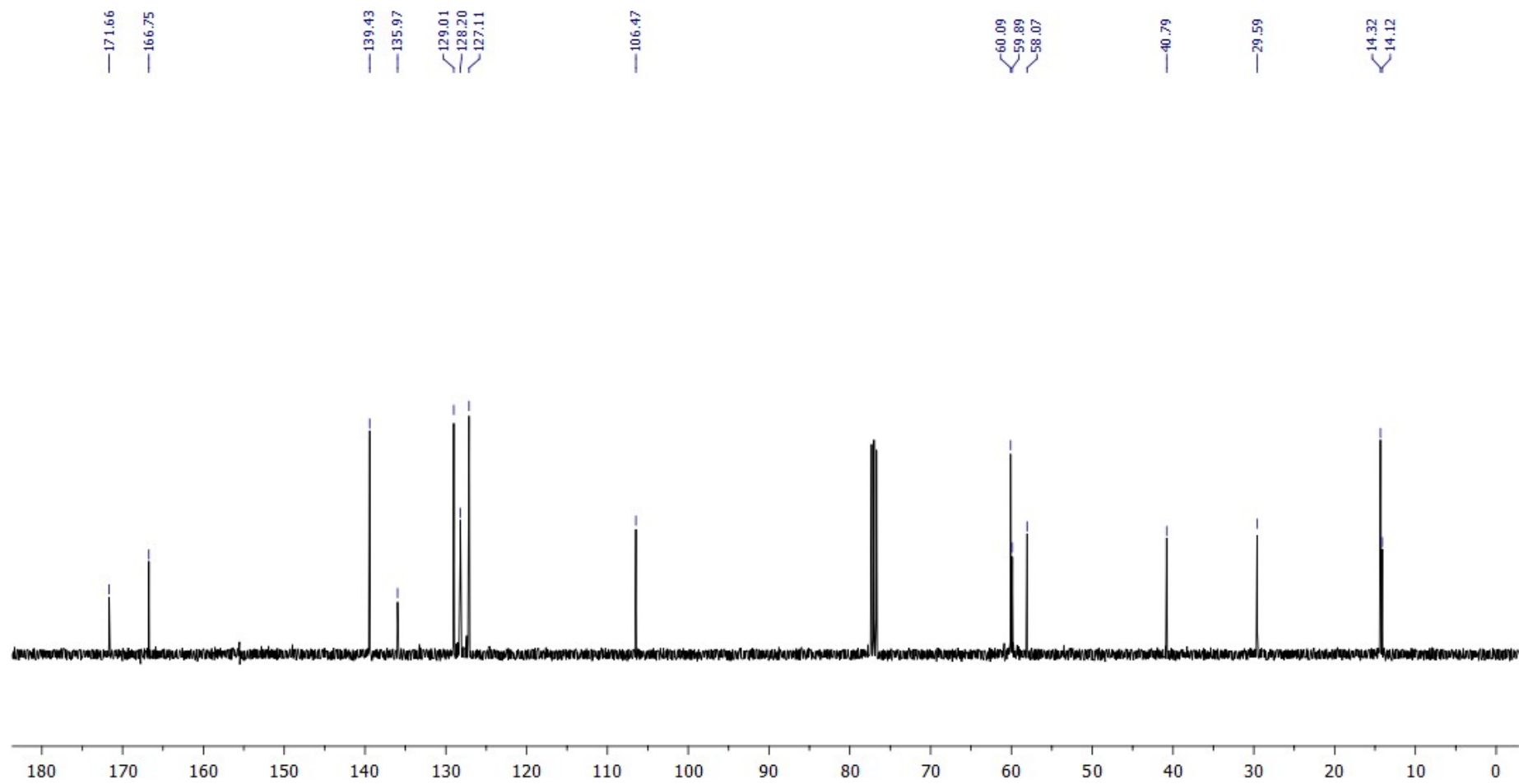
¹H NMR (400.1 MHz, CDCl₃)



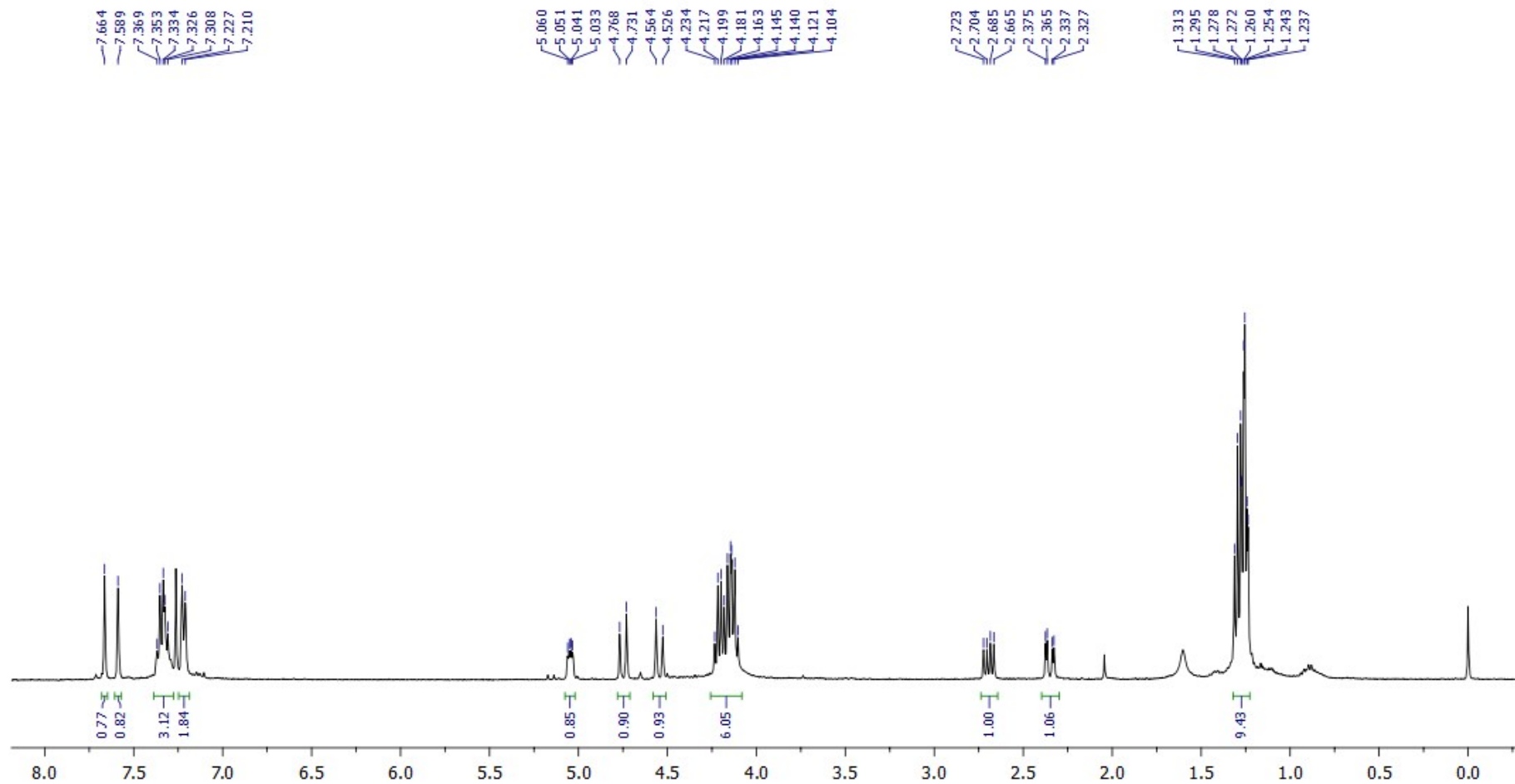
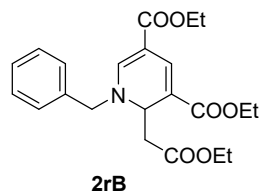
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



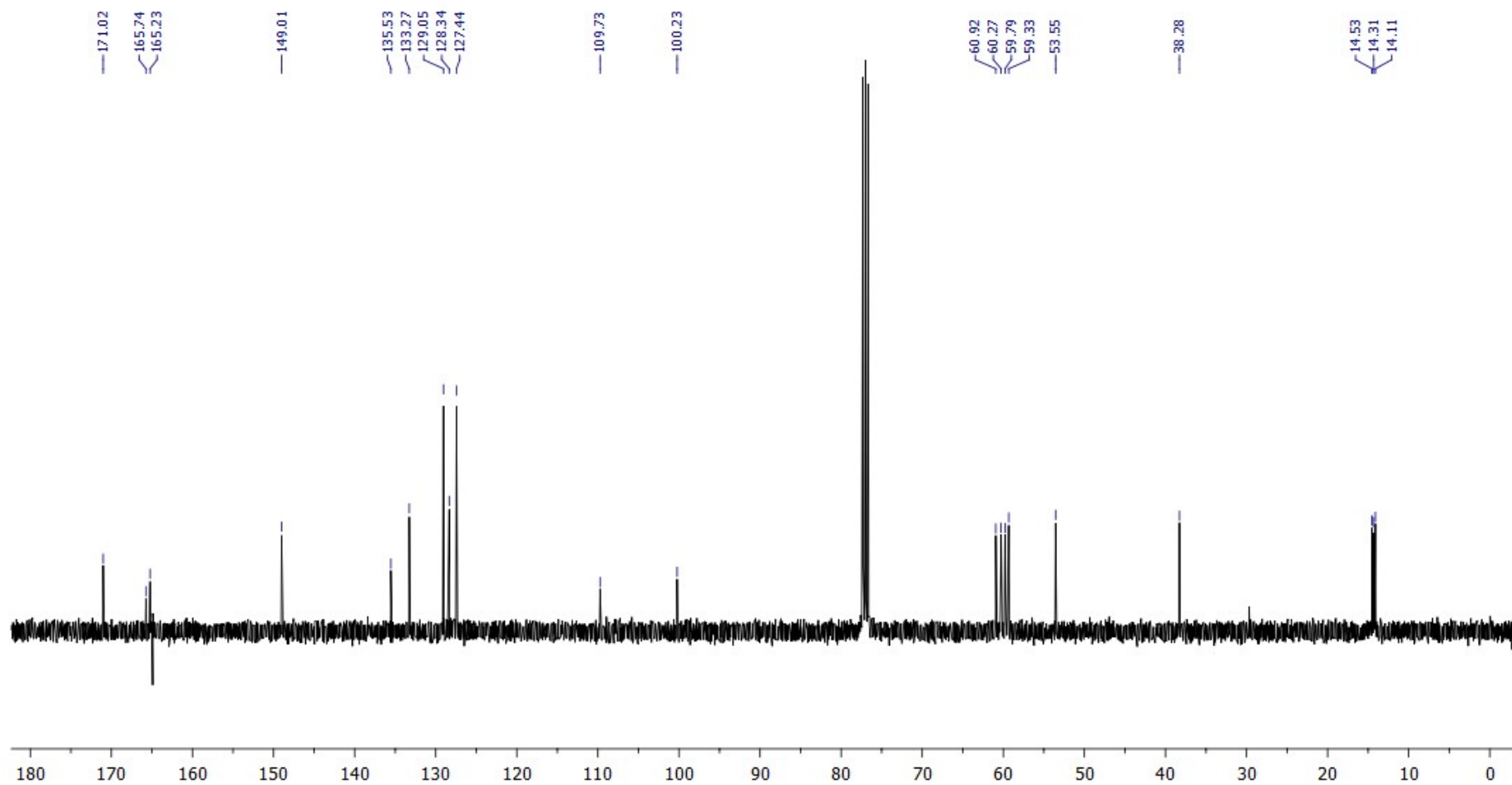
$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



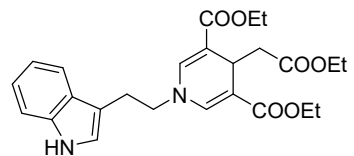
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



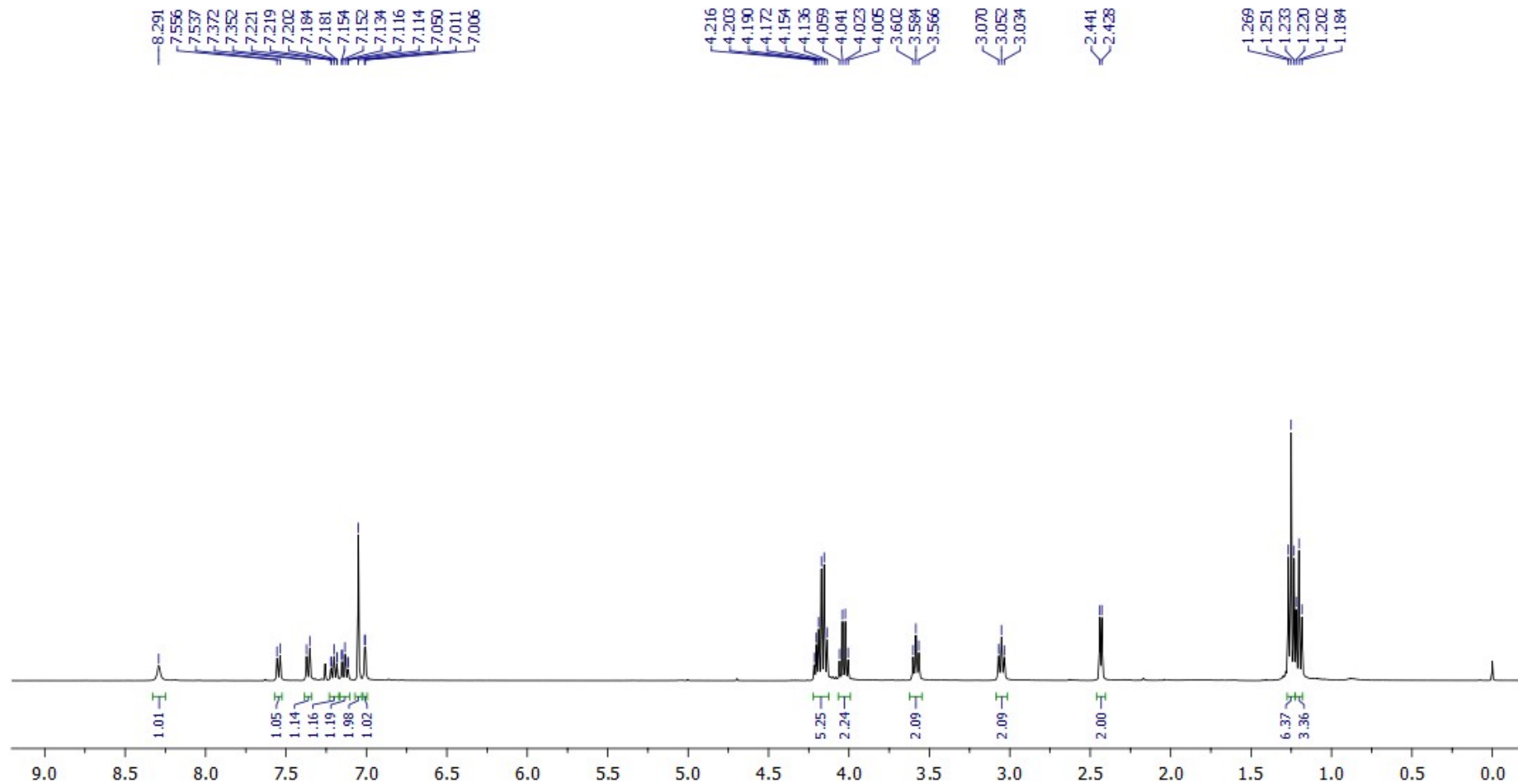
$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



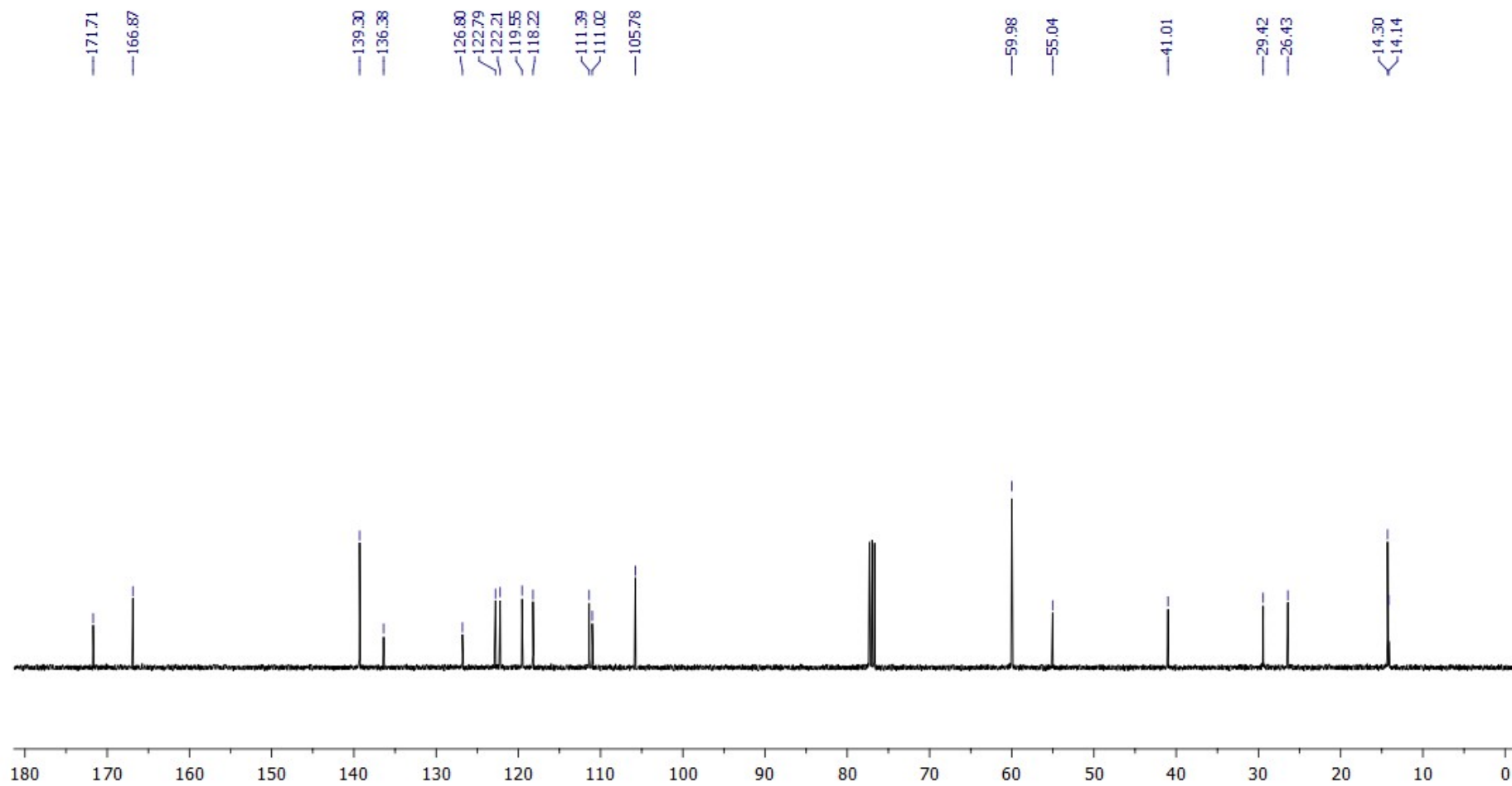
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



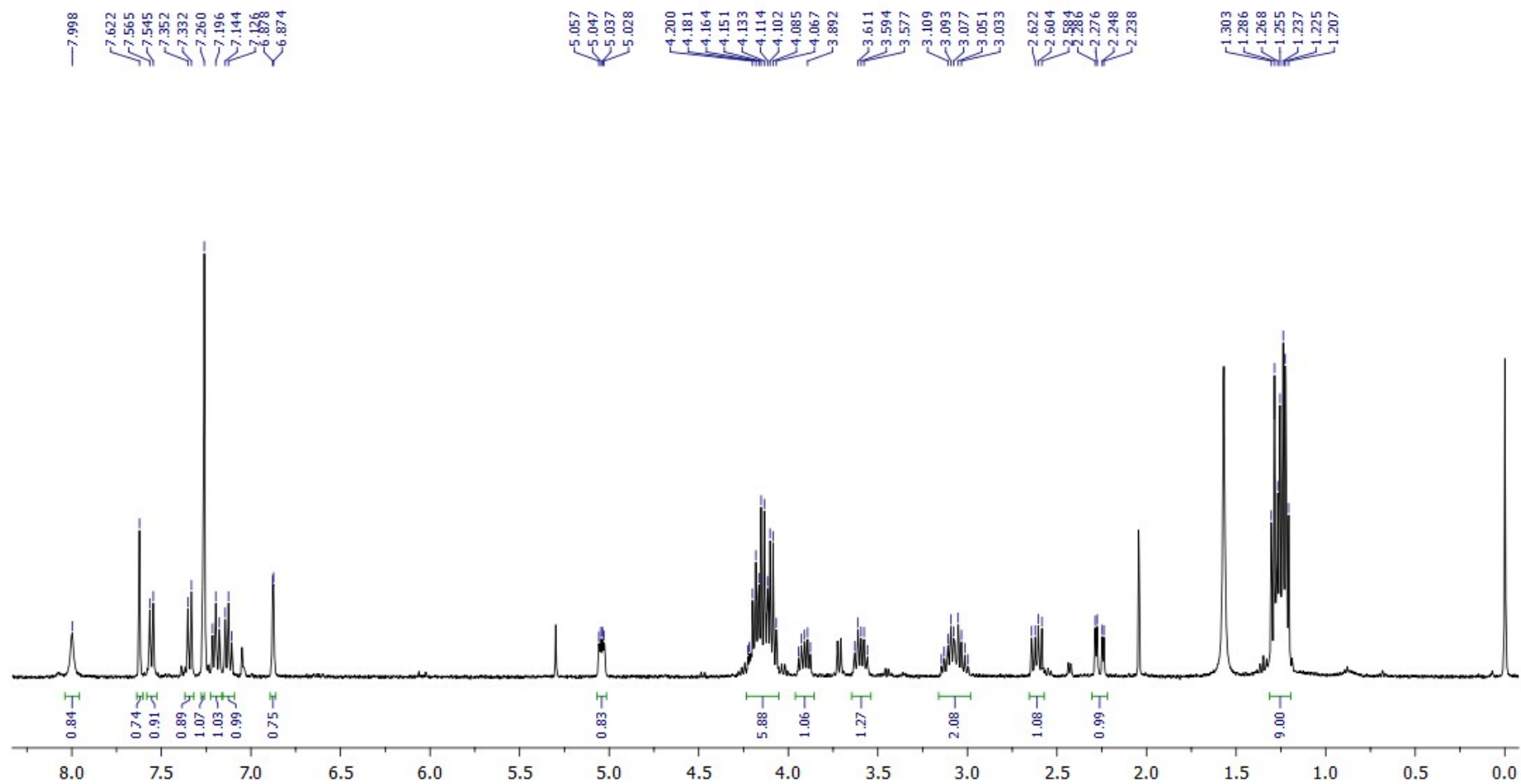
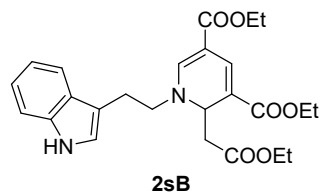
2sA



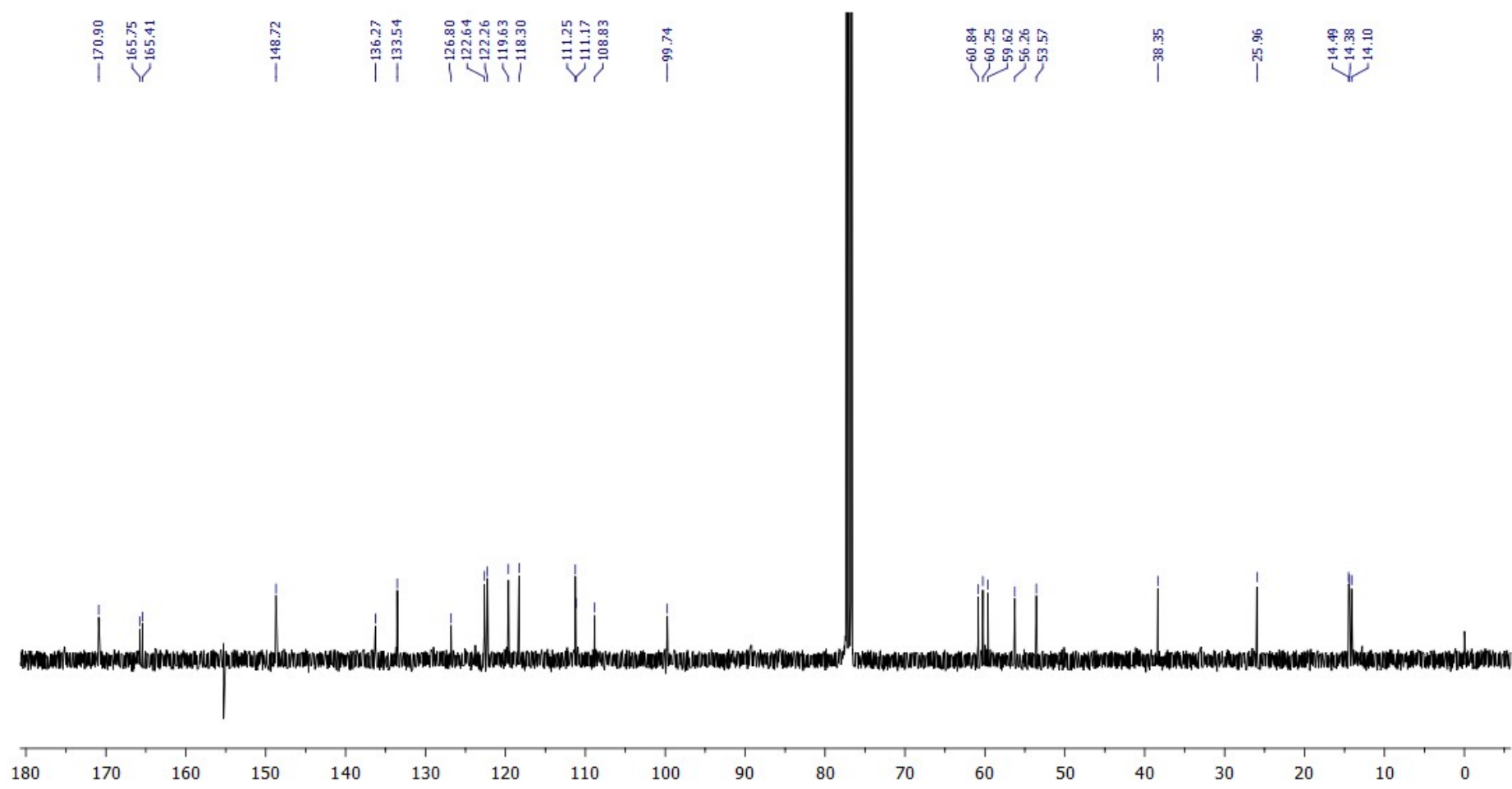
¹H NMR (400.1 MHz, CDCl₃)



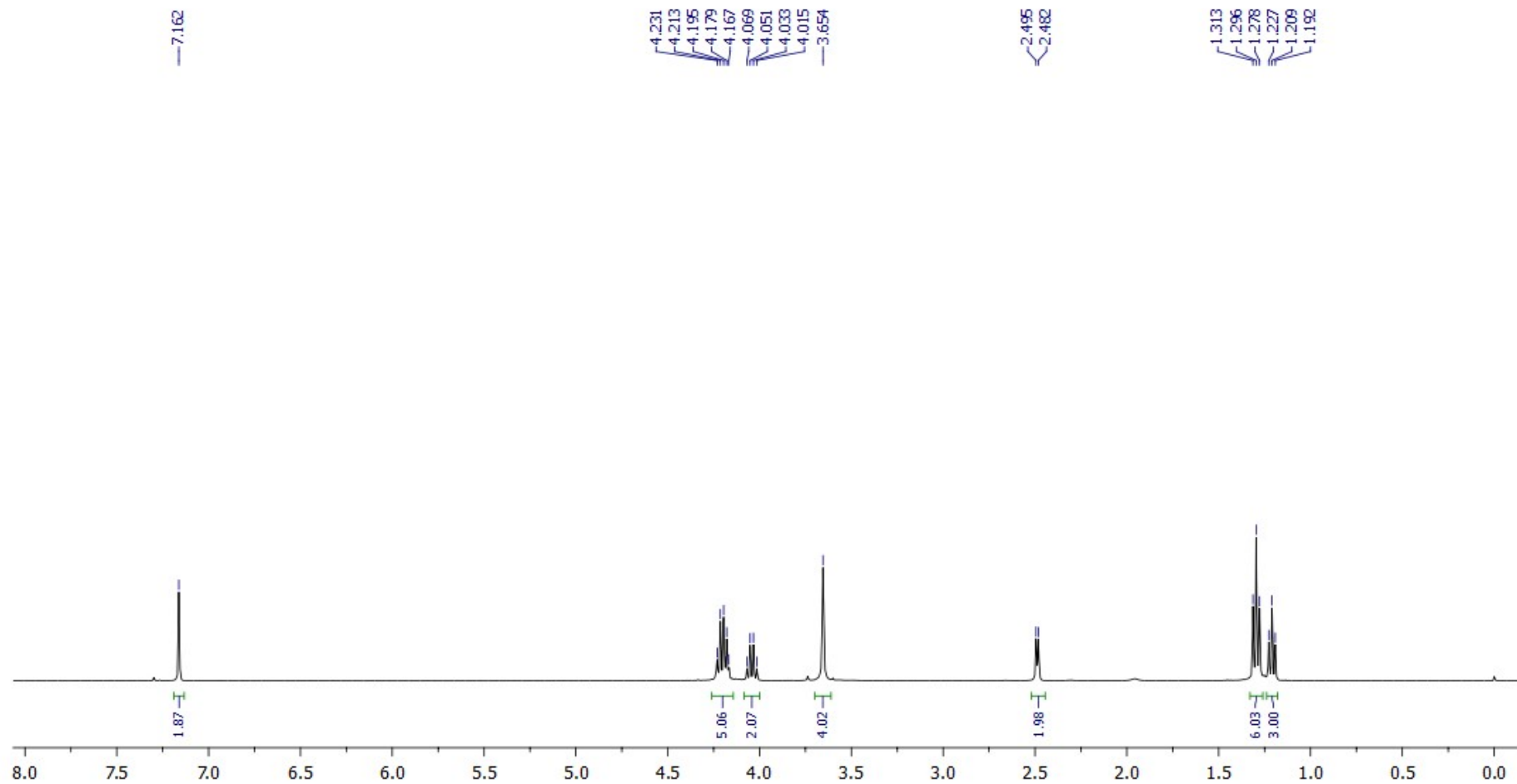
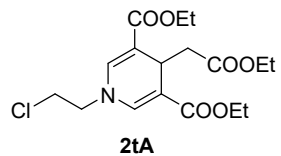
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



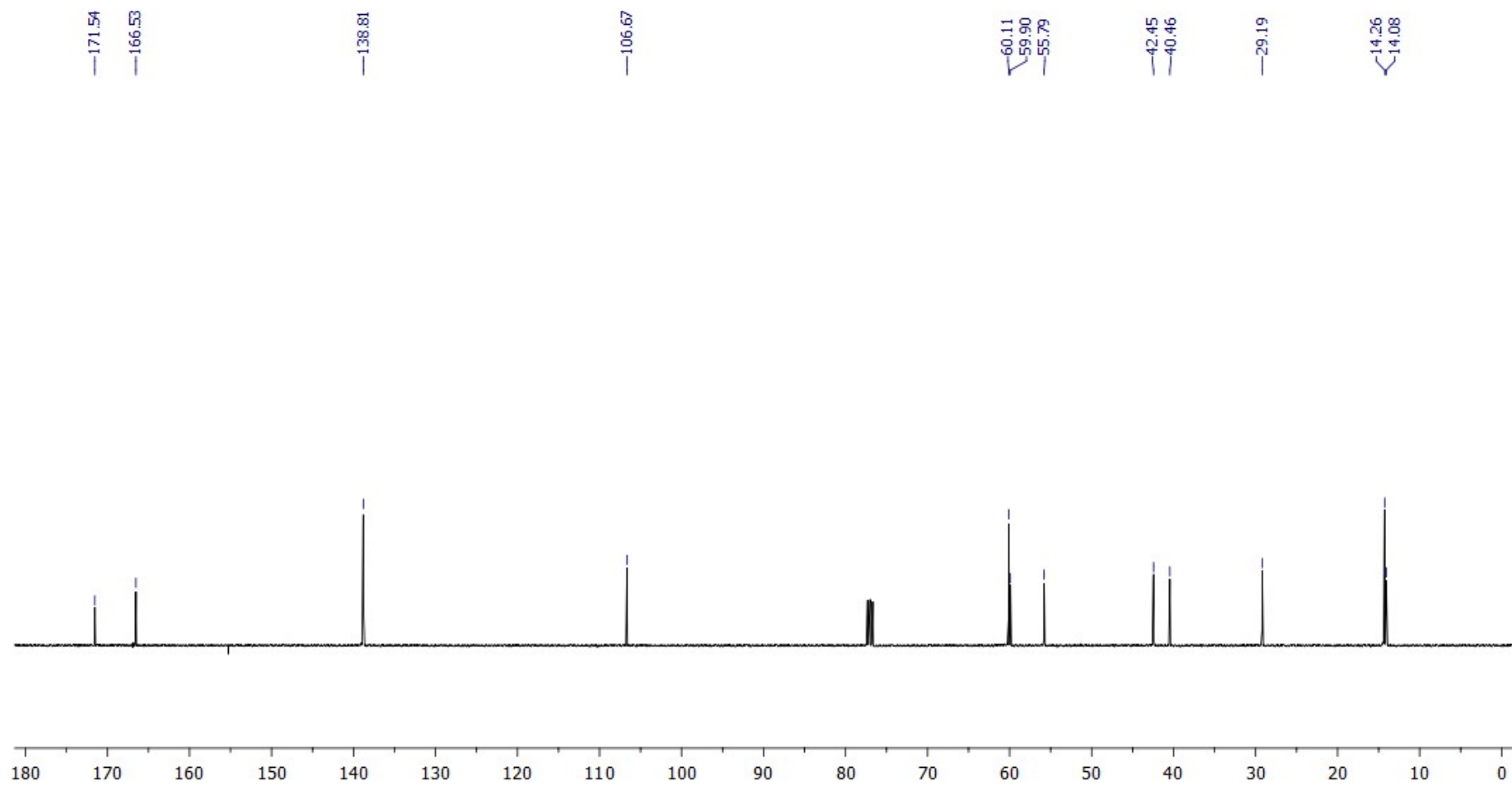
$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



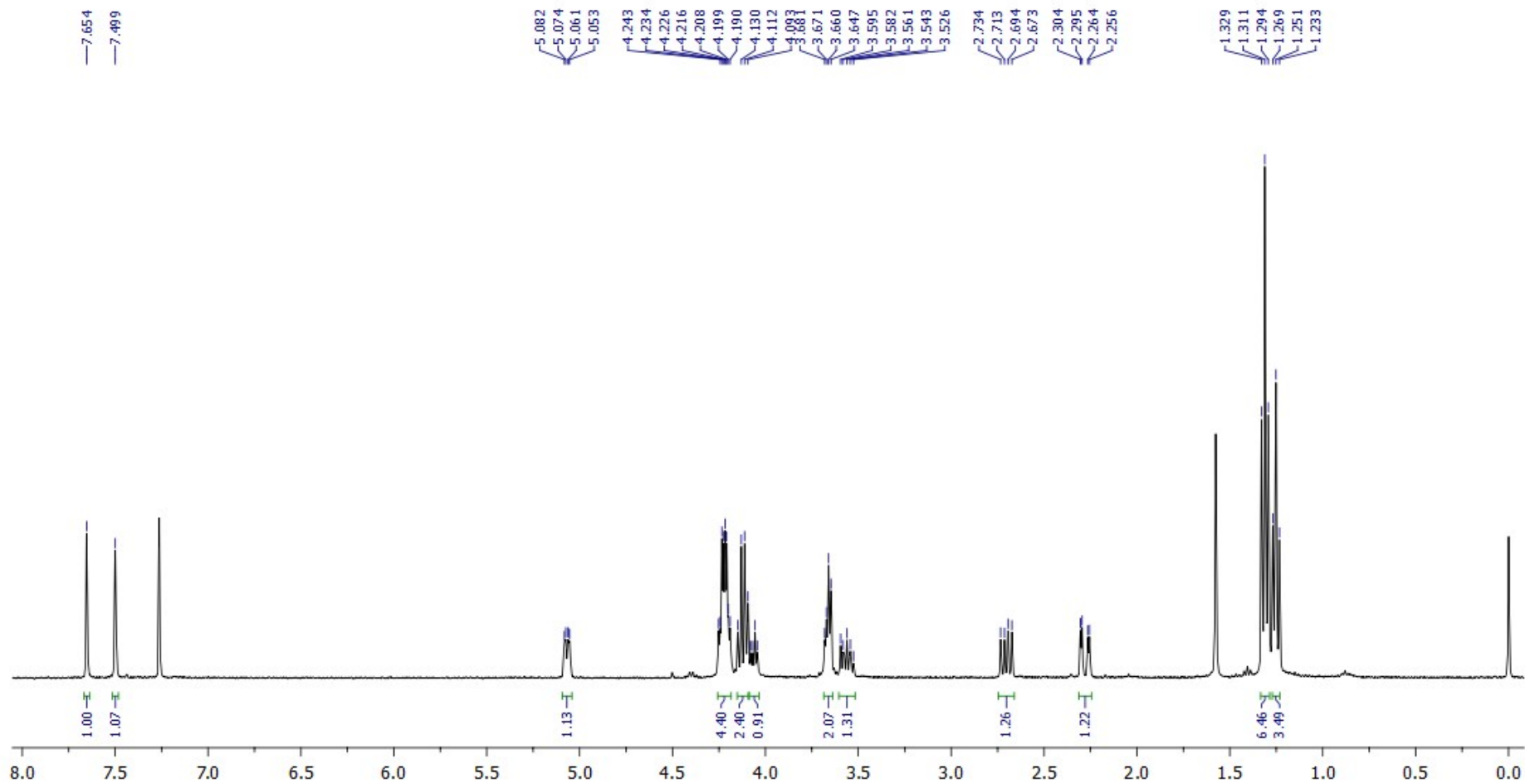
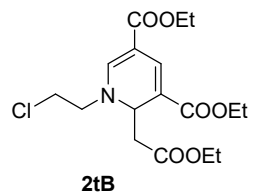
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



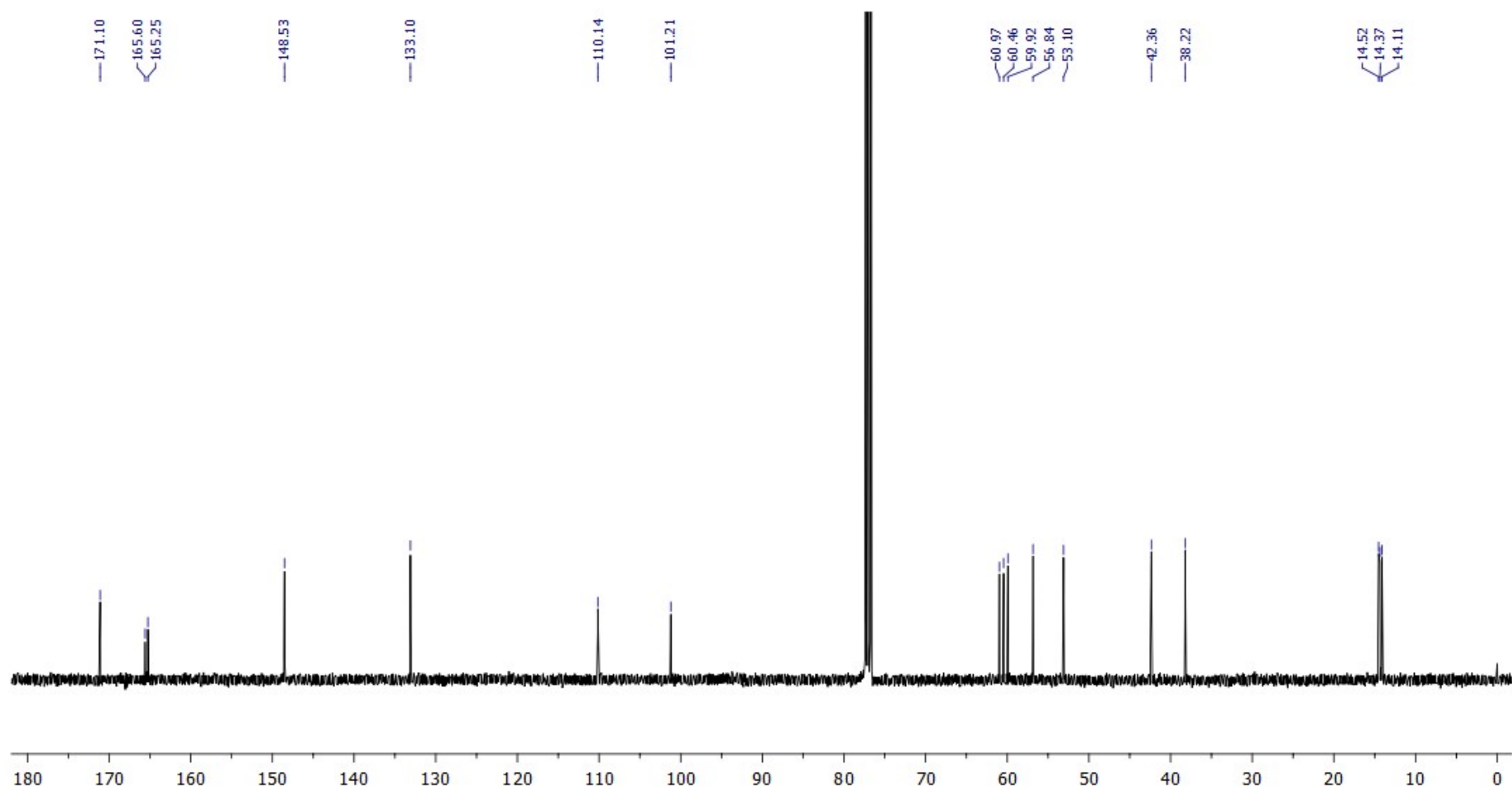
$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



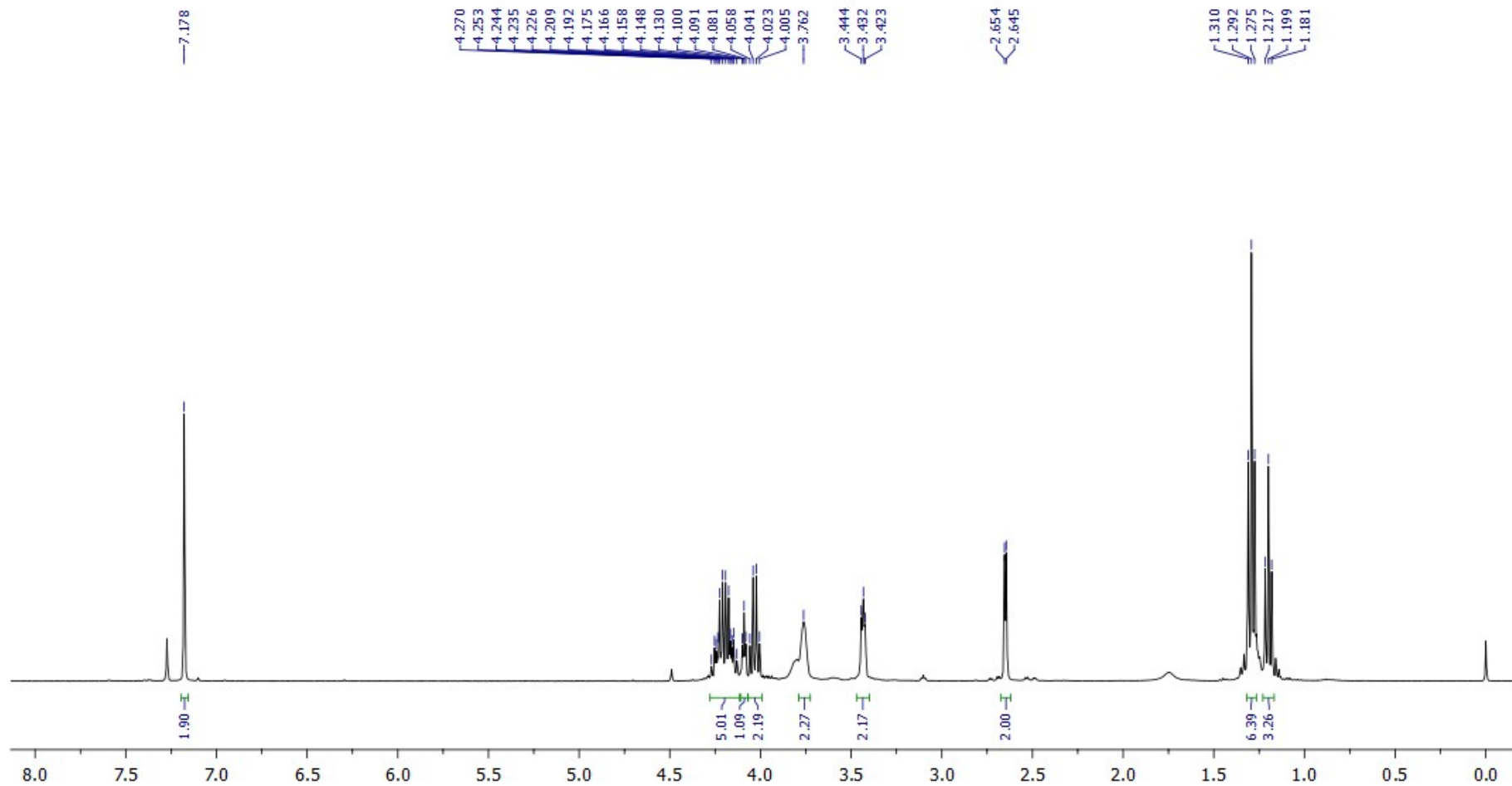
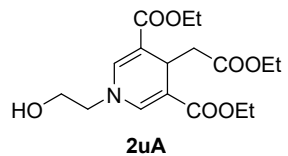
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



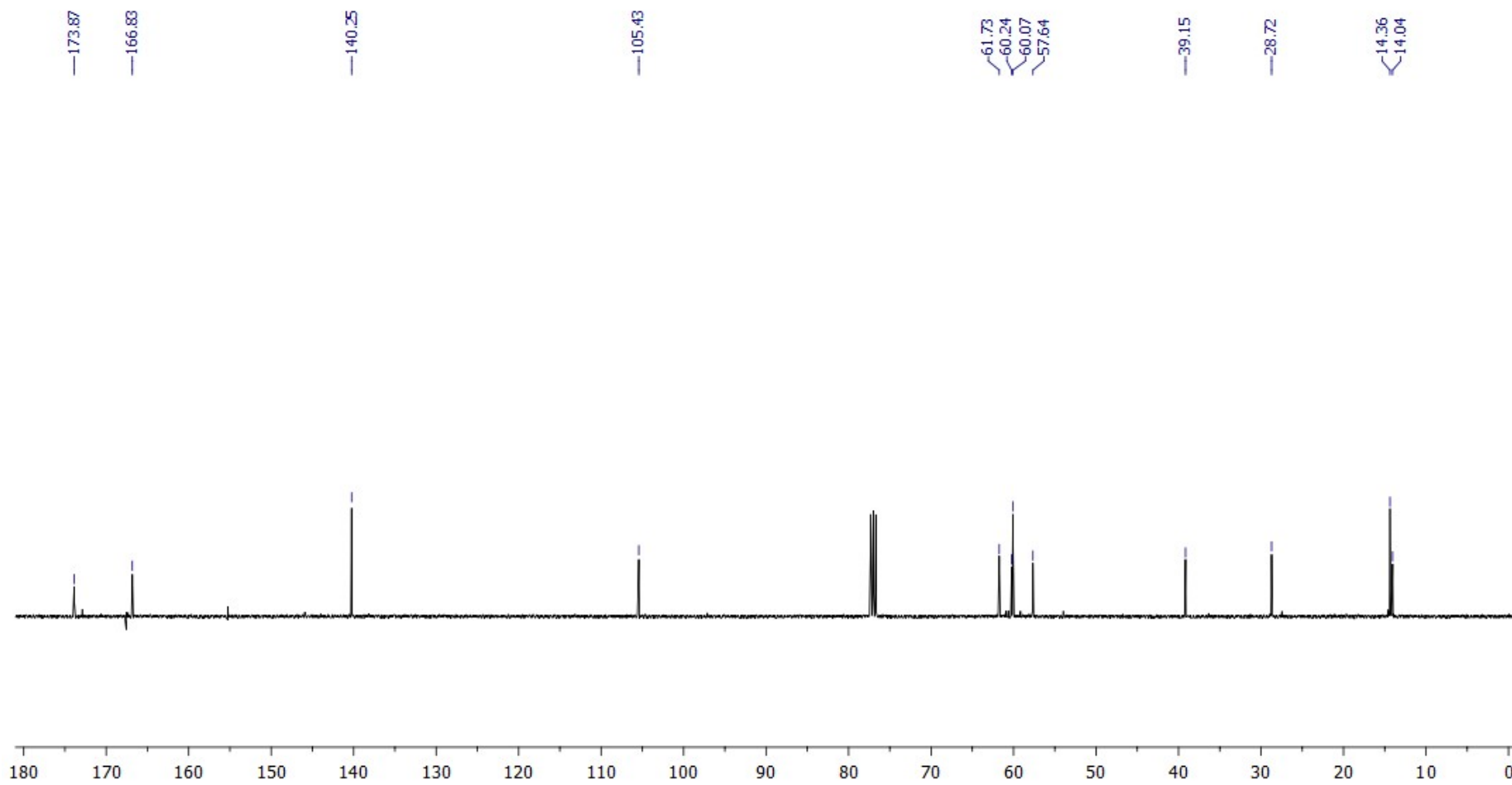
¹H NMR (400.1 MHz, CDCl₃)



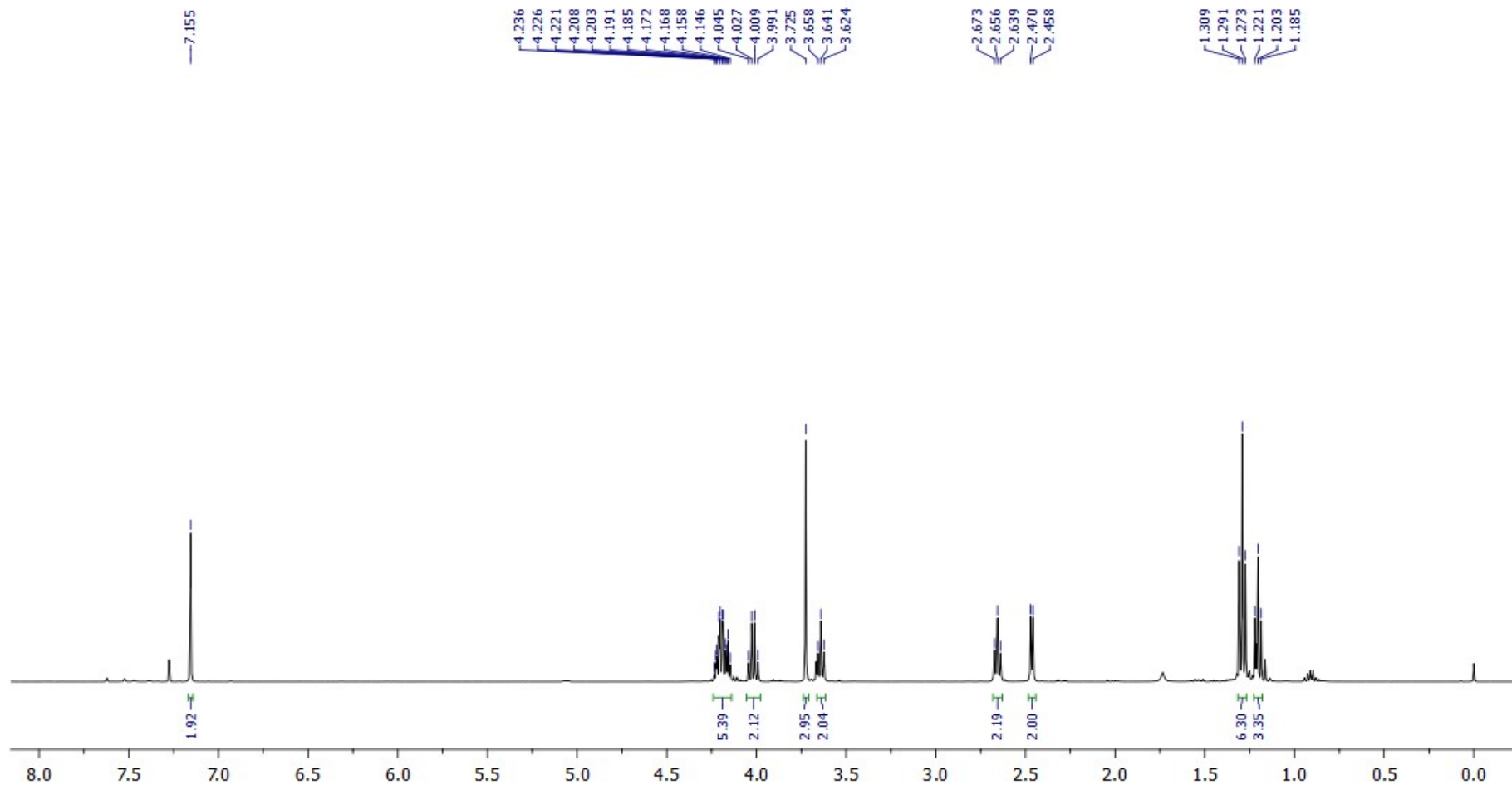
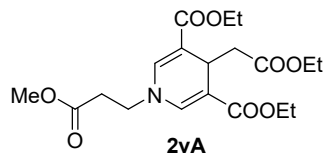
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



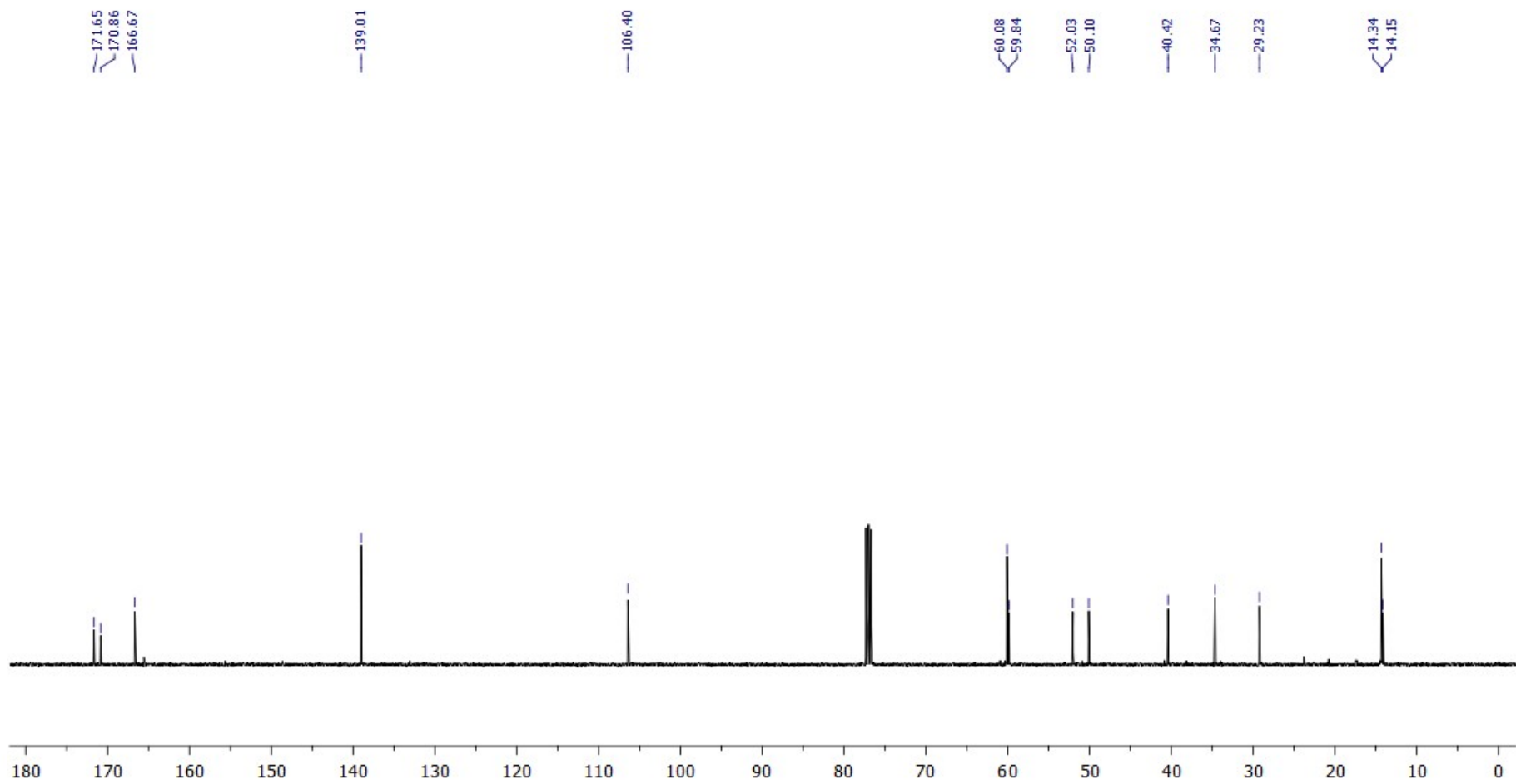
¹H NMR (400.1 MHz, CDCl₃)



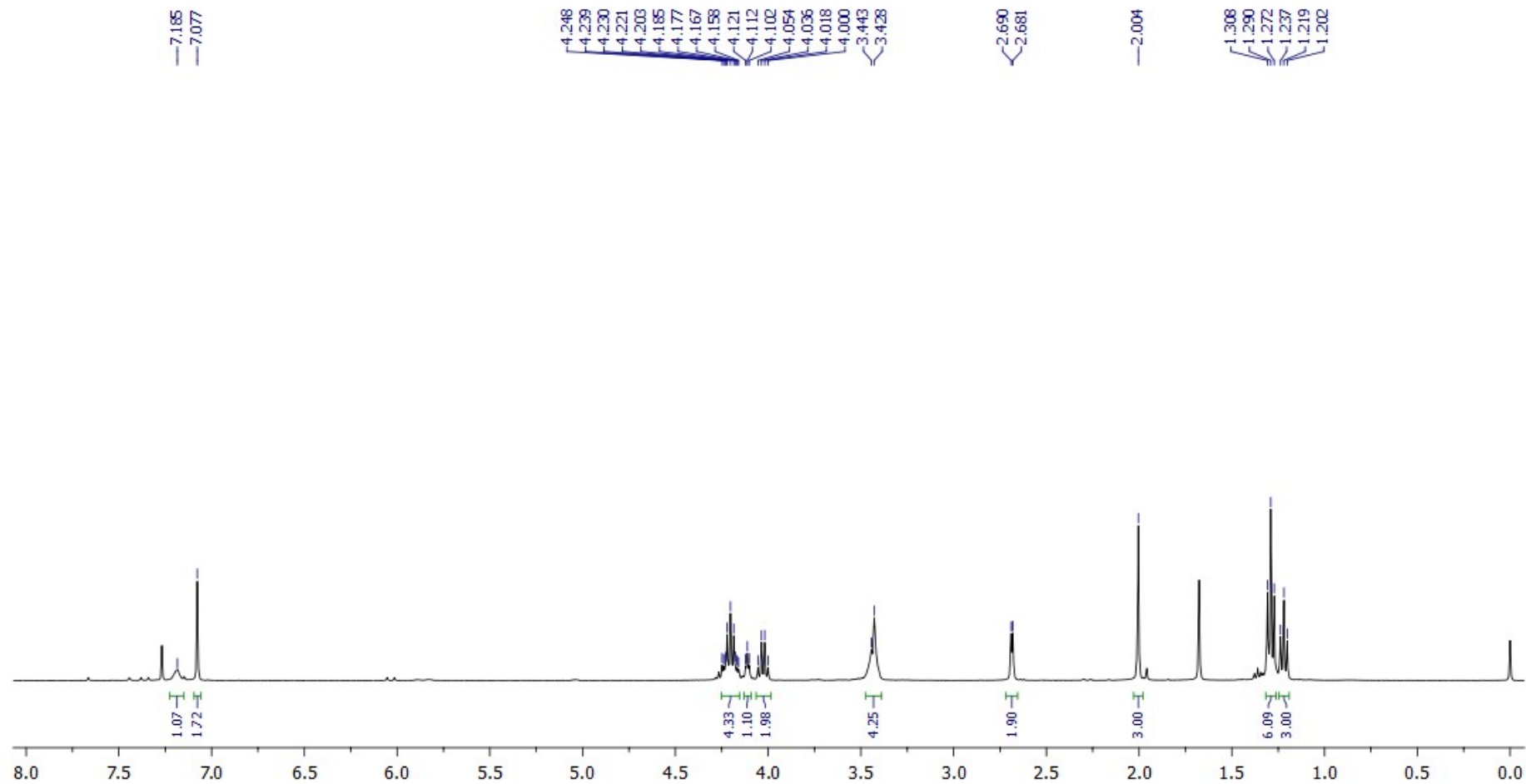
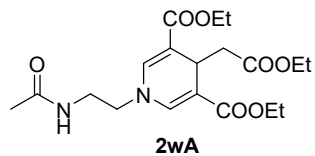
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



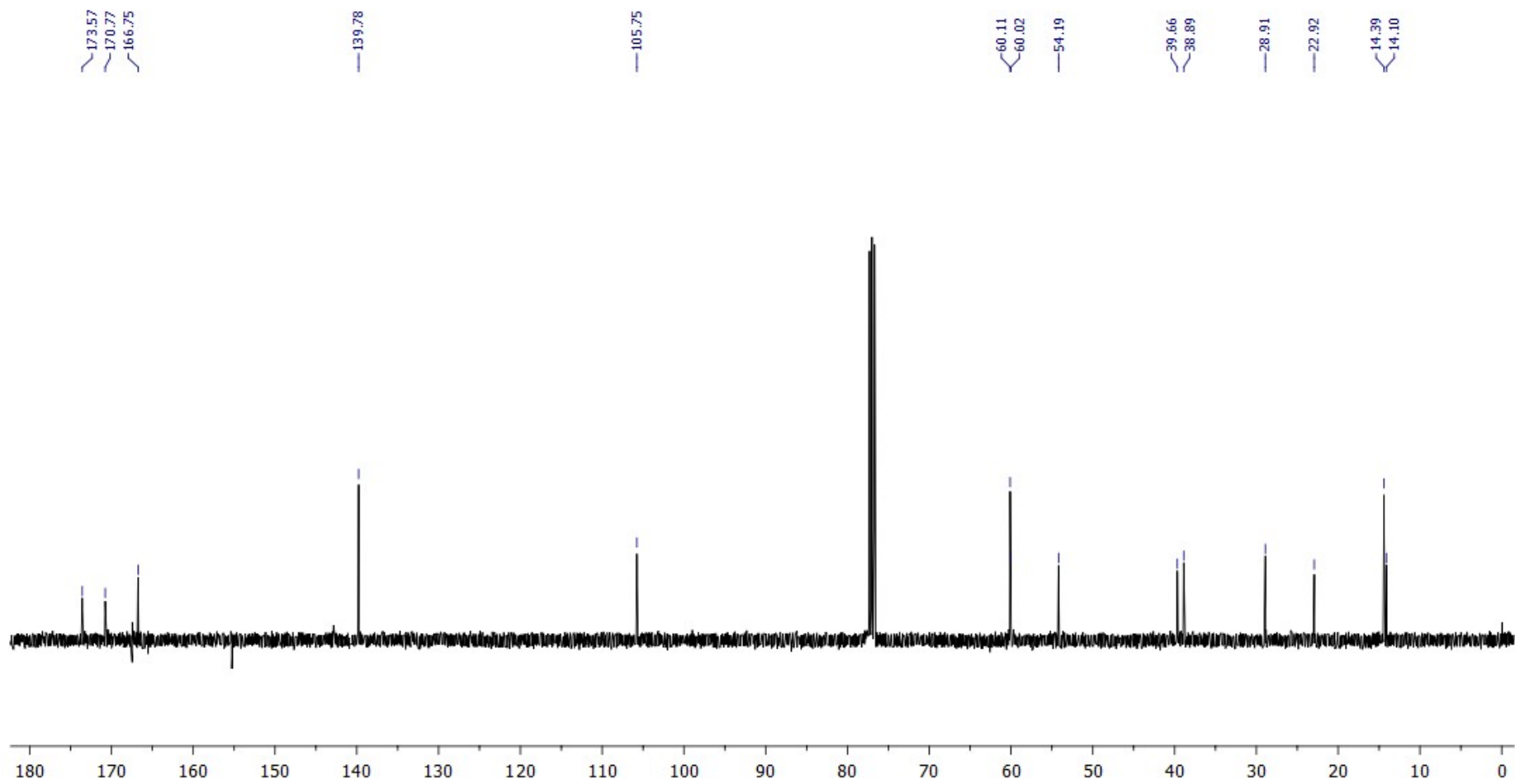
¹H NMR (400.1 MHz, CDCl₃)



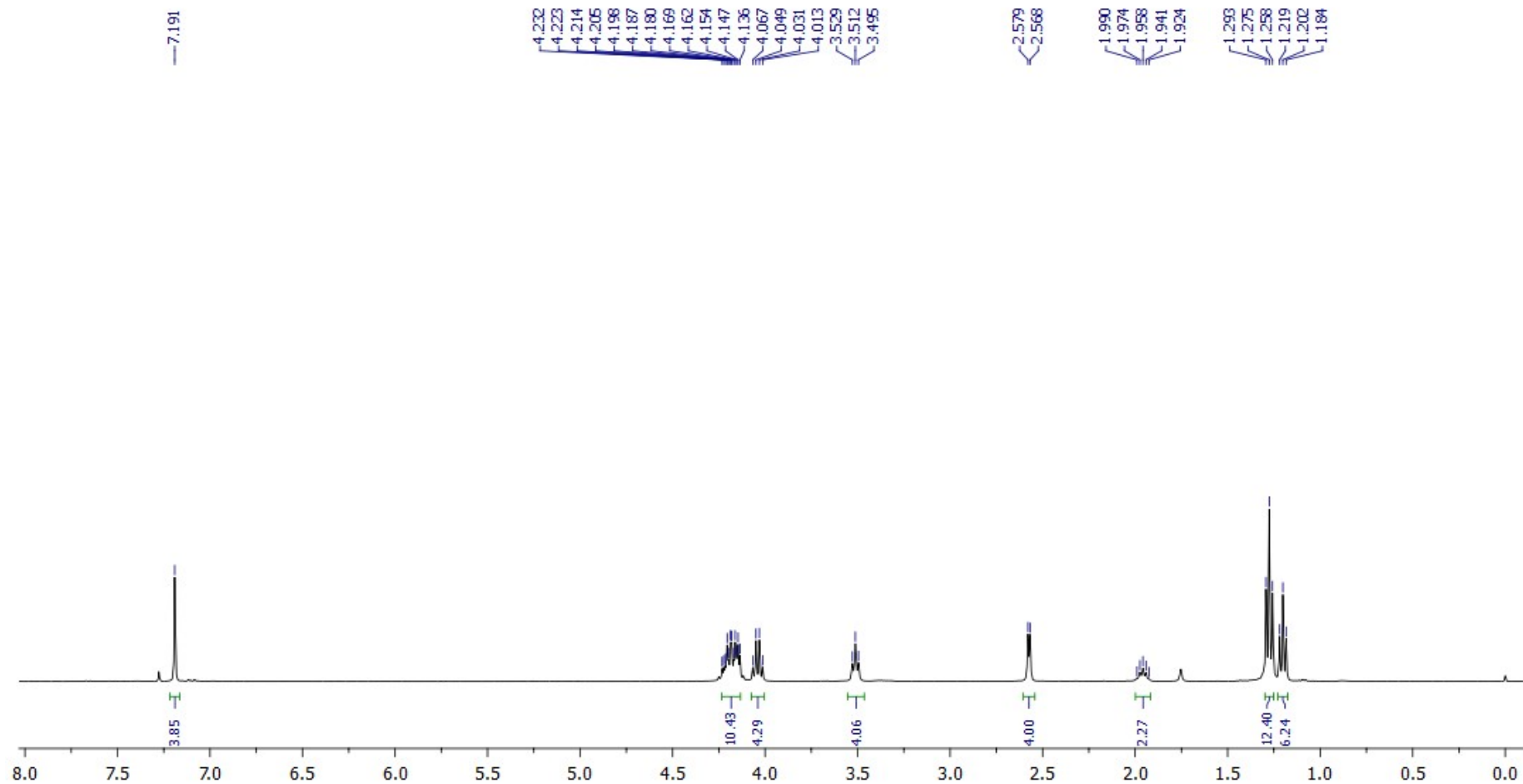
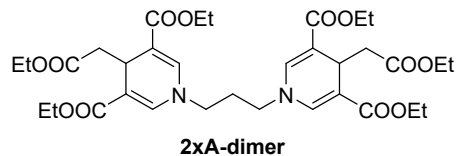
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



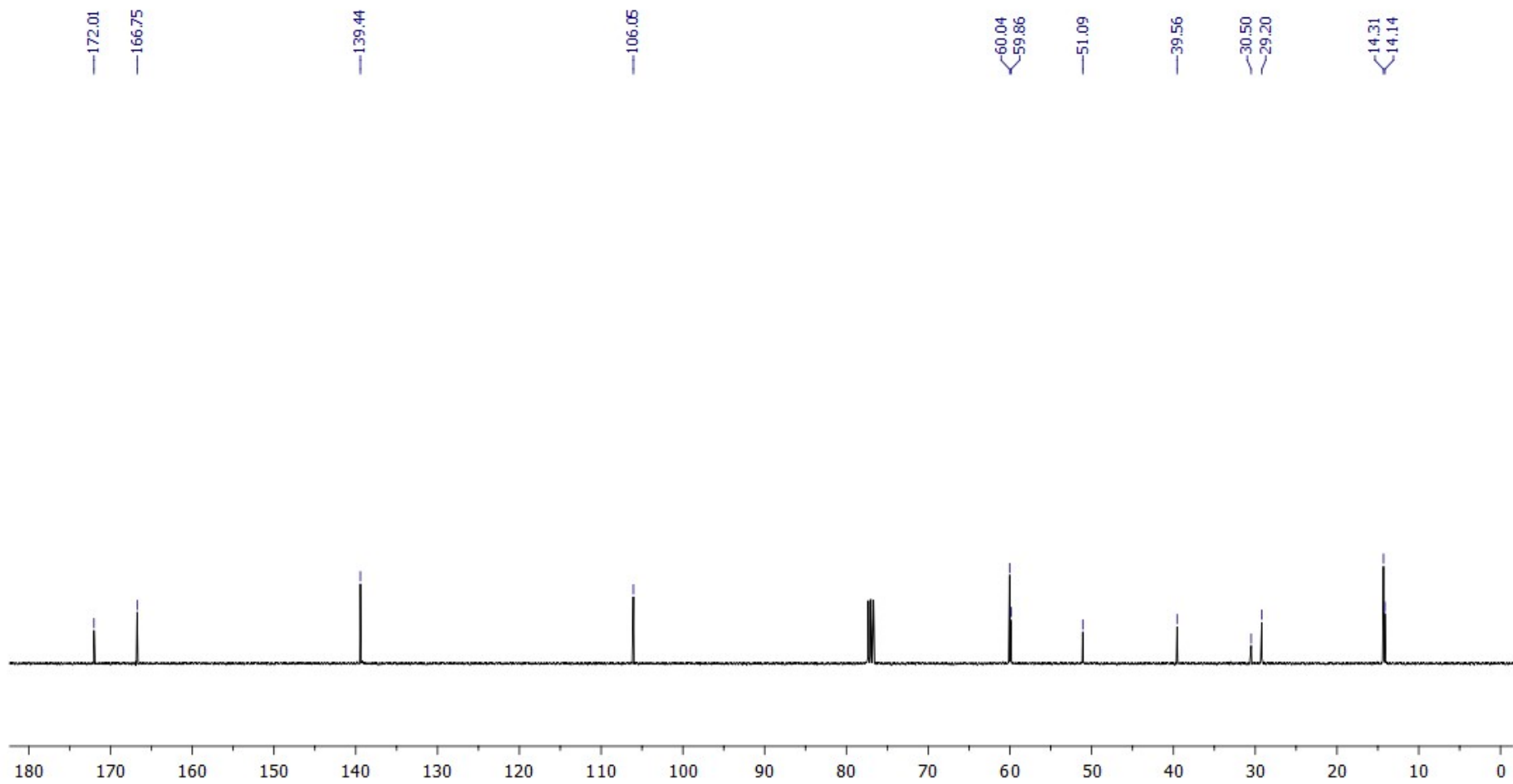
$^1\text{H NMR}$ (400.1 MHz, CDCl_3)



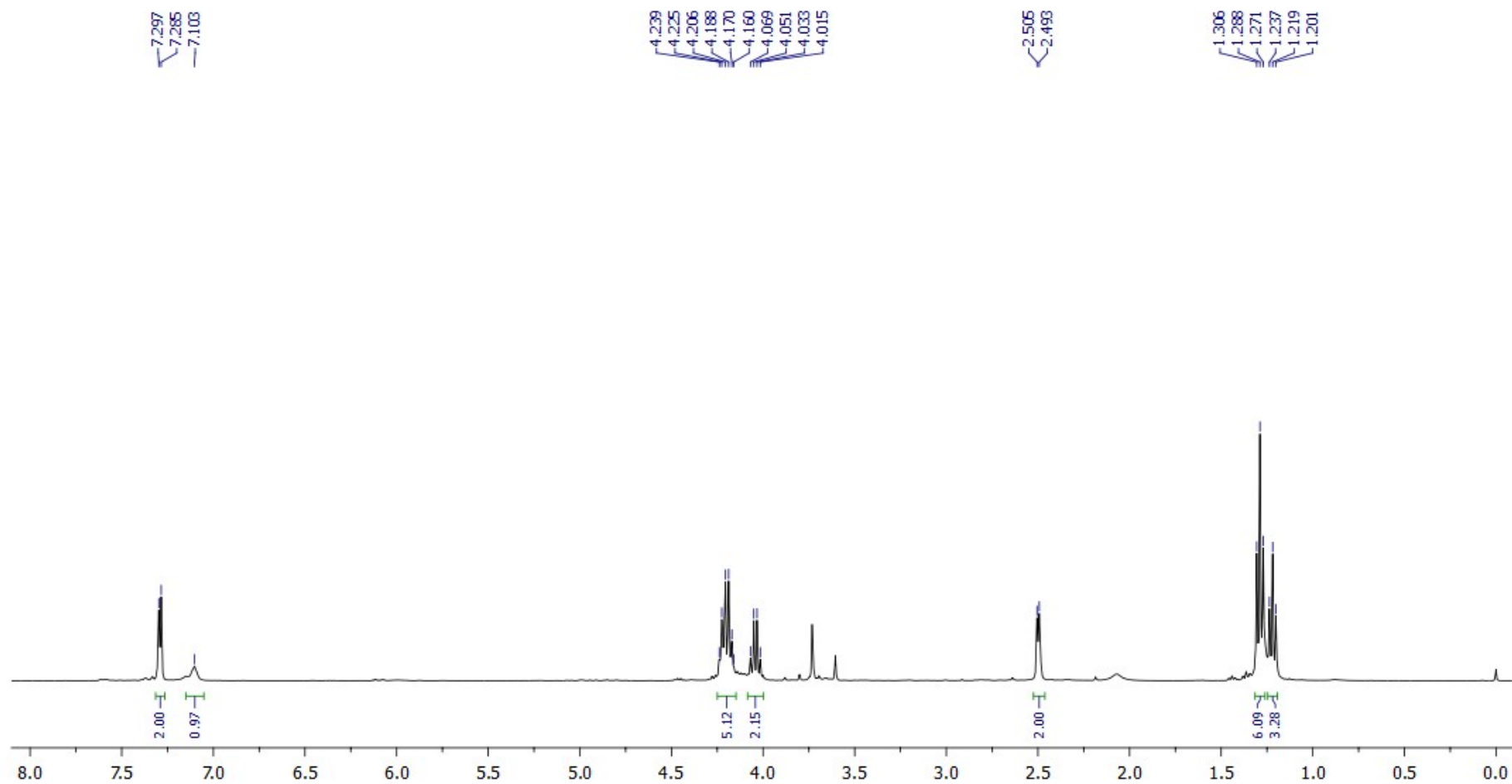
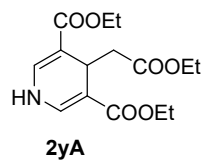
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



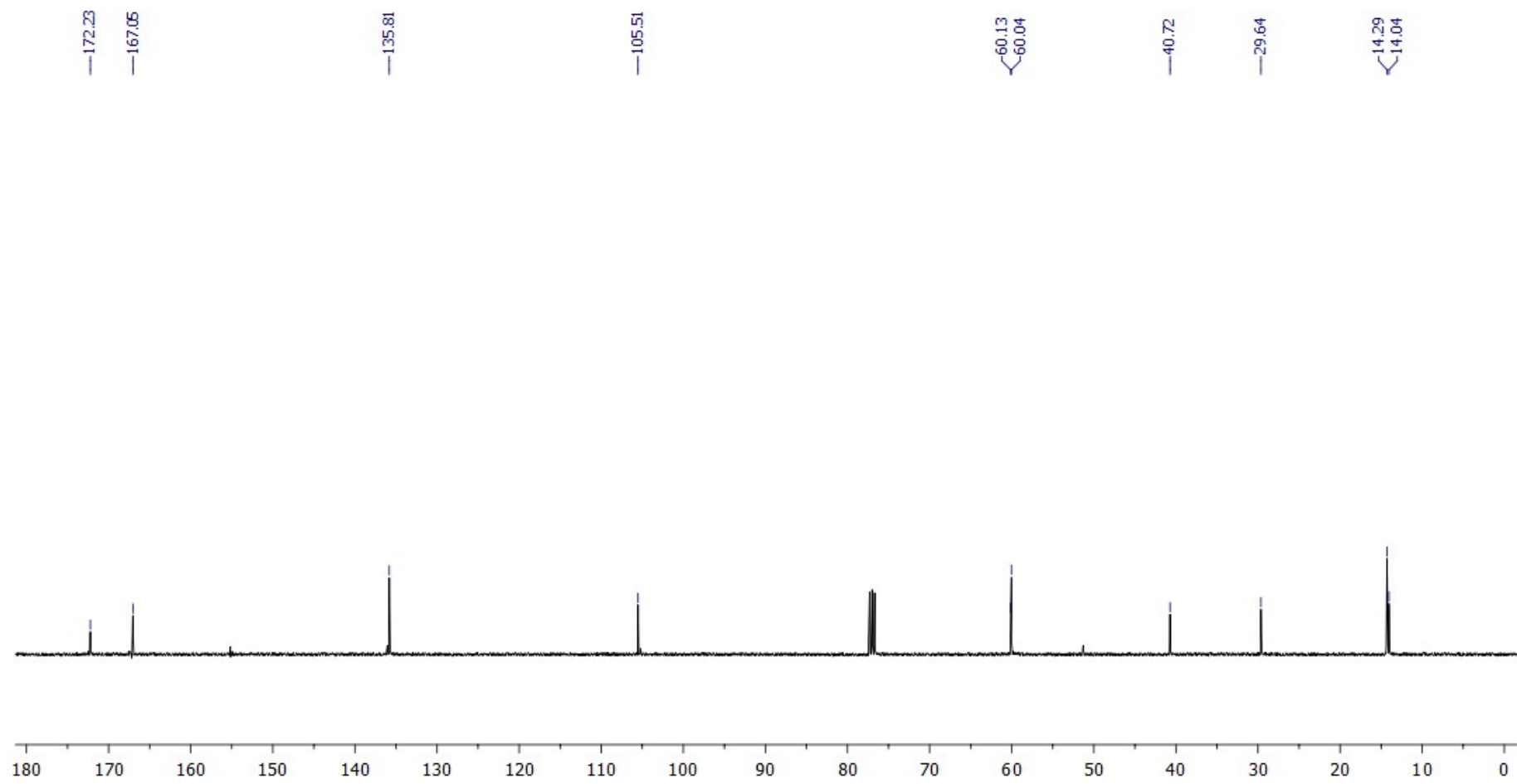
¹H NMR (400.1 MHz, CDCl₃)



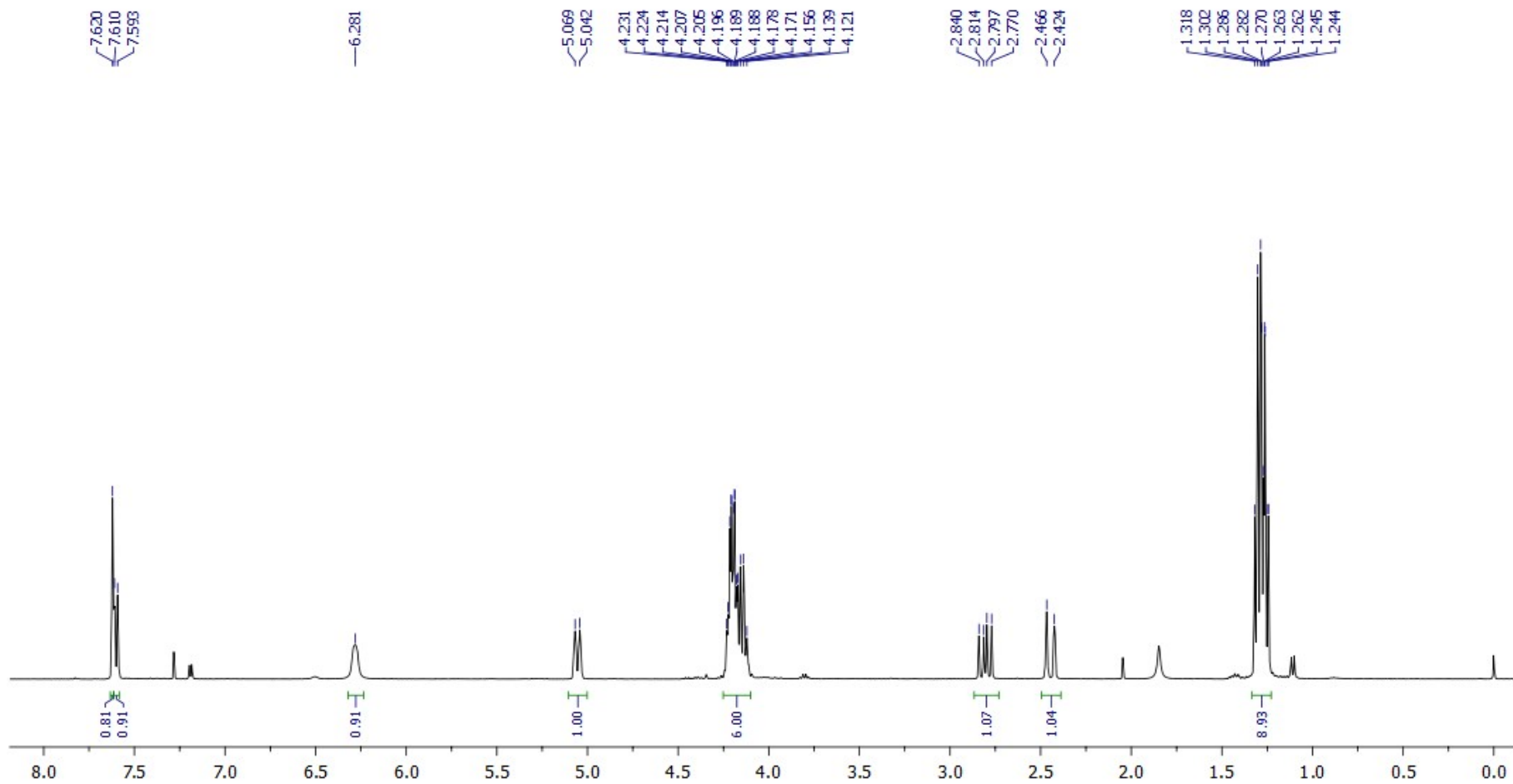
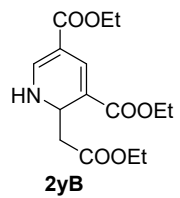
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



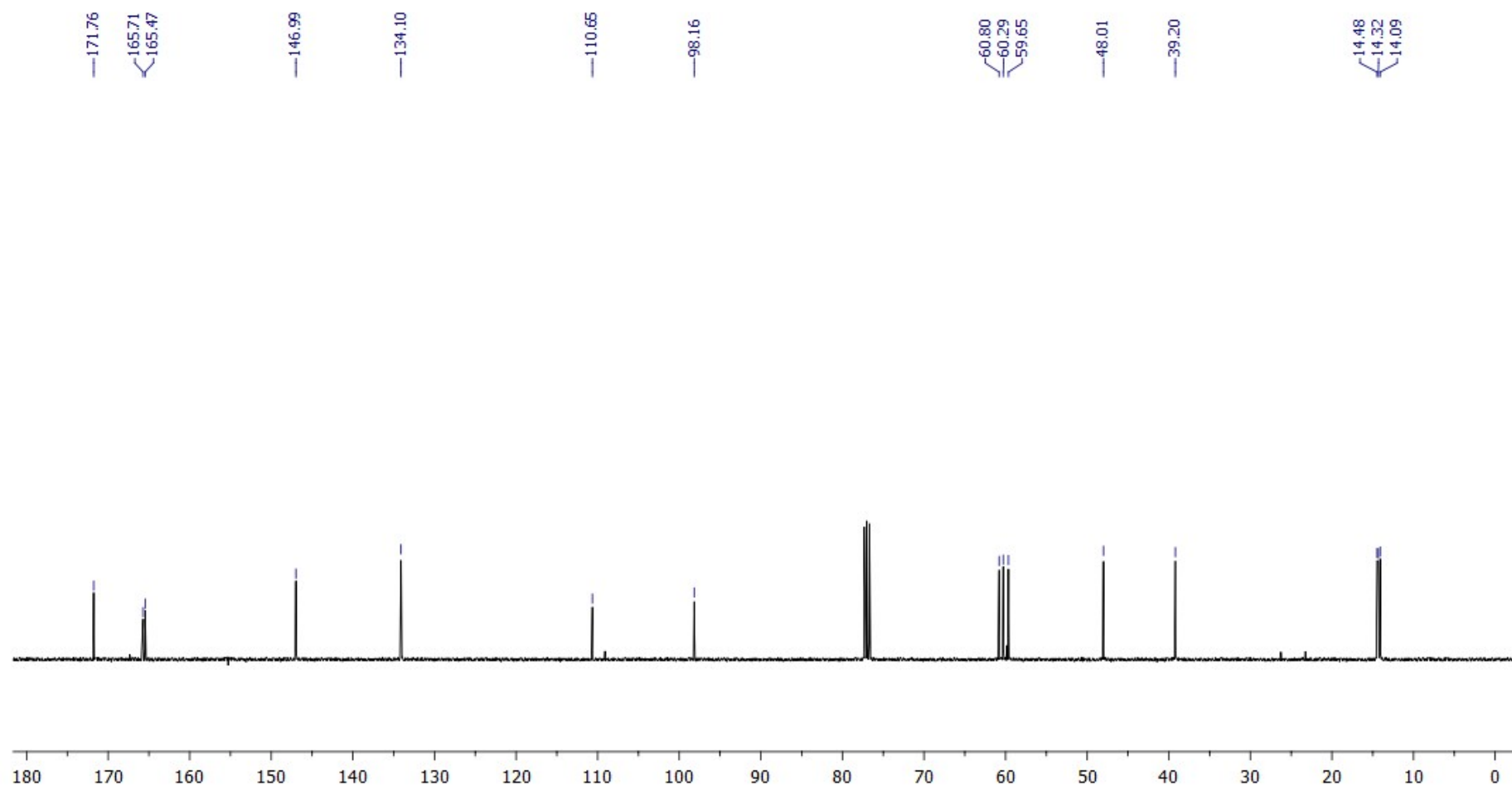
¹H NMR (400.1 MHz, CDCl₃)



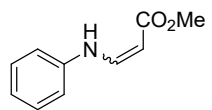
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl₃)



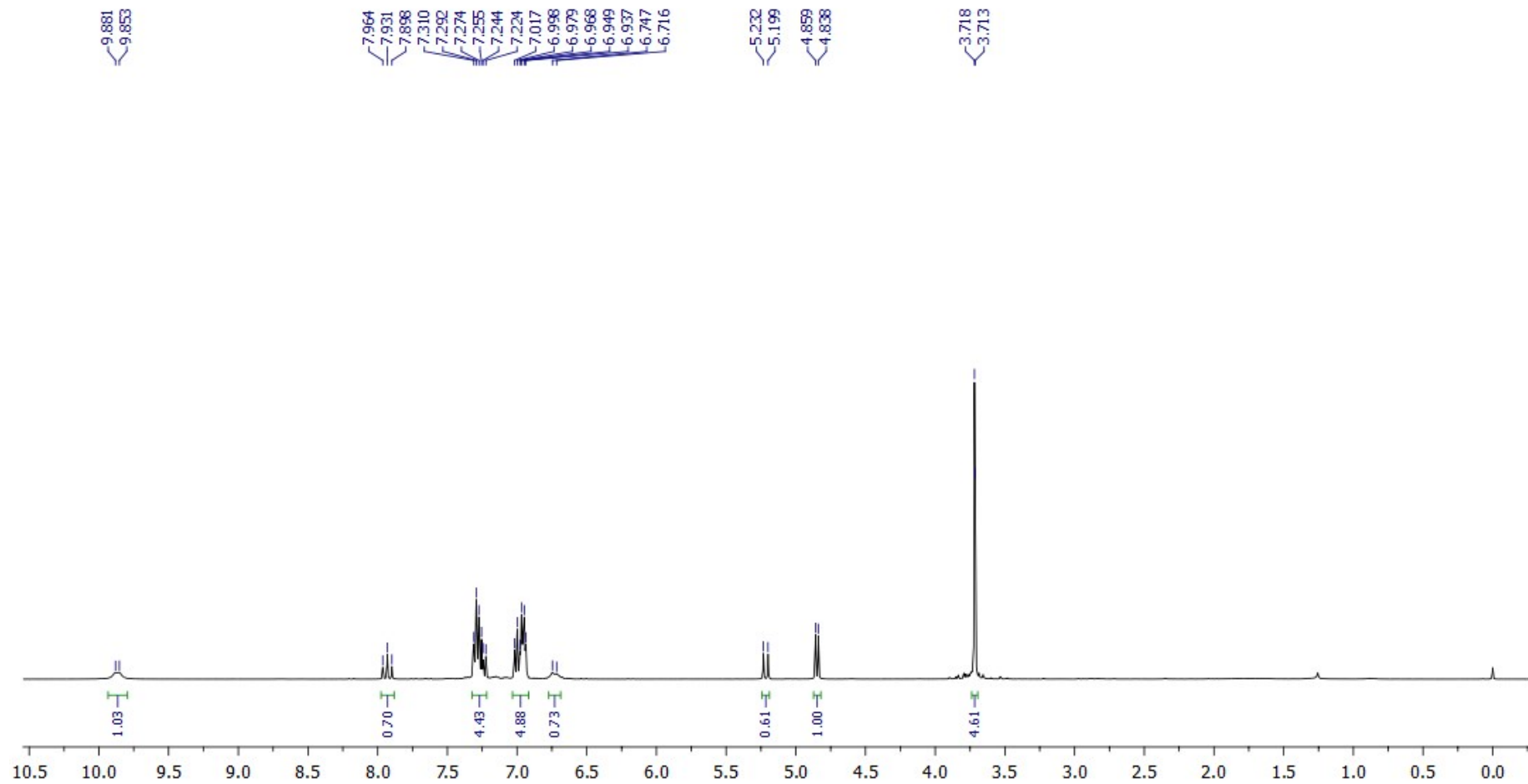
^1H NMR (400.1 MHz, CDCl_3)



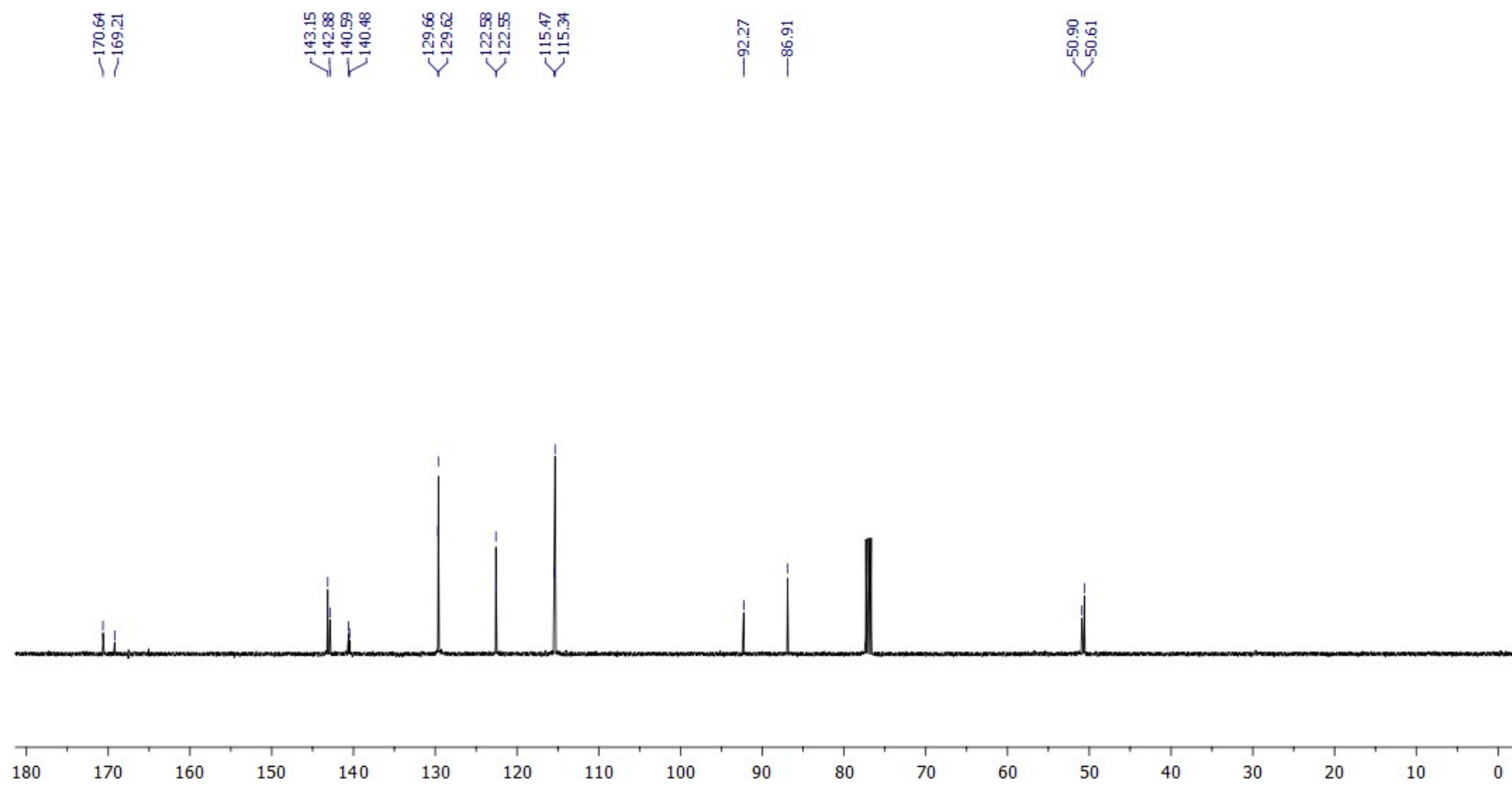
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)



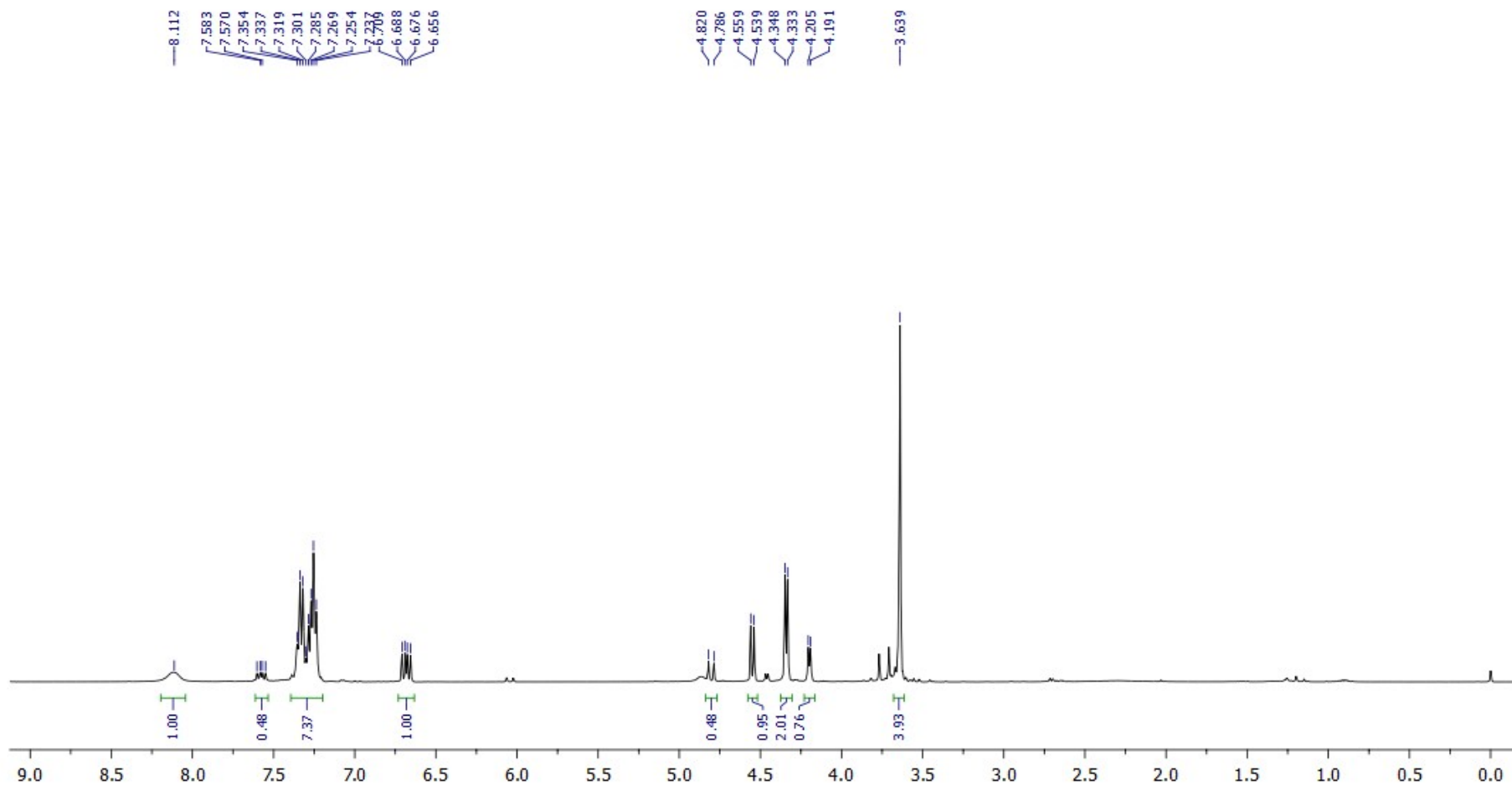
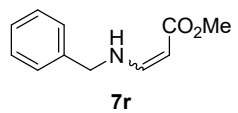
7a



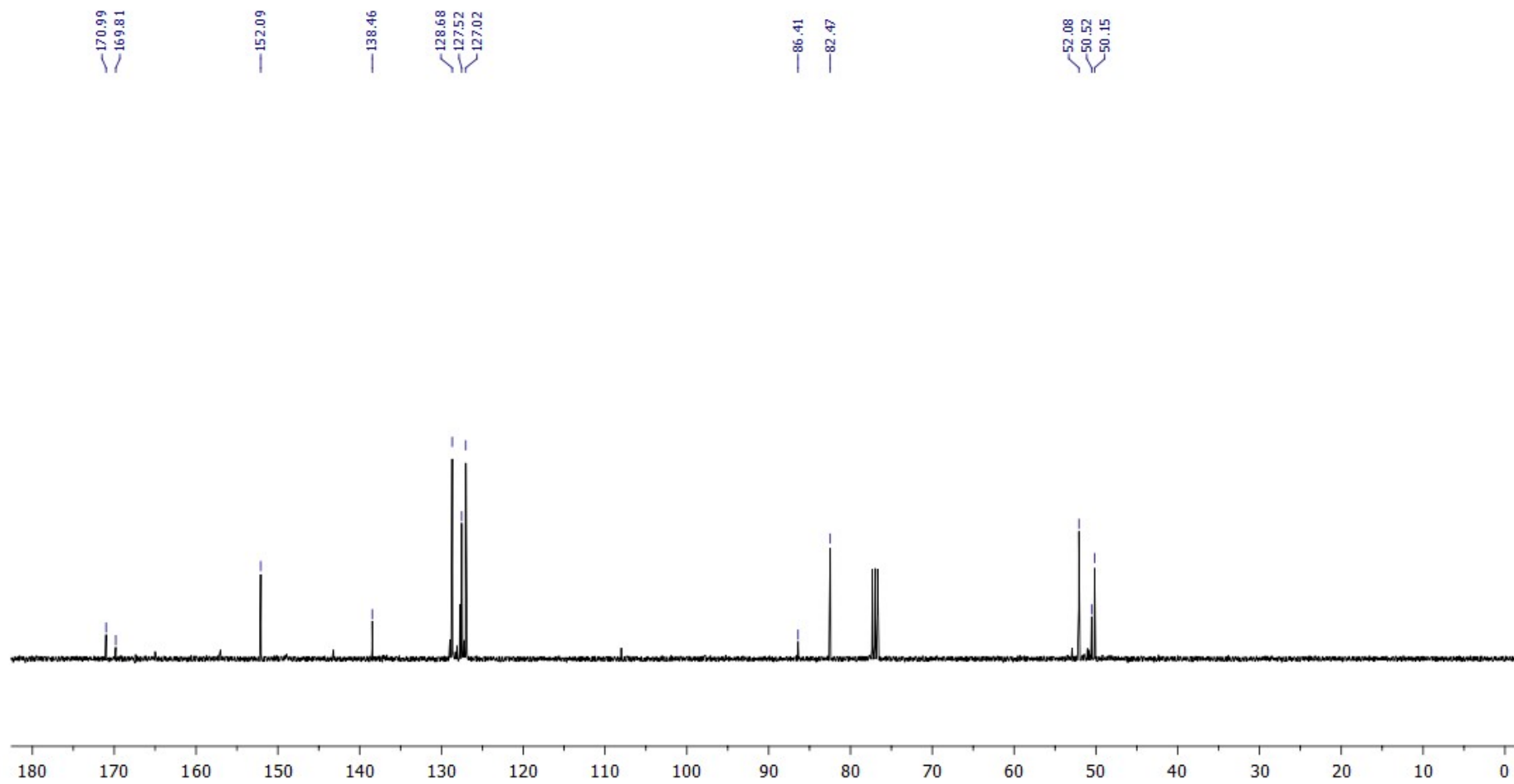
¹H NMR (400.1 MHz, CDCl₃)



$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)

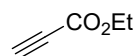


¹H NMR (400.1 MHz, CDCl₃)



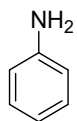
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.6 MHz, CDCl_3)

**Absolute energies and x, y, z coordinates of optimized structures
at the M062X/6-311+G(d,p) level of theory at 373.15 K**



E = -344.4776471 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.948330	-0.923994	0.000108
2	1	0	-3.873363	-1.451074	0.000032
3	6	0	-1.906935	-0.332055	0.000039
4	6	0	-0.671283	0.439867	-0.000143
5	8	0	-0.631536	1.638421	0.000166
6	8	0	0.395449	-0.359511	-0.000307
7	6	0	1.671157	0.309875	-0.000115
8	1	0	1.725753	0.949657	-0.883376
9	1	0	1.725423	0.949878	0.882994
10	6	0	2.736654	-0.760721	0.000205
11	1	0	2.649742	-1.391041	-0.885660
12	1	0	3.724061	-0.295916	0.000229
13	1	0	2.649504	-1.390619	0.886345



E = -287.553485 a.u.

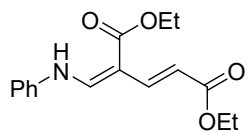
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.167566	-1.198432	0.003674

2	6	0	0.220880	-1.203898	-0.005982
3	6	0	0.933095	-0.000214	-0.008759
4	6	0	0.220843	1.203707	-0.005925
5	6	0	-1.167444	1.198634	0.003652
6	6	0	-1.874451	0.000038	0.008839
7	1	0	-1.700925	-2.142027	0.006935
8	1	0	0.763214	-2.143538	-0.016770
9	1	0	0.763486	2.143189	-0.016507
10	1	0	-1.700697	2.142281	0.006825
11	1	0	-2.956848	-0.000004	0.016594
12	7	0	2.327807	0.000039	-0.074025
13	1	0	2.772139	0.836404	0.273566
14	1	0	2.772838	-0.835589	0.274542

H₃C-NH₂

E = -95.8347391 a.u.

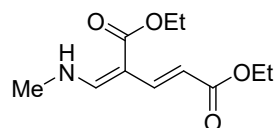
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.048717	0.705715	0.000000
2	1	0	0.589451	1.062228	0.878310
3	1	0	0.589451	1.062228	-0.878310
4	1	0	-0.946469	1.168703	0.000000
5	7	0	0.048717	-0.756055	0.000000
6	1	0	-0.432880	-1.117531	0.814524
7	1	0	-0.432880	-1.117531	-0.814524



E = -976.6724635 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.062372	-0.141258	-0.007137
2	1	0	0.992710	-1.222852	-0.009710
3	6	0	-0.118787	0.565258	-0.007670
4	6	0	-1.343067	-0.219655	-0.012835
5	1	0	-1.170935	-1.293635	-0.005658
6	6	0	-2.630351	0.161701	-0.027166
7	1	0	-2.947986	1.192312	-0.038296
8	6	0	-3.737512	-0.810164	-0.034080
9	6	0	-0.050289	2.032420	-0.001201
10	8	0	-4.902535	-0.496741	-0.064560
11	8	0	0.989844	2.670036	-0.001166
12	8	0	-3.337538	-2.099670	-0.002401
13	8	0	-1.240072	2.633615	0.007142
14	6	0	-4.386728	-3.074981	-0.011029
15	1	0	-5.054705	-2.883674	0.831570
16	1	0	-4.968883	-2.959460	-0.928327
17	6	0	-3.736258	-4.437180	0.078436
18	1	0	-4.501367	-5.215694	0.070265
19	1	0	-3.067072	-4.601302	-0.767663
20	1	0	-3.160521	-4.527663	1.000941
21	6	0	-1.231200	4.071697	0.020332
22	1	0	-0.701118	4.425004	-0.866435
23	1	0	-0.677702	4.408249	0.899180
24	6	0	-2.674232	4.521226	0.043724
25	1	0	-3.181051	4.141403	0.931987
26	1	0	-2.721558	5.611441	0.056782
27	1	0	-3.204398	4.161854	-0.839460
28	7	0	2.305703	0.359826	-0.004348
29	1	0	2.359123	1.376264	-0.003740

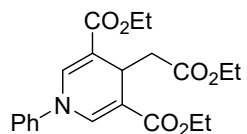
30	6	0	3.509469	-0.364253	-0.002865
31	6	0	4.698153	0.371218	-0.005789
32	6	0	3.568016	-1.759179	0.001667
33	6	0	5.923944	-0.276659	-0.004526
34	1	0	4.651340	1.454817	-0.009175
35	6	0	4.803073	-2.396691	0.002564
36	1	0	2.668914	-2.360935	0.004861
37	6	0	5.986069	-1.666734	-0.000496
38	1	0	6.834606	0.310258	-0.006780
39	1	0	4.834710	-3.479665	0.005996
40	1	0	6.942351	-2.174015	0.000408



E = -784.9612451 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.478031	-1.521482	0.000004
2	1	0	2.142420	-2.556348	-0.000020
3	6	0	1.506610	-0.538337	0.000014
4	6	0	0.129388	-0.987657	-0.000008
5	1	0	0.014962	-2.071431	-0.000056
6	6	0	-1.029907	-0.308411	0.000022
7	1	0	-1.103245	0.767099	0.000071
8	6	0	-2.283753	-1.079604	-0.000026
9	6	0	1.944952	0.856264	0.000034
10	8	0	-2.387724	-2.283780	-0.000110
11	8	0	3.113476	1.211934	0.000061
12	8	0	-3.357223	-0.262325	0.000033
13	8	0	0.944395	1.743035	0.000010

14	6	0	-4.633158	-0.912178	-0.000055
15	1	0	-4.702780	-1.553811	-0.881632
16	1	0	-4.702768	-1.554087	0.881322
17	6	0	-5.690385	0.168846	0.000124
18	1	0	-6.684305	-0.282664	-0.000001
19	1	0	-5.596010	0.798991	0.885842
20	1	0	-5.595949	0.799349	-0.885333
21	6	0	1.316934	3.129132	0.000000
22	1	0	1.927610	3.329962	-0.882715
23	1	0	1.927491	3.330006	0.882788
24	6	0	0.032494	3.927315	-0.000105
25	1	0	-0.561618	3.696929	0.885658
26	1	0	0.257480	4.995242	-0.000122
27	1	0	-0.561503	3.696878	-0.885933
28	7	0	3.798916	-1.367187	0.000019
29	1	0	4.133506	-0.407891	0.000041
30	6	0	4.740205	-2.468243	0.000000
31	1	0	5.374440	-2.436299	-0.888198
32	1	0	5.374383	-2.436385	0.888242
33	1	0	4.191609	-3.410011	-0.000065

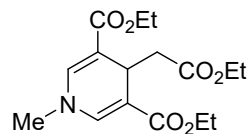


E = -1321.2537305 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.166877	0.865172	-0.552527
2	6	0	-1.200649	-0.373564	-1.069681
3	6	0	0.031225	-1.245432	-1.160194
4	6	0	1.258429	-0.372826	-1.014217
5	6	0	1.203460	0.867357	-0.500457
6	7	0	0.010839	1.483329	-0.182581

7	1	0	-2.061778	1.464852	-0.450203
8	1	0	2.099318	1.443168	-0.312407
9	6	0	0.009493	-2.403226	-0.145751
10	1	0	-0.860240	-3.038475	-0.336010
11	1	0	0.890304	-3.034757	-0.287879
12	6	0	-0.034496	-1.979085	1.300694
13	6	0	2.549211	-0.957918	-1.410128
14	6	0	-2.467570	-0.948401	-1.547949
15	8	0	2.669311	-2.077787	-1.847760
16	8	0	-2.565317	-2.063483	-2.003338
17	8	0	-0.087075	-0.851431	1.719640
18	8	0	3.598064	-0.127304	-1.245080
19	8	0	-0.011570	-3.051729	2.108833
20	8	0	-3.522132	-0.117623	-1.429843
21	6	0	-4.781946	-0.646229	-1.866569
22	1	0	-4.698435	-0.933912	-2.916786
23	1	0	-5.004914	-1.547757	-1.291518
24	6	0	-5.819465	0.433253	-1.655028
25	1	0	-6.798116	0.075360	-1.979693
26	1	0	-5.882452	0.706045	-0.600442
27	1	0	-5.568435	1.325281	-2.230953
28	6	0	4.878018	-0.663273	-1.608304
29	1	0	5.070676	-1.555801	-1.008722
30	1	0	4.847762	-0.967438	-2.656767
31	6	0	5.904662	0.418851	-1.360857
32	1	0	6.898184	0.055991	-1.629999
33	1	0	5.684105	1.301924	-1.962651
34	1	0	5.914497	0.707749	-0.308674
35	6	0	-0.050414	-2.781377	3.517468
36	1	0	0.808950	-2.160202	3.779868
37	1	0	-0.954489	-2.210938	3.742171
38	6	0	-0.027592	-4.113557	4.231836
39	1	0	-0.049945	-3.956190	5.311705
40	1	0	-0.892857	-4.715317	3.950115
41	1	0	0.877079	-4.668703	3.980064
42	1	0	0.051904	-1.727386	-2.142344
43	6	0	-0.018153	2.716598	0.524141

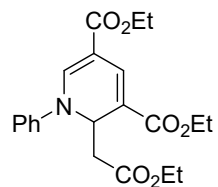
44	6	0	0.827367	3.763429	0.161138
45	6	0	-0.908582	2.869131	1.584913
46	6	0	0.779625	4.960123	0.865790
47	1	0	1.500555	3.648264	-0.680247
48	6	0	-0.963205	4.077315	2.269077
49	1	0	-1.526326	2.029582	1.882189
50	6	0	-0.118105	5.124117	1.916156
51	1	0	1.435437	5.773655	0.579837
52	1	0	-1.656568	4.192237	3.093504
53	1	0	-0.156981	6.061591	2.457003



E = -1129.542389 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.152457	-1.247045	1.128232
2	6	0	1.206843	-0.891144	-0.167529
3	6	0	-0.017632	-0.419051	-0.921660
4	6	0	-1.253881	-0.857691	-0.166387
5	6	0	-1.208287	-1.215915	1.128884
6	7	0	-0.029260	-1.353989	1.819239
7	1	0	2.046679	-1.505919	1.681708
8	1	0	-2.108721	-1.451814	1.682492
9	6	0	-0.028892	-1.399213	3.271350
10	1	0	0.847118	-1.949450	3.615951
11	1	0	-0.010332	-0.389731	3.690922
12	1	0	-0.923649	-1.917261	3.617407
13	6	0	0.004237	1.096589	-1.186890
14	1	0	0.879137	1.352641	-1.790747
15	1	0	-0.871440	1.378961	-1.778318
16	6	0	0.025633	1.961537	0.048555

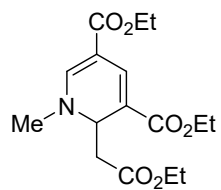
17	6	0	-2.531607	-0.829932	-0.891355
18	6	0	2.484104	-0.899747	-0.893858
19	8	0	-2.641583	-0.481834	-2.043523
20	8	0	2.602654	-0.556101	-2.046454
21	8	0	0.003056	1.589119	1.193858
22	8	0	-3.587657	-1.225918	-0.150629
23	8	0	0.075141	3.261472	-0.287823
24	8	0	3.529268	-1.324948	-0.153766
25	6	0	4.801788	-1.320145	-0.814034
26	1	0	4.741489	-1.950382	-1.703885
27	1	0	5.025672	-0.302451	-1.142149
28	6	0	5.822759	-1.833506	0.176312
29	1	0	6.813034	-1.843447	-0.282546
30	1	0	5.856769	-1.194419	1.060116
31	1	0	5.576640	-2.849166	0.489997
32	6	0	-4.859873	-1.184812	-0.810218
33	1	0	-5.054292	-0.161129	-1.138599
34	1	0	-4.817887	-1.816626	-1.699982
35	6	0	-5.894923	-1.668306	0.180418
36	1	0	-6.885267	-1.648157	-0.277995
37	1	0	-5.679161	-2.691083	0.493392
38	1	0	-5.909720	-1.029059	1.064643
39	6	0	0.102376	4.195919	0.800300
40	1	0	-0.804927	4.069377	1.395763
41	1	0	0.956375	3.964560	1.440721
42	6	0	0.199873	5.580932	0.201744
43	1	0	0.227321	6.328136	0.997047
44	1	0	1.107357	5.676160	-0.396162
45	1	0	-0.659643	5.785366	-0.438104
46	1	0	-0.024628	-0.882323	-1.912854



E = -1321.2538851 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.268974	0.579547	0.068972
2	6	0	-0.994990	1.353920	-0.215184
3	6	0	-2.184777	0.721803	-0.188397
4	6	0	-2.239025	-0.712110	-0.093984
5	6	0	-1.081552	-1.410424	-0.315056
6	7	0	0.115680	-0.807467	-0.428451
7	1	0	-3.100284	1.289983	-0.306657
8	1	0	-1.118584	-2.481018	-0.482615
9	6	0	-3.485956	-1.483874	-0.006819
10	8	0	-3.555387	-2.690381	-0.013628
11	8	0	-4.565719	-0.689253	0.086883
12	6	0	-5.830531	-1.360564	0.182640
13	1	0	-5.809517	-2.025391	1.048737
14	1	0	-5.969470	-1.977289	-0.708071
15	6	0	-6.894674	-0.294088	0.309488
16	1	0	-7.877992	-0.760123	0.395099
17	1	0	-6.721186	0.315943	1.197160
18	1	0	-6.893754	0.357578	-0.565420
19	6	0	-0.948084	2.814136	-0.412729
20	8	0	-1.900155	3.530433	-0.591087
21	8	0	0.318253	3.280823	-0.355354
22	6	0	0.470222	4.698235	-0.522739
23	1	0	-0.096612	5.205732	0.260879
24	1	0	0.040047	4.986553	-1.484205
25	6	0	1.948929	5.003662	-0.443915
26	1	0	2.491921	4.484212	-1.235108

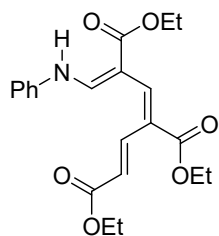
27	1	0	2.112659	6.076604	-0.558658
28	1	0	2.355937	4.691443	0.519114
29	1	0	1.119244	1.028542	-0.439419
30	6	0	0.563956	0.565502	1.583494
31	1	0	0.717386	1.600692	1.899330
32	1	0	-0.278411	0.136904	2.127781
33	6	0	1.798839	-0.243905	1.892814
34	8	0	1.829062	-1.235220	2.571378
35	8	0	2.869393	0.258723	1.261254
36	6	0	4.066769	-0.535723	1.318310
37	1	0	4.350259	-0.671681	2.364013
38	1	0	3.842681	-1.517876	0.893157
39	6	0	5.126988	0.194171	0.526328
40	1	0	6.052736	-0.384253	0.526897
41	1	0	4.803020	0.327869	-0.507093
42	1	0	5.328912	1.174553	0.960979
43	6	0	1.275870	-1.555668	-0.797140
44	6	0	1.504359	-2.814109	-0.242334
45	6	0	2.180757	-1.026867	-1.717677
46	6	0	2.615926	-3.552299	-0.633339
47	1	0	0.832595	-3.197258	0.516533
48	6	0	3.299678	-1.763022	-2.086739
49	1	0	1.999383	-0.051745	-2.154541
50	6	0	3.518130	-3.030911	-1.554216
51	1	0	2.784109	-4.529091	-0.195988
52	1	0	3.995277	-1.349342	-2.807594
53	1	0	4.387454	-3.604738	-1.851380



E = -1129.5397447 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.716345	-0.112141	-0.279751
2	6	0	-0.314957	0.991885	-0.235364
3	6	0	-1.627738	0.690860	-0.159270
4	6	0	-2.072713	-0.665017	-0.306622
5	6	0	-1.163577	-1.577864	-0.781348
6	7	0	0.132094	-1.291662	-0.940809
7	1	0	-2.353781	1.487647	-0.044969
8	1	0	-1.500491	-2.559272	-1.100275
9	6	0	1.037066	-2.244237	-1.568353
10	1	0	1.773377	-1.699070	-2.161516
11	1	0	1.560850	-2.857287	-0.828810
12	1	0	0.468077	-2.898309	-2.227891
13	6	0	-3.470943	-1.091114	-0.196182
14	8	0	-3.873147	-2.213804	-0.397373
15	8	0	-4.280941	-0.078579	0.161175
16	6	0	-5.671533	-0.404908	0.292286
17	1	0	-5.778942	-1.191467	1.042400
18	1	0	-6.031827	-0.801074	-0.659567
19	6	0	-6.393042	0.862835	0.689996
20	1	0	-7.459704	0.661962	0.805198
21	1	0	-6.007402	1.243956	1.636779
22	1	0	-6.265067	1.633373	-0.071705
23	6	0	0.113156	2.399300	-0.164198
24	8	0	-0.615190	3.357445	-0.102338
25	8	0	1.461177	2.505145	-0.157441
26	6	0	1.983620	3.838878	-0.074600
27	1	0	1.588832	4.314063	0.826012
28	1	0	1.627761	4.410057	-0.934878
29	6	0	3.491581	3.729770	-0.046851
30	1	0	3.861028	3.253516	-0.956315
31	1	0	3.934130	4.724687	0.028071
32	1	0	3.818285	3.140069	0.811336
33	1	0	1.582078	0.194984	-0.868213
34	6	0	1.195974	-0.450550	1.148256

35	1	0	1.581683	0.475814	1.583279
36	1	0	0.361345	-0.811805	1.750393
37	6	0	2.294106	-1.481680	1.183369
38	8	0	2.266225	-2.515633	1.794981
39	8	0	3.332590	-1.112642	0.412277
40	6	0	4.425593	-2.041869	0.340576
41	1	0	4.824429	-2.193443	1.345656
42	1	0	4.044204	-3.003411	-0.013302
43	6	0	5.453405	-1.457225	-0.600914
44	1	0	6.304817	-2.134555	-0.686265
45	1	0	5.026768	-1.310618	-1.594678
46	1	0	5.811121	-0.495170	-0.231517

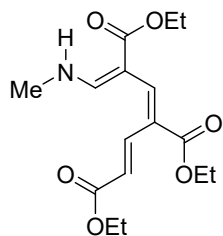


E = -1321.2314655 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.388259	0.970376	-0.297672
2	1	0	-0.379020	0.919005	-0.690004
3	6	0	-2.072625	-0.208823	-0.070531
4	6	0	-1.464980	-1.501193	-0.285615
5	1	0	-2.144876	-2.306341	-0.544149
6	6	0	-0.148696	-1.838103	-0.209174
7	6	0	0.166208	-3.240792	-0.610694
8	6	0	-3.491481	-0.133483	0.299778
9	8	0	-0.642946	-4.032541	-1.026155
10	8	0	-4.107565	0.903648	0.474635
11	8	0	1.460987	-3.552835	-0.449900

12	8	0	-4.069088	-1.331753	0.434902
13	6	0	1.828015	-4.898251	-0.790098
14	1	0	1.253202	-5.585686	-0.165918
15	1	0	1.553799	-5.085287	-1.830535
16	6	0	3.316595	-5.026121	-0.558256
17	1	0	3.642519	-6.040545	-0.794945
18	1	0	3.867864	-4.329830	-1.192426
19	1	0	3.562599	-4.815713	0.483620
20	6	0	-5.464006	-1.329012	0.779899
21	1	0	-6.013108	-0.780594	0.011677
22	1	0	-5.588172	-0.797291	1.725462
23	6	0	-5.902244	-2.772427	0.874242
24	1	0	-5.333196	-3.298113	1.642054
25	1	0	-6.961587	-2.819634	1.133032
26	1	0	-5.753986	-3.282474	-0.078501
27	7	0	-1.857541	2.209676	-0.140839
28	1	0	-2.832681	2.290217	0.140180
29	6	0	0.858609	-0.911575	0.294728
30	1	0	0.476269	-0.154283	0.978015
31	6	0	2.171582	-0.846148	0.036772
32	1	0	2.692700	-1.539535	-0.606540
33	6	0	2.958773	0.241996	0.649929
34	8	0	2.511373	1.167130	1.288791
35	8	0	4.268564	0.102799	0.393960
36	6	0	5.125354	1.121615	0.929308
37	1	0	4.806232	2.089970	0.536735
38	1	0	5.004293	1.146871	2.014458
39	6	0	6.540206	0.780247	0.520717
40	1	0	6.631853	0.757523	-0.566113
41	1	0	7.230739	1.529458	0.912071
42	1	0	6.828392	-0.195650	0.913800
43	6	0	-1.084746	3.377638	-0.330659
44	6	0	-1.721819	4.539053	-0.766664
45	6	0	0.283701	3.382699	-0.060644
46	6	0	-0.984452	5.700396	-0.951648
47	1	0	-2.786934	4.521153	-0.968817
48	6	0	1.012135	4.548490	-0.265718

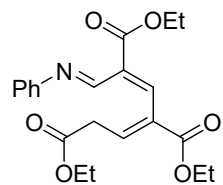
49	1	0	0.777187	2.506601	0.348066
50	6	0	0.386771	5.707957	-0.712061
51	1	0	-1.482761	6.600089	-1.292217
52	1	0	2.073519	4.548596	-0.047789
53	1	0	0.959492	6.614946	-0.860866



E = -1129.5164056 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.364810	-1.813386	0.721149
2	1	0	-0.370648	-1.660288	1.130303
3	6	0	-2.074287	-0.702828	0.285997
4	6	0	-1.504168	0.620761	0.296818
5	1	0	-2.209164	1.437589	0.412863
6	6	0	-0.193944	0.978162	0.181905
7	6	0	0.078582	2.432417	0.365862
8	6	0	-3.477694	-0.882706	-0.092305
9	8	0	-0.762875	3.266595	0.592213
10	8	0	-4.046859	-1.960125	-0.153836
11	8	0	1.379500	2.740380	0.244457
12	8	0	-4.105835	0.264651	-0.376684
13	6	0	1.710227	4.130253	0.376785
14	1	0	1.193455	4.688229	-0.407088
15	1	0	1.342155	4.490663	1.339528
16	6	0	3.213493	4.243291	0.259130
17	1	0	3.514150	5.289546	0.338743
18	1	0	3.706256	3.681406	1.054465

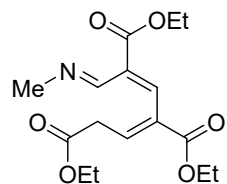
19	1	0	3.554641	3.855982	-0.702103
20	6	0	-5.488585	0.155590	-0.748802
21	1	0	-6.030960	-0.342826	0.057258
22	1	0	-5.561143	-0.472558	-1.639223
23	6	0	-5.994967	1.558047	-0.996246
24	1	0	-5.428121	2.036852	-1.795774
25	1	0	-7.046600	1.525017	-1.286950
26	1	0	-5.902630	2.164792	-0.094435
27	7	0	-1.779297	-3.071849	0.738840
28	1	0	-2.714643	-3.241826	0.378809
29	6	0	-0.985337	-4.171283	1.252664
30	1	0	-0.871267	-4.942774	0.489696
31	1	0	0.005219	-3.803638	1.519092
32	1	0	-1.452853	-4.610067	2.136603
33	6	0	0.835208	0.012016	-0.180612
34	1	0	0.460841	-0.860949	-0.713177
35	6	0	2.158955	0.022413	0.030279
36	1	0	2.685439	0.821851	0.529665
37	6	0	2.947885	-1.136419	-0.433015
38	8	0	2.502415	-2.156857	-0.903598
39	8	0	4.264871	-0.935609	-0.248476
40	6	0	5.125227	-2.006510	-0.659101
41	1	0	4.857896	-2.906749	-0.100776
42	1	0	4.952522	-2.210099	-1.718216
43	6	0	6.547731	-1.571876	-0.388451
44	1	0	6.692984	-1.368273	0.673428
45	1	0	7.239872	-2.360680	-0.688720
46	1	0	6.786839	-0.668184	-0.950828



E = -1321.2107736 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.958330	1.484186	1.216759
2	6	0	-1.865002	0.987400	0.362814
3	6	0	-2.104164	-0.440609	0.097174
4	6	0	-1.153839	-1.328181	-0.234413
5	6	0	0.252306	-0.940445	-0.453359
6	7	0	1.201434	-1.739270	-0.182118
7	1	0	-3.135859	-0.772941	0.142495
8	1	0	0.428902	0.078153	-0.821006
9	6	0	-1.529155	-2.751535	-0.520585
10	8	0	-0.965469	-3.454126	-1.311999
11	8	0	-2.606004	-3.135727	0.181406
12	6	0	-3.090175	-4.458978	-0.102520
13	1	0	-2.283536	-5.171622	0.080533
14	1	0	-3.351787	-4.514585	-1.161613
15	6	0	-4.282601	-4.702219	0.793626
16	1	0	-4.687430	-5.698744	0.608482
17	1	0	-3.993966	-4.635235	1.843543
18	1	0	-5.066633	-3.968536	0.600382
19	6	0	-2.816434	1.898547	-0.349001
20	8	0	-3.733903	1.494934	-1.016147
21	8	0	-2.552029	3.197560	-0.169584
22	6	0	-3.440347	4.112594	-0.834543
23	1	0	-4.451088	3.955178	-0.452063
24	1	0	-3.445759	3.879885	-1.901150
25	6	0	-2.936080	5.509690	-0.556532
26	1	0	-1.925121	5.638570	-0.945638
27	1	0	-3.588538	6.239559	-1.038872
28	1	0	-2.926298	5.710491	0.515658
29	1	0	-0.905226	2.564134	1.308230
30	6	0	-0.060768	0.704014	2.124018
31	1	0	-0.241316	1.019694	3.157085
32	1	0	-0.246240	-0.369980	2.085083
33	6	0	1.428686	0.919299	1.898928

34	8	0	2.276217	0.467009	2.616989
35	8	0	1.678206	1.683817	0.830915
36	6	0	3.066251	1.987843	0.576575
37	1	0	3.459395	2.528945	1.440532
38	1	0	3.617331	1.052577	0.479573
39	6	0	3.115705	2.812834	-0.687756
40	1	0	4.154955	3.033139	-0.939665
41	1	0	2.672263	2.259160	-1.516899
42	1	0	2.578308	3.754533	-0.563308
43	6	0	2.522936	-1.348737	-0.474098
44	6	0	2.865304	-0.698990	-1.664166
45	6	0	3.524185	-1.684527	0.441253
46	6	0	4.191551	-0.365021	-1.917607
47	1	0	2.097314	-0.497612	-2.402747
48	6	0	4.843005	-1.334778	0.188311
49	1	0	3.242983	-2.199745	1.351372
50	6	0	5.182538	-0.673353	-0.991226
51	1	0	4.451444	0.127341	-2.847719
52	1	0	5.610752	-1.582943	0.911403
53	1	0	6.215546	-0.416462	-1.193422

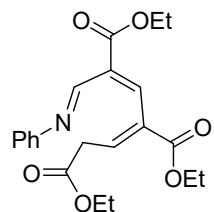


E = -1129.491794 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.177211	0.489742	1.081582
2	6	0	0.317305	1.251207	0.390168
3	6	0	-1.104196	0.948814	0.149641
4	6	0	-1.562325	-0.203665	-0.357230

5	6	0	-0.665828	-1.292851	-0.810313
6	7	0	-0.947720	-2.502143	-0.582034
7	1	0	-1.810115	1.742138	0.370352
8	1	0	0.257107	-0.987831	-1.323970
9	6	0	-0.031995	-3.512317	-1.066266
10	1	0	0.322466	-4.099181	-0.214409
11	1	0	-0.579167	-4.190383	-1.724747
12	1	0	0.825372	-3.092241	-1.610340
13	6	0	-3.030477	-0.391464	-0.594336
14	8	0	-3.493715	-1.120767	-1.426702
15	8	0	-3.774647	0.386185	0.207104
16	6	0	0.746484	2.586678	-0.134657
17	8	0	-0.015101	3.364149	-0.649419
18	8	0	2.051497	2.835141	0.030185
19	1	0	2.194329	0.855780	1.174785
20	6	0	0.867267	-0.775230	1.817737
21	1	0	1.116497	-0.637525	2.875535
22	1	0	-0.187273	-1.049421	1.775169
23	6	0	1.670935	-1.987744	1.378923
24	8	0	1.650012	-3.042245	1.950179
25	8	0	2.421976	-1.744124	0.295859
26	6	0	-5.193034	0.323240	-0.011910
27	1	0	-5.398676	0.581202	-1.053057
28	1	0	-5.524277	-0.704862	0.149238
29	6	0	-5.839600	1.289611	0.953875
30	1	0	-5.485636	2.306125	0.775628
31	1	0	-6.923145	1.272233	0.824359
32	1	0	-5.608750	1.016067	1.984441
33	6	0	3.289913	-2.811241	-0.128903
34	1	0	2.702967	-3.724862	-0.231696
35	1	0	4.035121	-2.977939	0.652379
36	6	0	3.917315	-2.381651	-1.434922
37	1	0	3.150574	-2.218863	-2.194699
38	1	0	4.479189	-1.455424	-1.307095
39	1	0	4.598688	-3.155915	-1.791456
40	6	0	2.510628	4.108116	-0.455587
41	1	0	1.961395	4.897693	0.061318

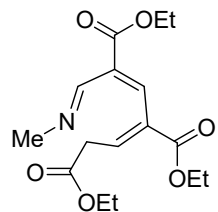
42	1	0	2.277252	4.179660	-1.519853
43	6	0	3.996801	4.179662	-0.190591
44	1	0	4.389613	5.133206	-0.547838
45	1	0	4.202514	4.099104	0.877754
46	1	0	4.519407	3.374088	-0.708492



E = -1321.2130765 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.087380	1.439241	1.270400
2	6	0	-1.110164	1.419481	0.405769
3	6	0	-2.065523	0.315246	0.220107
4	6	0	-1.819111	-0.967919	-0.107679
5	6	0	-0.520956	-1.547935	-0.508073
6	7	0	0.564939	-0.892015	-0.453721
7	1	0	-3.108830	0.601297	0.312088
8	1	0	-0.570183	-2.565874	-0.906635
9	6	0	-2.967075	-1.923440	-0.235937
10	8	0	-2.845635	-3.059782	-0.618519
11	8	0	-4.142425	-1.395353	0.119617
12	6	0	-5.285462	-2.256765	-0.016488
13	1	0	-5.144614	-3.126213	0.629175
14	1	0	-5.335009	-2.609407	-1.048493
15	6	0	-6.502301	-1.447839	0.370019
16	1	0	-7.397998	-2.065939	0.287409
17	1	0	-6.419348	-1.094230	1.398644
18	1	0	-6.613946	-0.584759	-0.287654

19	6	0	-1.469357	2.642356	-0.373922
20	8	0	-2.475817	2.733207	-1.030623
21	8	0	-0.566675	3.625718	-0.273137
22	6	0	-0.864304	4.824255	-1.008013
23	1	0	-1.806813	5.234824	-0.639435
24	1	0	-1.001419	4.564271	-2.059617
25	6	0	0.291534	5.775799	-0.800889
26	1	0	1.220107	5.340046	-1.172370
27	1	0	0.104679	6.706224	-1.339833
28	1	0	0.414979	6.007978	0.257893
29	1	0	0.506460	2.344625	1.330955
30	6	0	0.261872	0.339689	2.215663
31	1	0	0.255341	0.746018	3.235511
32	1	0	-0.451115	-0.481927	2.186045
33	6	0	1.641872	-0.267507	2.038428
34	8	0	1.919975	-1.379726	2.396682
35	8	0	2.519413	0.588006	1.509556
36	6	0	3.866879	0.095453	1.362147
37	1	0	4.268402	-0.108996	2.357568
38	1	0	3.839646	-0.842981	0.805057
39	6	0	4.654749	1.160720	0.636299
40	1	0	5.681008	0.819484	0.487461
41	1	0	4.211077	1.356986	-0.340977
42	1	0	4.674975	2.090274	1.207702
43	6	0	1.762819	-1.488479	-0.888217
44	6	0	2.173069	-2.750455	-0.451763
45	6	0	2.603770	-0.728873	-1.706272
46	6	0	3.408668	-3.249609	-0.849595
47	1	0	1.548671	-3.301918	0.241415
48	6	0	3.826978	-1.242311	-2.113603
49	1	0	2.277092	0.259717	-2.007449
50	6	0	4.236420	-2.503100	-1.682948
51	1	0	3.731225	-4.221061	-0.494068
52	1	0	4.469702	-0.652730	-2.757411
53	1	0	5.198646	-2.896199	-1.988147



E = -1129.4841736 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.069537	-0.090012	-0.356031
2	6	0	-0.089159	0.823365	-0.294607
3	6	0	1.329738	0.417909	-0.297338
4	6	0	1.857876	-0.545498	0.469525
5	6	0	1.131466	-1.332279	1.513646
6	7	0	0.473196	-0.903955	2.506567
7	1	0	1.984267	0.960086	-0.972321
8	1	0	1.223481	-2.415417	1.416308
9	6	0	0.349579	0.516480	2.767618
10	1	0	-0.659686	0.837185	2.487662
11	1	0	0.447486	0.671060	3.843198
12	1	0	1.075629	1.146468	2.242398
13	6	0	3.284986	-0.954501	0.303649
14	8	0	3.794174	-1.833419	0.951032
15	8	0	3.938702	-0.254824	-0.631236
16	6	0	5.324499	-0.593410	-0.809087
17	1	0	5.392477	-1.644278	-1.098383
18	1	0	5.836596	-0.475974	0.148115
19	6	0	5.878242	0.328697	-1.870678
20	1	0	6.934788	0.109911	-2.034905
21	1	0	5.346652	0.194747	-2.813775
22	1	0	5.783552	1.370619	-1.562027
23	6	0	-0.282166	2.303183	-0.270873
24	8	0	0.623431	3.087287	-0.393605
25	8	0	-1.554320	2.673075	-0.078393
26	6	0	-1.798838	4.091642	-0.038543

27	1	0	-1.453514	4.529602	-0.977097
28	1	0	-1.206287	4.523093	0.770763
29	6	0	-3.283362	4.281659	0.171630
30	1	0	-3.601835	3.828967	1.111881
31	1	0	-3.517930	5.346900	0.204510
32	1	0	-3.850389	3.828402	-0.643094
33	1	0	-0.759227	-1.129681	-0.386431
34	6	0	-2.551770	0.134313	-0.379125
35	1	0	-2.882814	0.494044	0.603262
36	1	0	-2.845137	0.914587	-1.080159
37	6	0	-3.391512	-1.087977	-0.685825
38	8	0	-4.512526	-1.023932	-1.112179
39	8	0	-2.775063	-2.237577	-0.393668
40	6	0	-3.541799	-3.438458	-0.598826
41	1	0	-4.442448	-3.382758	0.015931
42	1	0	-3.851445	-3.477155	-1.645084
43	6	0	-2.658649	-4.603428	-0.216357
44	1	0	-3.202695	-5.539651	-0.351914
45	1	0	-1.764408	-4.630448	-0.840894
46	1	0	-2.352249	-4.527626	0.827806

Ph-TS

E = -1321.1987921 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.163859	0.997951	0.902755
2	6	0	-1.027147	1.479651	0.393054
3	6	0	-2.159615	0.635064	0.225531
4	6	0	-2.025793	-0.689176	-0.111690
5	6	0	-0.781096	-1.244077	-0.606353
6	7	0	0.385358	-0.776226	-0.350710
7	1	0	-3.148855	1.080512	0.198074
8	1	0	-0.900287	-2.068877	-1.313745
9	6	0	-3.219341	-1.536110	-0.363296

10	8	0	-3.184450	-2.613426	-0.906356
11	8	0	-4.350613	-0.981935	0.091091
12	6	0	-5.551336	-1.739729	-0.130591
13	1	0	-5.434043	-2.721562	0.332489
14	1	0	-5.676516	-1.889654	-1.205156
15	6	0	-6.693860	-0.955351	0.472226
16	1	0	-7.630646	-1.495806	0.325821
17	1	0	-6.539455	-0.812053	1.542572
18	1	0	-6.781677	0.023760	-0.000862
19	6	0	-1.132619	2.844136	-0.165254
20	8	0	-2.163985	3.349033	-0.534530
21	8	0	0.050942	3.486224	-0.212630
22	6	0	0.017014	4.812680	-0.760260
23	1	0	-0.644090	5.428452	-0.146826
24	1	0	-0.406984	4.767369	-1.765596
25	6	0	1.436492	5.332964	-0.763145
26	1	0	2.077875	4.699065	-1.377614
27	1	0	1.459159	6.345307	-1.170270
28	1	0	1.839712	5.358588	0.250297
29	1	0	1.053761	1.600842	0.742994
30	6	0	0.241191	0.086938	2.095342
31	1	0	0.297336	0.737620	2.978593
32	1	0	-0.638418	-0.545006	2.196157
33	6	0	1.467841	-0.799588	2.104184
34	8	0	1.469322	-1.958794	2.415738
35	8	0	2.563954	-0.123418	1.738979
36	6	0	3.780531	-0.888350	1.642152
37	1	0	3.958291	-1.382957	2.599053
38	1	0	3.642836	-1.657751	0.878137
39	6	0	4.885614	0.076376	1.280771
40	1	0	5.825697	-0.466274	1.165701
41	1	0	4.658121	0.575773	0.337914
42	1	0	5.012673	0.831664	2.058219
43	6	0	1.535379	-1.281475	-0.989489
44	6	0	1.797524	-2.653543	-1.015145
45	6	0	2.470902	-0.382678	-1.506219
46	6	0	2.981571	-3.118137	-1.576558

47	1	0	1.092506	-3.339341	-0.559681
48	6	0	3.647157	-0.858517	-2.069939
49	1	0	2.260165	0.680014	-1.459454
50	6	0	3.909343	-2.226375	-2.106076
51	1	0	3.183683	-4.182630	-1.586192
52	1	0	4.366209	-0.157420	-2.478154
53	1	0	4.832415	-2.593433	-2.537841

Me-TS

E = -1129.480488 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.947347	0.272385	-0.553526
2	6	0	0.111221	1.143077	-0.395246
3	6	0	1.450320	0.667255	-0.278461
4	6	0	1.730494	-0.508360	0.367074
5	6	0	0.757846	-1.177292	1.216927
6	7	0	-0.511714	-1.131348	1.073500
7	1	0	2.271821	1.318494	-0.557776
8	1	0	1.197620	-1.681716	2.082430
9	6	0	-1.369592	-1.615013	2.139410
10	1	0	-2.060160	-0.817711	2.422447
11	1	0	-1.962147	-2.455732	1.769790
12	1	0	-0.805522	-1.930438	3.023554
13	6	0	3.133688	-0.951654	0.564411
14	8	0	3.474111	-1.805665	1.346599
15	8	0	3.995568	-0.305485	-0.232227
16	6	0	-0.097348	2.587519	-0.165881
17	8	0	0.792959	3.399086	-0.095830
18	8	0	-1.397759	2.924250	-0.056089
19	1	0	-1.943413	0.659539	-0.358506
20	6	0	-0.905041	-0.900658	-1.490290
21	1	0	-1.220620	-0.527503	-2.474745
22	1	0	0.093982	-1.317230	-1.596234

23	6	0	-1.847190	-2.022706	-1.127021
24	8	0	-1.611434	-3.190241	-1.271901
25	8	0	-3.020292	-1.559950	-0.662283
26	6	0	5.378351	-0.662971	-0.077937
27	1	0	5.676086	-0.470063	0.955030
28	1	0	5.484561	-1.733997	-0.262129
29	6	0	6.168045	0.167927	-1.063132
30	1	0	6.031641	1.232021	-0.865232
31	1	0	7.230285	-0.067649	-0.977274
32	1	0	5.847920	-0.039849	-2.085092
33	6	0	-4.014375	-2.552651	-0.362593
34	1	0	-3.584770	-3.291100	0.317843
35	1	0	-4.278163	-3.071588	-1.286930
36	6	0	-5.196758	-1.835733	0.247482
37	1	0	-4.904959	-1.327755	1.168261
38	1	0	-5.597676	-1.094795	-0.445652
39	1	0	-5.984857	-2.553342	0.481927
40	6	0	-1.661074	4.314364	0.182382
41	1	0	-1.285066	4.893333	-0.664092
42	1	0	-1.111198	4.629810	1.071488
43	6	0	-3.155604	4.465666	0.353964
44	1	0	-3.403151	5.512907	0.536677
45	1	0	-3.682466	4.136524	-0.542925
46	1	0	-3.506799	3.874372	1.201101
