Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information to Accompany:

Activation of a CH bond in polypyridine systems by acetyl hypofluorite made from F_2

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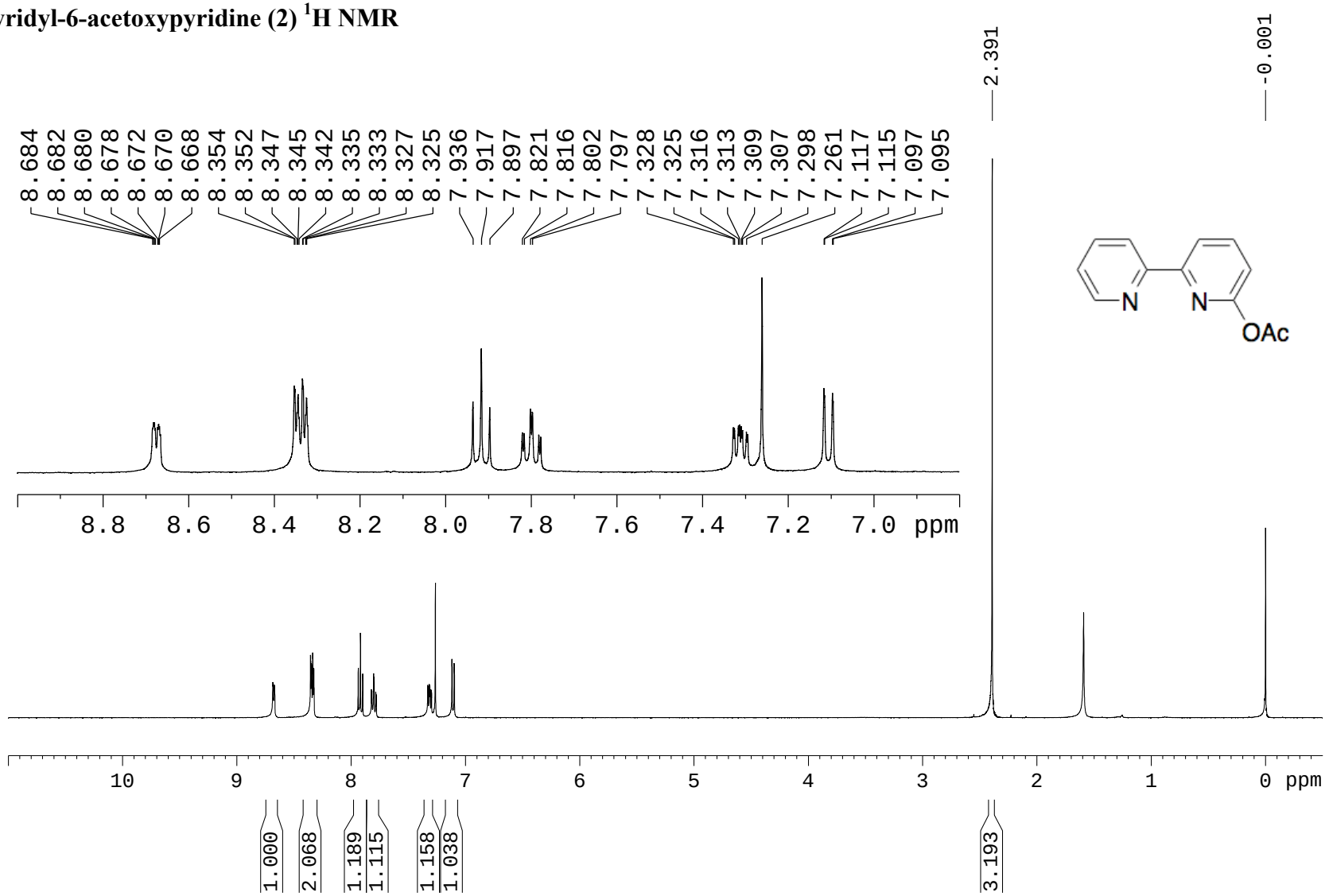
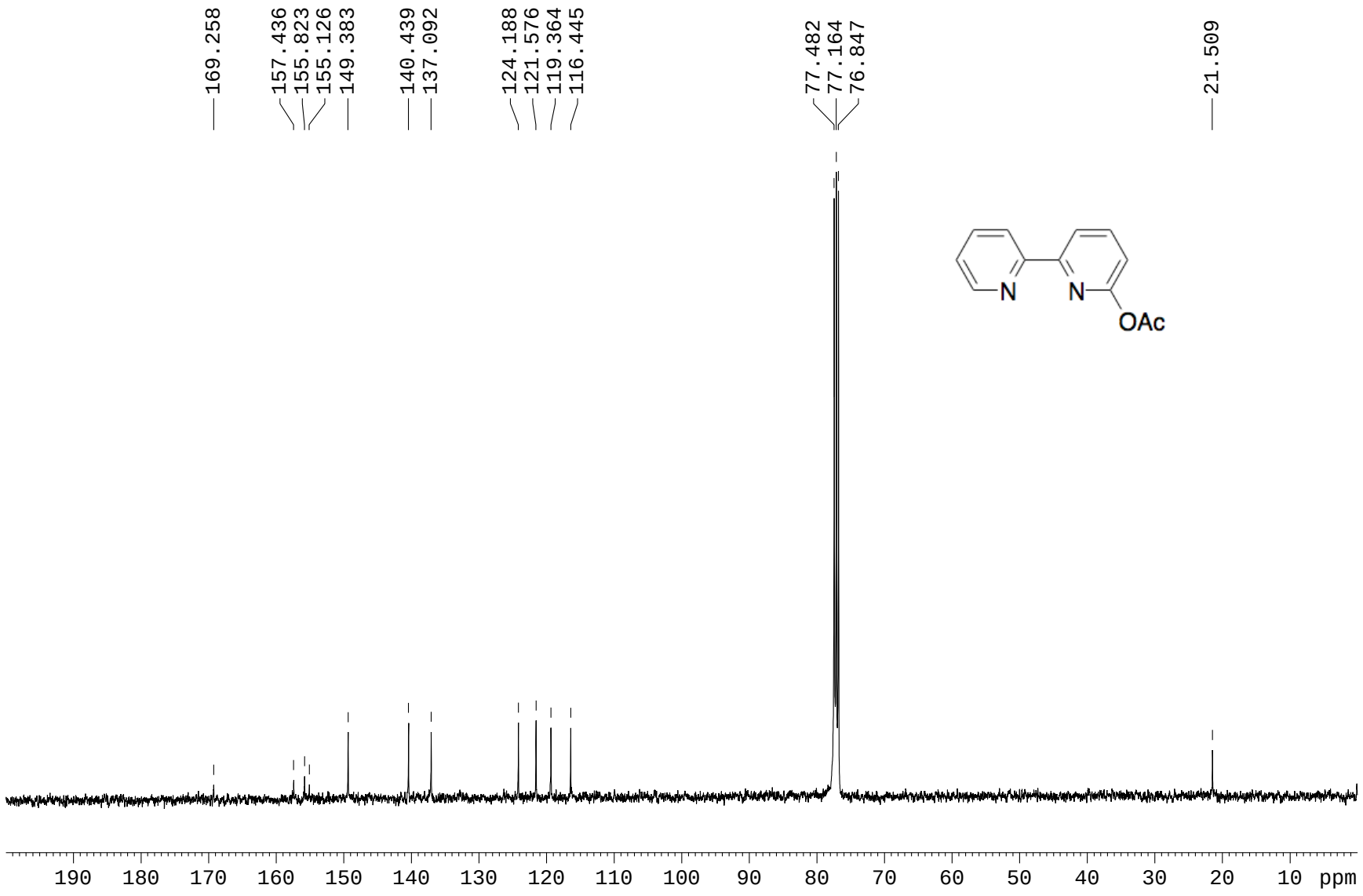
Proton and carbon NMR spectra

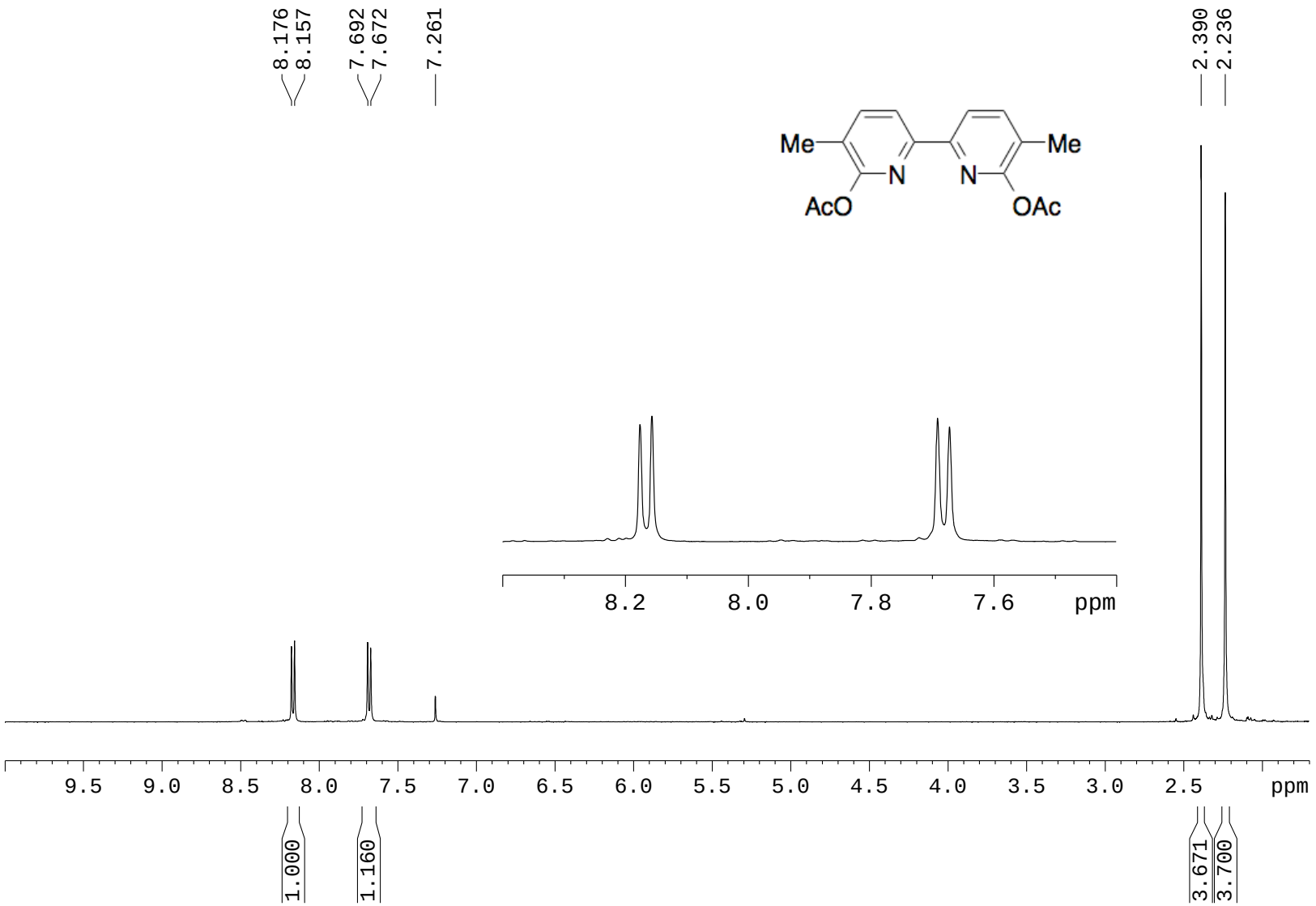
2-Pyridyl-6-acetoxypyridine (2) ^{1}H NMR



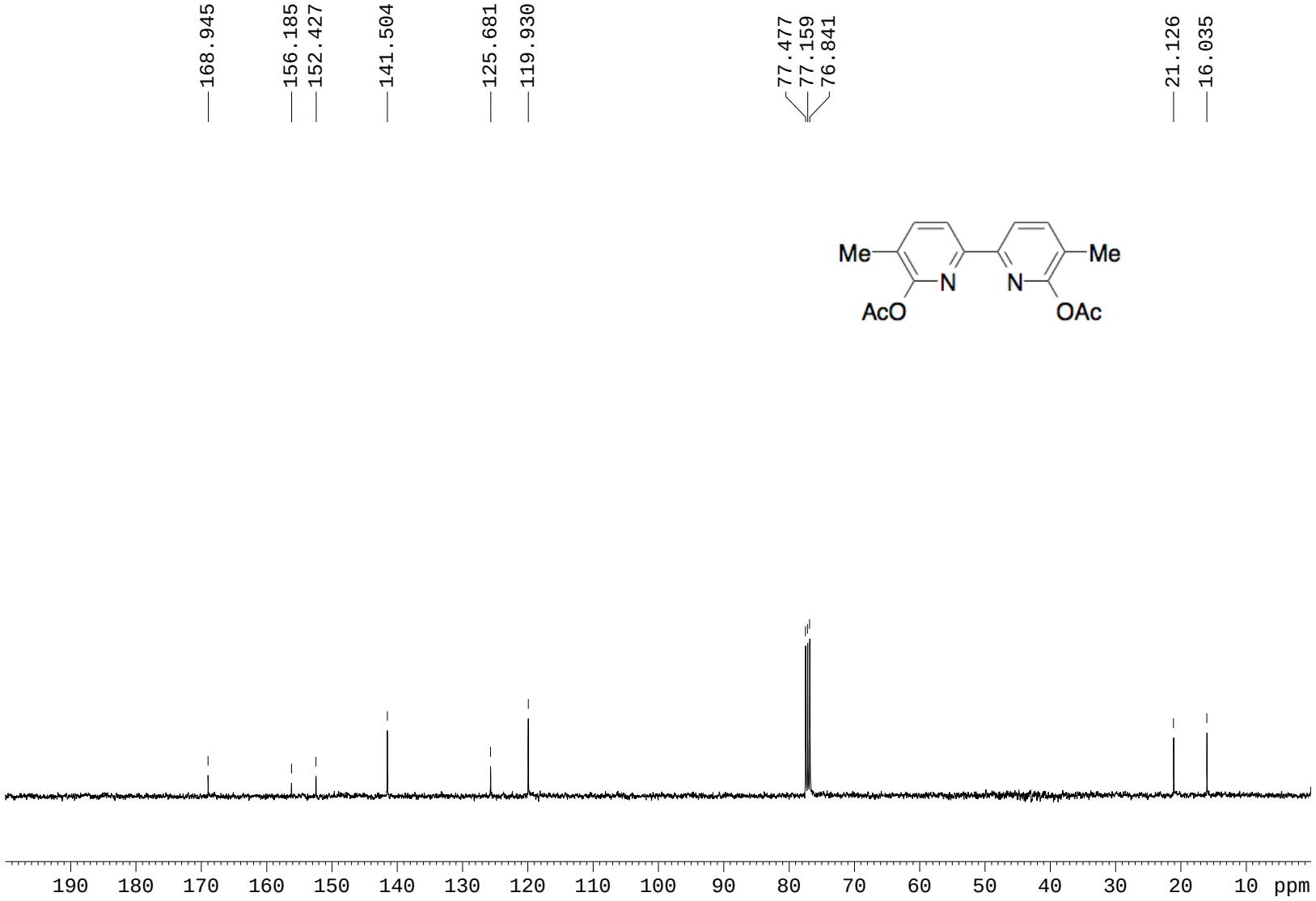
2-Pyridyl-6-acetoxypyridine (2) ^{13}C NMR



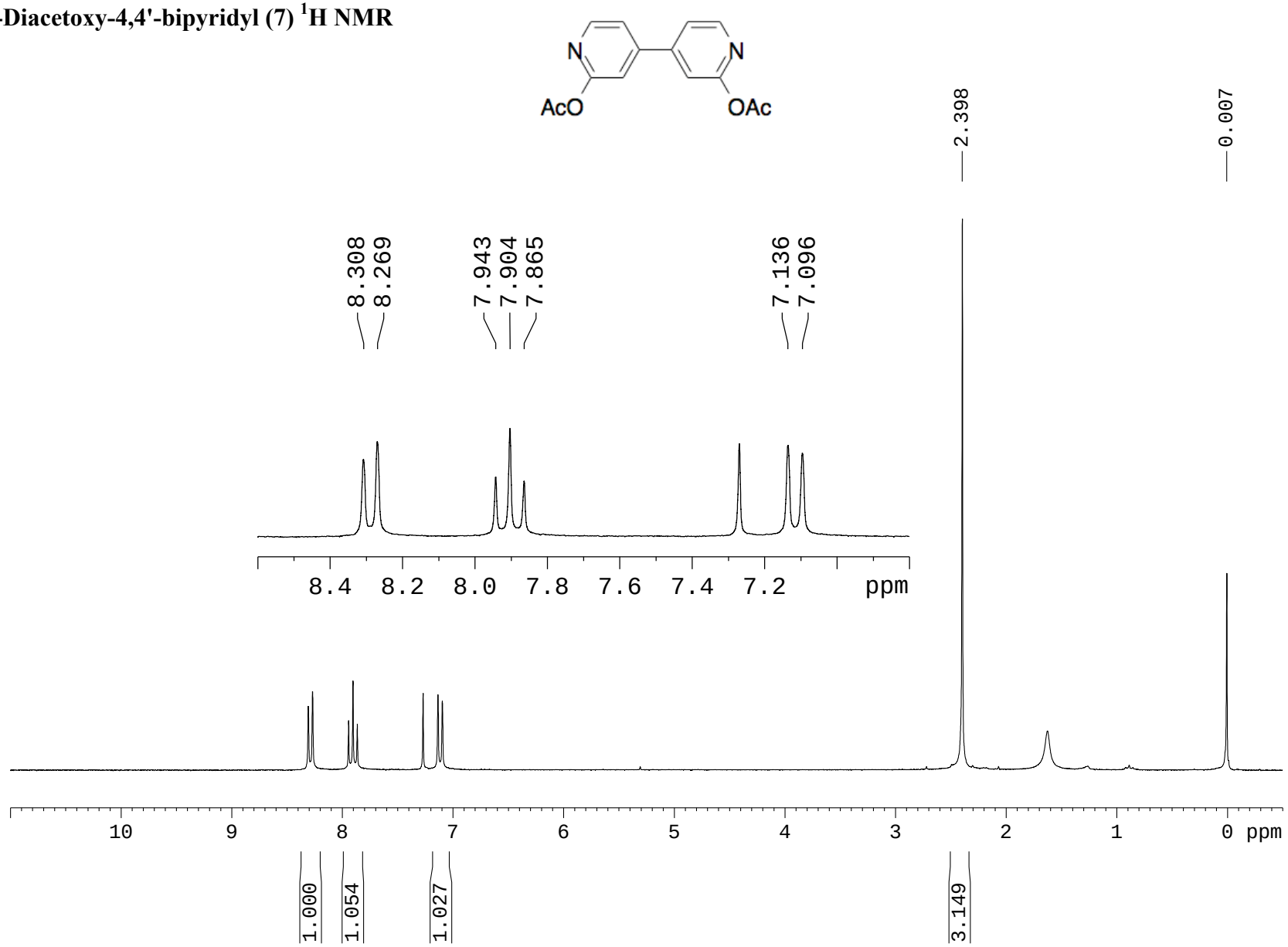
6,6'-Diacetoxy-5,5'-dimethyl-2,2'-bipyridyl (5) ^{1}H NMR



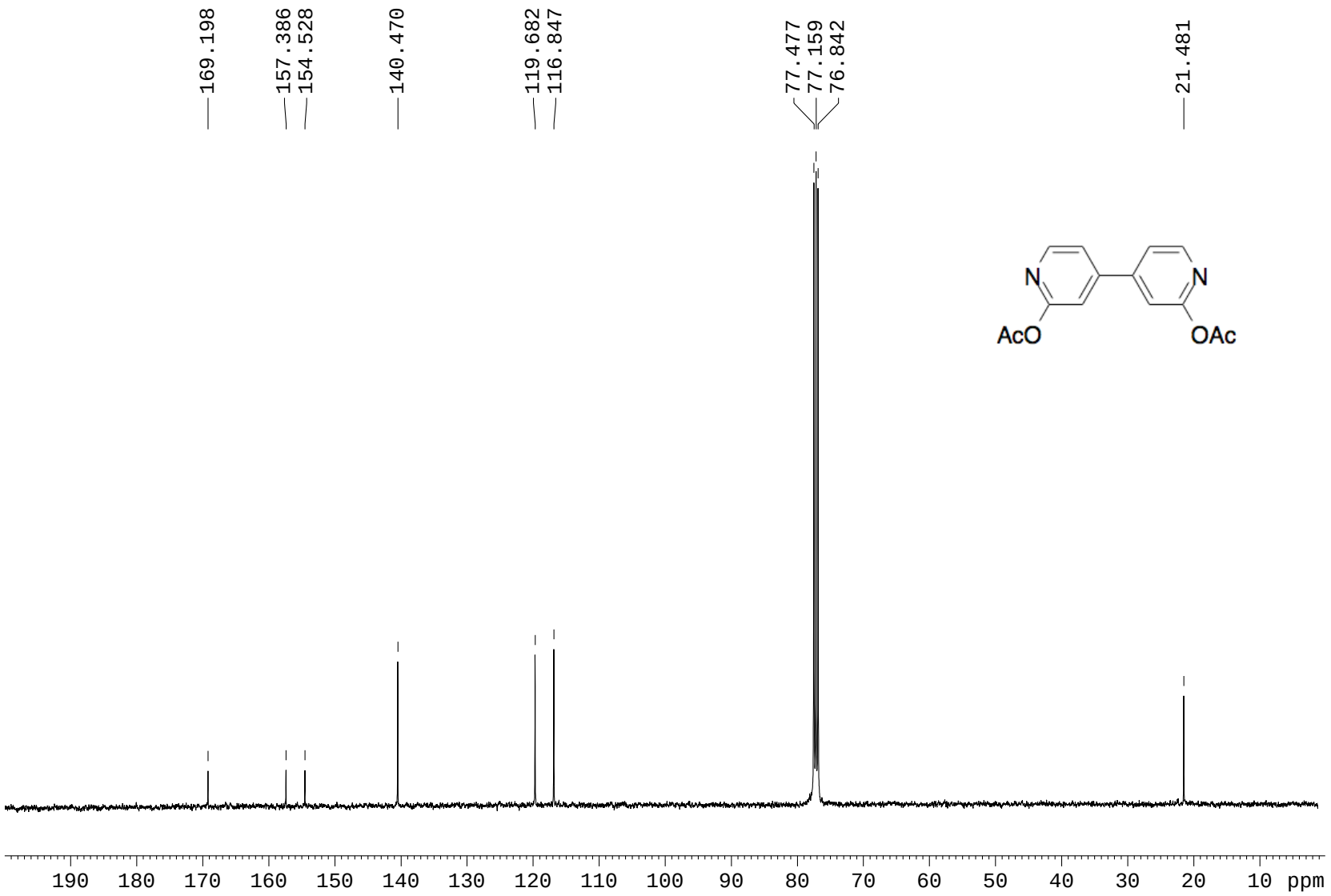
6,6'-Diacetoxy-5,5'-dimethyl-2,2'-bipyridyl (5) ^{13}C NMR



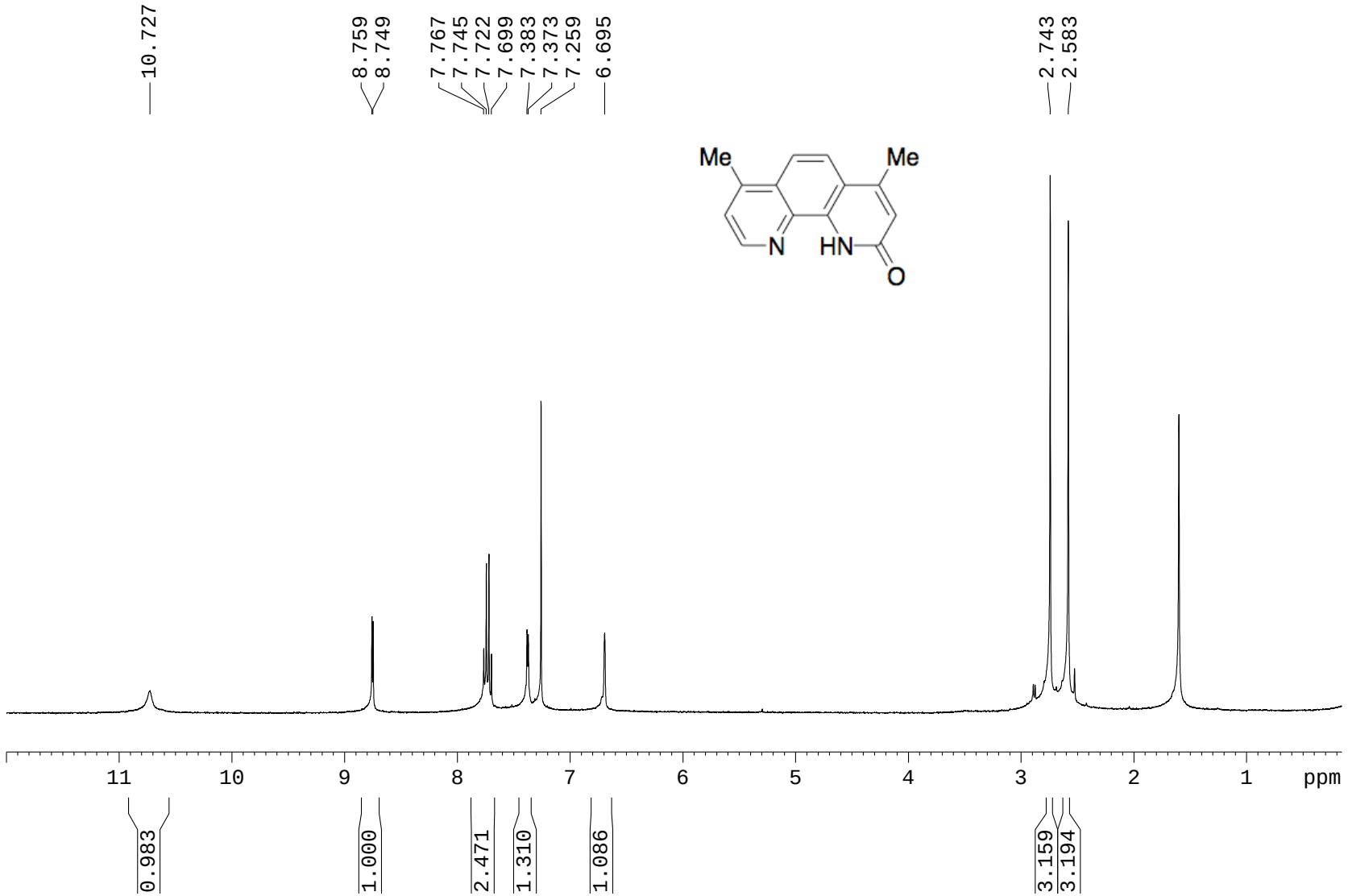
2,2'-Diacetoxy-4,4'-bipyridyl (7) ^{1}H NMR



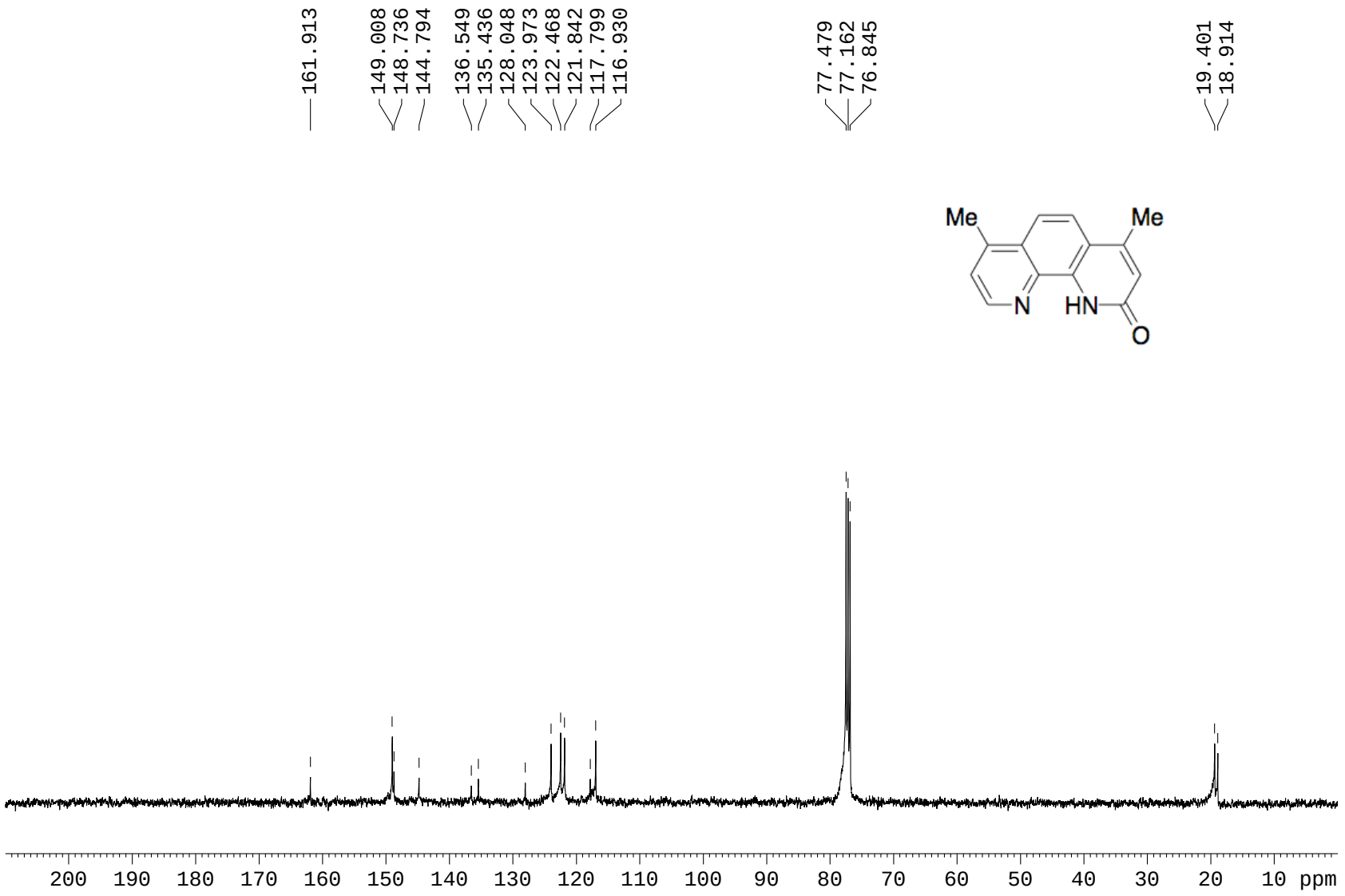
2,2'-Diacetoxy-4,4'-bipyridyl (7) ^{13}C NMR



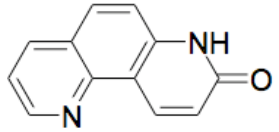
4,7-Dimethyl-1,10-phenanthrolin-2(1H)-one (12) ^{1}H NMR

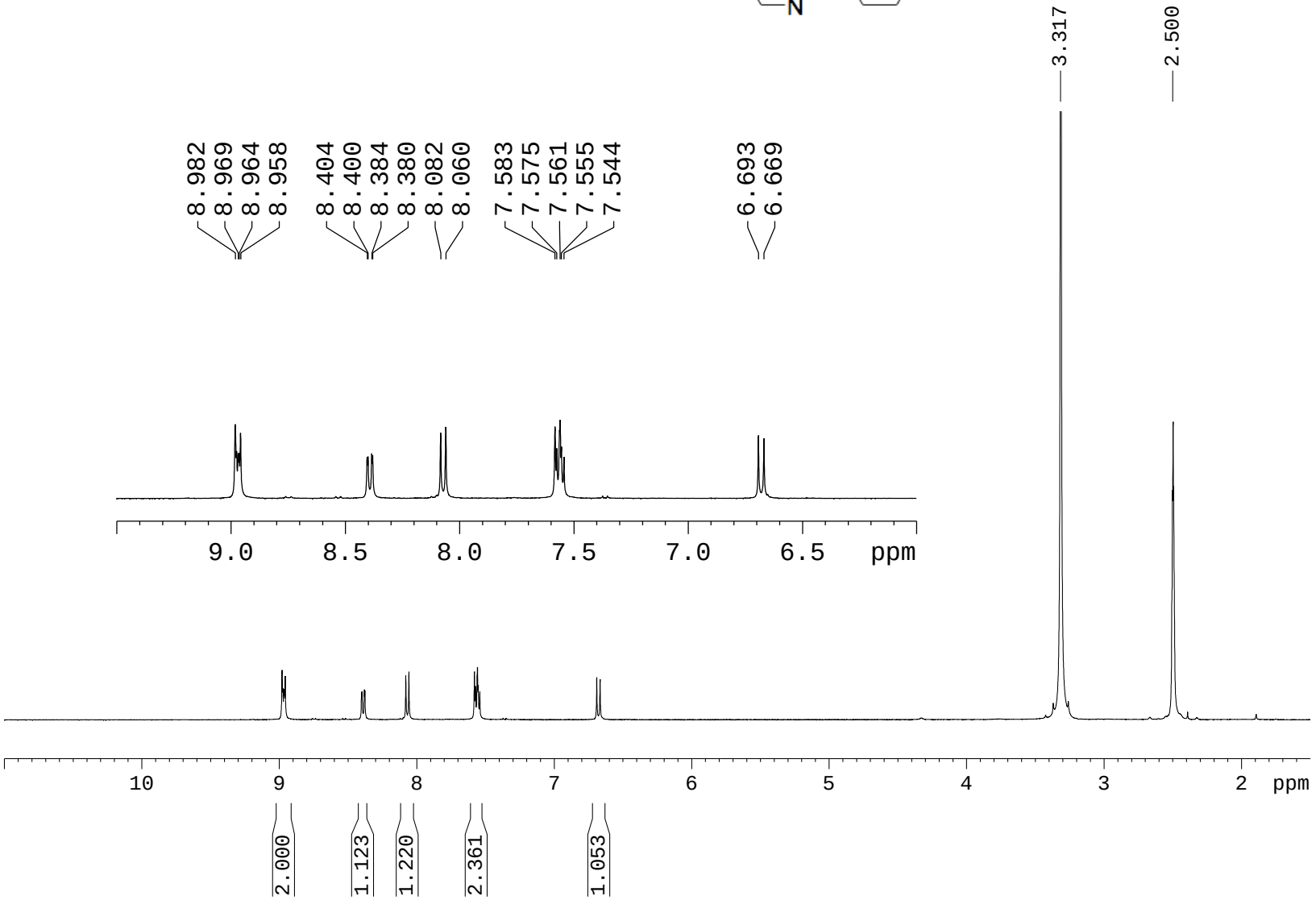


4,7-Dimethyl-1,10-phenanthrolin-2(1H)-one (12) ^{13}C NMR

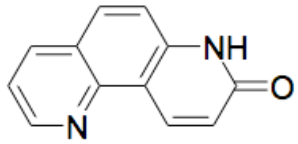


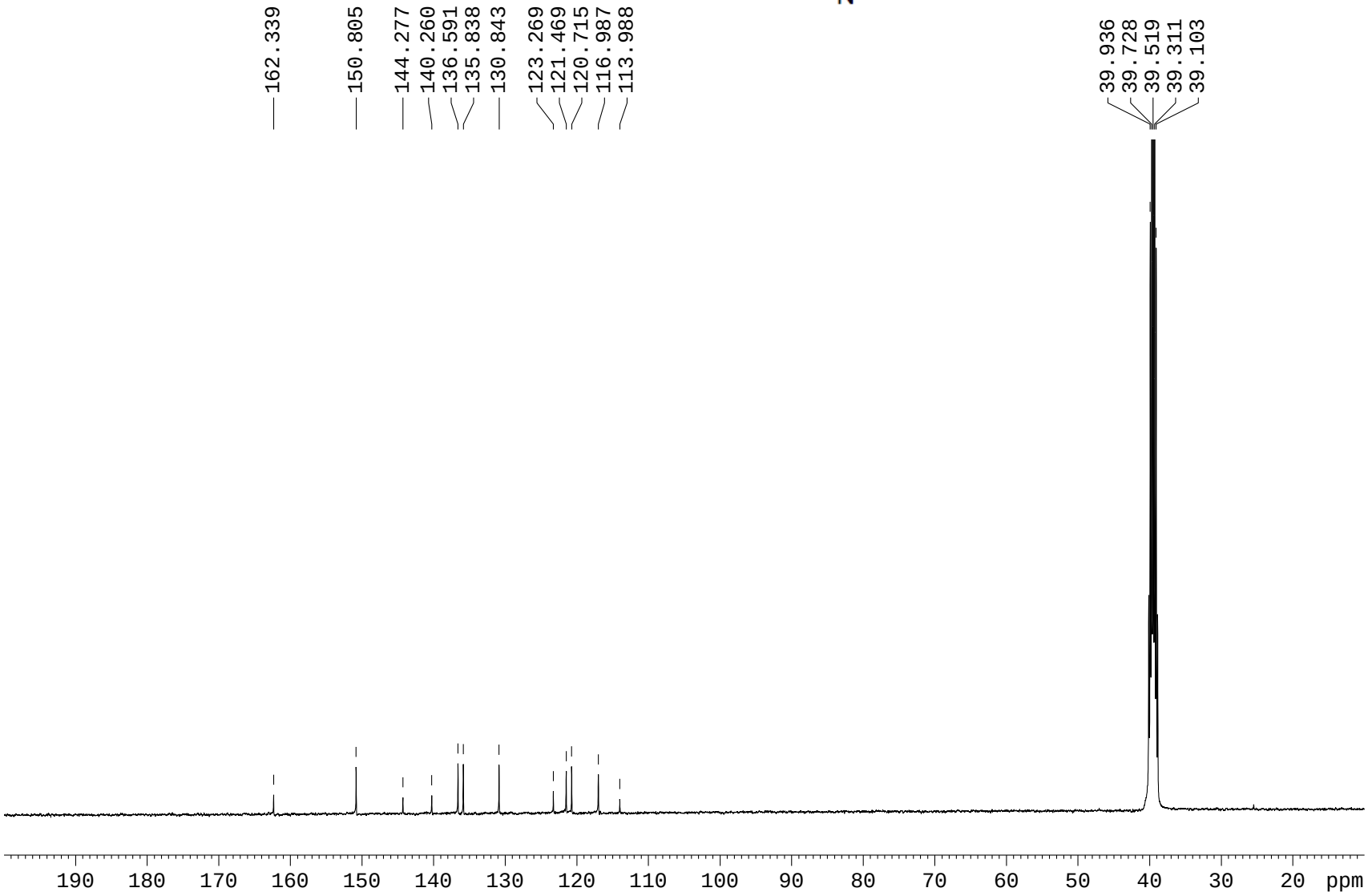
1,7-Phenanthrolin-8-one (15) ^{1}H NMR



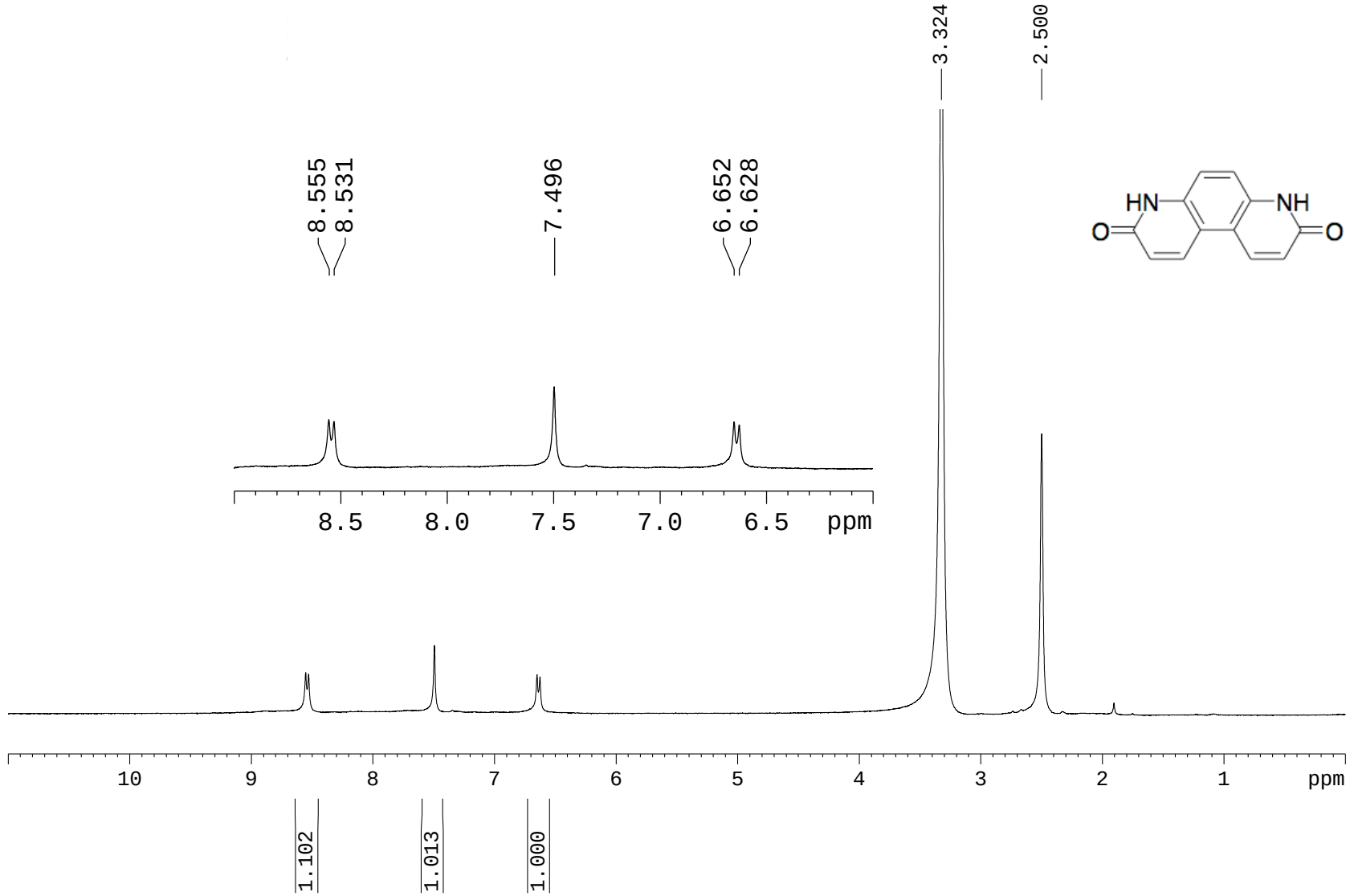


1,7-Phenanthrolin-8-one (15) ^{1}H NMR

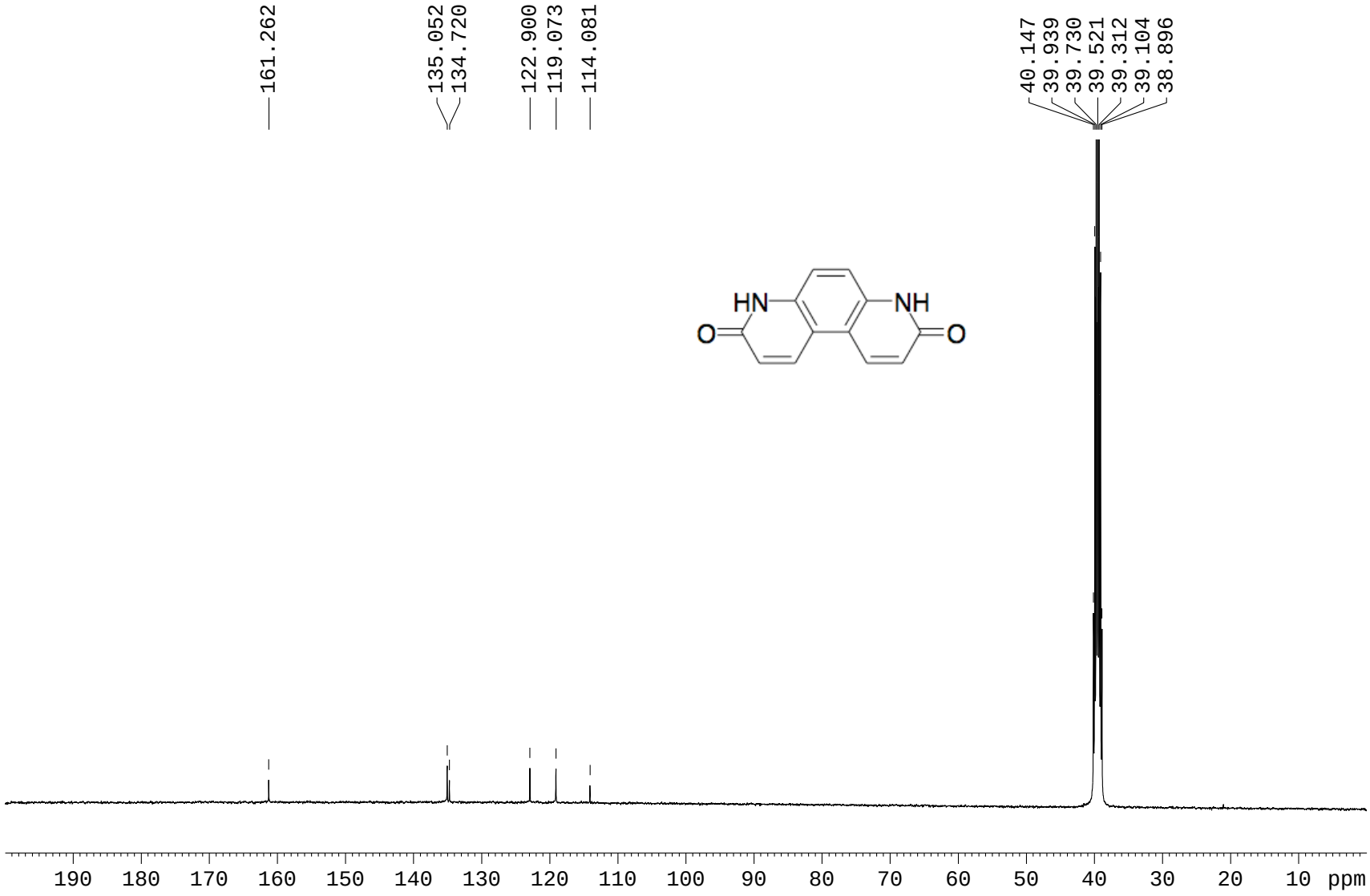




4,7-Phenanthroline-3,8(4H,7H)-dione (18) ^{1}H NMR

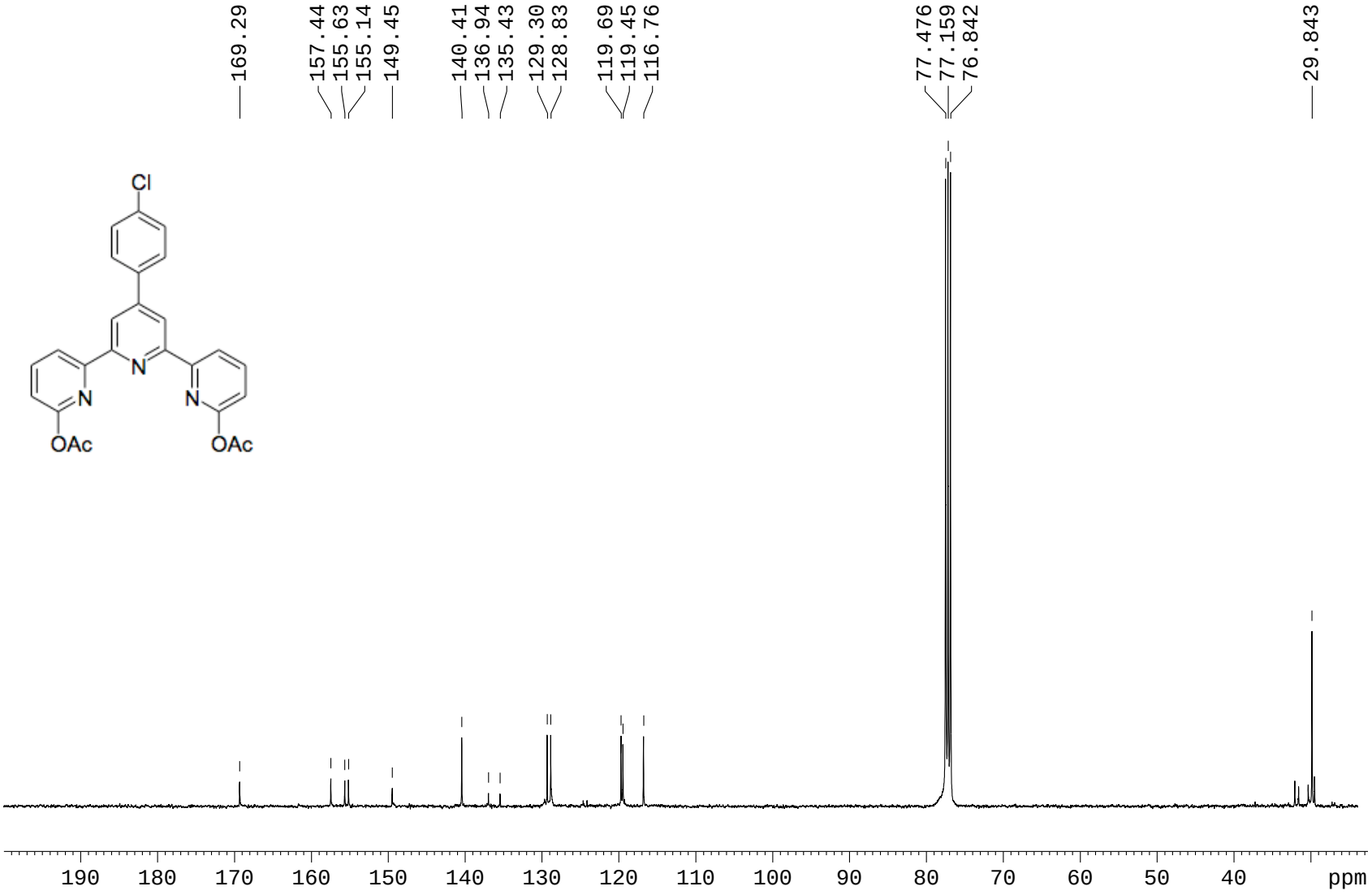


4,7-Phenanthroline-3,8(4H,7H)-dione (18) ^{13}C NMR



6,6″-Diacetoxy-4′-(4-chlorophenyl)-2,2′:6′,2″-terpyridine (23) ^{1}H NMR

6,6″-Diacetoxy-4′-(4-chlorophenyl)-2,2′:6′,2″-terpyridine (23) ^{13}C NMR



DFT calculations

All calculations were preformed using Gaussian 03 program.

5,6-Dimethyl-1,10-phenanthroline (**10**) - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.473667	-0.719465	0.000126
2	6	0	2.856249	0.519367	-0.000018
3	6	0	1.429865	0.542279	-0.000035
4	6	0	0.730670	-0.701130	-0.000018
5	6	0	2.688860	-1.890209	0.000136
6	6	0	0.682338	1.766452	-0.000019
7	6	0	-0.730670	-0.701130	0.000018
8	6	0	-1.429865	0.542279	0.000035
9	6	0	-0.682338	1.766452	0.000019
10	6	0	-2.856249	0.519367	0.000018
11	6	0	-3.473667	-0.719465	-0.000126
12	6	0	-2.688860	-1.890209	-0.000136
13	1	0	1.214814	2.712565	-0.000054
14	1	0	4.558248	-0.797700	0.000244
15	1	0	3.173844	-2.866222	0.000163
16	1	0	-1.214814	2.712565	0.000054
17	1	0	-4.558248	-0.797700	-0.000244
18	1	0	-3.173844	-2.866222	-0.000163
19	7	0	-1.367459	-1.896286	-0.000024

20	7	0	1.367459	-1.896286	0.000024
21	6	0	3.669832	1.790740	-0.000155
22	6	0	-3.669832	1.790740	0.000155
23	1	0	-4.740235	1.563998	0.000107
24	1	0	-3.458106	2.406423	0.883524
25	1	0	-3.458059	2.406735	-0.882977
26	1	0	3.458106	2.406423	-0.883524
27	1	0	4.740235	1.563998	-0.000107
28	1	0	3.458059	2.406735	0.882977

Energy

SCF Done: E(RB+HF-LYP) = -650.266478686 A.U. after 18 cycles
Predicted change in Energy=-9.242895D-09

4,7-dimethyl-1,10-phenanthrolin-2-yl ethanoate (**11**) - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.730138	-2.060425	-0.020863
2	6	0	3.828274	-0.686880	0.116573
3	6	0	2.618292	0.067257	0.055927
4	6	0	1.392217	-0.635133	-0.138869
5	6	0	2.466506	-2.655880	-0.212165
6	6	0	2.595532	1.495140	0.183324
7	6	0	0.143670	0.115847	-0.199966
8	6	0	0.169097	1.534018	-0.071749
9	6	0	1.425609	2.196068	0.120780
10	6	0	-1.068934	2.243490	-0.141938
11	6	0	-2.223404	1.507169	-0.328804
12	6	0	-2.116982	0.108646	-0.433729
13	1	0	3.528685	2.029325	0.332447
14	1	0	4.619160	-2.685308	0.017404
15	1	0	2.389243	-3.737408	-0.321107
16	1	0	1.445673	3.276843	0.220298
17	1	0	-3.197565	1.981970	-0.388925
18	7	0	1.332011	-1.981602	-0.271082
19	7	0	-1.008696	-0.574417	-0.380789
20	6	0	5.166959	-0.021316	0.322943
21	6	0	-1.129007	3.745639	-0.014958

22	1	0	5.389904	0.695981	-0.477019
23	1	0	5.969728	-0.764545	0.338168
24	1	0	5.202396	0.529223	1.271544
25	1	0	-2.161077	4.099745	-0.092065
26	1	0	-0.729663	4.082985	0.949621
27	1	0	-0.543875	4.240114	-0.800467
28	8	0	-3.282708	-0.622260	-0.686976
29	6	0	-3.969543	-1.125792	0.390226
30	6	0	-5.082136	-2.028886	-0.074804
31	1	0	-5.719396	-2.288770	0.771725
32	1	0	-4.649956	-2.941006	-0.502143
33	1	0	-5.670048	-1.544683	-0.860838
34	8	0	-3.694060	-0.862254	1.536087

Energy

SCF Done: E(RB+HF-LYP) = -878.158421245 A.U. after 12 cycles
Predicted change in Energy=-9.351624D-09

1,7-phenanthroline (**13**) - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.438198	3.149621	0.000000
2	6	0	-1.422214	0.850740	0.000000
3	6	0	0.000000	0.811286	0.000000
4	6	0	0.693795	2.039607	0.000000
5	6	0	-0.028398	3.217765	0.000000
6	6	0	-2.168710	-0.377587	0.000000
7	6	0	0.678263	-0.471542	0.000000
8	6	0	-0.098058	-1.665633	0.000000
9	6	0	-1.532005	-1.582975	0.000000
10	6	0	0.595972	-2.896207	0.000000
11	1	0	0.033415	-3.827585	0.000000
12	6	0	1.977378	-2.899024	0.000000
13	6	0	2.650173	-1.659115	0.000000
14	1	0	-3.251933	-0.302486	0.000000
15	1	0	-2.027635	4.065740	0.000000
16	1	0	1.778814	2.030318	0.000000
17	1	0	0.468478	4.183796	0.000000
18	1	0	-2.103563	-2.508673	0.000000
19	1	0	2.543028	-3.826203	0.000000
20	1	0	3.738971	-1.629737	0.000000
21	7	0	-2.123883	2.016258	0.000000

22	7	0	2.034229	-0.485798	0.000000

Energy

SCF Done: E(RB+HF-LYP) = -571.638106299 A.U. after 11 cycles
Predicted change in Energy=-5.392611D-05

1,7-phenanthrolin-8-yl ethanoate (**14**) - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.864427	-0.544373	0.193851
2	6	0	-4.281264	0.707337	0.231795
3	6	0	-2.878624	0.825735	0.110732
4	6	0	-2.127195	-0.374574	-0.046154
5	6	0	-4.028187	-1.669472	0.033332
6	6	0	-2.200731	2.090929	0.140047
7	6	0	-0.685864	-0.290915	-0.171135
8	6	0	-0.053846	0.980643	-0.137637
9	6	0	-0.844201	2.168609	0.020098
10	6	0	2.011957	0.041821	-0.393448
11	6	0	1.500987	-1.271814	-0.441640
12	6	0	0.135889	-1.429365	-0.326843
13	1	0	-2.794940	2.994028	0.261124
14	1	0	-5.939227	-0.672045	0.284043
15	1	0	-4.885843	1.603610	0.353590
16	1	0	-4.459401	-2.668927	-0.000866
17	1	0	-0.321625	3.120005	0.041147
18	1	0	2.168829	-2.117775	-0.556514
19	1	0	-0.324295	-2.411219	-0.354064
20	7	0	-2.710239	-1.598033	-0.083098
21	7	0	1.294920	1.125664	-0.250465

22	8	0	3.376160	0.261412	-0.590772
23	8	0	3.950835	-0.826205	1.324009
24	6	0	5.675709	0.168849	-0.060764
25	1	0	6.384080	-0.273706	0.640847
26	1	0	5.888335	-0.171794	-1.079404
27	1	0	5.778233	1.259699	-0.052795
28	6	0	4.272650	-0.209568	0.336422

Energy

SCF Done: E(RB+HF-LYP) = -799.529022794 A.U. after 17 cycles
Predicted change in Energy=-1.171799D-08

4,7-phenanthroline (**16**) - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.478822	-0.194717
2	6	0	0.000000	1.422037	0.838979
3	6	0	0.000000	0.726767	-0.406242
4	6	0	0.000000	1.515533	-1.577803
5	6	0	0.000000	2.894178	-1.477479
6	6	0	0.000000	0.680879	2.070066
7	6	0	0.000000	-0.726767	-0.406242
8	6	0	0.000000	-1.422037	0.838979
9	6	0	0.000000	-0.680879	2.070066
10	6	0	0.000000	-3.478822	-0.194717
11	6	0	0.000000	-2.894178	-1.477479
12	6	0	0.000000	-1.515533	-1.577803
13	1	0	0.000000	1.253996	2.992335
14	1	0	0.000000	4.562547	-0.086994
15	1	0	0.000000	1.049259	-2.558424
16	1	0	0.000000	3.521770	-2.364045
17	1	0	0.000000	-1.253996	2.992335
18	1	0	0.000000	-4.562547	-0.086994
19	1	0	0.000000	-3.521770	-2.364045
20	1	0	0.000000	-1.049259	-2.558424
21	7	0	0.000000	2.778564	0.928614

22	7	0	0.000000	-2.778564	0.928614

Energy

SCF Done: E(RB+HF-LYP) = -571.634642553 A.U. after 11 cycles
Predicted change in Energy=-9.526620D-08

4,7-phenanthroline-3-yl ethanoate - Standard basis: 6-31+G(d)

Geometry

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.877055	-0.373803	0.179556
2	6	0	2.891780	0.788215	0.106124
3	6	0	2.126307	-0.405674	-0.048717
4	6	0	2.842084	-1.623314	-0.082448
5	6	0	4.219281	-1.612385	0.031435
6	6	0	2.226870	2.060378	0.150530
7	6	0	0.682335	-0.309228	-0.161223
8	6	0	0.065780	0.973045	-0.110820
9	6	0	0.871264	2.150274	0.046500
10	6	0	-2.026606	0.081062	-0.353116
11	6	0	-1.540516	-1.239887	-0.422084
12	6	0	-0.176838	-1.421121	-0.321909
13	1	0	2.850547	2.941024	0.270617
14	1	0	5.961624	-0.337631	0.270943
15	1	0	2.320847	-2.569033	-0.195983
16	1	0	4.791342	-2.535463	0.008773
17	1	0	0.356387	3.105575	0.079306
18	1	0	-2.219806	-2.075665	-0.538020
19	1	0	0.224399	-2.428434	-0.369536
20	7	0	-1.280464	1.143913	-0.206852
21	7	0	4.246738	0.789113	0.217077

22	8	0	-3.384098	0.344605	-0.531640
23	6	0	-4.310244	-0.229679	0.304059
24	6	0	-5.695621	0.229662	-0.067922
25	1	0	-5.778070	1.311234	0.086645
26	1	0	-6.428878	-0.288852	0.551207
27	1	0	-5.889487	0.035866	-1.127987
28	8	0	-4.024703	-0.981489	1.205725

Energy

SCF Done: E(RB+HF-LYP) = -799.525554659 A.U. after 13 cycles
Predicted change in Energy=-1.802950D-08