Supporting Information

Emission Tuning of Fluorescent Kinase Inhibitors: Conjugation Length and Substituent Effects

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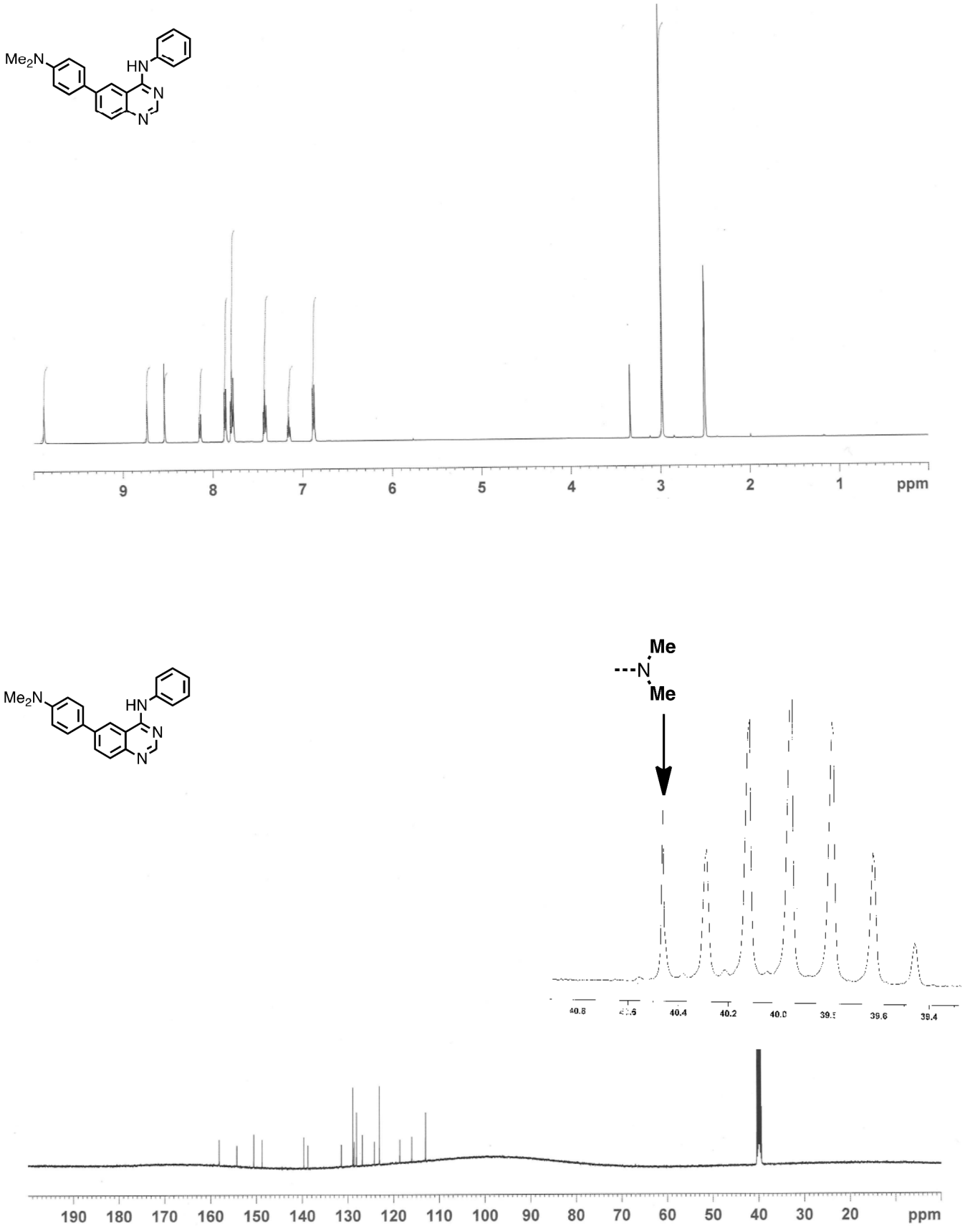

Figure S1. ^{1}H (top) and ^{13}C (bottom) NMRs of **1a**.

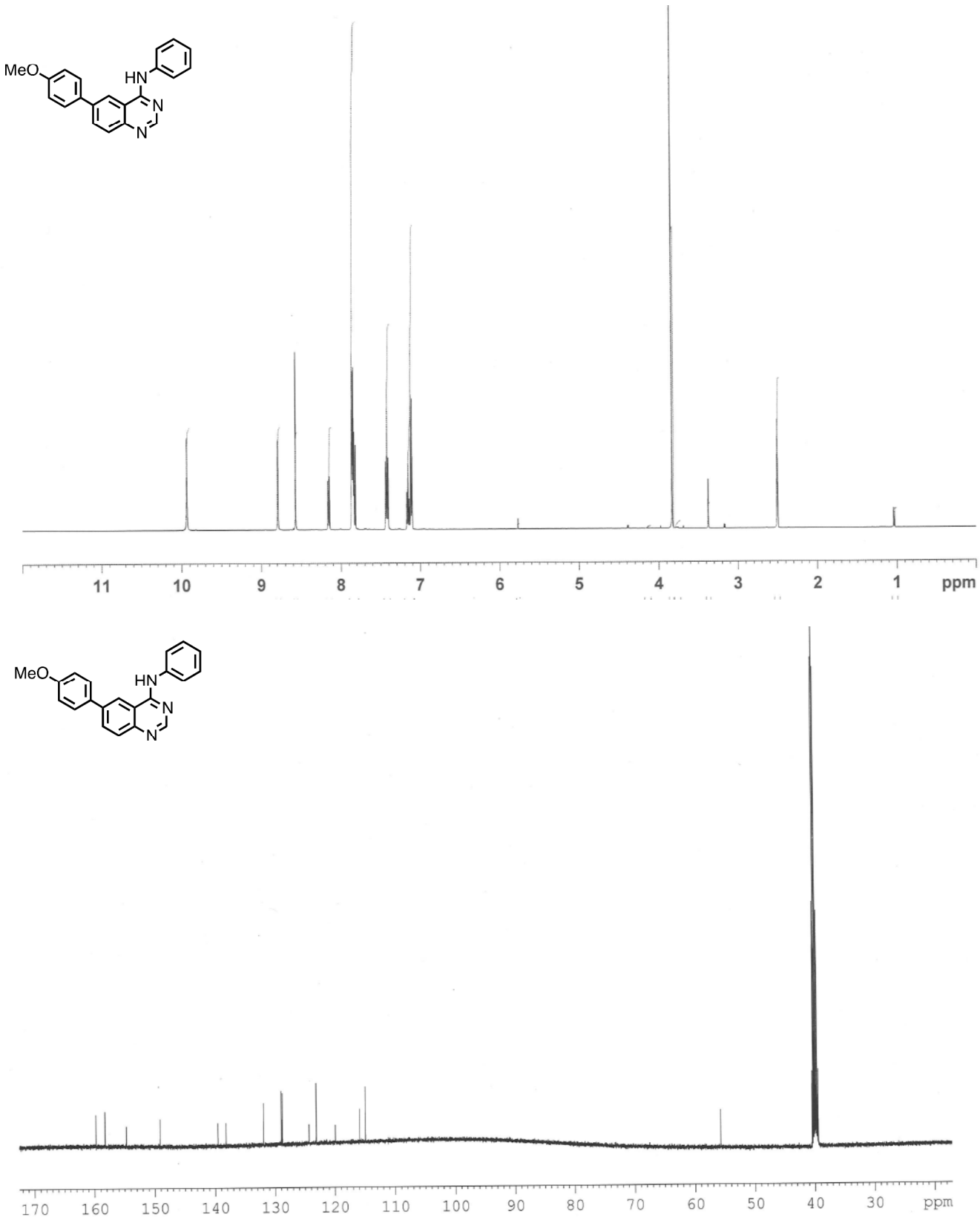

Figure S2. ^{1}H (top) and ^{13}C (bottom) NMRs of **1b**.

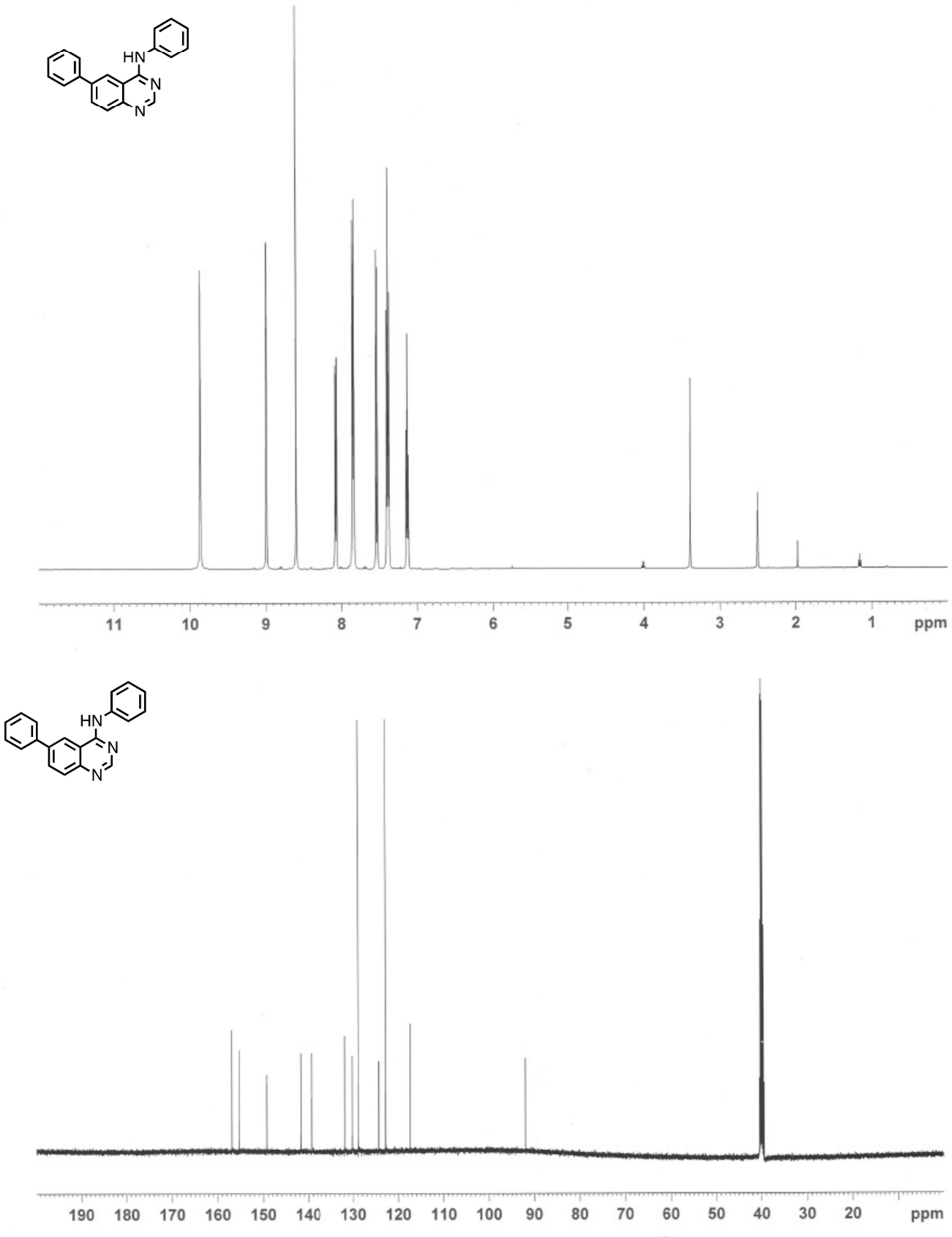

Figure S3. ^{1}H (top) and ^{13}C (bottom) NMRs of **1c**.

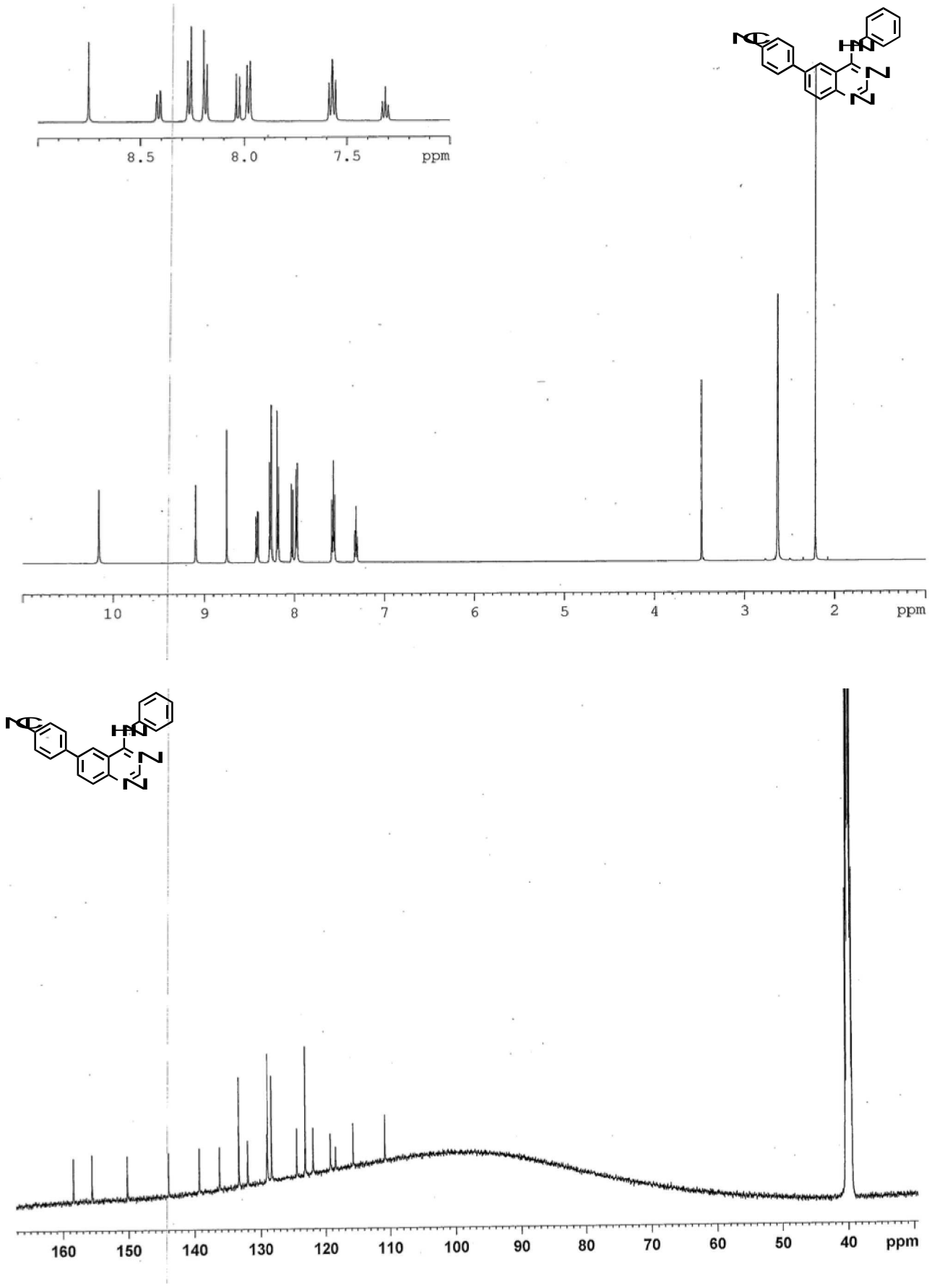

Figure S4. ^{1}H (top) and ^{13}C (bottom) NMRs of **1d**.

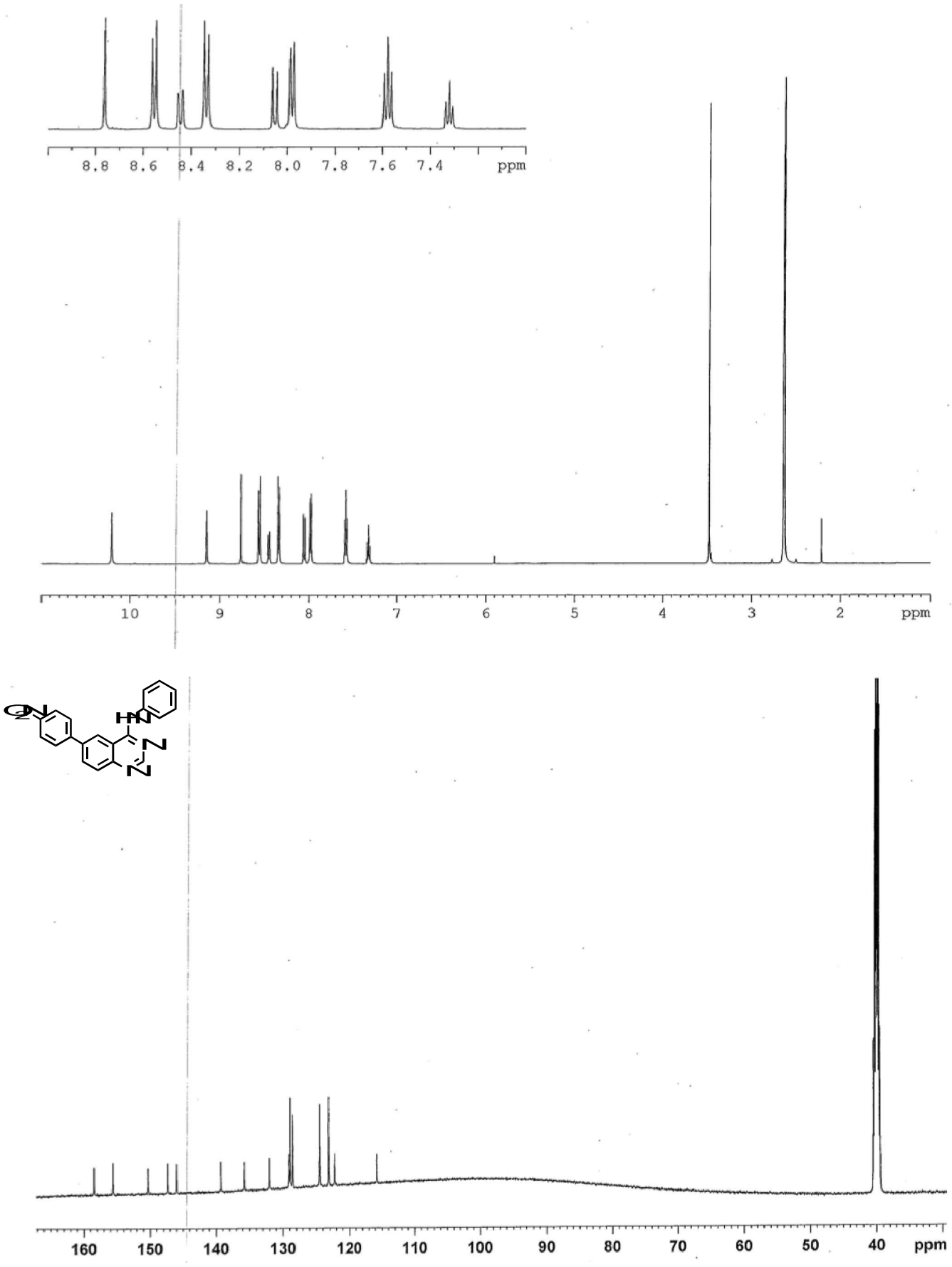

Figure S5. ^{1}H (top) and ^{13}C (bottom) NMRs of **1e**.

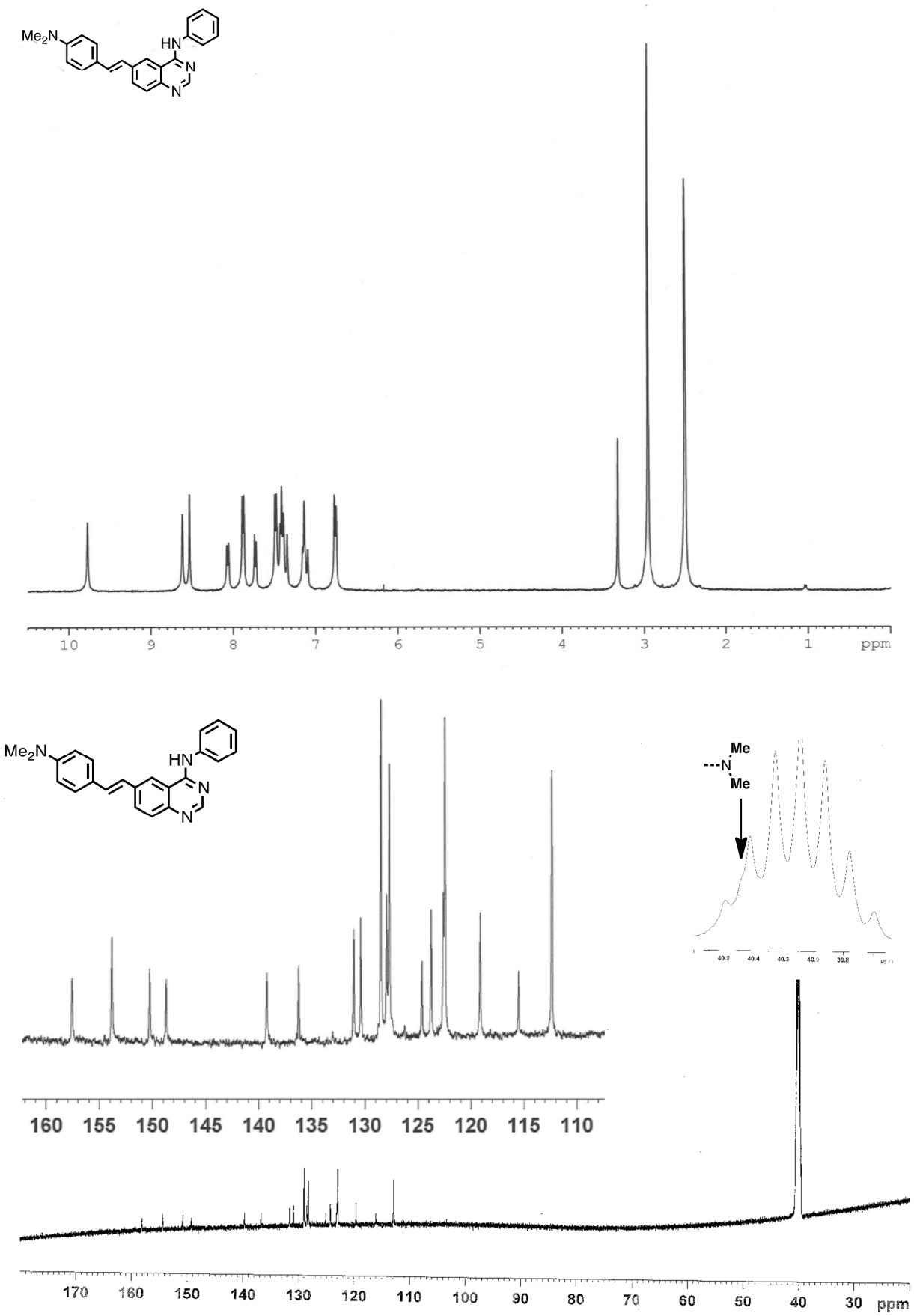

Figure S6. ^{1}H (top) and ^{13}C (bottom) NMRs of **2a**.

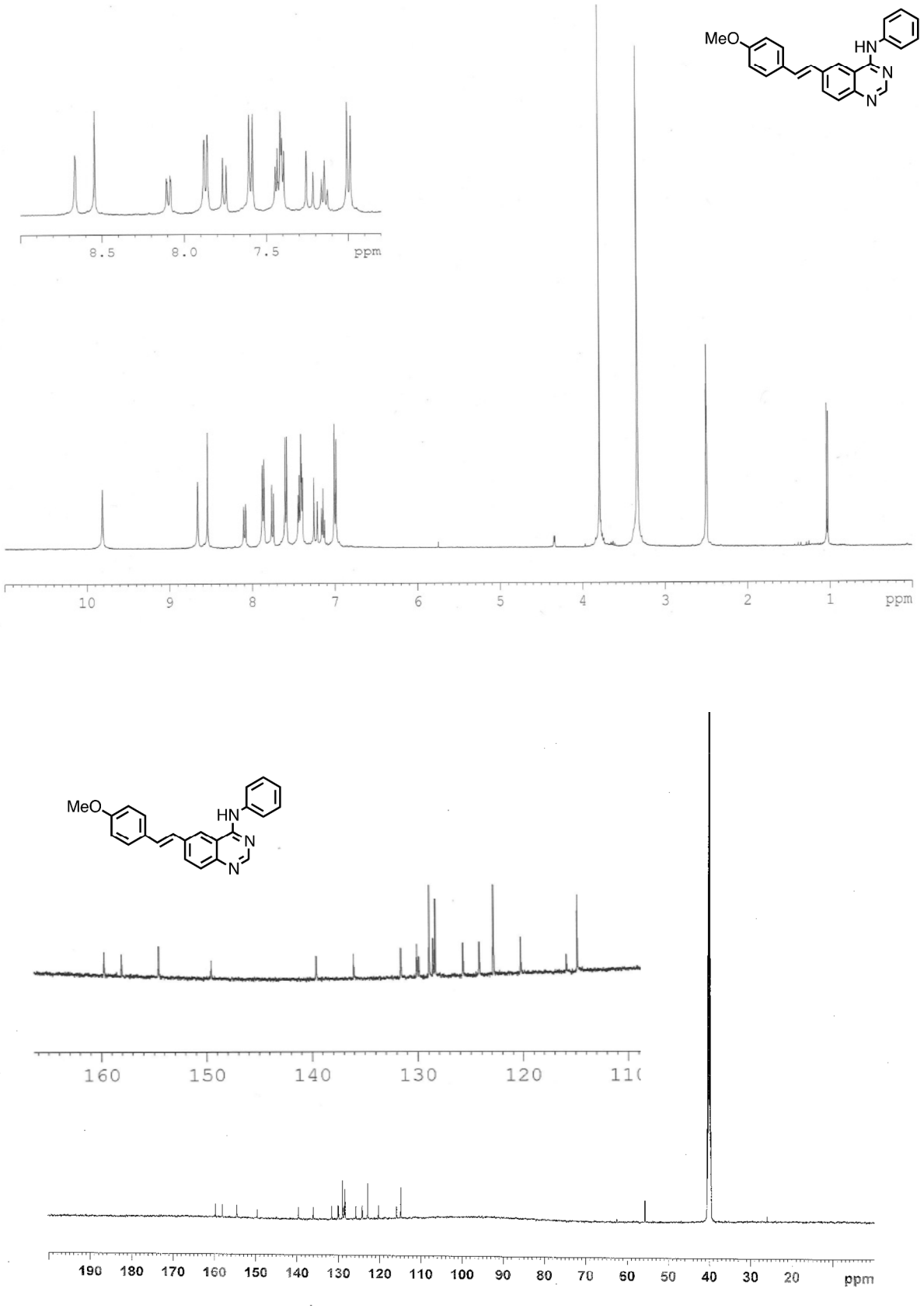

Figure S7. ^{1}H (top) and ^{13}C (bottom) NMRs of **2b** (cocrystalized with isopropanol, 1.03 and 4.33 ppm in ^{1}H spectrum and 27.0 and 62.4 ppm in ^{13}C spectrum).

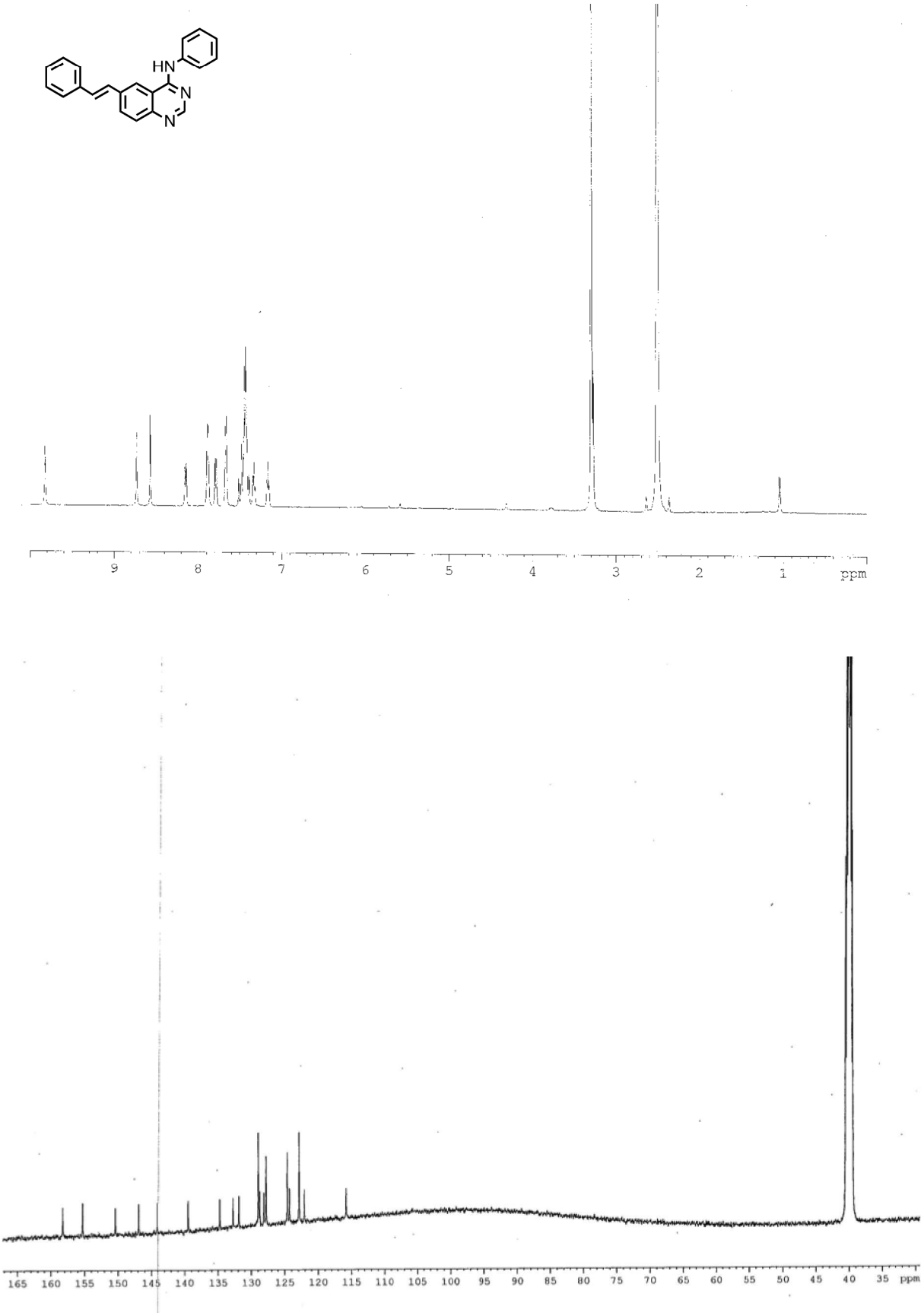

Figure S8. ^{1}H (top) and ^{13}C (bottom) NMRs of **2c**.

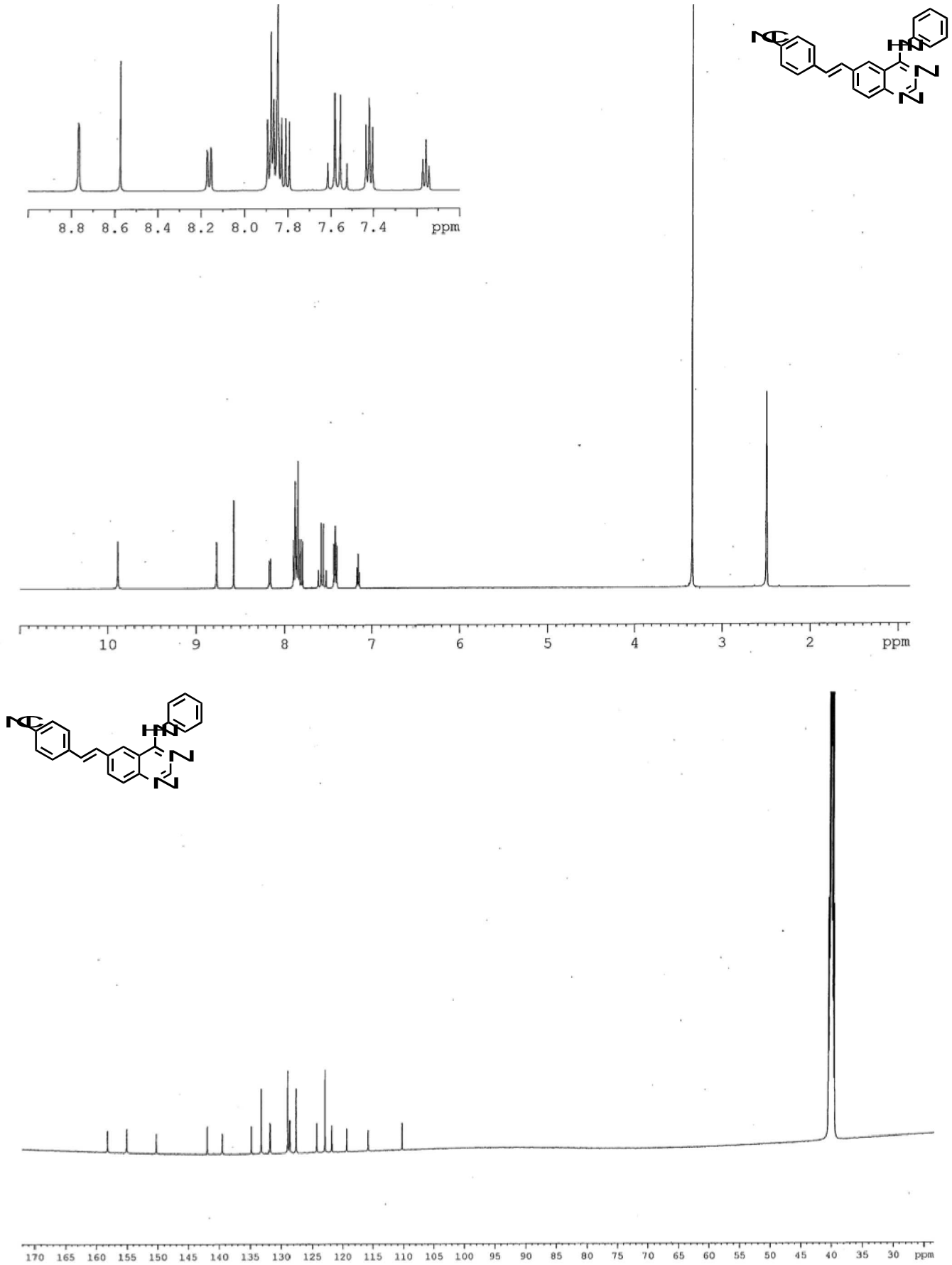

Figure S9. ^{1}H (top) and ^{13}C (bottom) NMRs of **2d**.

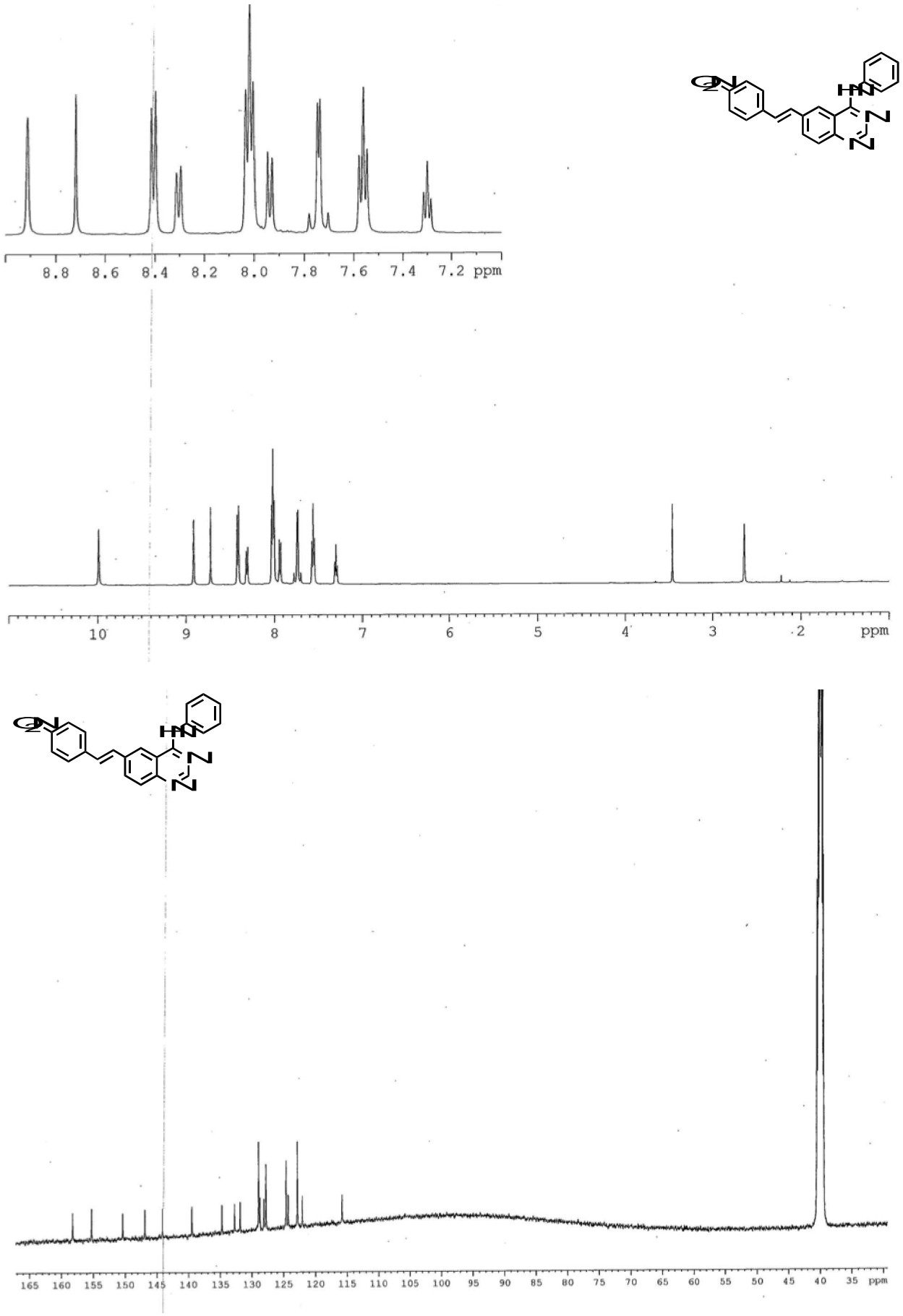

Figure S10. ^{1}H (top) and ^{13}C (bottom) NMRs of **2e**.

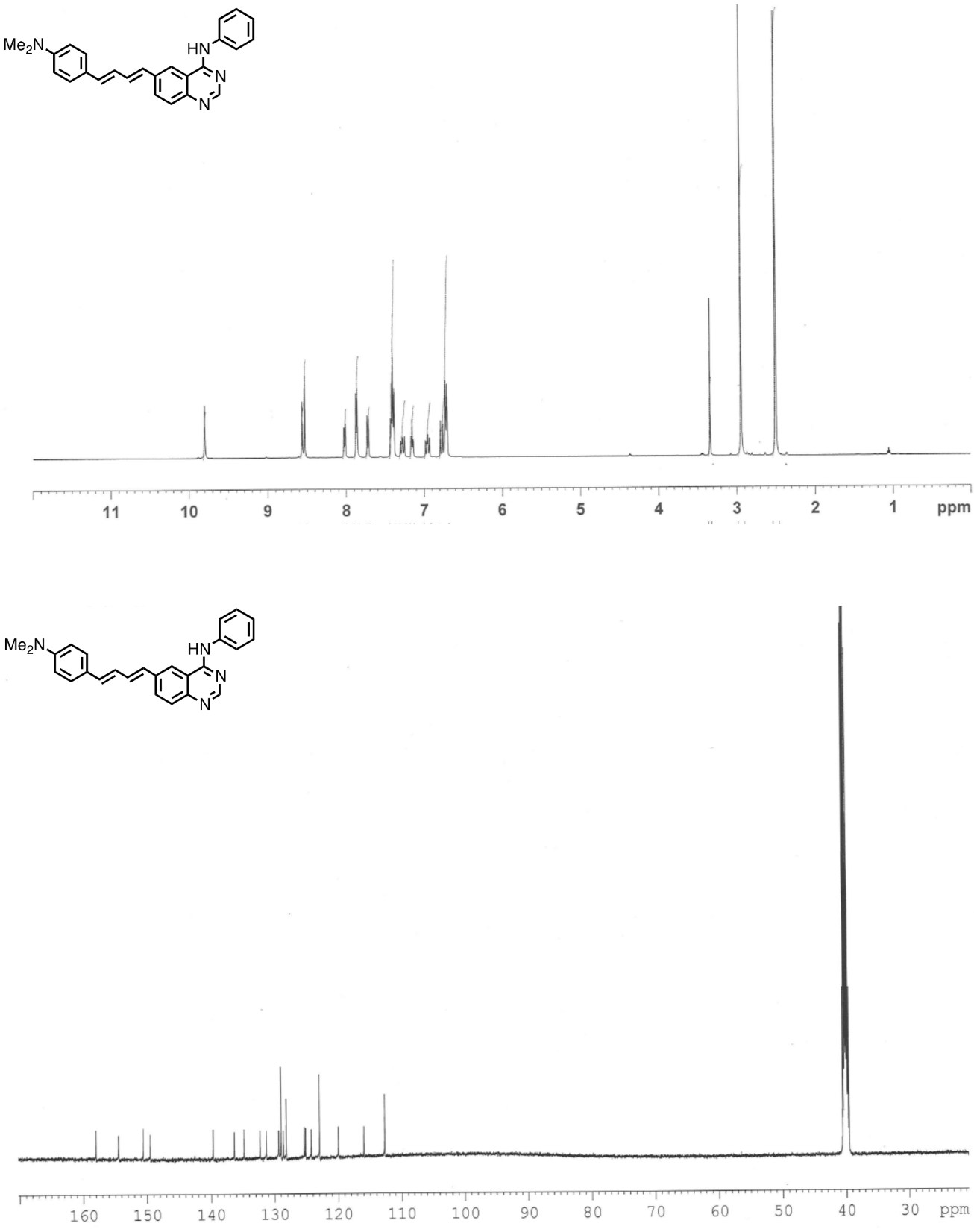

Figure S11. ^{1}H (top) and ^{13}C (bottom) NMRs of **3a**.

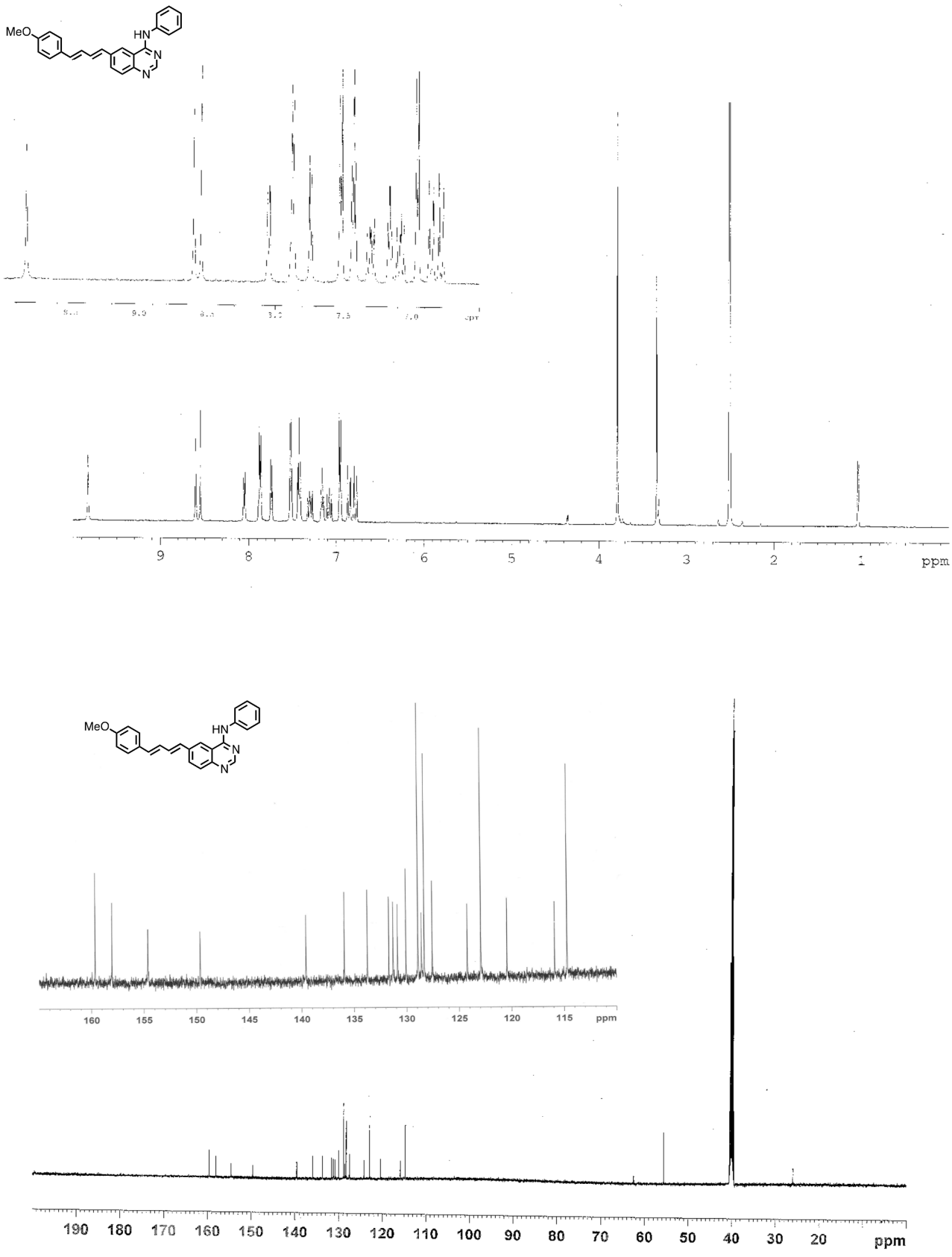

Figure S12. ^{1}H (top) and ^{13}C (bottom) NMRs of **3b**. (cocrystalized with isopropanol, 1.03 and 4.33 ppm in ^{1}H spectrum and 27.0 and 62.4 ppm in ^{13}C spectrum).

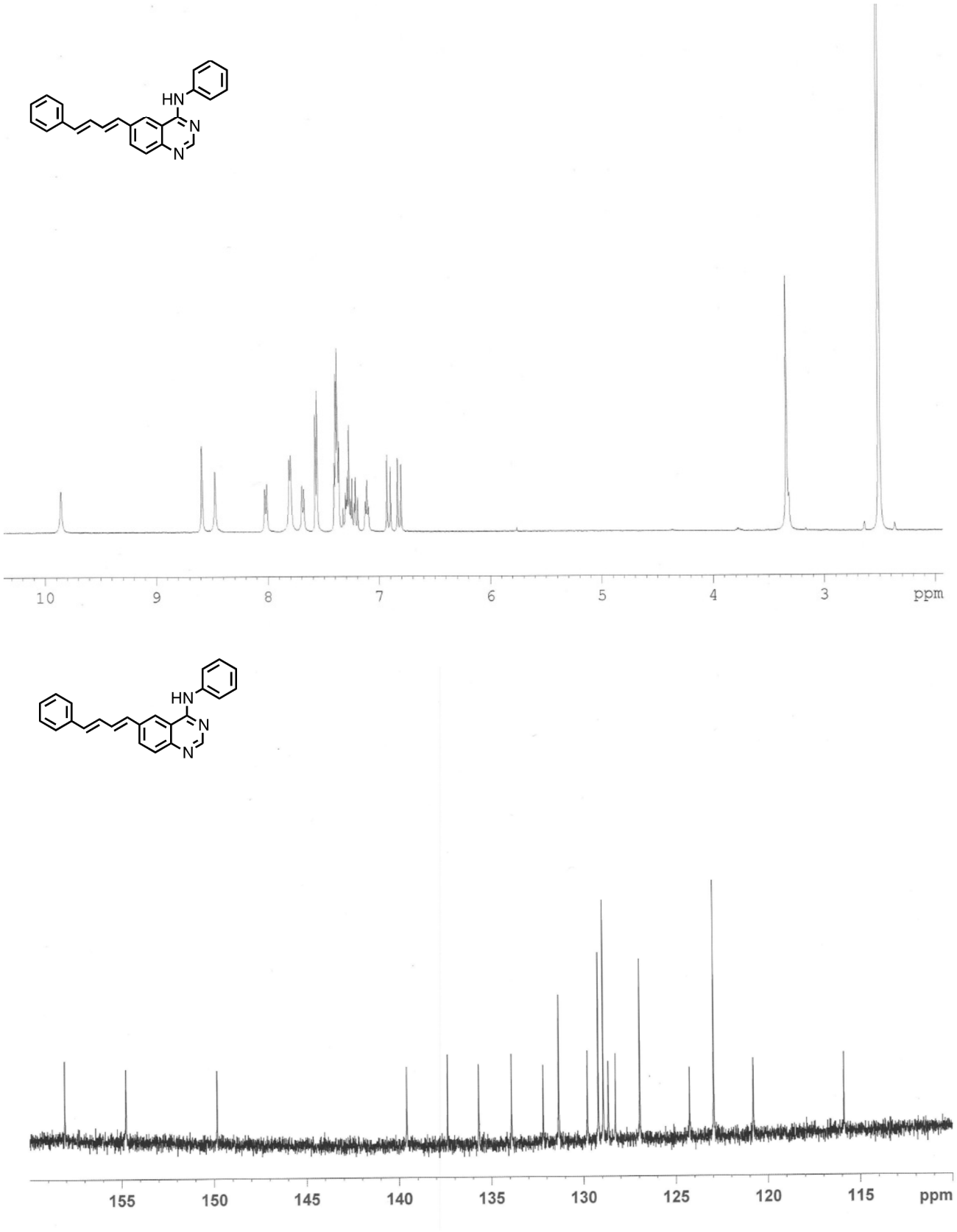

Figure S13. ^{1}H (top) and ^{13}C (bottom) NMRs of **3c**.

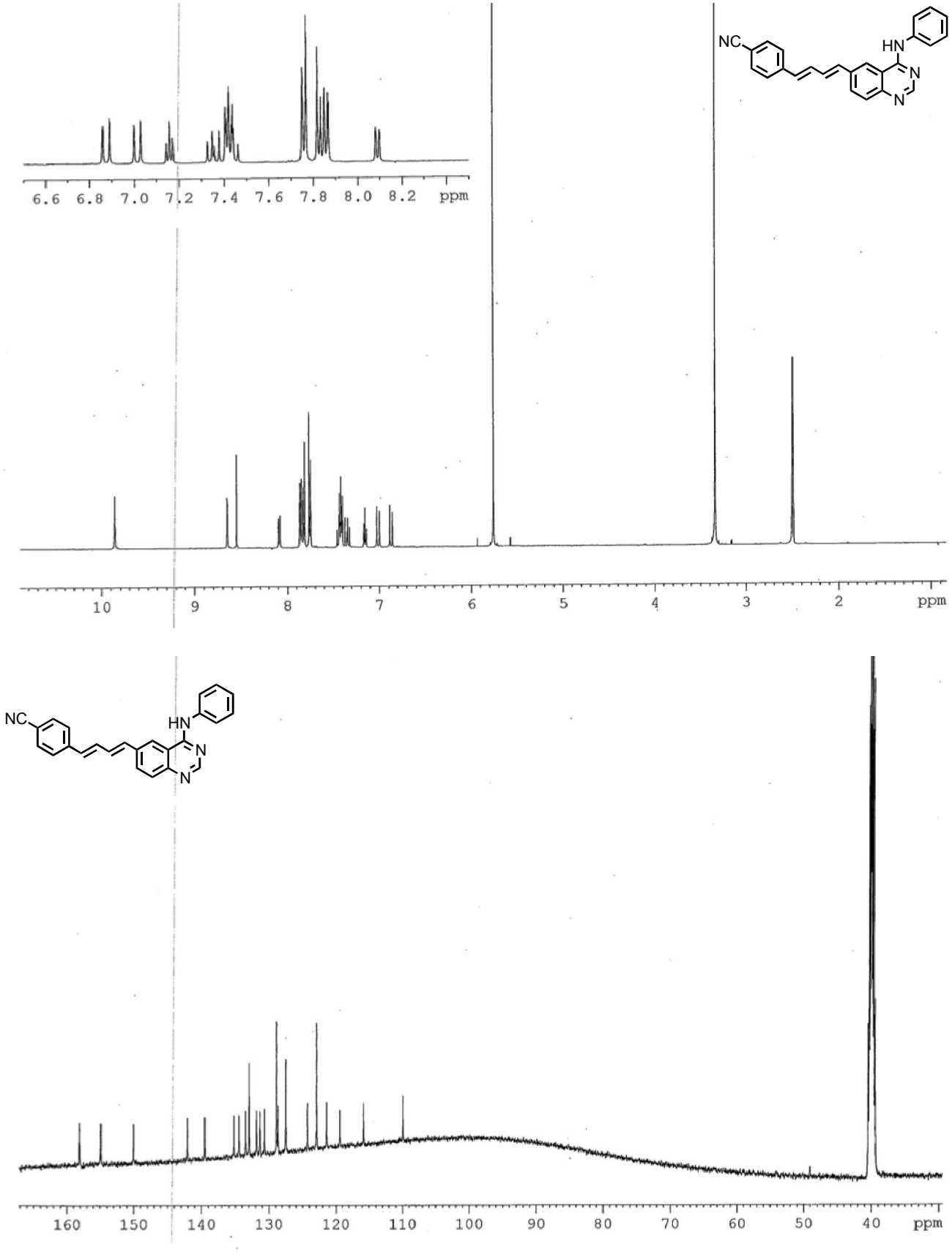

Figure S14. ^{1}H (top) and ^{13}C (bottom) NMRs of **3d**.

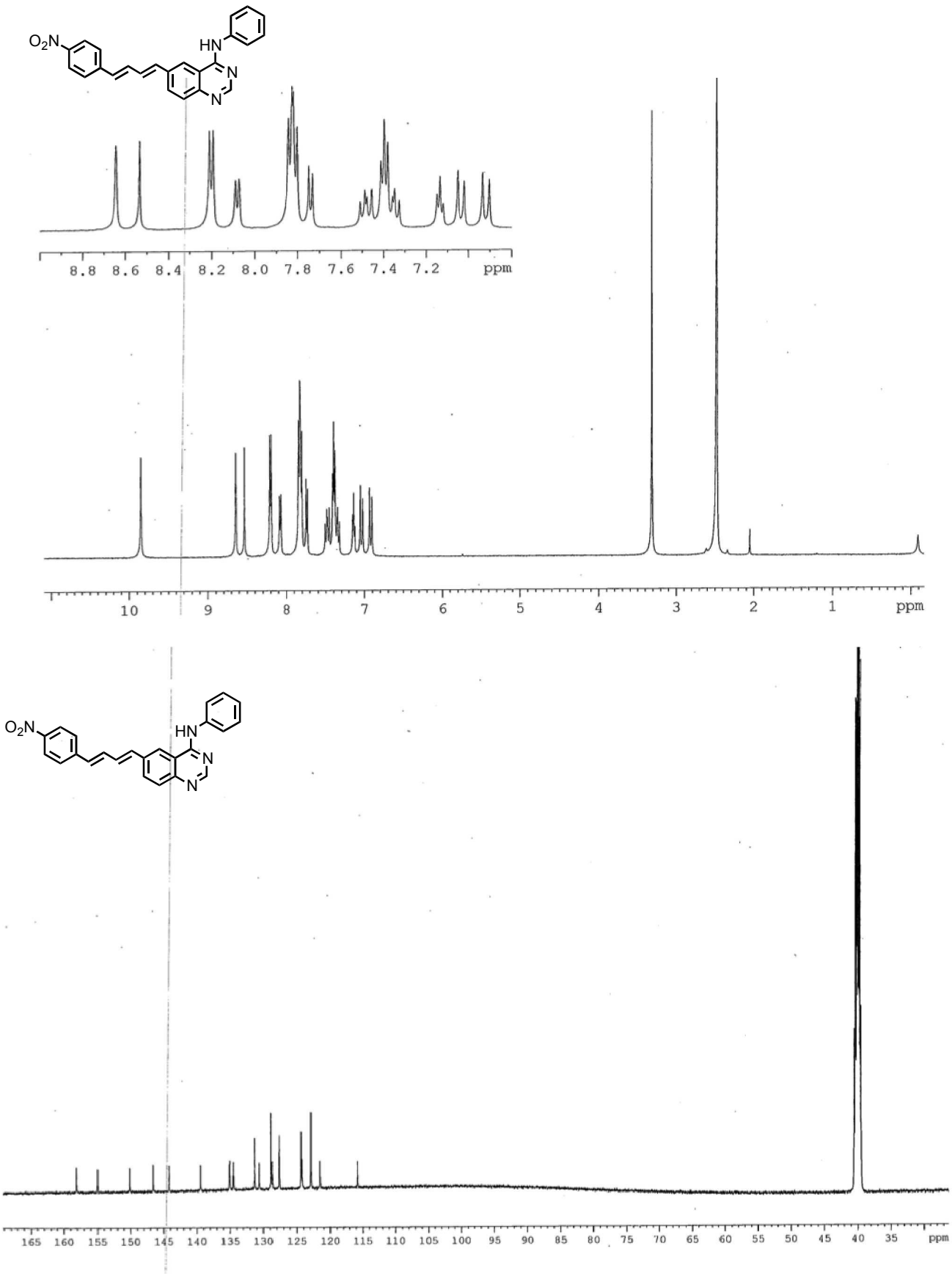

Figure S15. ^{1}H (top) and ^{13}C (bottom) NMRs of **3e**.

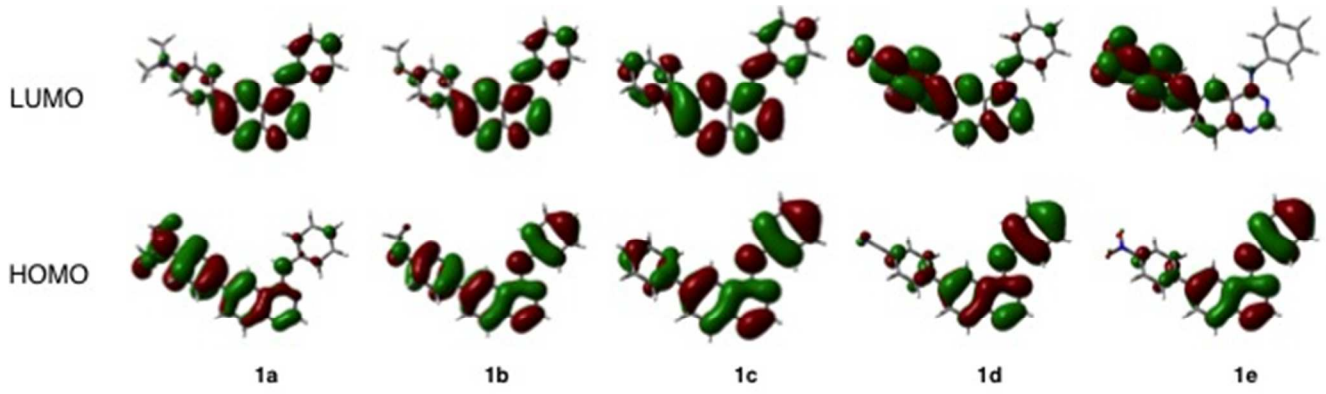

Figure S16. Frontier molecular orbitals of **1a-e** calculated at the CAM-B3LYP/6-31G* level: the polarization of the HOMO and LUMO shifts across the series (compare **1a** and **1e**).

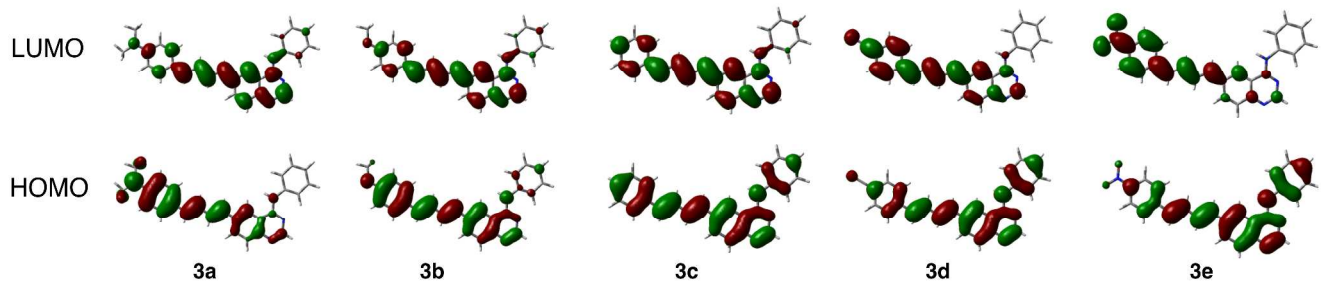

Figure S17. Frontier molecular orbitals of **3a-e** calculated at the CAM-B3LYP/6-31G* level**:** the polarization of the HOMO and LUMO shifts across the series (compare **3a** and **3e**).

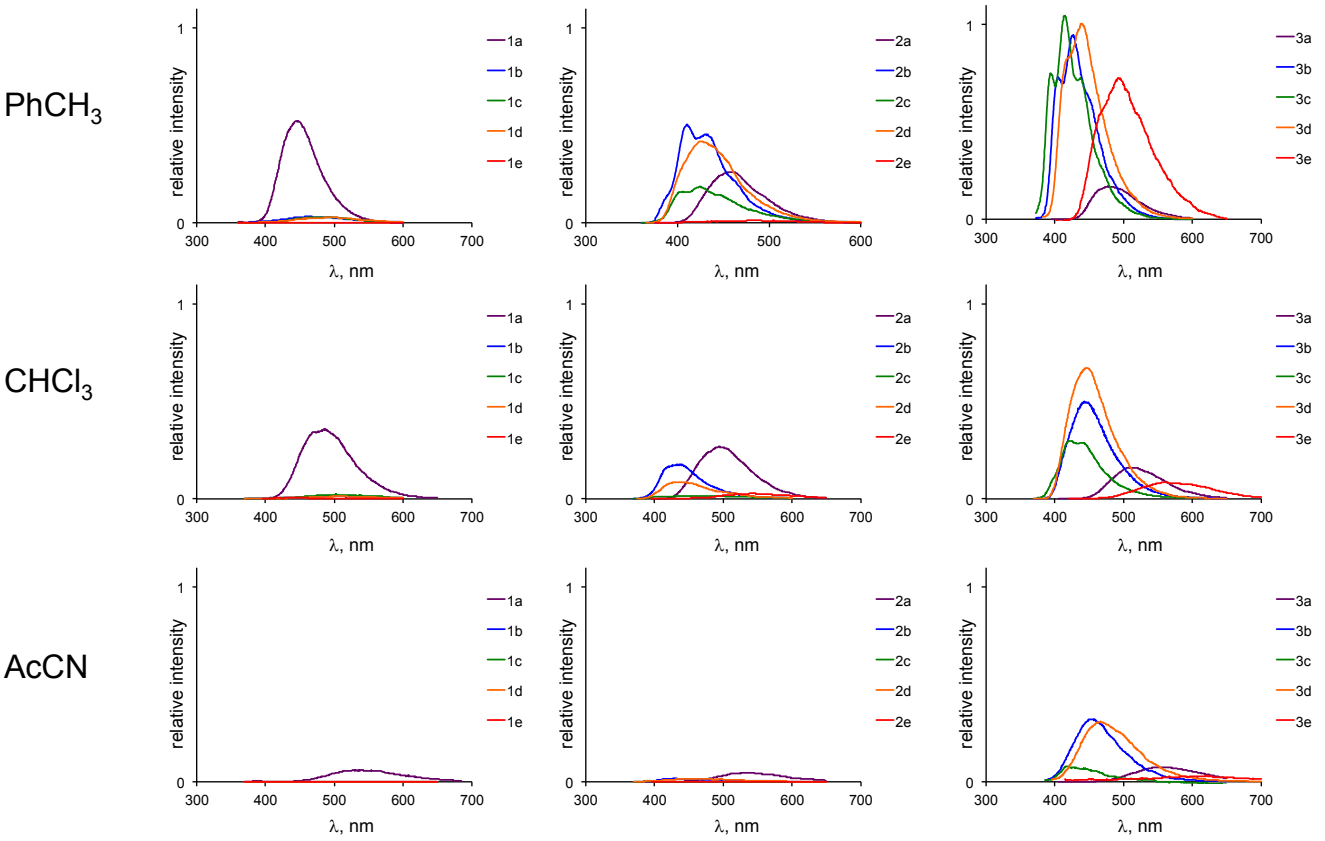

Figure S18. Emission spectra of **1a-3e** in toluene ($E_T(30)$ = 33.9 kcal/mol[a]), chloroform (($E_T(30)$ = 39.1 kcal/mol), and acetonitrile ($E_T(30)$ = 46.0 kcal/mol). With increasing polarity, emission intensity generally decreases along with a red shift in emission wavelengths.

[a] Reichardt, C. *Angew. Chem., Int. Ed.* **1979**, *18*, 98-110.

Table S1: Optimized geometry of **1a**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	3.76	-2.309	-1.02
2	C	3.717	-1.337	-0.546
3	C	3.536	1.18	0.582
4	C	2.53	-0.627	-0.599
5	C	4.856	-0.805	0.092
6	C	4.733	0.485	0.644
7	C	2.399	0.646	-0.034
8	H	1.688	-1.07	-1.123
9	H	5.575	0.953	1.138
10	H	3.487	2.16	1.047
11	C	1.122	1.395	-0.085
12	H	-0.092	-0.336	0.081
13	C	-0.096	0.743	-0.036
14	C	-0.054	3.52	-0.21
15	C	-1.315	1.449	-0.084
16	C	1.116	2.81	-0.182
17	C	-1.3	2.859	-0.156
18	C	-2.629	0.845	-0.047
19	H	2.061	3.339	-0.248
20	H	-0.058	4.603	-0.28
21	N	-3.718	1.59	-0.035
22	C	-3.562	2.93	-0.088
23	H	-4.488	3.501	-0.074
24	N	-2.449	3.604	-0.164
25	N	-2.731	-0.512	-0.031
26	H	-1.86	-1.013	-0.131
27	C	-3.851	-1.36	0.05
28	C	-5.929	-3.234	0.219
29	C	-5.16	-0.935	0.296
30	C	-3.597	-2.728	-0.11
31	C	-4.625	-3.654	-0.025
32	C	-6.181	-1.877	0.377
33	H	-5.367	0.117	0.415
34	H	-2.58	-3.061	-0.303
35	H	-4.403	-4.709	-0.152
36	H	-7.193	-1.532	0.569
37	H	-6.736	-3.956	0.285
38	N	6.035	-1.519	0.178
39	C	6.182	-2.736	-0.595
40	H	5.418	-3.471	-0.319
41	H	7.154	-3.18	-0.379
42	H	6.115	-2.564	-1.679
43	C	7.244	-0.838	0.6
44	H	7.138	-0.436	1.613
45	H	7.522	-0.011	-0.07
46	H	8.066	-1.553	0.619

Table S2: Optimized geometry of **1b**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	4.098	-2.407	-1.095
2	C	4.048	-1.461	-0.572
3	C	3.877	0.991	0.728
4	C	2.884	-0.702	-0.641
5	C	5.136	-0.986	0.159
6	C	5.042	0.25	0.806
7	C	2.768	0.53	0.004
8	H	2.054	-1.075	-1.234
9	H	5.894	0.604	1.377
10	H	3.819	1.937	1.258
11	C	1.514	1.317	-0.059
12	H	0.257	-0.383	0.072
13	C	0.28	0.697	-0.032
14	C	0.403	3.475	-0.176
15	C	-0.918	1.438	-0.083
16	C	1.553	2.732	-0.139
17	C	-0.861	2.847	-0.142
18	C	-2.25	0.872	-0.059
19	H	2.516	3.231	-0.184
20	H	0.43	4.558	-0.235
21	N	-3.316	1.649	-0.048
22	C	-3.12	2.984	-0.091
23	H	-4.029	3.583	-0.081
24	N	-1.987	3.626	-0.153
25	N	-2.392	-0.481	-0.053
26	H	-1.535	-1.007	-0.145
27	C	-3.537	-1.298	0.025
28	C	-5.664	-3.115	0.192
29	C	-4.84	-0.835	0.222
30	C	-3.312	-2.676	-0.09
31	C	-4.365	-3.573	-0.006
32	C	-5.886	-1.749	0.304
33	H	-5.024	0.225	0.306
34	H	-2.3	-3.04	-0.244
35	H	-4.165	-4.637	-0.096
36	H	-6.894	-1.375	0.459
37	H	-6.49	-3.816	0.258
38	O	6.316	-1.64	0.298
39	C	6.449	-2.919	-0.297
40	H	5.716	-3.627	0.108
41	H	7.454	-3.263	-0.05
42	H	6.344	-2.87	-1.387

Table S3: Optimized geometry of **1c**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	4.064	-3.602	-1.212
2	C	4.218	-2.672	-0.672
3	C	4.605	-0.278	0.679
4	C	3.235	-1.69	-0.7
5	C	5.4	-2.46	0.03
6	C	5.589	-1.259	0.705
7	C	3.41	-0.48	-0.021
8	H	2.33	-1.857	-1.275
9	H	6.506	-1.084	1.261
10	H	4.758	0.646	1.229
11	C	2.356	0.566	-0.042
12	H	0.761	-0.823	0.062
13	C	1.018	0.229	-0.008
14	C	1.741	2.914	-0.119
15	C	0.008	1.212	-0.032
16	C	2.703	1.939	-0.097
17	C	0.371	2.575	-0.087
18	C	-1.416	0.95	0.003
19	H	3.75	2.219	-0.143
20	H	2.002	3.965	-0.17
21	N	-2.286	1.943	-0.021
22	C	-1.804	3.202	-0.08
23	H	-2.561	3.982	-0.101
24	N	-0.557	3.582	-0.113
25	N	-1.853	-0.336	0.055
26	H	-1.129	-1.041	0.069
27	C	-3.153	-0.881	0.069
28	C	-5.637	-2.182	0.095
29	C	-4.335	-0.136	0.07
30	C	-3.23	-2.28	0.084
31	C	-4.457	-2.922	0.097
32	C	-5.56	-0.795	0.082
33	H	-4.286	0.942	0.059
34	H	-2.314	-2.866	0.084
35	H	-4.491	-4.007	0.107
36	H	-6.471	-0.202	0.082
37	H	-6.6	-2.681	0.105
38	H	6.169	-3.226	0.049

Table S4: Optimized geometry of **1d**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-4.106	-2.626	1.247
2	C	-4.077	-1.69	0.701
3	C	-4.026	0.725	-0.683
4	C	-2.948	-0.889	0.741
5	C	-5.19	-1.28	-0.039
6	C	-5.162	-0.065	-0.73
7	C	-2.901	0.326	0.049
8	H	-2.097	-1.201	1.337
9	H	-6.024	0.248	-1.308
10	H	-4.005	1.655	-1.24
11	C	-1.682	1.17	0.08
12	H	-0.361	-0.481	-0.051
13	C	-0.426	0.598	0.039
14	C	-0.667	3.372	0.155
15	C	0.74	1.39	0.059
16	C	-1.786	2.581	0.142
17	C	0.621	2.796	0.106
18	C	2.095	0.881	0.021
19	H	-2.769	3.039	0.195
20	H	-0.738	4.453	0.204
21	N	3.125	1.706	-0.011
22	C	2.871	3.03	0.023
23	H	3.752	3.667	-0.005
24	N	1.711	3.624	0.094
25	N	2.296	-0.462	0.024
26	H	1.462	-1.023	0.118
27	C	3.474	-1.232	-0.035
28	C	5.677	-2.96	-0.147
29	C	4.762	-0.715	-0.198
30	C	3.303	-2.619	0.07
31	C	4.393	-3.472	0.015
32	C	5.846	-1.585	-0.252
33	H	4.904	0.352	-0.276
34	H	2.302	-3.026	0.195
35	H	4.236	-4.543	0.098
36	H	6.842	-1.17	-0.379
37	H	6.533	-3.626	-0.191
38	C	-6.363	-2.103	-0.085
39	N	-7.311	-2.765	-0.125

Table S5: Optimized geometry of **1e**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	3.911	-2.266	-1.276
2	C	3.807	-1.339	-0.727
3	C	3.6	1.055	0.687
4	C	2.633	-0.606	-0.767
5	C	4.866	-0.856	0.028
6	C	4.782	0.335	0.736
7	C	2.508	0.597	-0.06
8	H	1.807	-0.96	-1.374
9	H	5.627	0.679	1.319
10	H	3.518	1.975	1.256
11	C	1.241	1.366	-0.095
12	H	0.017	-0.361	0.017
13	C	0.021	0.72	-0.065
14	C	0.099	3.504	-0.173
15	C	-1.189	1.442	-0.089
16	C	1.262	2.781	-0.153
17	C	-1.154	2.853	-0.134
18	C	-2.51	0.852	-0.054
19	H	2.216	3.297	-0.197
20	H	0.105	4.587	-0.219
21	N	-3.588	1.613	-0.026
22	C	-3.414	2.951	-0.062
23	H	-4.331	3.534	-0.04
24	N	-2.292	3.613	-0.128
25	N	-2.631	-0.501	-0.052
26	H	-1.769	-1.017	-0.151
27	C	-3.764	-1.335	0.038
28	C	-5.861	-3.184	0.228
29	C	-5.068	-0.892	0.271
30	C	-3.522	-2.708	-0.1
31	C	-4.56	-3.621	-0.005
32	C	-6.1	-1.822	0.363
33	H	-5.265	0.164	0.373
34	H	-2.509	-3.055	-0.283
35	H	-4.349	-4.681	-0.114
36	H	-7.109	-1.464	0.546
37	H	-6.676	-3.897	0.303
38	N	6.108	-1.622	0.077
39	O	6.16	-2.674	-0.547
40	O	7.035	-1.176	0.739

Table S6: Optimized geometry of **2a**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	5.147	2.549	-0.051
2	C	5.123	1.466	-0.045
3	C	4.979	-1.291	-0.009
4	C	3.895	0.832	-0.031
5	C	6.328	0.73	-0.053
6	C	6.219	-0.675	-0.021
7	C	3.782	-0.566	-0.016
8	H	3.002	1.45	-0.029
9	H	7.108	-1.292	-0.008
10	H	4.938	-2.377	0.011
11	C	0.005	-1.479	-0.003
12	H	-1.098	0.326	-0.006
13	C	-1.175	-0.757	-0.002
14	C	-1.294	-3.533	0.007
15	C	-2.435	-1.388	0.003
16	C	-0.083	-2.897	0.001
17	C	-2.502	-2.797	0.007
18	C	-3.711	-0.705	0.004
19	H	0.824	-3.492	0
20	H	-1.363	-4.616	0.01
21	N	-4.842	-1.386	0.008
22	C	-4.765	-2.733	0.012
23	H	-5.723	-3.247	0.015
24	N	-3.691	-3.474	0.012
25	C	1.278	-0.752	-0.011
26	H	1.173	0.331	-0.024
27	C	2.509	-1.286	-0.005
28	H	2.612	-2.37	0.009
29	N	-3.733	0.654	0.001
30	H	-2.828	1.101	-0.001
31	C	-4.796	1.576	0.001
32	C	-6.746	3.589	0
33	C	-6.152	1.238	0.002
34	C	-4.429	2.928	0
35	C	-5.394	3.923	0
36	C	-7.109	2.249	0.001
37	H	-6.443	0.199	0.003
38	H	-3.375	3.195	-0.001
39	H	-5.086	4.964	-0.001
40	H	-8.159	1.972	0.002
41	H	-7.504	4.366	0
42	N	7.553	1.356	-0.096
43	C	7.63	2.794	0.071
44	H	7.07	3.315	-0.713
45	H	8.672	3.106	-0.009
46	H	7.246	3.129	1.045
47	C	8.76	0.573	0.076
48	H	8.848	-0.192	-0.704
49	H	8.804	0.07	1.052
50	H	9.626	1.23	-0.008

Table S7: Optimized geometry of **2b**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-5.502	2.666	0.063
2	C	-5.484	1.583	0.03
3	C	-5.385	-1.188	-0.054
4	C	-4.262	0.923	0.023
5	C	-6.67	0.847	-0.006
6	C	-6.61	-0.548	-0.049
7	C	-4.179	-0.472	-0.018
8	H	-3.357	1.522	0.053
9	H	-7.538	-1.109	-0.077
10	H	-5.356	-2.274	-0.086
11	C	-0.415	-1.444	-0.001
12	H	0.712	0.345	0.017
13	C	0.774	-0.738	0.009
14	C	0.854	-3.516	-0.011
15	C	2.025	-1.386	0.009
16	C	-0.348	-2.863	-0.011
17	C	2.072	-2.796	0
18	C	3.31	-0.722	0.015
19	H	-1.263	-3.446	-0.018
20	H	0.908	-4.599	-0.017
21	N	4.431	-1.418	0.018
22	C	4.335	-2.764	0.011
23	H	5.286	-3.292	0.014
24	N	3.251	-3.491	0.001
25	C	-1.678	-0.699	0
26	H	-1.558	0.382	0.019
27	C	-2.915	-1.216	-0.022
28	H	-3.035	-2.297	-0.044
29	N	3.352	0.638	0.018
30	H	2.455	1.099	0.009
31	C	4.433	1.541	0.005
32	C	6.419	3.518	-0.022
33	C	5.781	1.18	0.074
34	C	4.092	2.897	-0.079
35	C	5.075	3.874	-0.091
36	C	6.756	2.173	0.058
37	H	6.053	0.138	0.135
38	H	3.044	3.181	-0.139
39	H	4.786	4.918	-0.156
40	H	7.8	1.879	0.112
41	H	7.191	4.281	-0.033
42	O	-7.912	1.39	-0.003
43	C	-8.03	2.8	0.07
44	H	-7.585	3.194	0.991
45	H	-9.1	3.013	0.072
46	H	-7.568	3.288	-0.795

Table S8: Optimized geometry of **2c**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	5.857	-3.676	0.057
2	C	5.961	-2.595	0.044
3	C	6.211	0.164	0.01
4	C	4.826	-1.798	0.027
5	C	7.229	-2.018	0.044
6	C	7.349	-0.633	0.027
7	C	4.93	-0.4	0.01
8	H	3.848	-2.27	0.027
9	H	8.331	-0.17	0.027
10	H	6.311	1.246	-0.004
11	C	1.323	1.045	-0.021
12	H	-0.037	-0.576	0.033
13	C	0.049	0.506	-0.005
14	C	0.35	3.271	-0.056
15	C	-1.101	1.321	-0.018
16	C	1.451	2.459	-0.053
17	C	-0.954	2.724	-0.032
18	C	-2.466	0.841	-0.01
19	H	2.438	2.907	-0.069
20	H	0.446	4.351	-0.071
21	N	-3.48	1.686	0.027
22	C	-3.198	3.005	0.027
23	H	-4.066	3.661	0.058
24	N	-2.025	3.575	-0.013
25	C	2.477	0.141	-0.002
26	H	2.217	-0.915	0.019
27	C	3.769	0.499	-0.008
28	H	4.027	1.555	-0.027
29	N	-2.695	-0.499	-0.042
30	H	-1.871	-1.073	-0.145
31	C	-3.89	-1.243	-0.016
32	C	-6.134	-2.922	0.028
33	C	-5.167	-0.702	0.155
34	C	-3.75	-2.63	-0.16
35	C	-4.86	-3.458	-0.139
36	C	-6.272	-1.548	0.174
37	H	-5.285	0.365	0.264
38	H	-2.758	-3.057	-0.29
39	H	-4.727	-4.53	-0.255
40	H	-7.258	-1.113	0.306
41	H	-7.005	-3.569	0.044
42	H	8.115	-2.645	0.058

Table S9: Optimized geometry of **2d**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-5.567	2.896	-0.307
2	C	-5.558	1.821	-0.17
3	C	-5.55	-0.935	0.172
4	C	-4.362	1.128	-0.175
5	C	-6.765	1.133	0.008
6	C	-6.755	-0.253	0.179
7	C	-4.332	-0.264	0
8	H	-3.441	1.68	-0.322
9	H	-7.688	-0.788	0.315
10	H	-5.548	-2.012	0.306
11	C	-0.606	-1.344	-0.04
12	H	0.571	0.411	-0.032
13	C	0.603	-0.674	-0.03
14	C	0.594	-3.453	-0.029
15	C	1.834	-1.36	-0.016
16	C	-0.586	-2.764	-0.042
17	C	1.833	-2.772	-0.015
18	C	3.141	-0.739	-0.003
19	H	-1.52	-3.315	-0.059
20	H	0.616	-4.537	-0.032
21	N	4.238	-1.473	0.007
22	C	4.093	-2.814	0.006
23	H	5.025	-3.376	0.015
24	N	2.986	-3.506	-0.003
25	C	-1.846	-0.565	-0.05
26	H	-1.697	0.511	-0.104
27	C	-3.094	-1.05	0.01
28	H	-3.246	-2.123	0.083
29	N	3.23	0.618	0
30	H	2.35	1.109	-0.002
31	C	4.344	1.483	0.014
32	C	6.406	3.38	0.039
33	C	5.678	1.067	-0.008
34	C	4.056	2.852	0.049
35	C	5.076	3.79	0.061
36	C	6.691	2.021	0.005
37	H	5.906	0.013	-0.034
38	H	3.02	3.184	0.068
39	H	4.828	4.846	0.088
40	H	7.723	1.684	-0.013
41	H	7.207	4.111	0.048
42	C	-8.006	1.851	0.012
43	N	-9.007	2.431	0.015

Table S10: Optimized geometry of **2e**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-5.199	2.626	0
2	C	-5.153	1.545	0
3	C	-5.093	-1.236	0
4	C	-3.941	0.88	0
5	C	-6.328	0.801	0
6	C	-6.315	-0.586	0
7	C	-3.884	-0.523	0
8	H	-3.03	1.467	0
9	H	-7.246	-1.139	0
10	H	-5.069	-2.321	0
11	C	-0.126	-1.489	0
12	H	0.975	0.318	0
13	C	1.052	-0.765	0
14	C	1.167	-3.542	0
15	C	2.311	-1.396	0
16	C	-0.044	-2.906	0
17	C	2.374	-2.805	0
18	C	3.587	-0.713	0
19	H	-0.952	-3.5	0
20	H	1.236	-4.625	0
21	N	4.717	-1.396	0
22	C	4.637	-2.742	0
23	H	5.594	-3.259	0
24	N	3.562	-3.484	0
25	C	-1.395	-0.756	0
26	H	-1.282	0.325	0
27	C	-2.628	-1.281	0
28	H	-2.753	-2.36	0
29	N	3.612	0.645	0
30	H	2.709	1.095	0
31	C	4.679	1.565	0
32	C	6.63	3.575	0
33	C	6.033	1.224	0
34	C	4.313	2.917	0
35	C	5.279	3.911	0
36	C	6.991	2.234	0
37	H	6.324	0.185	0
38	H	3.258	3.185	0
39	H	4.972	4.952	0
40	H	8.041	1.956	0
41	H	7.389	4.351	0
42	N	-7.607	1.499	0
43	O	-7.596	2.724	0
44	O	-8.631	0.829	0

Table S11: Optimized geometry of **3a**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	6.652	2.581	-0.06
2	C	6.586	1.5	-0.055
3	C	6.334	-1.25	-0.021
4	C	5.334	0.914	-0.046
5	C	7.761	0.717	-0.057
6	C	7.597	-0.683	-0.028
7	C	5.165	-0.478	-0.031
8	H	4.465	1.566	-0.048
9	H	8.461	-1.334	-0.012
10	H	6.25	-2.334	-0.002
11	C	1.418	-1.338	-0.01
12	H	1.527	-2.421	-0.008
13	C	0.195	-0.777	-0.006
14	H	0.136	0.311	-0.009
15	C	-1.097	-1.463	0.001
16	H	-2.149	0.373	-0.004
17	C	-2.257	-0.708	0.001
18	C	-2.45	-3.481	0.012
19	C	-3.533	-1.305	0.006
20	C	-1.223	-2.878	0.007
21	C	-3.637	-2.712	0.011
22	C	-4.792	-0.59	0.006
23	H	-0.332	-3.497	0.009
24	H	-2.549	-4.561	0.017
25	N	-5.94	-1.241	0.01
26	C	-5.898	-2.589	0.013
27	H	-6.869	-3.079	0.016
28	N	-4.844	-3.358	0.015
29	C	2.647	-0.575	-0.018
30	H	2.542	0.509	-0.023
31	C	3.866	-1.144	-0.021
32	H	3.913	-2.233	-0.015
33	N	-4.78	0.77	0.003
34	H	-3.863	1.193	0.001
35	C	-5.822	1.717	0.002
36	C	-7.726	3.774	-0.001
37	C	-7.185	1.41	0.002
38	C	-5.425	3.061	0.001
39	C	-6.367	4.077	-0.001
40	C	-8.119	2.442	0
41	H	-7.501	0.378	0.003
42	H	-4.365	3.306	0.001
43	H	-6.036	5.111	-0.002
44	H	-9.175	2.188	0
45	H	-8.467	4.567	-0.002
46	N	9.011	1.295	-0.09
47	C	9.141	2.728	0.078
48	H	8.602	3.269	-0.707
49	H	10.193	3.002	0.002
50	H	8.766	3.077	1.051
51	C	10.182	0.466	0.113
52	H	10.257	-0.309	-0.657
53	H	10.184	-0.028	1.096
54	H	11.075	1.087	0.042

Table S12: Optimized geometry of **3b**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-7.022	2.671	0.055
2	C	-6.964	1.59	0.025
3	C	-6.763	-1.177	-0.046
4	C	-5.718	0.975	0.022
5	C	-8.121	0.81	-0.008
6	C	-8.01	-0.582	-0.044
7	C	-5.583	-0.417	-0.015
8	H	-4.836	1.607	0.05
9	H	-8.918	-1.177	-0.068
10	H	-6.693	-2.261	-0.073
11	C	-1.845	-1.335	-0.011
12	H	-1.964	-2.416	-0.019
13	C	-0.621	-0.78	0
14	H	-0.558	0.308	0.007
15	C	0.67	-1.47	0.005
16	H	1.724	0.365	-0.001
17	C	1.83	-0.715	0.004
18	C	2.02	-3.489	0.015
19	C	3.106	-1.314	0.007
20	C	0.793	-2.885	0.012
21	C	3.207	-2.722	0.013
22	C	4.365	-0.6	0.006
23	H	-0.099	-3.502	0.016
24	H	2.117	-4.57	0.021
25	N	5.513	-1.253	0.009
26	C	5.468	-2.602	0.013
27	H	6.439	-3.093	0.014
28	N	4.413	-3.369	0.015
29	C	-3.067	-0.557	-0.011
30	H	-2.947	0.525	-0.004
31	C	-4.293	-1.108	-0.018
32	H	-4.358	-2.196	-0.028
33	N	4.355	0.759	0.002
34	H	3.439	1.183	0.002
35	C	5.398	1.705	-0.003
36	C	7.305	3.76	-0.016
37	C	6.761	1.396	-0.007
38	C	5.003	3.049	-0.005
39	C	5.946	4.064	-0.011
40	C	7.696	2.427	-0.013
41	H	7.076	0.364	-0.005
42	H	3.944	3.295	-0.002
43	H	5.616	5.099	-0.013
44	H	8.752	2.173	-0.017
45	H	8.047	4.552	-0.021
46	O	-9.383	1.307	-0.007
47	C	-9.552	2.713	0.049
48	H	-9.122	3.134	0.965
49	H	-10.629	2.886	0.046
50	H	-9.107	3.207	-0.823

Table S13: Optimized geometry of **3c**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	7.6	3.527	-0.178
2	C	7.617	2.444	-0.097
3	C	7.646	-0.32	0.106
4	C	6.423	1.739	-0.094
5	C	8.833	1.772	0.002
6	C	8.843	0.386	0.103
7	C	6.415	0.34	0.009
8	H	5.487	2.282	-0.177
9	H	9.784	-0.149	0.18
10	H	7.66	-1.403	0.185
11	C	2.765	-0.877	-0.003
12	H	2.971	-1.945	0.035
13	C	1.499	-0.428	-0.034
14	H	1.342	0.649	-0.066
15	C	0.277	-1.232	-0.026
16	H	-0.945	0.493	-0.026
17	C	-0.95	-0.593	-0.021
18	C	-0.873	-3.371	-0.016
19	C	-2.163	-1.31	-0.011
20	C	0.29	-2.652	-0.024
21	C	-2.129	-2.722	-0.009
22	C	-3.485	-0.722	-0.003
23	H	1.237	-3.18	-0.032
24	H	-0.867	-4.456	-0.016
25	N	-4.565	-1.482	0.002
26	C	-4.387	-2.82	0.001
27	H	-5.306	-3.403	0.004
28	N	-3.264	-3.484	-0.003
29	C	3.921	-0.005	-0.015
30	H	3.718	1.063	-0.053
31	C	5.185	-0.457	0.02
32	H	5.338	-1.535	0.063
33	H	9.766	2.328	-0.001
34	N	-3.607	0.634	0.002
35	H	-2.737	1.144	0.005
36	C	-4.74	1.471	0.01
37	C	-6.846	3.32	0.025
38	C	-6.064	1.024	-0.002
39	C	-4.484	2.848	0.029
40	C	-5.526	3.761	0.036
41	C	-7.099	1.954	0.006
42	H	-6.267	-0.035	-0.016
43	H	-3.456	3.203	0.038
44	H	-5.303	4.823	0.051
45	H	-8.123	1.593	-0.003
46	H	-7.664	4.032	0.031

Table S14: Optimized geometry of **3d**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	7.027	2.909	0
2	C	6.999	1.825	0
3	C	6.946	-0.953	0
4	C	5.789	1.158	0
5	C	8.197	1.099	0
6	C	8.165	-0.297	0
7	C	5.736	-0.245	0
8	H	4.874	1.74	0
9	H	9.092	-0.861	0
10	H	6.926	-2.038	0
11	C	2.039	-1.304	0
12	H	2.18	-2.383	0
13	C	0.808	-0.765	0
14	H	0.734	0.321	0
15	C	-0.477	-1.466	0
16	H	-1.541	0.363	0
17	C	-1.64	-0.718	0
18	C	-1.812	-3.493	0
19	C	-2.912	-1.324	0
20	C	-0.589	-2.882	0
21	C	-3.005	-2.732	0
22	C	-4.175	-0.617	0
23	H	0.307	-3.493	0
24	H	-1.904	-4.574	0
25	N	-5.319	-1.277	0
26	C	-5.265	-2.625	0
27	H	-6.233	-3.122	0
28	N	-4.205	-3.387	0
29	C	3.238	-0.493	0
30	H	3.084	0.584	0
31	C	4.482	-1.002	0
32	H	4.596	-2.085	0
33	N	-4.174	0.742	0
34	H	-3.261	1.173	0
35	C	-5.223	1.682	0
36	C	-7.139	3.727	0
37	C	-6.584	1.366	0
38	C	-4.834	3.028	0
39	C	-5.782	4.038	0
40	C	-7.524	2.392	0
41	H	-6.893	0.332	0
42	H	-3.775	3.279	0
43	H	-5.457	5.074	0
44	H	-8.579	2.132	0
45	H	-7.885	4.515	0
46	C	9.452	1.791	0
47	N	10.464	2.351	0

Table S15: Optimized geometry of **3e**; CAM-B3LYP/6-31G(d), SMD solvent model ($CHCl_3$).

atom	nucleus	x	y	z
1	H	-6.655	2.648	-0.001
2	C	-6.582	1.568	0
3	C	-6.457	-1.211	0.001
4	C	-5.355	0.933	0
5	C	-7.74	0.797	0
6	C	-7.694	-0.59	0.001
7	C	-5.265	-0.47	0.001
8	H	-4.457	1.539	0
9	H	-8.612	-1.163	0.001
10	H	-6.408	-2.295	0.002
11	C	-1.543	-1.425	0.001
12	H	-1.656	-2.507	0.001
13	C	-0.326	-0.853	0
14	H	-0.281	0.235	-0.001
15	C	0.975	-1.521	0
16	H	1.995	0.334	0
17	C	2.121	-0.744	0
18	C	2.359	-3.515	-0.001
19	C	3.407	-1.32	0
20	C	1.121	-2.934	-0.001
21	C	3.532	-2.726	0
22	C	4.654	-0.584	0
23	H	0.241	-3.567	-0.001
24	H	2.477	-4.594	-0.001
25	N	5.812	-1.219	0
26	C	5.79	-2.567	0
27	H	6.768	-3.043	0
28	N	4.748	-3.353	0
29	C	-2.763	-0.648	0
30	H	-2.64	0.433	0
31	C	-3.993	-1.192	0.001
32	H	-4.076	-2.277	0.002
33	N	4.623	0.774	0
34	H	3.7	1.184	0
35	C	5.653	1.736	0
36	C	7.53	3.818	0
37	C	7.02	1.447	0
38	C	5.238	3.074	0
39	C	6.167	4.103	0
40	C	7.94	2.491	0
41	H	7.35	0.419	0
42	H	4.176	3.306	0
43	H	5.822	5.132	0
44	H	8.999	2.251	0
45	H	8.26	4.62	0.001
46	N	-9.034	1.465	-0.001
47	O	-9.053	2.69	-0.001
48	O	-10.043	0.77	0