Supporting Information to Accompany:

One probe, two-channel imaging of nuclear and cytosolic compartments with orange and red emissive dyes

*Demar R. G. Pitter,[a] Adrienne S. Brown,[a] James D. Baker,[b] James N. Wilson[a]**

[a]Department of Chemistry, University of Miami, 1301 Memorial Drive, Coral Gables, FL 33146, United States.

[b]Department of Biology, University of Miami, 1301 Memorial Drive, Coral Gables, FL 33146, United States.

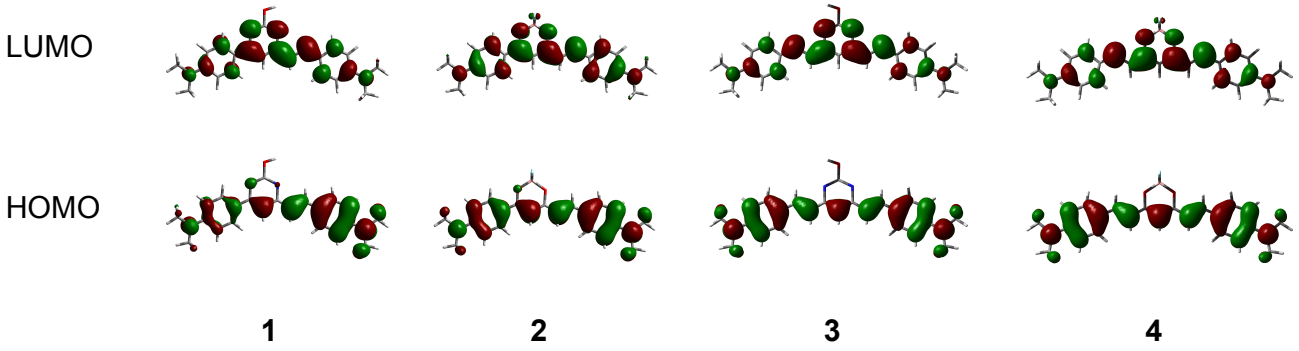

Figure S1. HOMO and LUMO densities of **1**-**4**.

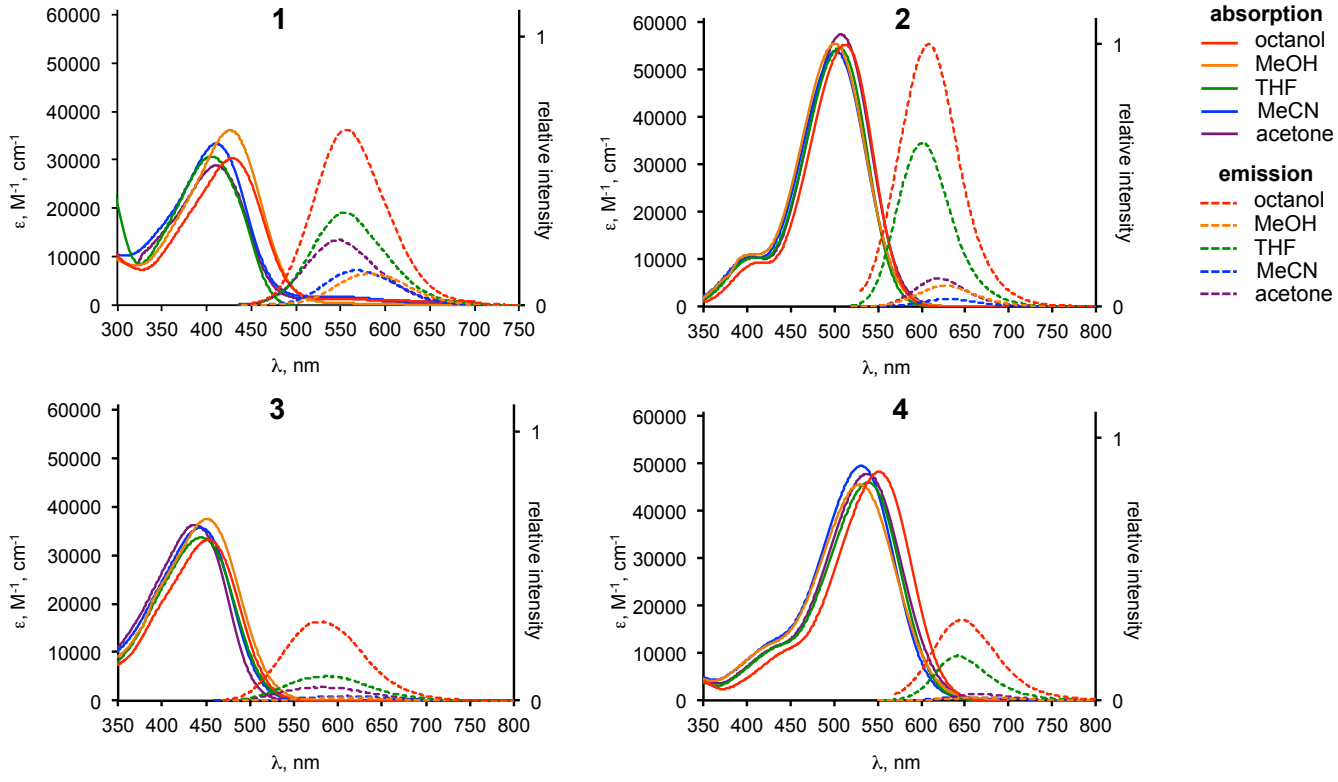

Figure S2. Absorption (solid line) and emission (dashed line) spectra of **1**-**4** in several protic (octanol, methanol) and aprotic (acetone, acetonitrile, THF) solvents. Emission intensity is highly sensitive to solvent polarity and viscosity with emission highest in octanol (red) and THF (green); this effect is consistent for both protic (octanol versus methanol) and aprotic solvents (THF versus acetone/acetonitrile).

Table S1. Summary of photophysical parameters in organic solvents.

	1	**2**	**3**	**4**
acetone				
$\lambda_{max, abs}$ / nm	410	507	436	538
ε / cm^{-1} M^{-1}	28,800	57,500	36,200	47,900
$\lambda_{max, em}$ / nm	552	624	585	661
ϕ	0.05	0.004	0.005	0.001
acetonitrile				
$\lambda_{max, abs}$ / nm	410	501	444	531
ε / cm^{-1} M^{-1}	33,300	54,000	35,600	49,500
$\lambda_{max, em}$ / nm	570	627	613	652
ϕ	0.02	0.001	0.002	~10^{-4}
tetrahydrofuran				
$\lambda_{max, abs}$ / nm	405	506	445	539
ε / cm^{-1} M^{-1}	30,700	54,600	33,600	46,000
$\lambda_{max, em}$ / nm	558	602	598	638
ϕ	0.05	0.02	0.009	0.008
octanol				
$\lambda_{max, abs}$ / nm	427	512	453	551
ε / cm^{-1} M^{-1}	30,300	55,300	33,100	48,200
$\lambda_{max, em}$ / nm	556	609	580	675
ϕ	0.14	0.04	0.03	0.01
methanol				
$\lambda_{max, abs}$ / nm (calculated)	438	521	478	572
$\lambda_{max, abs}$ / nm (observed)	426	500	452	529
ε / cm^{-1} M^{-1}	36,100	55,600	37,400	45,600
$\lambda_{max, em}$	579	628	627	675
ϕ	0.01	0.003	0.001	~10^{-4}

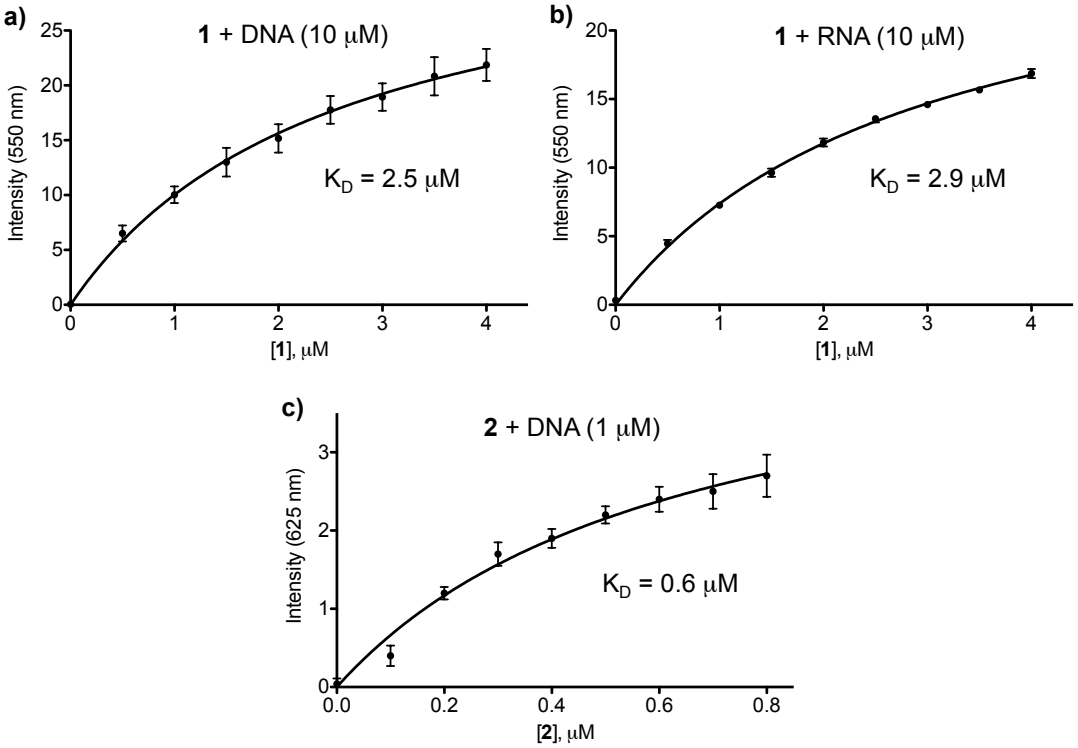

Figure S3. Determination of K_D values for a) **1** + DNA, b) **1** + RNA and c) **2** + DNA. Fluorescence was monitored at 550 nm for **1** and 625 nm for **2**. Data was plotted and analyzed with Prism 5. No saturation was observed for **2** + RNA over the concentration range tested; inner filter effects preclude measurements for [**2**] > 5 μM, as A > 0.2.

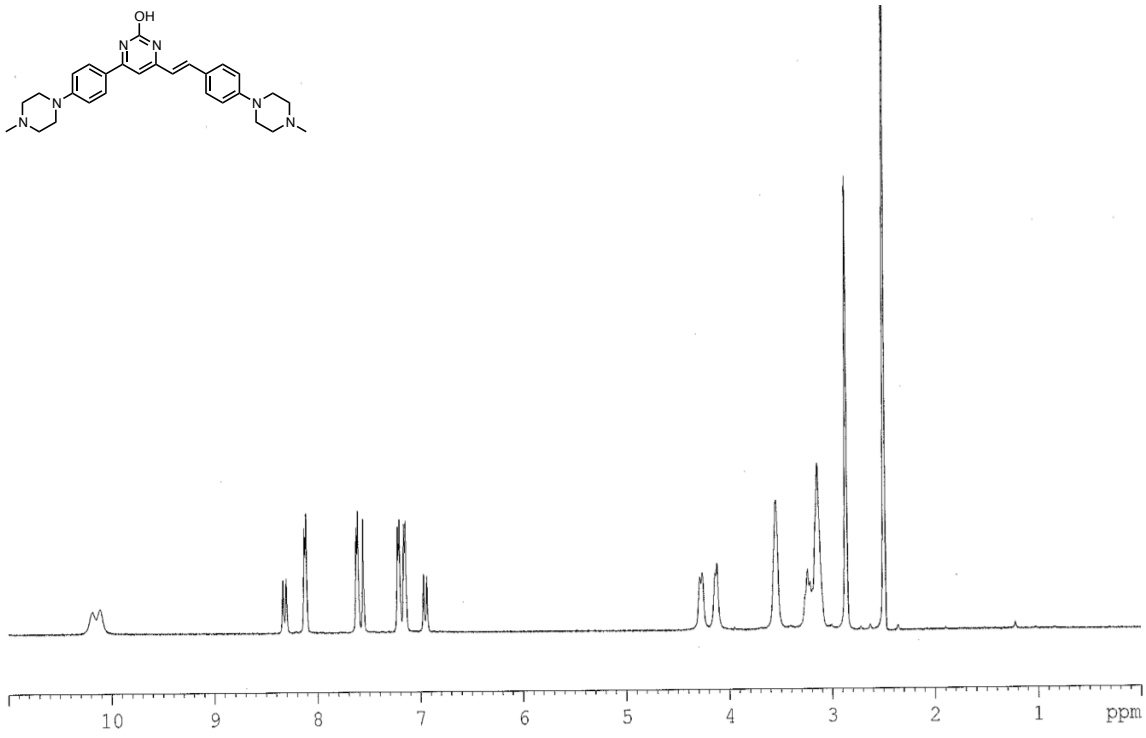

Figure S4. ^{1}H NMR of **1**.

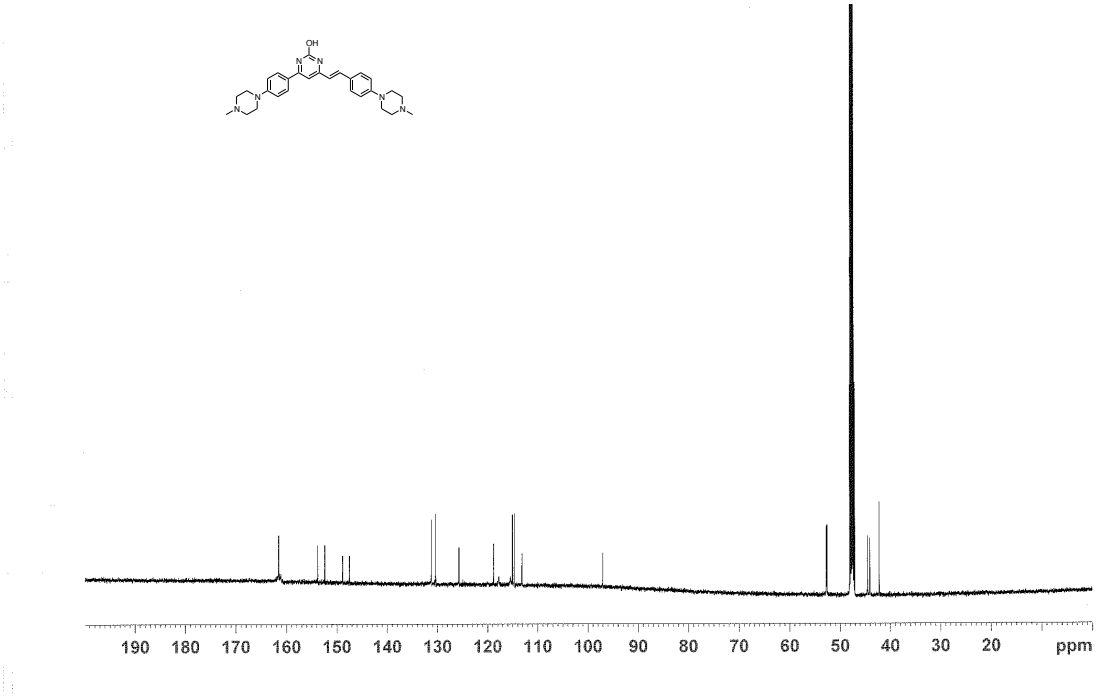

Figure S5. ^{13}C NMR of **1**.

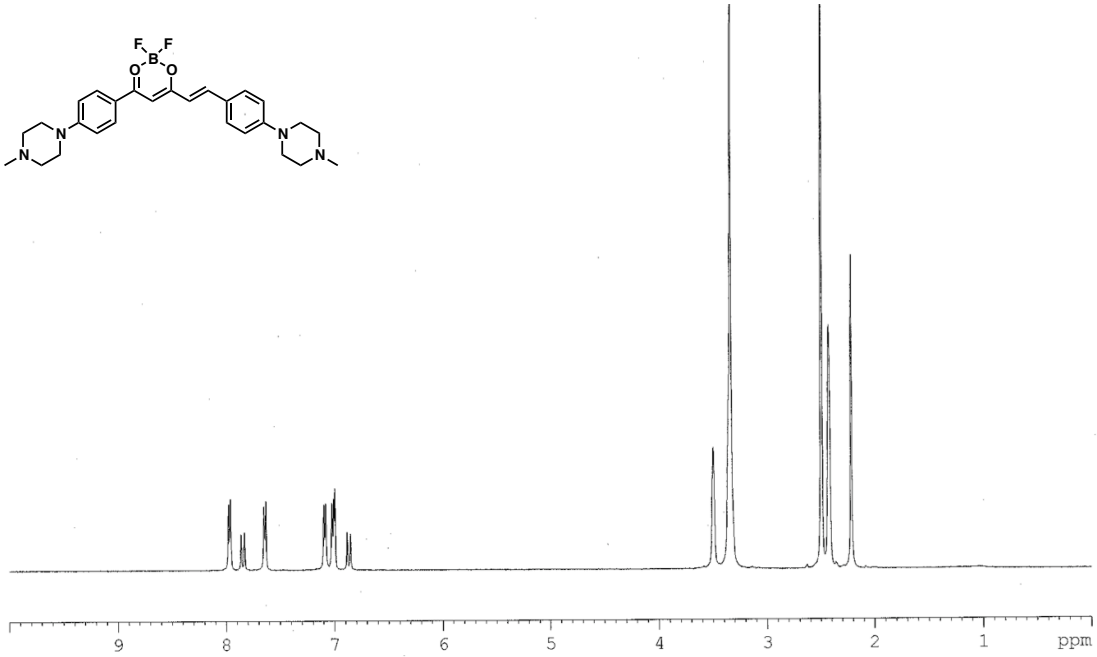

Figure S6. ^{1}H NMR of **2**.

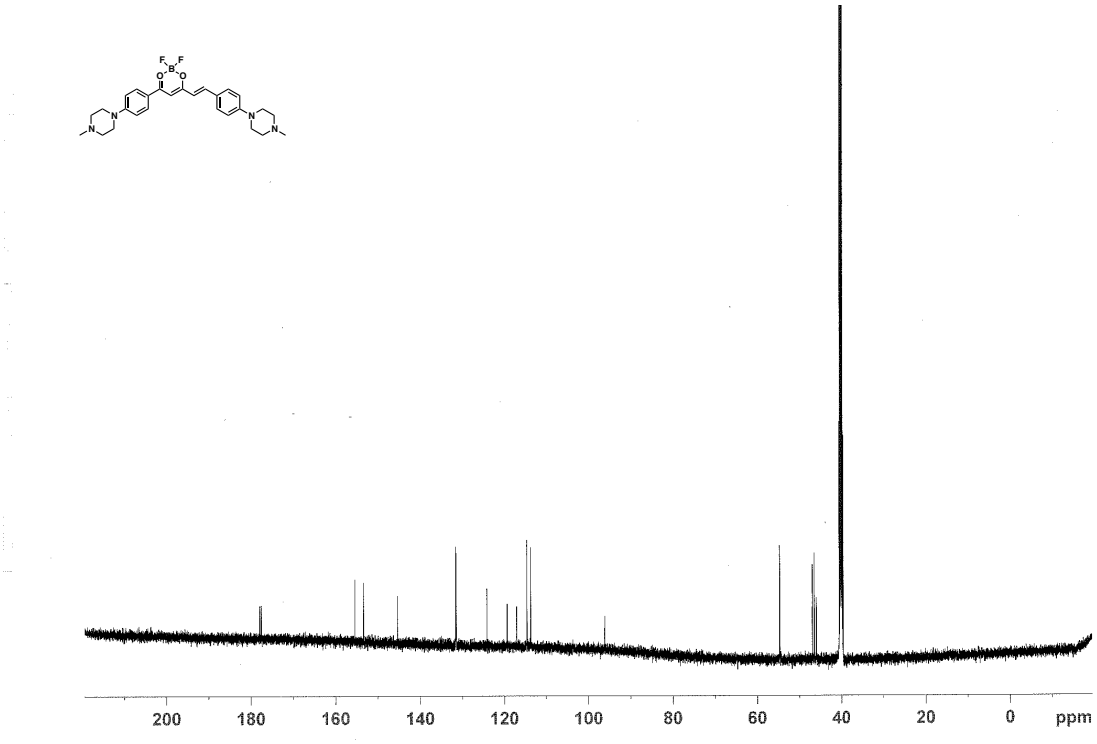

Figure S7. ^{13}C NMR of **2**.

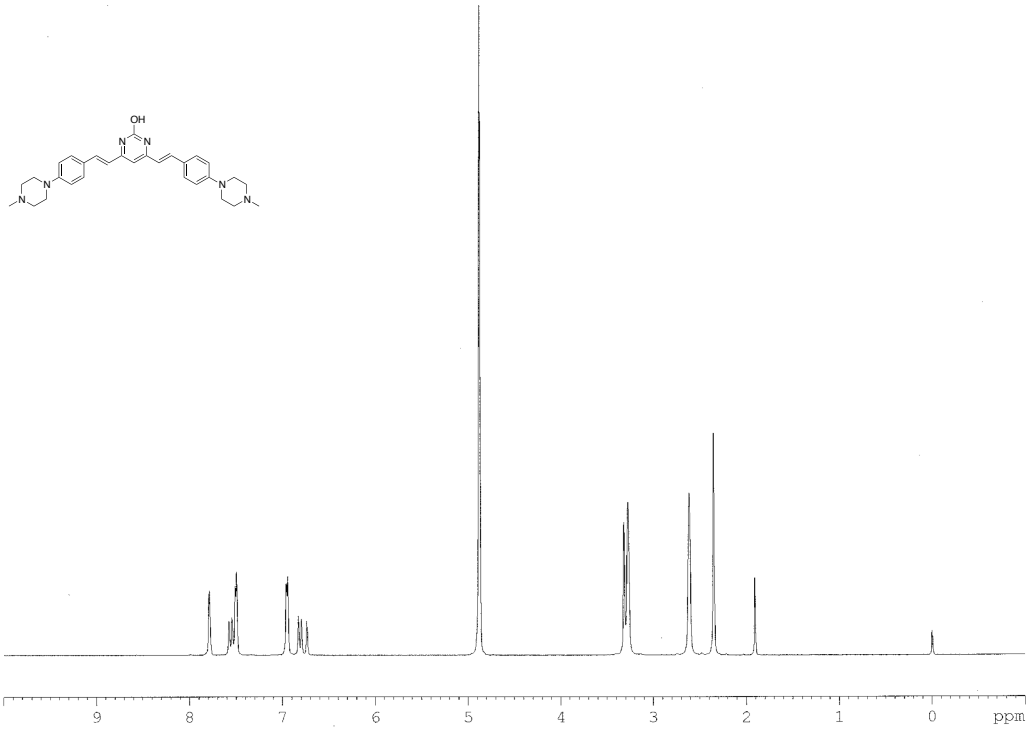

Figure S8. ^{1}H NMR of **3**.

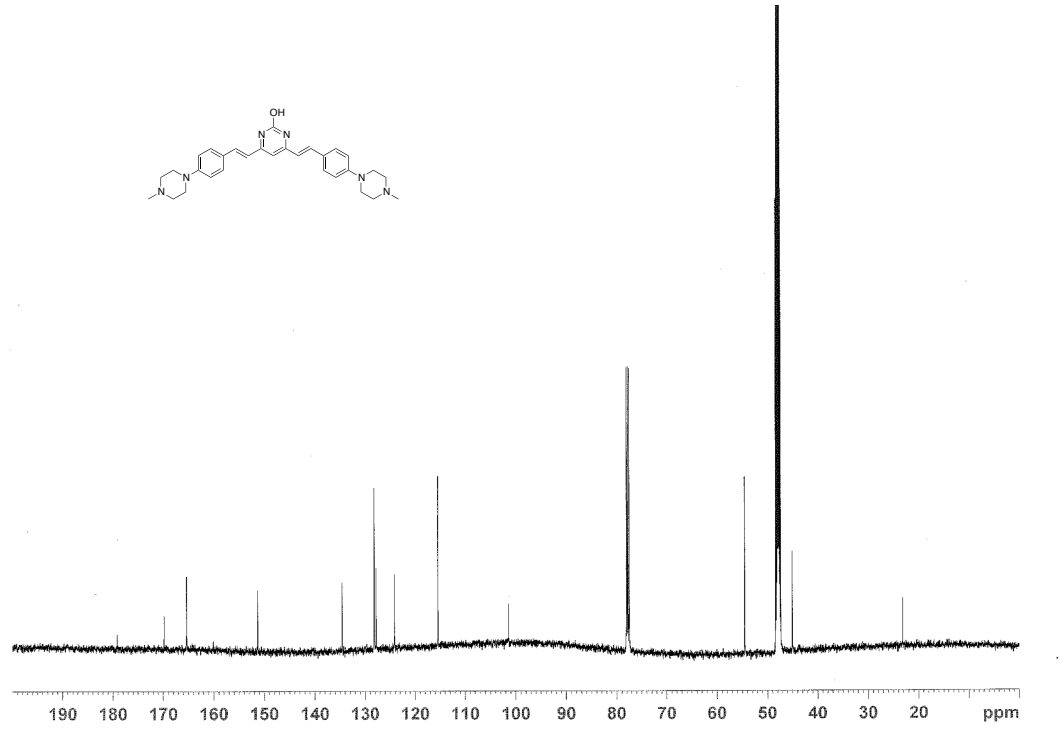

Figure S9. ^{13}C NMR of **3**.

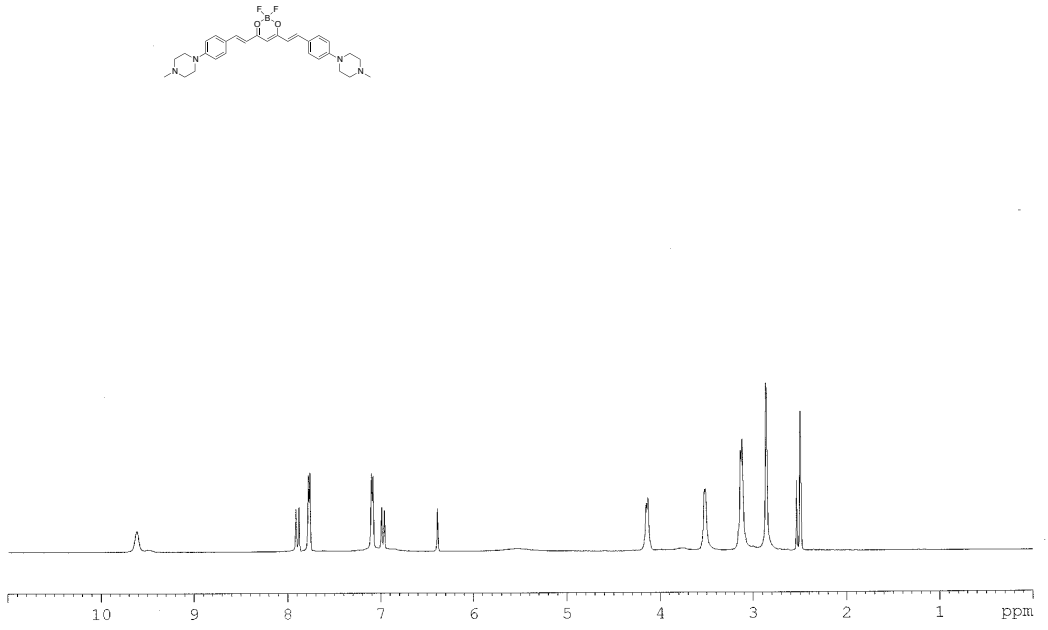

Figure S10. ^{1}H NMR of **4**.

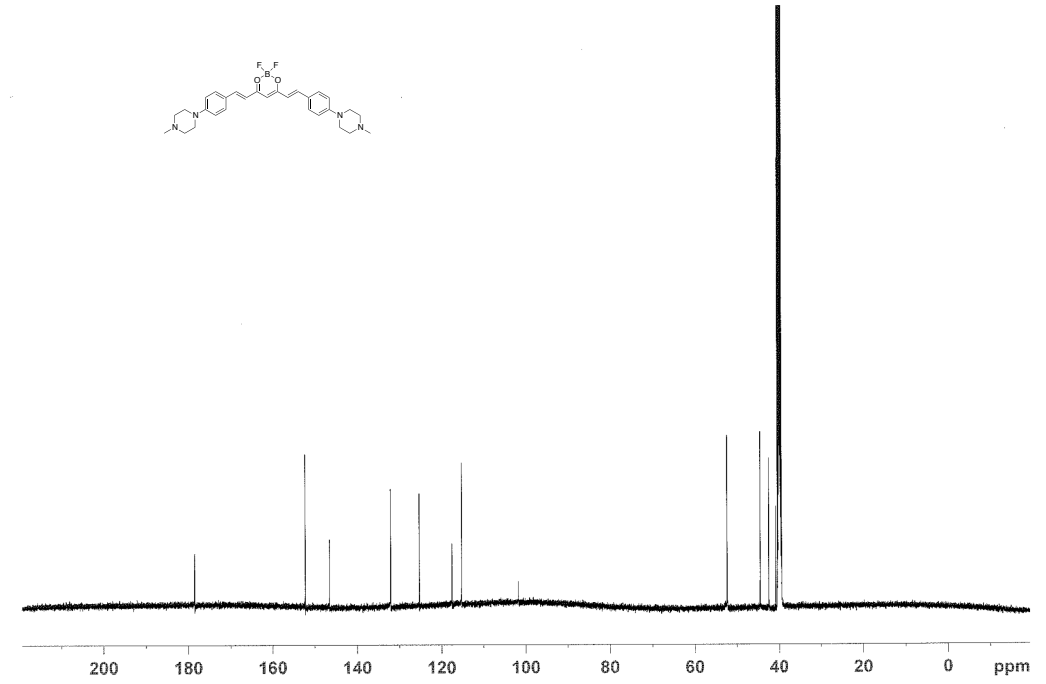

Figure S11. ^{13}C NMR of **4**.

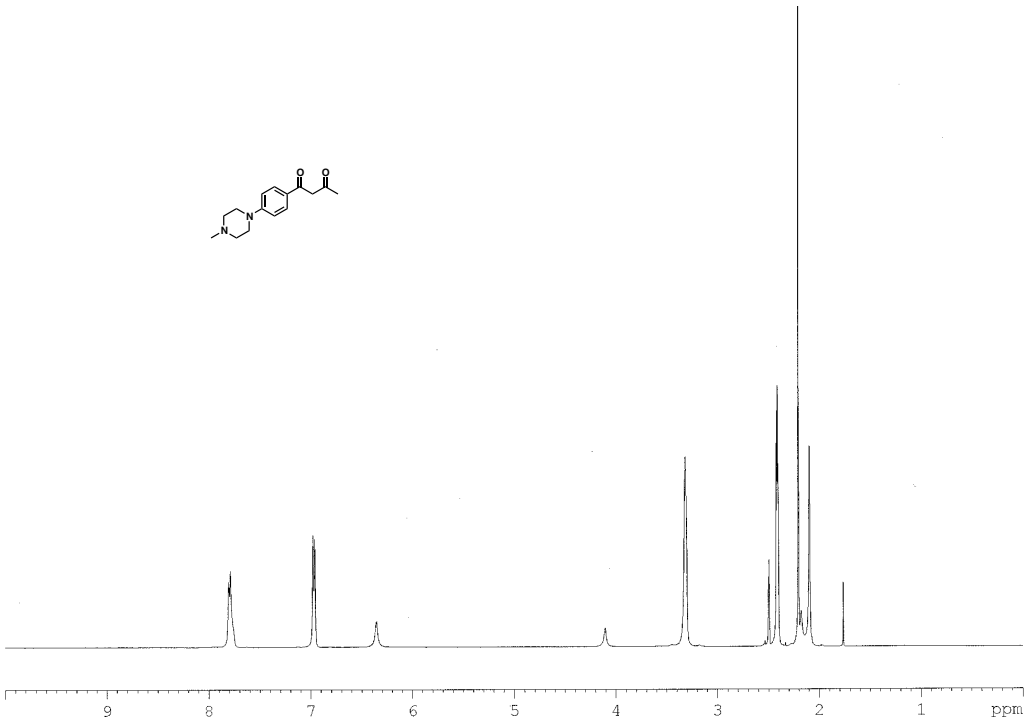

Figure S12. ^{1}H NMR of **5**.

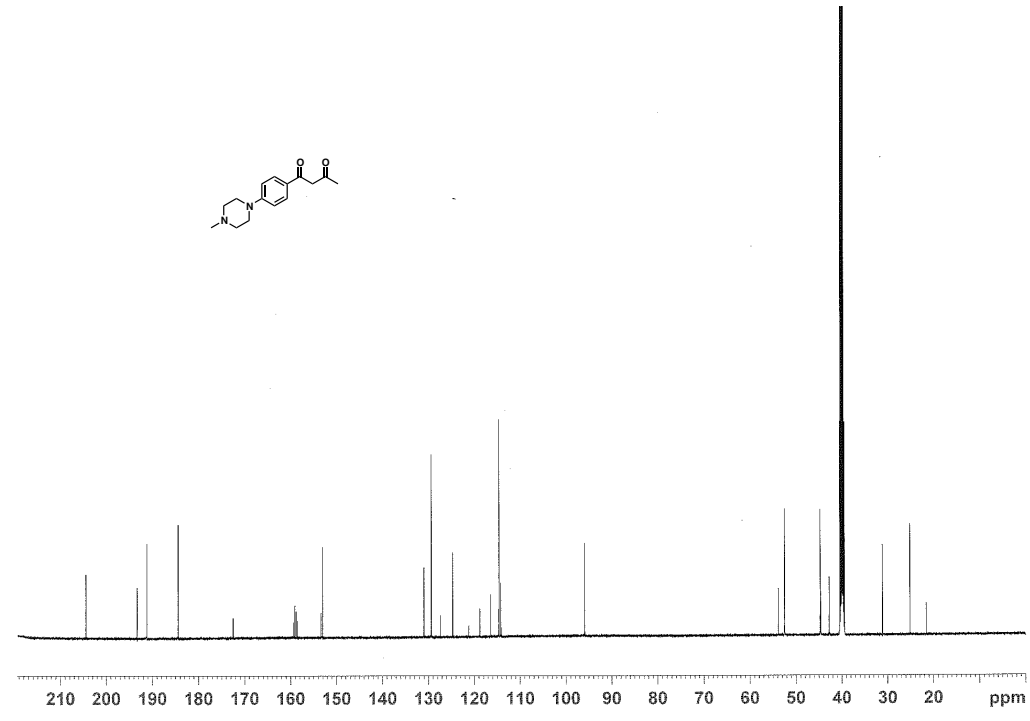

Figure S13. ^{13}C NMR of **5**.

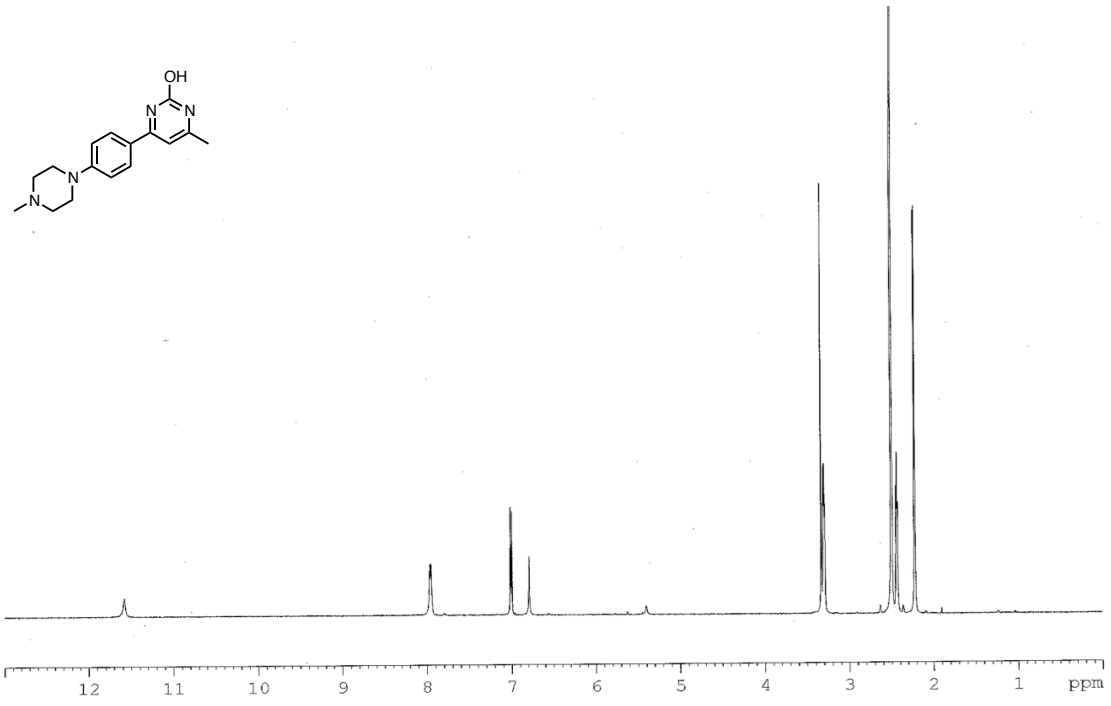

Figure S14. ^{1}H NMR of **6**.

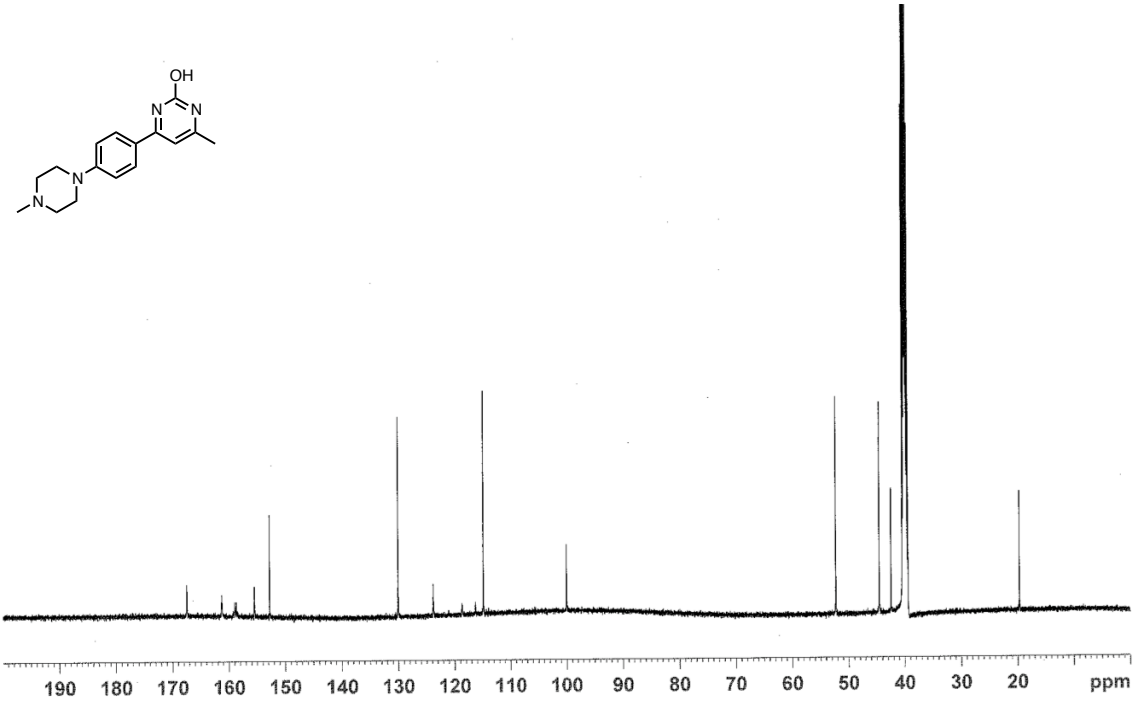

Figure S15. ^{13}C NMR of **6**.

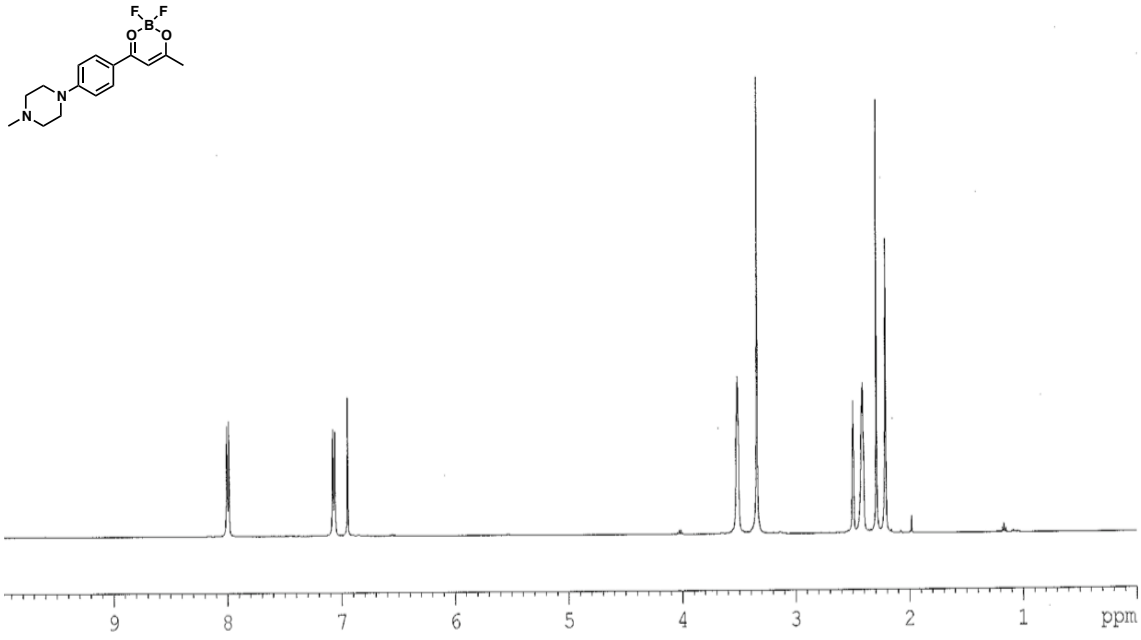

Figure S16. ^{1}H NMR of **7**.

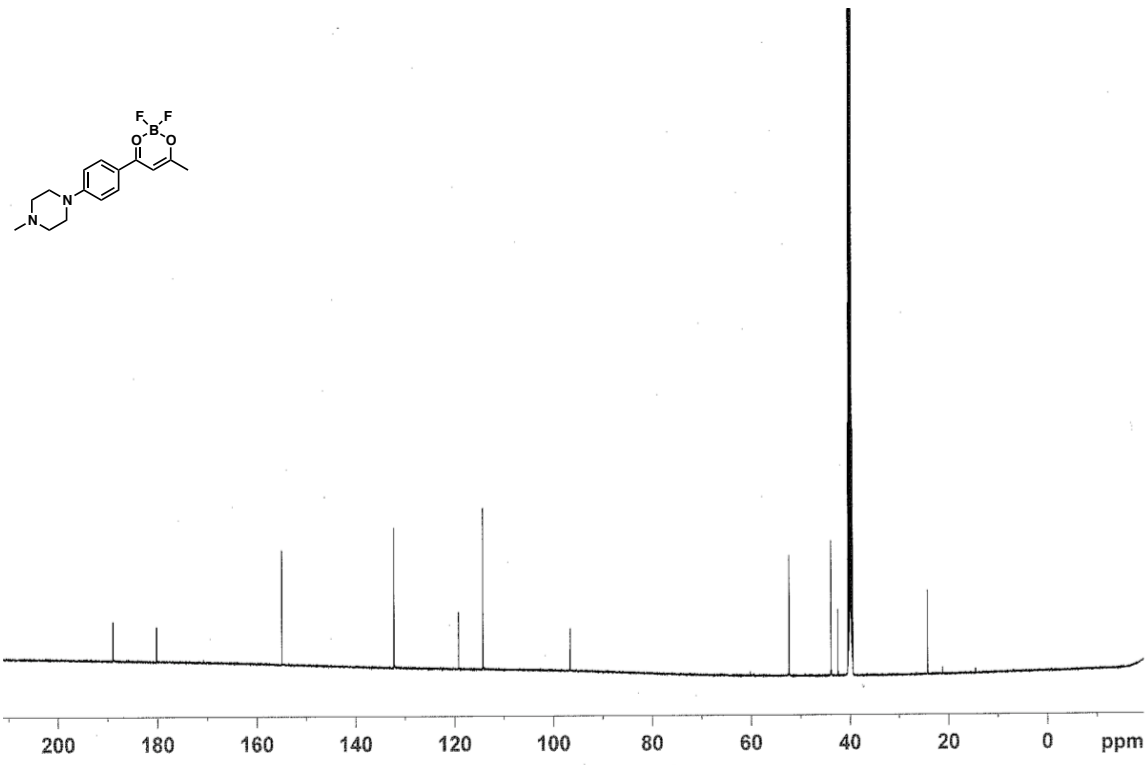

Figure S17. ^{13}C NMR of **7**.

Table S2: Optimized geometry of **1**; B3LYP/6-31G(d), SMD solvent model (MeOH); E = -1146.955 a.u.

atom	nucleus	x	y	z
1	C	1.118578	2.876965	-0.054545
2	C	1.091957	0.231865	-0.051602
3	N	2.31137	2.28752	-0.050583
4	N	-0.086373	2.317693	-0.06374
5	C	-0.105033	0.960143	-0.05851
6	C	2.307217	0.932631	-0.052363
7	H	1.057243	-0.850346	-0.028719
8	C	-1.386476	0.268542	-0.052197
9	H	-1.327674	-0.817389	-0.050921
10	C	-2.586279	0.900268	-0.045062
11	H	-2.571886	1.989484	-0.048523
12	C	3.61825	0.260227	-0.045192
13	C	6.193375	-1.003255	-0.026707
14	C	4.797735	0.989234	0.202113
15	C	3.764016	-1.121115	-0.277688
16	C	5.004603	-1.740688	-0.268683
17	C	6.045364	0.386744	0.2227
18	H	4.72511	2.054791	0.393501
19	H	2.893845	-1.736455	-0.485791
20	H	5.050628	-2.806856	-0.456195
21	H	6.913052	0.999715	0.435754
22	C	-3.909888	0.303042	-0.032073
23	C	-6.57809	-0.75527	-0.007609
24	C	-4.154444	-1.088246	-0.009585
25	C	-5.04404	1.142097	-0.033034
26	C	-6.337412	0.643332	-0.017088
27	C	-5.438028	-1.606149	0.005463
28	H	-3.320516	-1.785215	0.002447
29	H	-4.899387	2.220522	-0.042515
30	H	-7.165888	1.341612	-0.01271
31	H	-5.562904	-2.682193	0.029927
32	N	7.431245	-1.604505	-0.045756
33	N	-7.854312	-1.266646	-0.016975
34	C	8.604672	-0.860547	0.398159
35	H	8.545674	-0.57349	1.458918
36	H	8.741869	0.049412	-0.196122
37	H	9.49072	-1.482211	0.260228
38	C	7.529363	-3.057789	-0.117046
39	H	7.078397	-3.554238	0.755448
40	H	8.582471	-3.339734	-0.163259
41	H	7.042308	-3.442812	-1.019892
42	C	-8.066889	-2.699693	0.143848
43	H	-7.710796	-3.070933	1.116457
44	H	-7.559431	-3.266055	-0.645692
45	H	-9.134783	-2.910656	0.069667
46	C	-8.994688	-0.372908	0.144381
47	H	-8.976244	0.159169	1.107022
48	H	-9.914249	-0.957552	0.09396
49	H	-9.029199	0.374445	-0.657105
50	O	1.168353	4.232076	-0.053062
51	H	0.248144	4.555346	-0.058087

Table S3: Optimized geometry of **2**; B3LYP/6-31G(d), SMD solvent model (MeOH); E = -1298.708 a.u.

atom	nucleus	x	y	z
1	H	-1.39568	-1.03525	0.11472
2	C	-2.63195	0.71106	-0.01575
3	H	-2.5897	1.7975	-0.0772
4	C	3.55249	0.03624	0.0049
5	C	6.14009	-1.18453	-0.0129
6	C	4.73505	0.81096	0.02298
7	C	3.70386	-1.36925	-0.02873
8	C	4.9491	-1.96609	-0.03771
9	C	5.98753	0.23083	0.01678
10	H	4.65852	1.89266	0.04856
11	H	2.8317	-2.01436	-0.06171
12	H	5.00784	-3.04736	-0.06967
13	H	6.86025	0.87198	0.03717
14	C	-3.95812	0.1514	-0.00976
15	C	-6.64815	-0.83831	-0.00499
16	C	-4.23652	-1.23607	0.05518
17	C	-5.07225	1.02109	-0.07243
18	C	-6.37378	0.5562	-0.07114
19	C	-5.5291	-1.7203	0.05756
20	H	-3.41926	-1.95052	0.10274
21	H	-4.8972	2.09353	-0.12312
22	H	-7.18634	1.2709	-0.12047
23	H	-5.68462	-2.79126	0.10656
24	N	7.3738	-1.76527	-0.0193
25	N	-7.92825	-1.31459	-0.0021
26	C	8.57764	-0.93967	-0.01356
27	H	8.63183	-0.31212	0.88533
28	H	8.62385	-0.28638	-0.89446
29	H	9.45341	-1.58877	-0.02666
30	C	7.50797	-3.21829	-0.05078
31	H	7.02825	-3.68615	0.81809
32	H	8.56694	-3.477	-0.03308
33	H	7.06726	-3.64644	-0.96048
34	C	-8.18265	-2.75046	0.05581
35	H	-7.76835	-3.19745	0.96853
36	H	-7.75304	-3.27283	-0.80891
37	H	-9.2594	-2.92157	0.0542
38	C	-9.05715	-0.39332	-0.08141
39	H	-9.06601	0.30815	0.76267
40	H	-9.98487	-0.9654	-0.05606
41	H	-9.0396	0.18883	-1.01232
42	C	2.25414	0.68535	0.01241
43	C	1.03157	0.01486	0.10159
44	H	0.99305	-1.0609	0.19919
45	C	-0.1734	0.72216	0.02688
46	O	2.27493	2.00536	-0.08205
47	O	-0.1788	2.04215	-0.0811
48	B	1.05837	2.8525	0.00779
49	F	1.07459	3.74964	-1.05208
50	F	1.07222	3.53006	1.22401

Table S4: Optimized geometry of **3**; B3LYP/6-31G(d), SMD solvent model (MeOH). -1224.371 a. u.

atom	nucleus	x	y	z
1	C	0.003772	2.805433	0.015851
2	C	0.00438	0.16031	-0.011043
3	N	1.204464	2.235575	0.010596
4	N	-1.195966	2.229516	0.009109
5	C	-1.203082	0.871914	-0.004654
6	C	1.2092	0.878725	-0.003508
7	H	0.00693	-0.924699	-0.021991
8	C	-2.476766	0.167166	-0.013102
9	H	-2.407159	-0.918095	-0.024132
10	C	-3.682431	0.788267	-0.008709
11	H	-3.676587	1.877531	0.001185
12	C	5.007802	0.187849	-0.01636
13	C	7.668298	-0.889512	-0.043529
14	C	6.148003	1.018774	-0.013613
15	C	5.242402	-1.205394	-0.024161
16	C	6.522282	-1.732503	-0.033798
17	C	7.437689	0.510674	-0.02261
18	H	6.011057	2.098136	-0.00046
19	H	4.403504	-1.896468	-0.018041
20	H	6.639636	-2.8097	-0.032528
21	H	8.271	1.20307	-0.014296
22	C	-5.001142	0.181282	-0.017512
23	C	-7.661968	-0.895131	-0.042927
24	C	-5.23615	-1.211923	-0.024661
25	C	-6.141078	1.012623	-0.014706
26	C	-7.430903	0.505045	-0.022924
27	C	-6.516187	-1.738553	-0.033483
28	H	-4.397422	-1.903205	-0.01864
29	H	-6.00377	2.091961	-0.00212
30	H	-8.264012	1.197683	-0.014606
31	H	-6.633972	-2.815694	-0.031786
32	N	8.940607	-1.409621	-0.079029
33	N	-8.934314	-1.414721	-0.077049
34	C	10.089301	-0.526603	0.082813
35	H	10.09006	-0.014655	1.056492
36	H	10.115536	0.236779	-0.7036
37	H	11.004094	-1.115687	0.005119
38	C	9.145048	-2.846083	0.061431
39	H	8.79712	-3.227006	1.03321
40	H	10.21059	-3.063216	-0.027519
41	H	8.625243	-3.399175	-0.729466
42	C	-9.139329	-2.851223	0.062375
43	H	-8.789949	-3.23304	1.033237
44	H	-8.621102	-3.403953	-0.729838
45	H	-10.205132	-3.067687	-0.024861
46	C	-10.08285	-0.531066	0.082372
47	H	-10.083501	-0.016713	1.054763
48	H	-10.997756	-1.120144	0.006177
49	H	-10.108909	0.23043	-0.70591
50	O	0.029595	4.161592	0.030196
51	H	-0.896616	4.467184	0.032748
52	C	2.483575	0.17399	-0.011485
53	H	2.414515	-0.911314	-0.0226
54	C	3.689088	0.795156	-0.007121
55	H	3.682583	1.884385	0.002866

Table S5: Optimized geometry of **4**; B3LYP/6-31G(d), SMD solvent model (MeOH); E = -1376.125 a. u.

atom	nucleus	x	y	z
1	C	-2.473583	-0.057153	0.000288
2	H	-2.418108	-1.141475	0.024229
3	C	-3.672809	0.596578	-0.024001
4	H	-3.641105	1.685006	-0.040753
5	C	4.993166	0.023759	-0.000545
6	C	7.674167	-0.990387	0.01049
7	C	5.258469	-1.367678	0.021273
8	C	6.115814	0.884664	-0.019095
9	C	7.412978	0.407941	-0.014976
10	C	6.546565	-1.863574	0.025382
11	H	4.434385	-2.075768	0.03303
12	H	5.950943	1.959721	-0.03853
13	H	8.23231	1.116347	-0.032375
14	H	6.691784	-2.937002	0.039913
15	C	-4.993448	0.024376	-0.026118
16	C	-7.67411	-0.990706	-0.024468
17	C	-5.258301	-1.367287	-0.019574
18	C	-6.116382	0.885082	-0.03131
19	C	-7.413411	0.407912	-0.028127
20	C	-6.546242	-1.863603	-0.018008
21	H	-4.434034	-2.075252	-0.015631
22	H	-5.951882	1.960365	-0.034574
23	H	-8.233067	1.116169	-0.027769
24	H	-6.691082	-2.937155	-0.011635
25	N	8.94996	-1.47848	0.020627
26	N	-8.94981	-1.479344	-0.028283
27	C	9.190727	-2.917292	-0.015116
28	H	8.78377	-3.376175	-0.926081
29	H	8.745603	-3.420558	0.852122
30	H	10.265698	-3.098388	0.005278
31	C	10.088021	-0.567203	-0.03868
32	H	10.093796	0.017444	-0.968736
33	H	11.010071	-1.147363	0.004876
34	H	10.086598	0.131826	0.806804
35	C	-9.190152	-2.917235	0.035931
36	H	-8.79023	-3.357388	0.959294
37	H	-8.737795	-3.437554	-0.817253
38	H	-10.264826	-3.099501	0.010479
39	C	-10.088046	-0.567575	0.018737
40	H	-10.092939	0.030945	0.939955
41	H	-11.009944	-1.148656	-0.015074
42	H	-10.088012	0.118494	-0.837275
43	C	1.214042	0.629061	0.008962
44	C	-0.000408	-0.063096	0.043228
45	H	-0.000816	-1.145257	0.082468
46	C	-1.214313	0.629569	0.000539
47	O	1.230461	1.953058	-0.041331
48	O	-1.23004	1.95358	-0.049079
49	B	0.000258	2.780985	0.013684
50	F	0.003877	3.646778	-1.074078
51	F	-0.003292	3.497997	1.207496
52	C	3.672458	0.595648	-0.0058
53	H	3.64069	1.683941	-0.029418
54	C	2.473104	-0.05794	0.017523
55	H	2.417389	-1.142168	0.045137