Supporting Information

Fluoride recognition by a chiral urea receptor linked to a phthalimide chromophore

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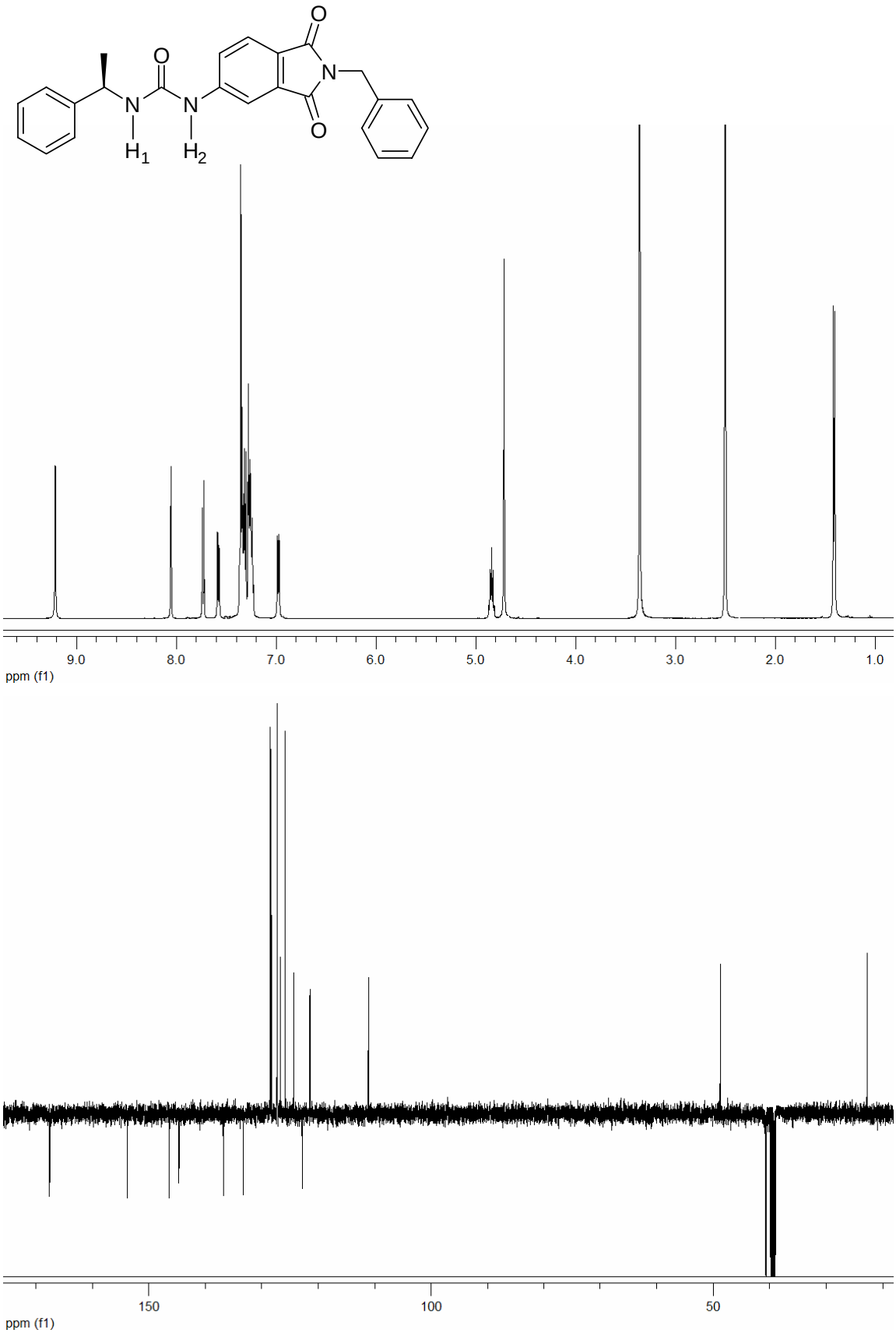
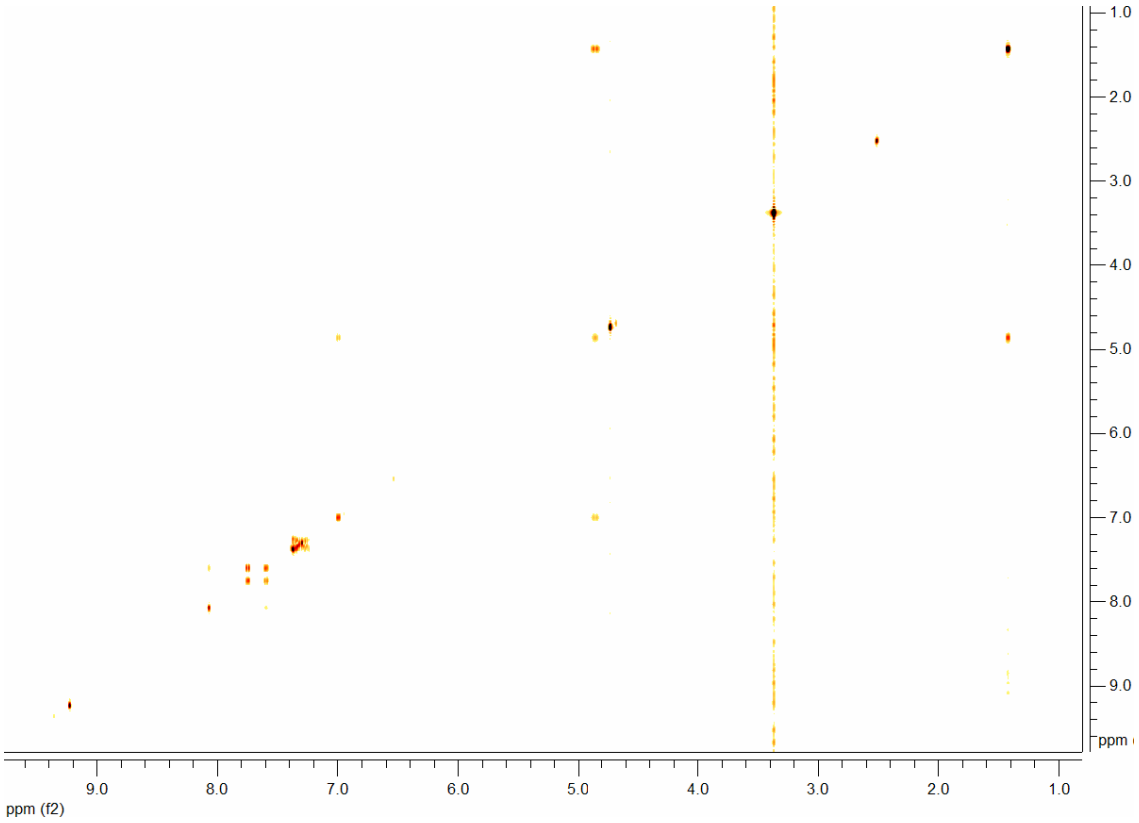
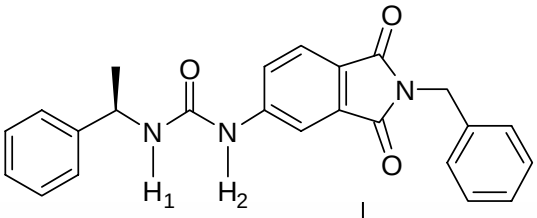
^{1}H-NMR and ^{13}C-APT-NMR of **1** (DMSO-d^{6}, 600 MHz)

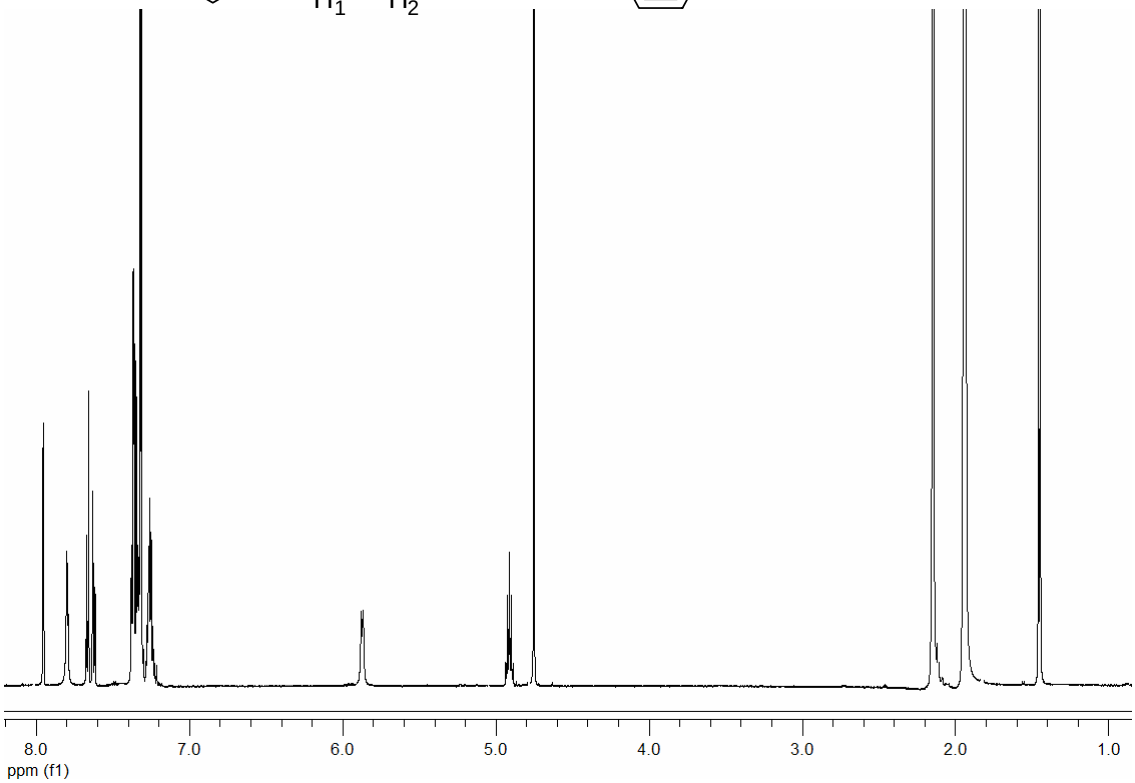


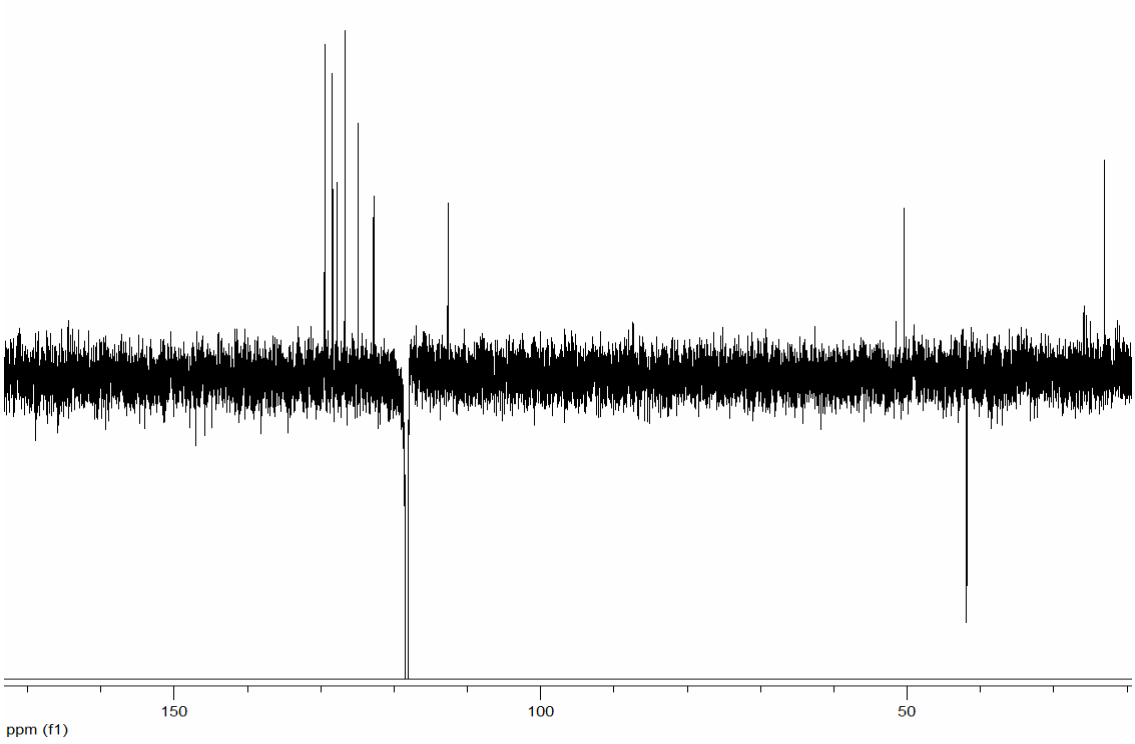
$^{1}H/^{1}H$ NMR NOEDIFF (DMSO-d^{6}, 600 MHz)



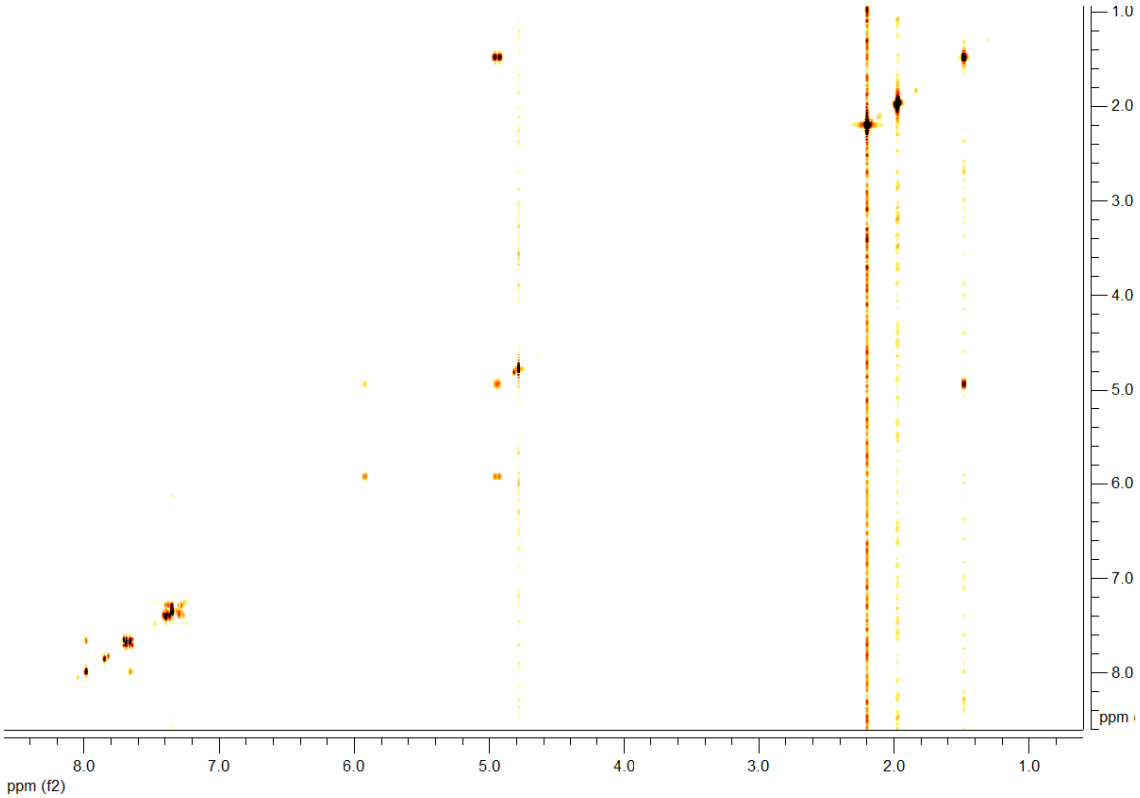
^{1}H-NMR and ^{13}C-APT-NMR of **1** (CD_3CN, 600 MHz)







Significant correlations in the $^{1}H/^{1}H$ NMR NOEDIFF (CD_3CN, 600 MHz)



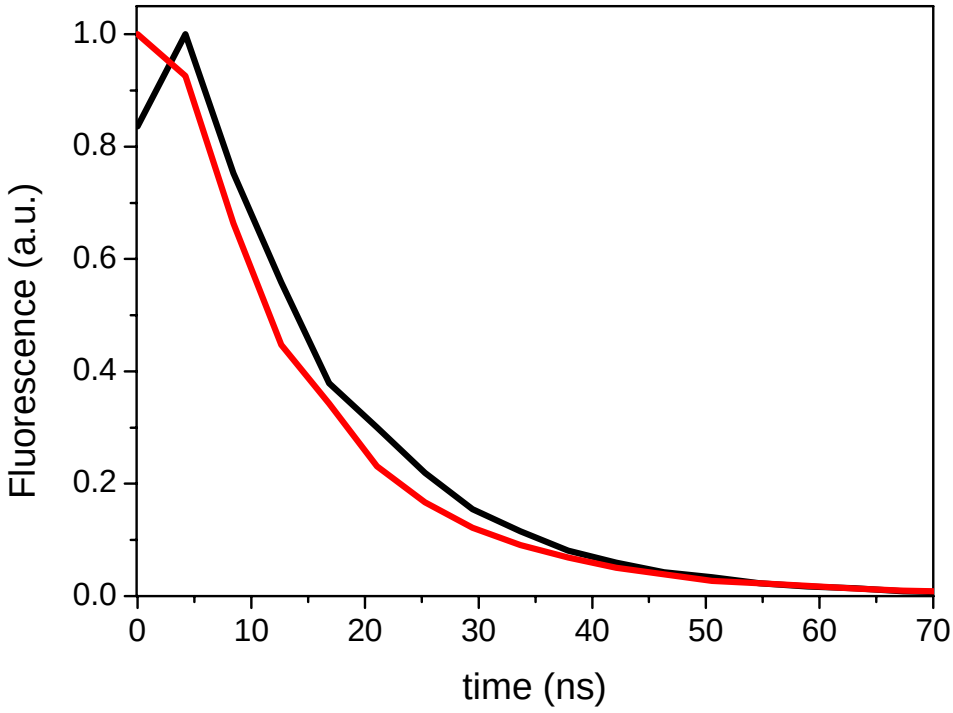


Figure S1: Normalized fluorescence decay traces of **1** (3.3 x 10^{-6} M) in the absence (—) and in the presence of fluoride anion (3 x 10^{-4} M) (—) in acetonitrile.

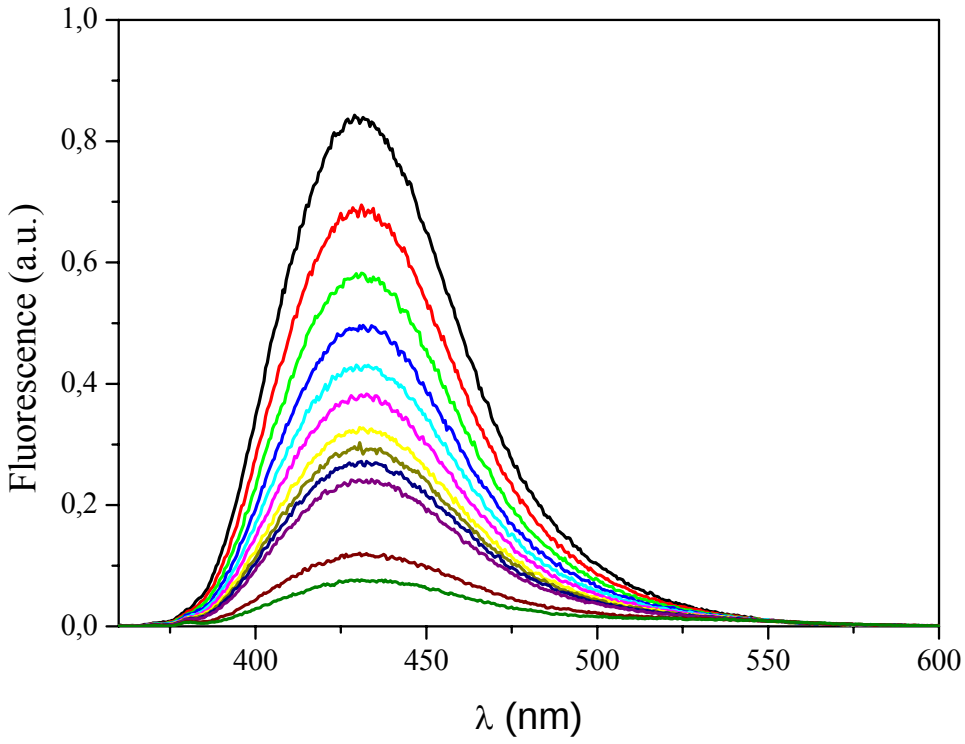
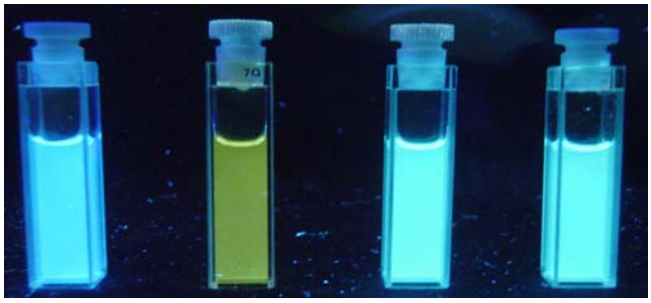


Figure S2. Emission spectra of **1** (λ_{exc} = 340 nm) in the presence of increasing amounts of DBU (0, 0.033 → 0.3 mM) in acetonitrile.



1 **1**+F^- **1**+F^-+MeOH **1**+MeOH

Figure S3. Colour changes observed in the emission on addition of F^- in the absence/presence of methanol (10%) to an acetonitrile solution of **1**.

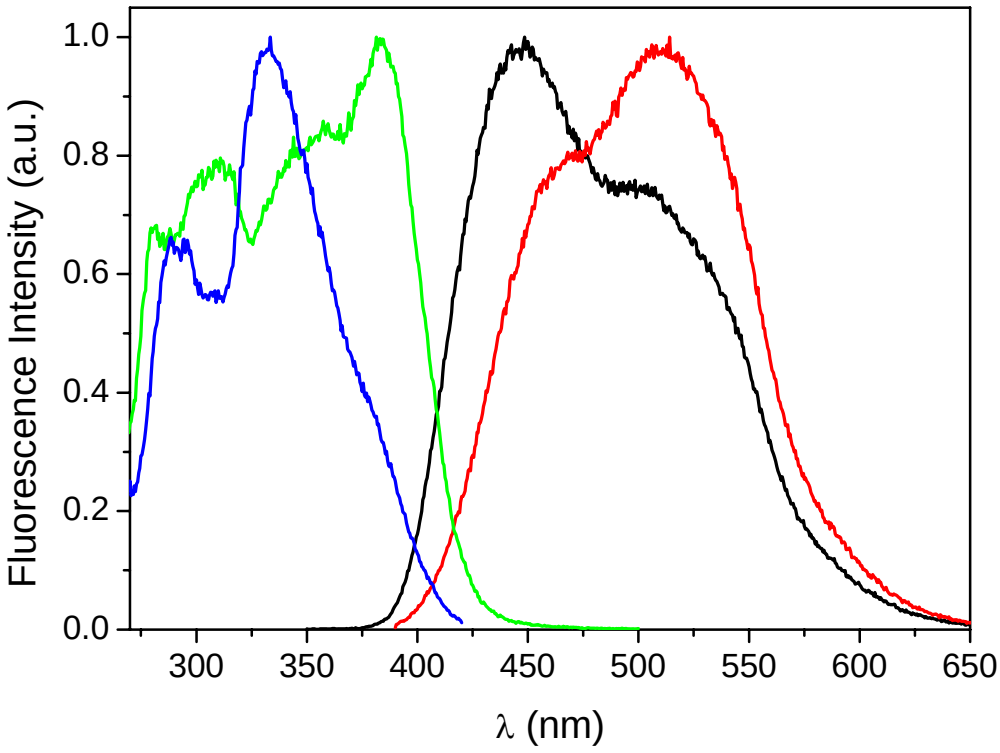


Figure S4: Normalized emission spectra (—, λ_{exc} = 340 nm and —, λ_{exc} = 380 nm) and excitation spectra (—, λ_{em} = 430 nm and —, λ_{exc} = 520 nm) of **1** (10^{-4} M) and F^- (3.4 x 10^{-3} M) in acetonitrile

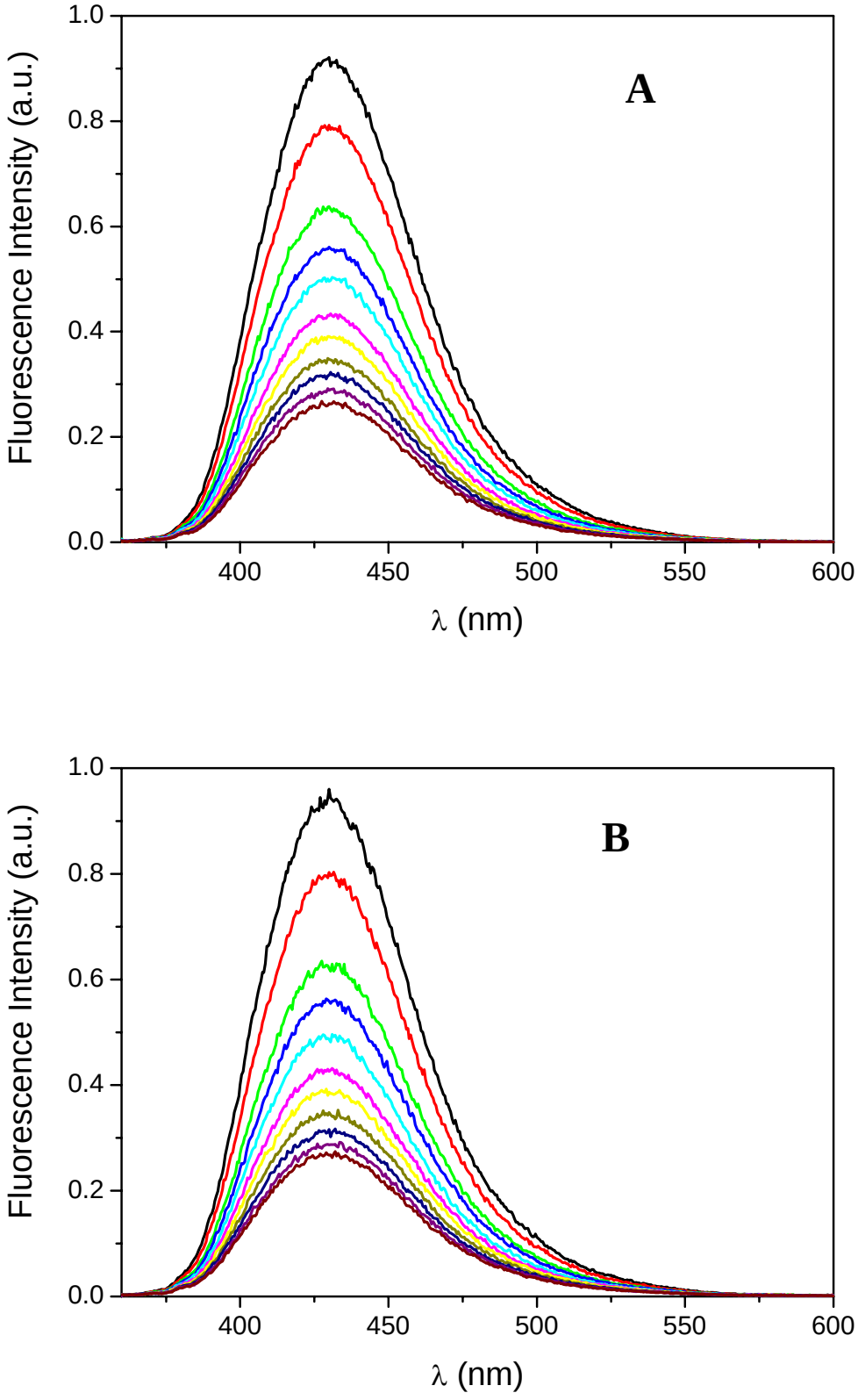


Figure S5: Emission spectra of **1** (λ_{exc} = 340 nm) in acetonitrile in the presence of increasing amounts of: A) *R*-methylbenzylamine (0 → 0.05 M) and B) *S*-methylbenzylamine (0 → 0.05 M)

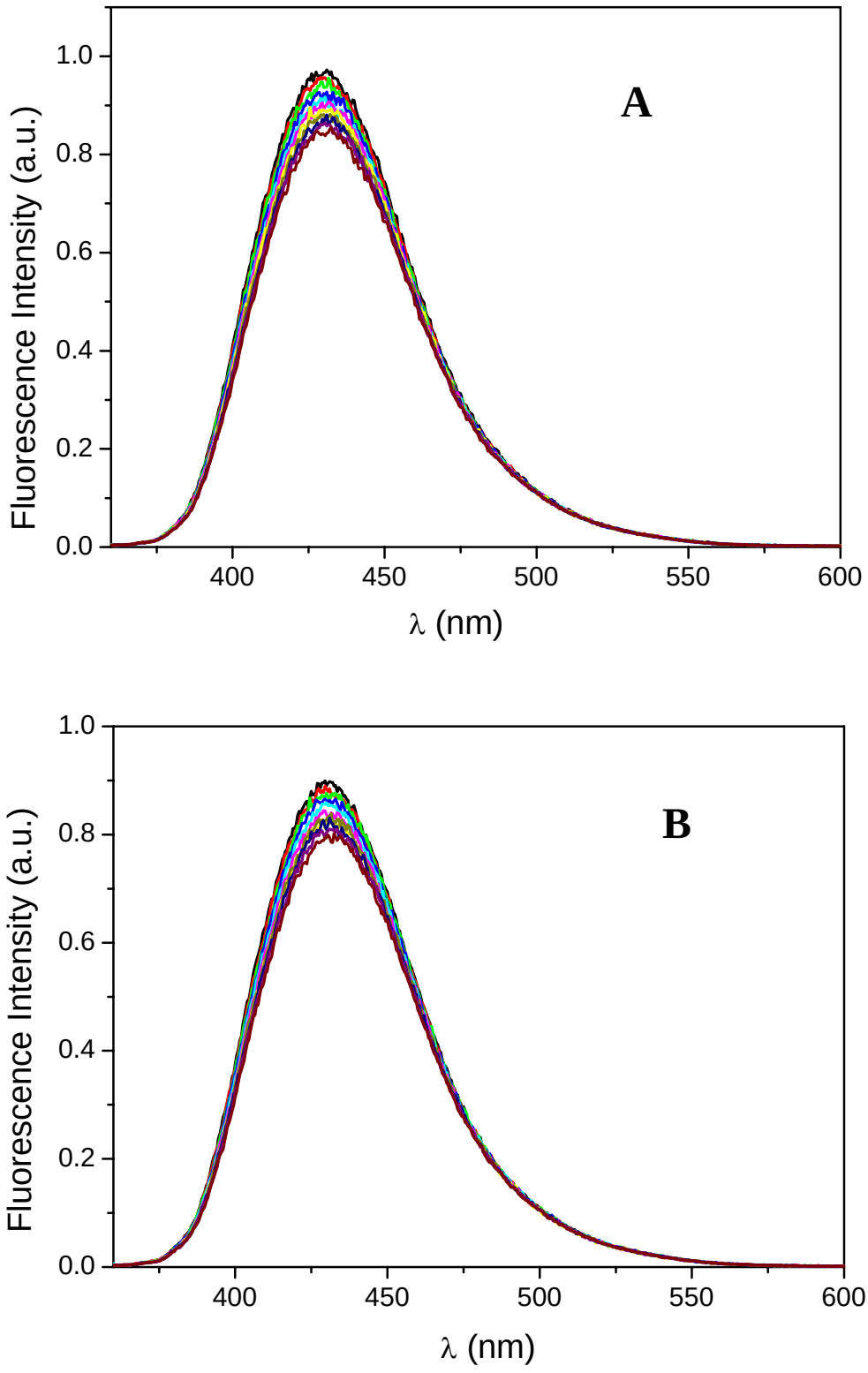


Figure S6: Emission spectra of **1** (λ_{exc} = 340 nm) in acetonitrile in the presence of increasing amounts of: A) *R*-1-phenylethanol (0 → 0.05 M) and B) *S*-1-phenylethanol (0 → 0.05 M)

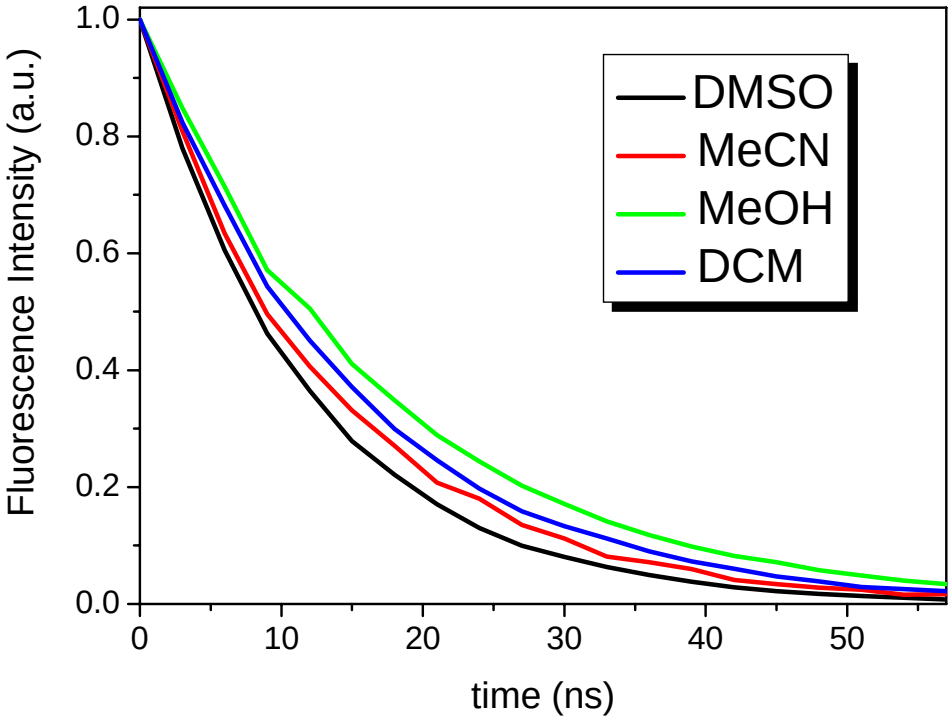


Figure S7: Normalized fluorescence decay traces of **1** (3.3 x 10^{-6} M) in different solvents

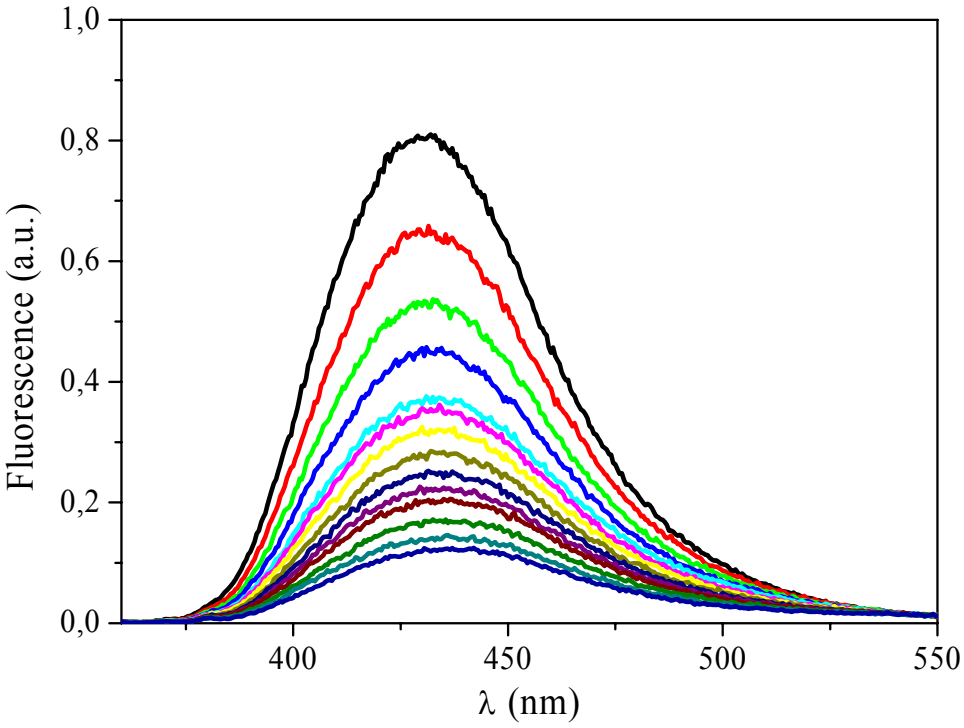


Figure S8. Emission spectra of **1** (λ_{exc} = 340 nm) in the presence of increasing amounts of $H_2PO_4^-$ (0, 0.025 → 0.33 mM) in acetonitrile

Optimised geometry coordinates of model system before complexation with F^-

Standard orientation

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.719906	0.088344	-0.034325
2	8	0	-1.707162	1.324958	-0.044103
3	7	0	-0.581201	-0.701616	-0.022295
4	1	0	-0.730298	-1.714601	-0.039448
5	7	0	-2.883163	-0.634336	-0.067140
6	1	0	-2.845307	-1.635475	0.134844
7	6	0	-4.167031	0.030152	0.077461
8	1	0	-4.954148	-0.649954	-0.257879
9	1	0	-4.375801	0.327463	1.114896
10	1	0	-4.183966	0.927609	-0.544564
11	6	0	0.766094	-0.302121	-0.009073
12	6	0	1.192885	1.037735	0.000188
13	6	0	1.734203	-1.324479	-0.002535
14	6	0	2.559017	1.328667	0.016717
15	1	0	0.458257	1.830854	-0.006723
16	6	0	3.092497	-1.017363	0.013190
17	1	0	1.409939	-2.365542	-0.009676
18	6	0	3.518471	0.314269	0.023364
19	1	0	2.871387	2.372385	0.023897
20	1	0	3.820653	-1.827370	0.017727
21	1	0	4.579737	0.555396	0.035872

Optimised geometry coordinates of model system after complexation with F^-

B3LYP/6-31G* SCFR = (CPCM, solvent = acetonitrile)

Standard orientation

Centre Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.493489	-0.587225	0.000119
2	8	0	-1.367959	-1.830498	0.007171
3	7	0	-0.448772	0.320116	-0.005711
4	1	0	-0.779880	1.317748	-0.001336
5	7	0	-2.700717	0.036840	-0.002594
6	1	0	-2.668483	1.070913	-0.007745
7	6	0	-3.945248	-0.705202	0.016765
8	1	0	-4.770441	0.009151	0.042582
9	1	0	-4.061802	-1.335308	-0.873918
10	1	0	-4.020650	-1.351987	0.899524
11	6	0	0.922718	0.078042	-0.001851
12	6	0	1.517506	-1.199632	-0.018156
13	6	0	1.766522	1.210118	0.018334
14	6	0	2.908740	-1.323310	-0.015523
15	1	0	0.887812	-2.077766	-0.032027
16	6	0	3.151442	1.070164	0.020151
17	1	0	1.316412	2.199398	0.035035
18	6	0	3.739058	-0.200035	0.002559
19	1	0	3.344792	-2.319315	-0.025847
20	1	0	3.774979	1.960372	0.036296
21	1	0	4.819572	-0.309646	0.004660
22	9	0	-1.806190	2.547133	-0.023428