Electronic Supplementary Information for

N-(cyano(naphthalen-1-yl)methyl)benzamides: synthesis, crystal structures, and colorimetric sensing for fluoride anion

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1. Synthesis of Compound 5

2-Amino-2-(naphthalene-1-yl)acetonitrile) (**5**) was prepared according to the literature procedures[1] with slight modifications. A cooled mixture (at 0 ^{o}C) of 1-naphthaldehyde (0.18 g, 1.0 mmol) in ammonium hydroxide (20 mL) and ethanol (20 mL) was stirred for 10 minutes. Sodium cyanide (NaCN) (0.050 g, 1.0 mmol) was added in portions with continuous stirring. Ammonium chloride (0.053 g, 1.0 mmol) was then added to the solution. The flask was securely stoppered, and left under continuous stirring for 24 hours at room temperature. The resulting product was extracted with chloroform (2 ×15 mL). The organic layers were combined and dried over anhydrous $MgSO_4$. The organic solvent was removed under reduced pressure to give aminonitrile (**5**) as an orange semi-solid in a quantitative yield. The aminonitrile (**5**) was used for the next step without any further purification. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.4 Hz, 1H), 7.93 (t, *J* = 7.8 Hz, 2H), 7.83 (d, *J* = 7.1 Hz, 1H), 7.67-7.49 (m, 3H), 5.59(s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.09, 131.69, 130.11, 130.01, 129.13, 127.15, 126.37, 125.28, 124.97, 122.84, 121.04, 45.38 ppm.

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1) K. Mai and G. Patil, *Organic Preparations and Procedures International*, 1985, **17**, 183–186.

2. NMR Spectra of Compounds 7a-c

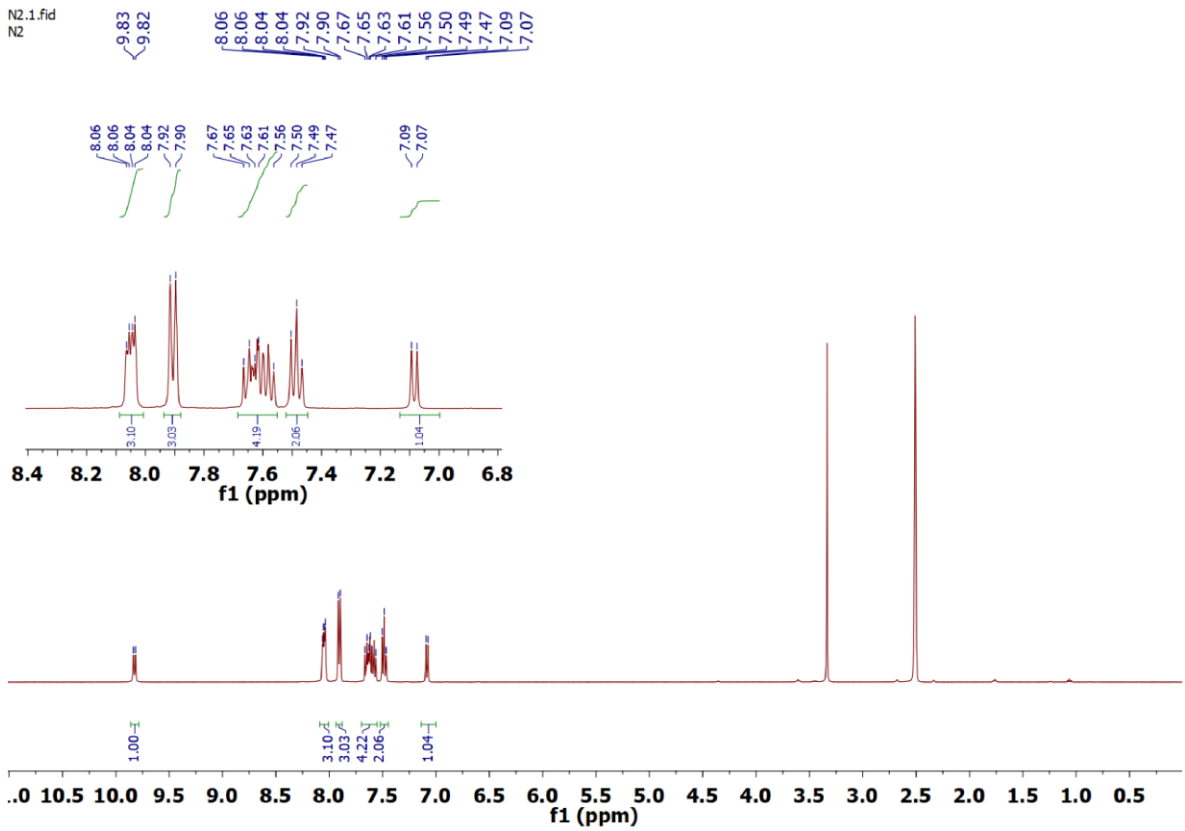

Fig. S-1: ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **7a**.

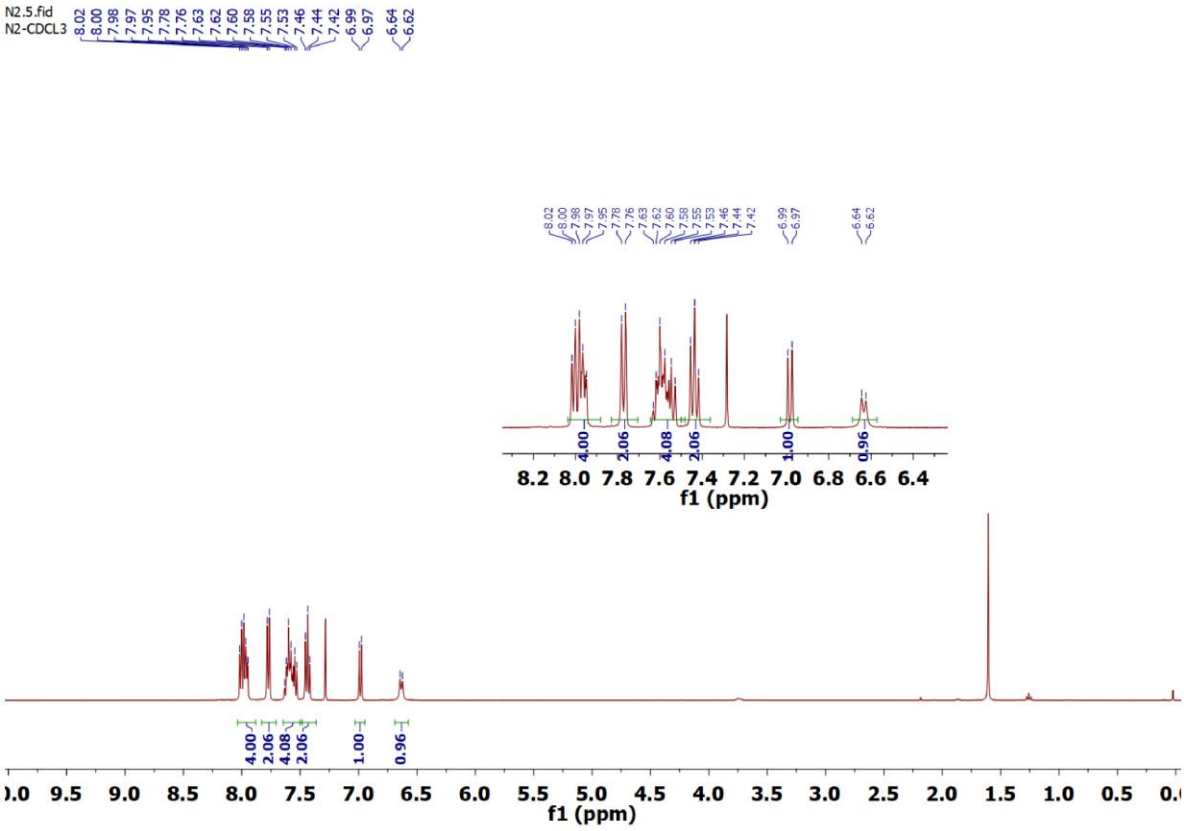

Fig. S-2: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7a**.

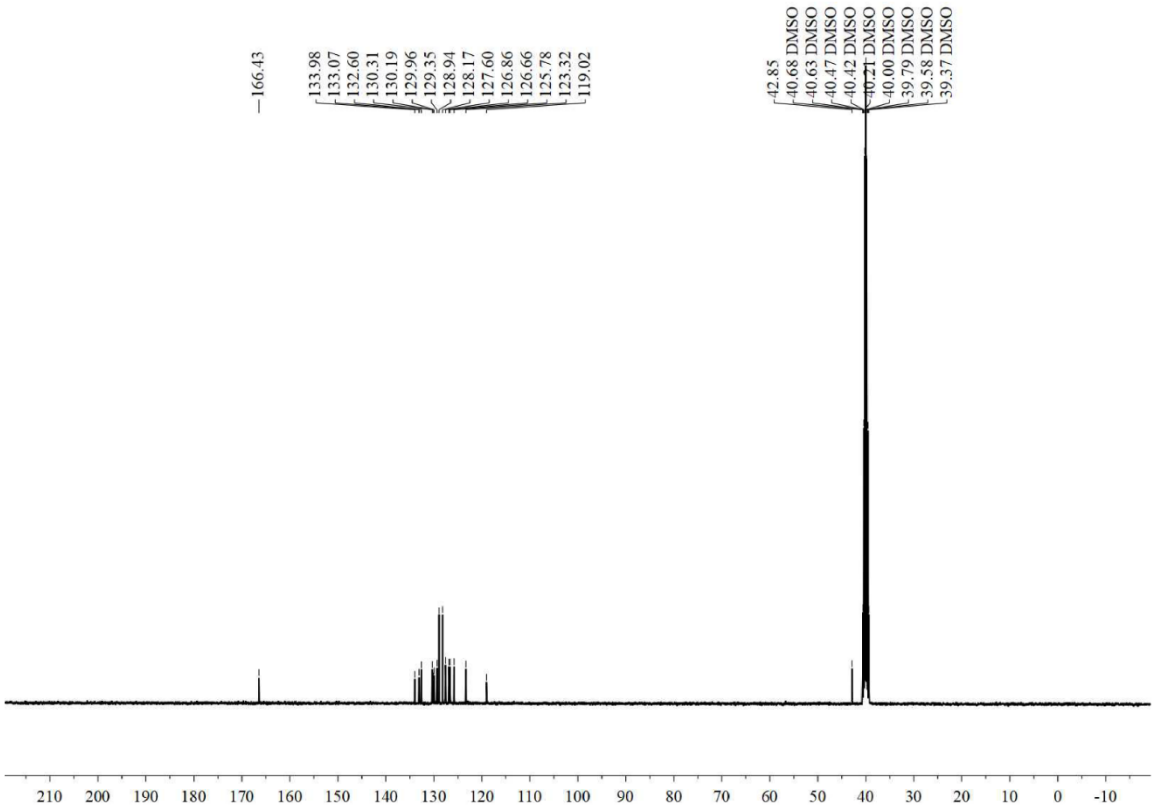

Fig. S-3: ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **7a**.

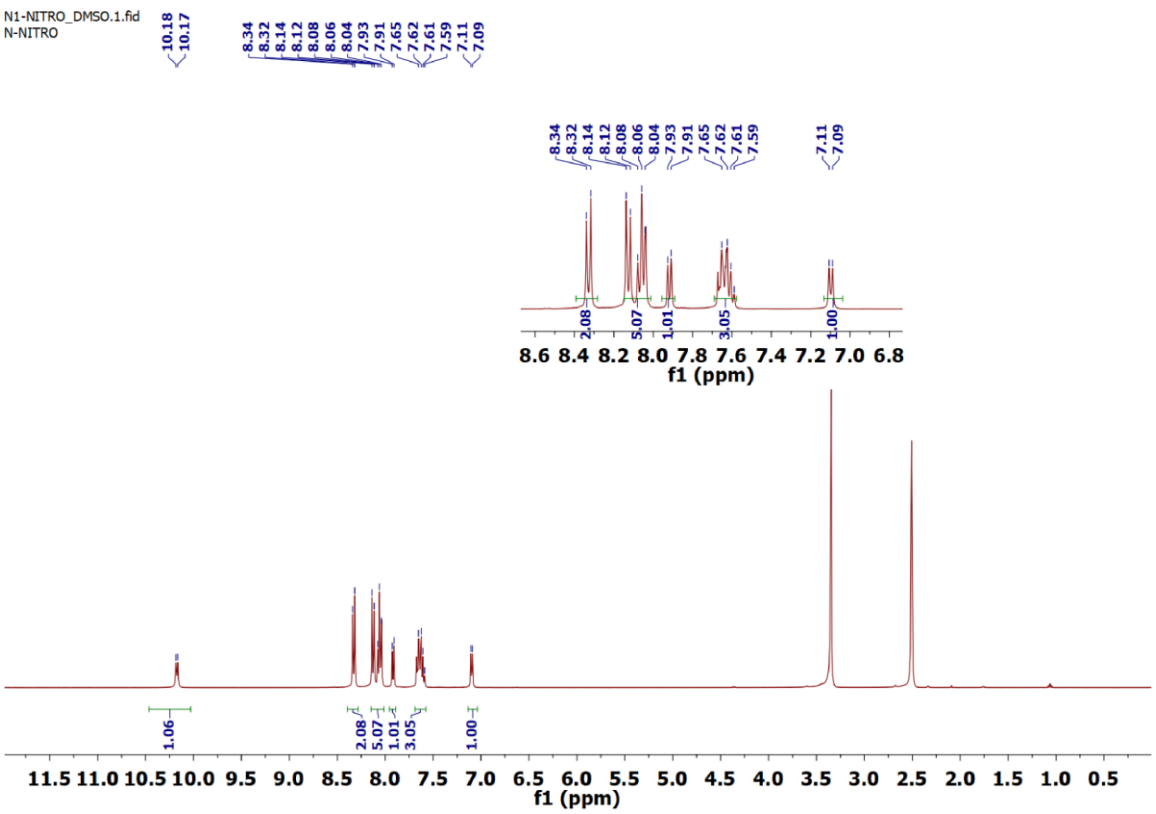

Fig. S-4: ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **7b**.

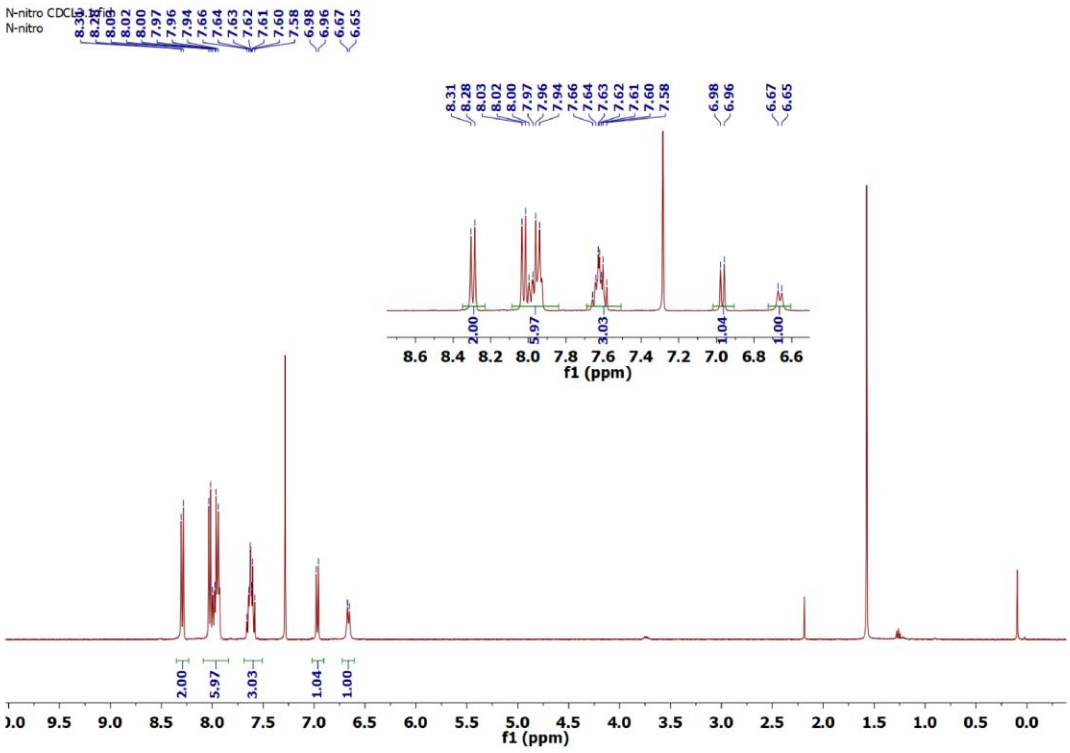

Fig. S-5: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7b**.

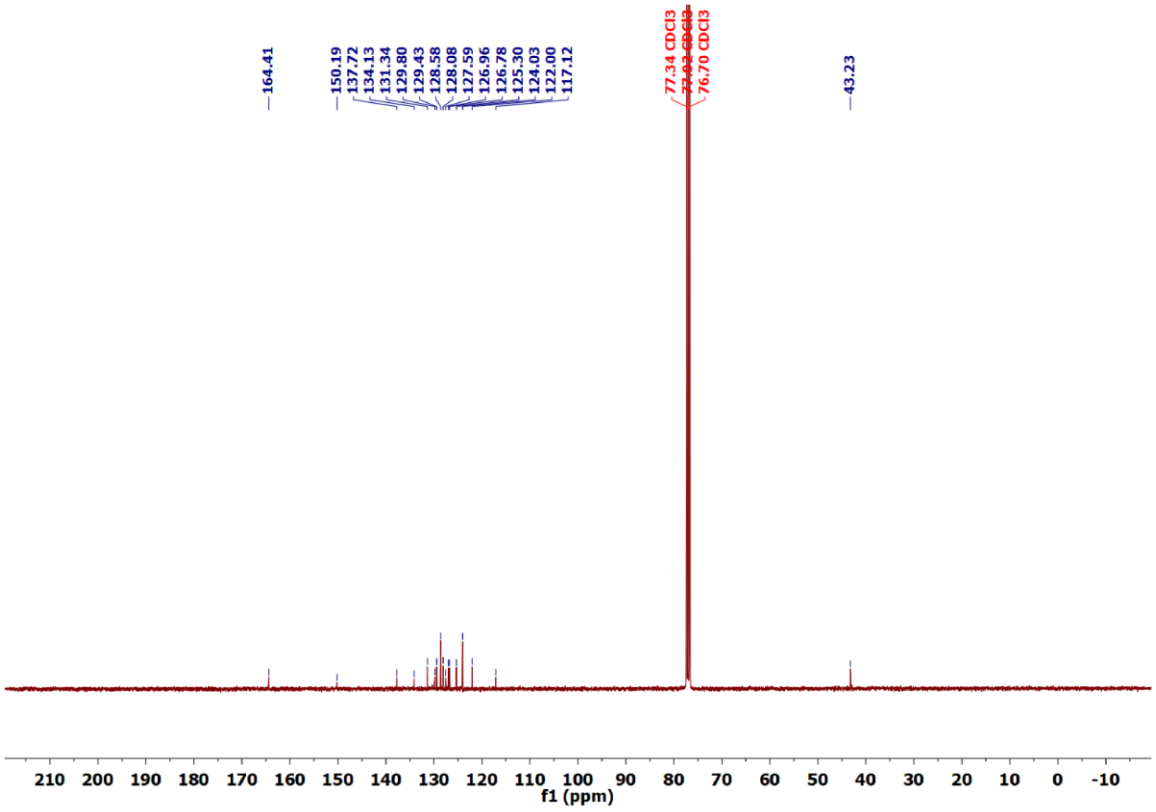

Fig. S-6: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7b**.

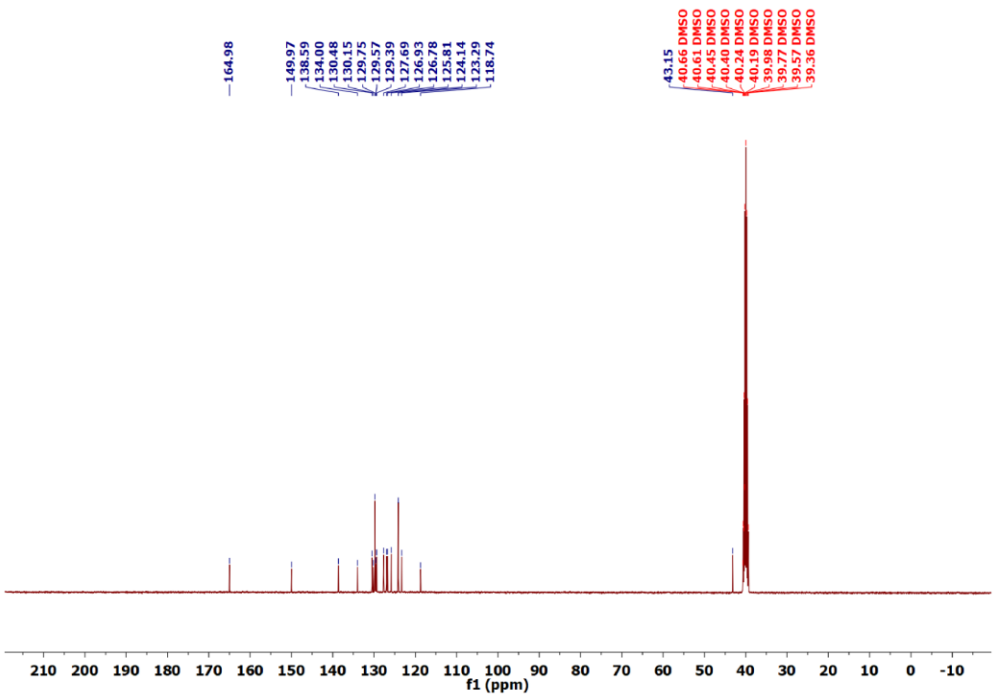

Fig. S-7: ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **7b**.

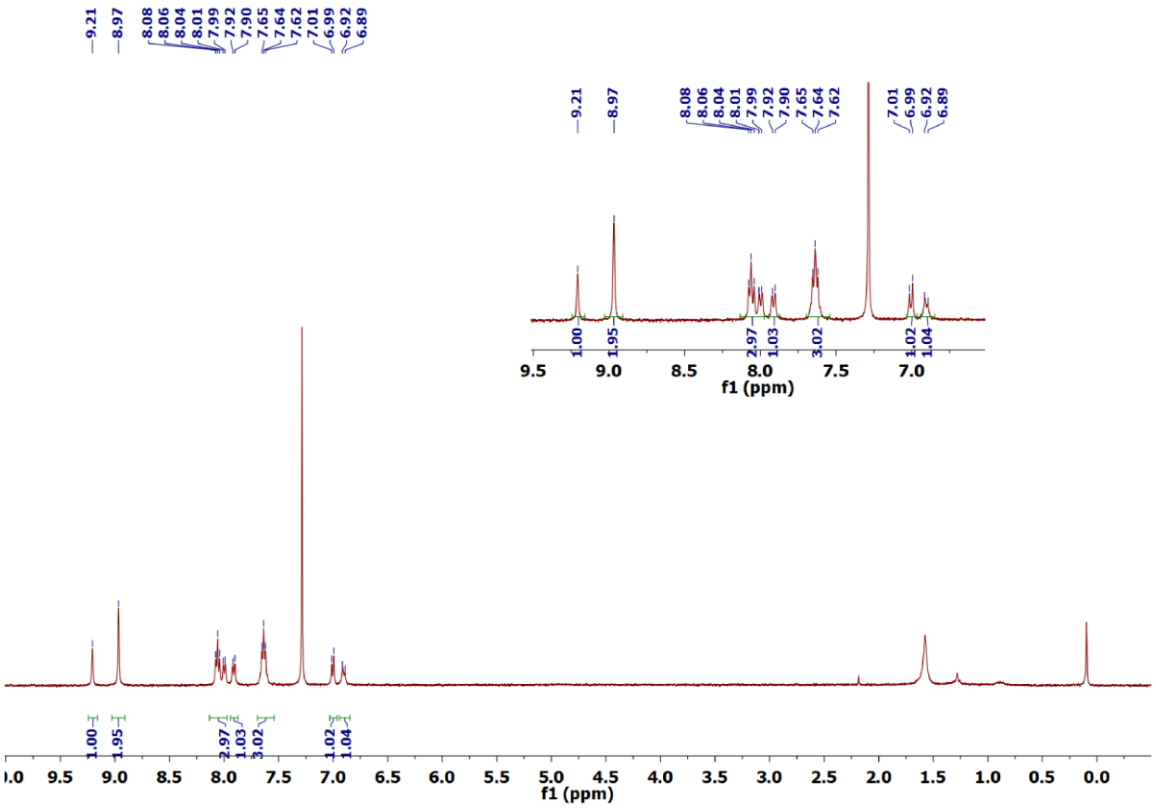

Fig. S-8: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **7c**.

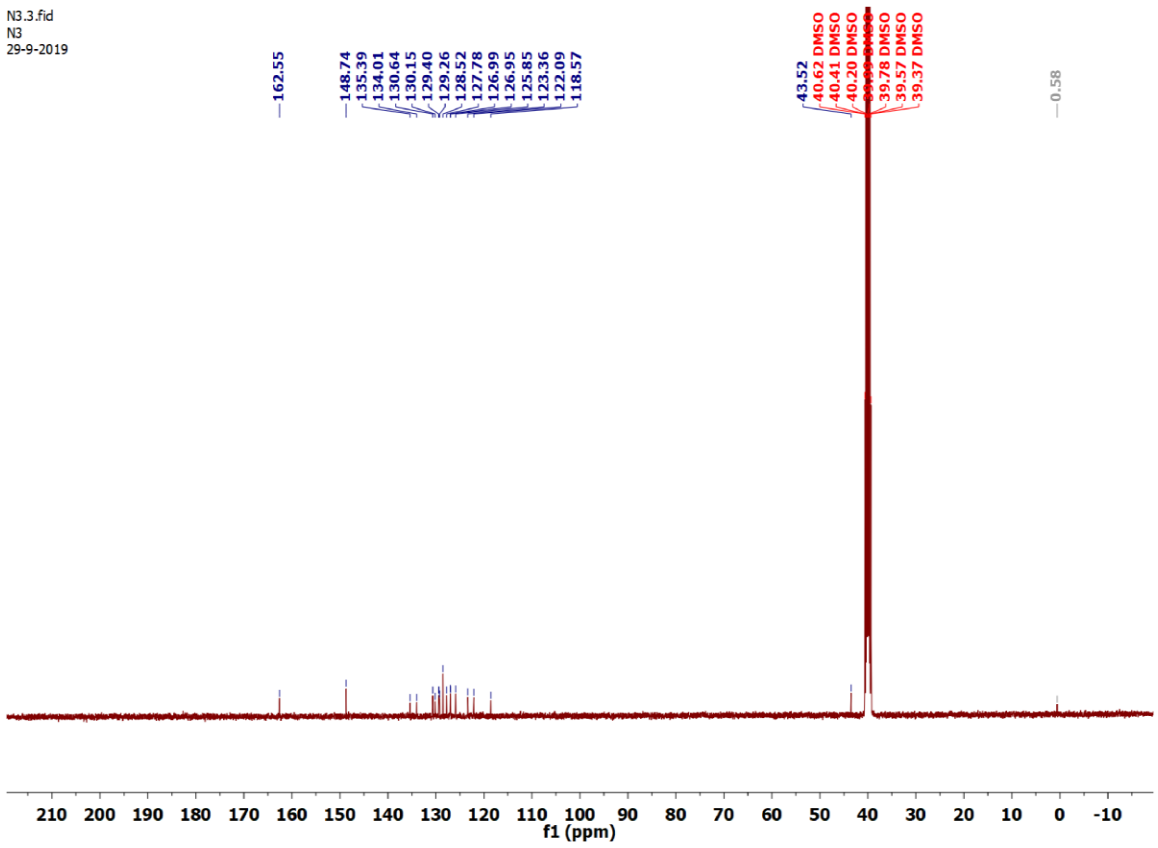

Fig. S-9: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **7c**.

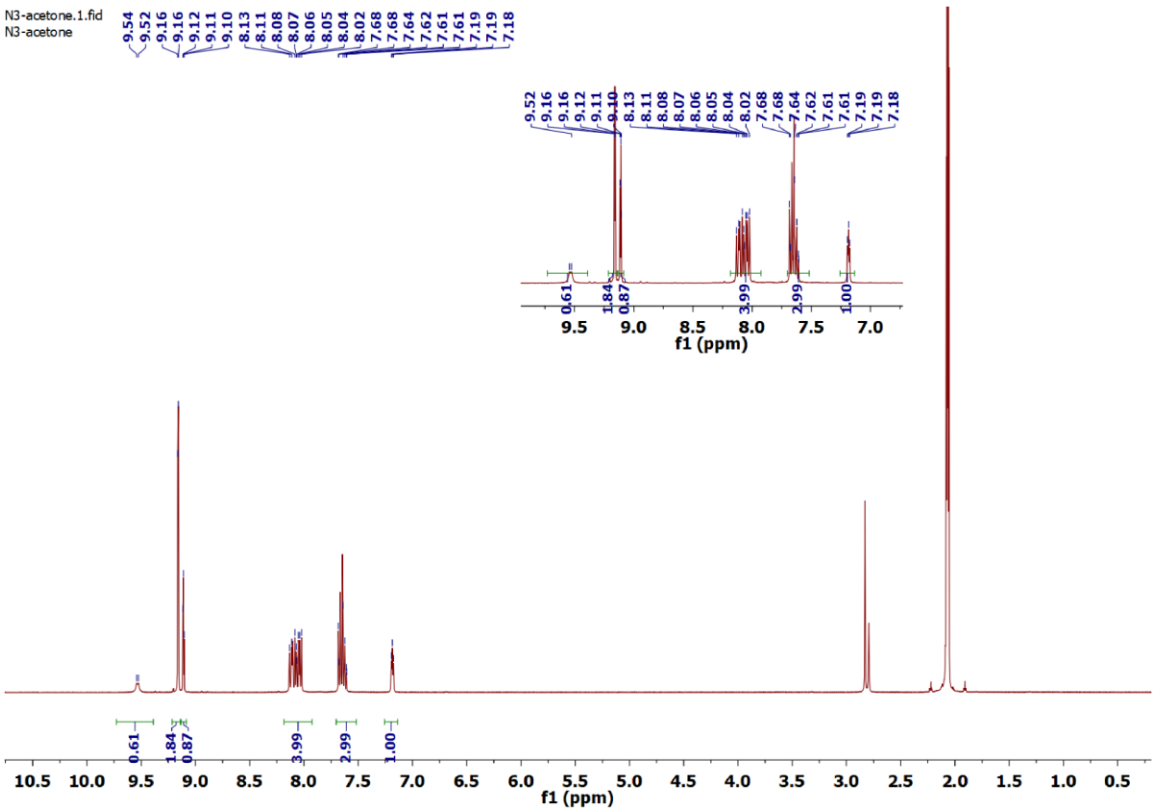

Fig. S-10: ^{1}H NMR (400 MHz, acetone-d_6) spectrum of compound **7c**.

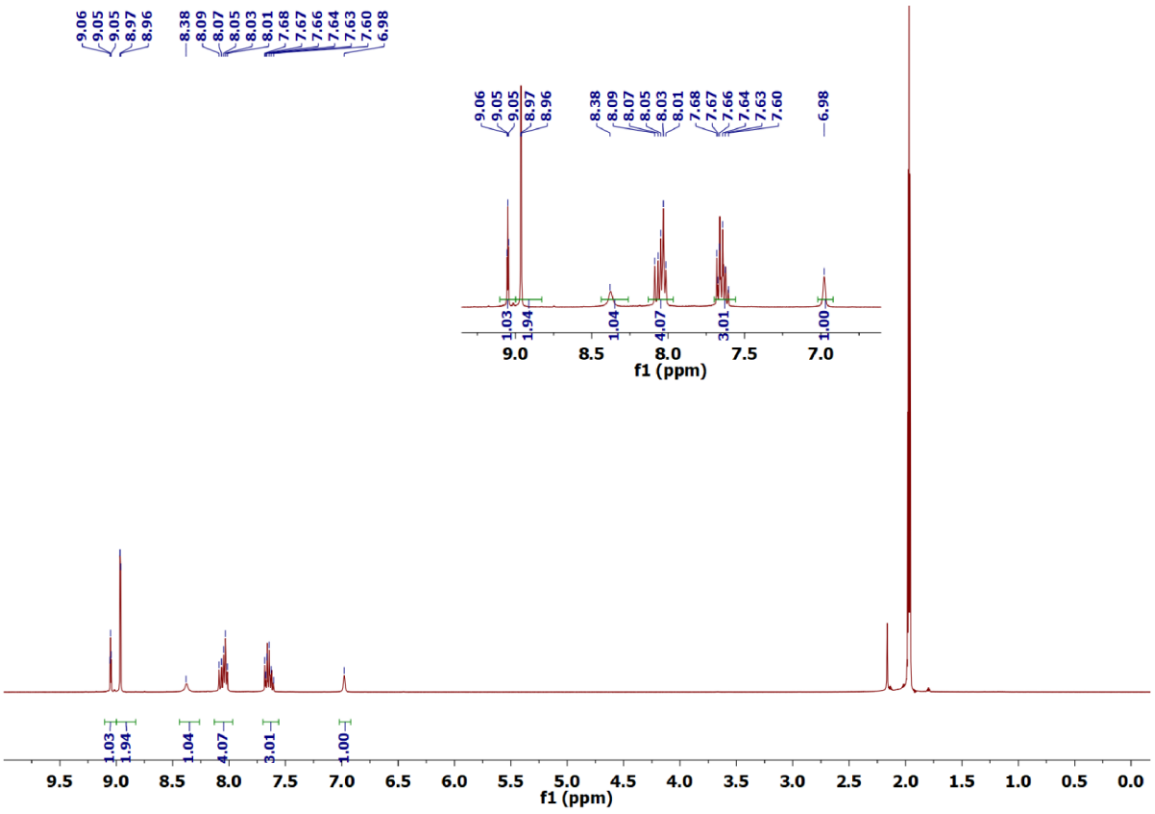

Fig. S-11: ^{1}H NMR (400 MHz, acetonitrile-d_3) spectrum of compound **7c**.

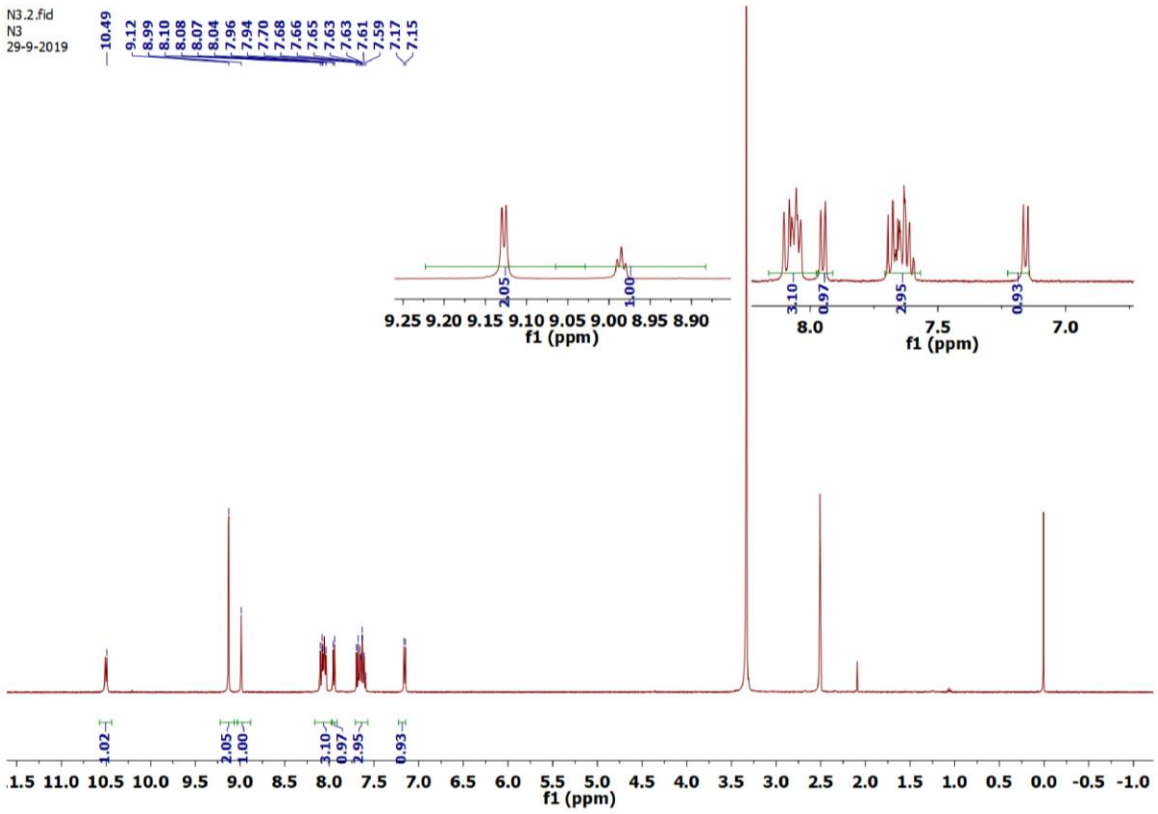

Fig. S-12: ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **7c**.

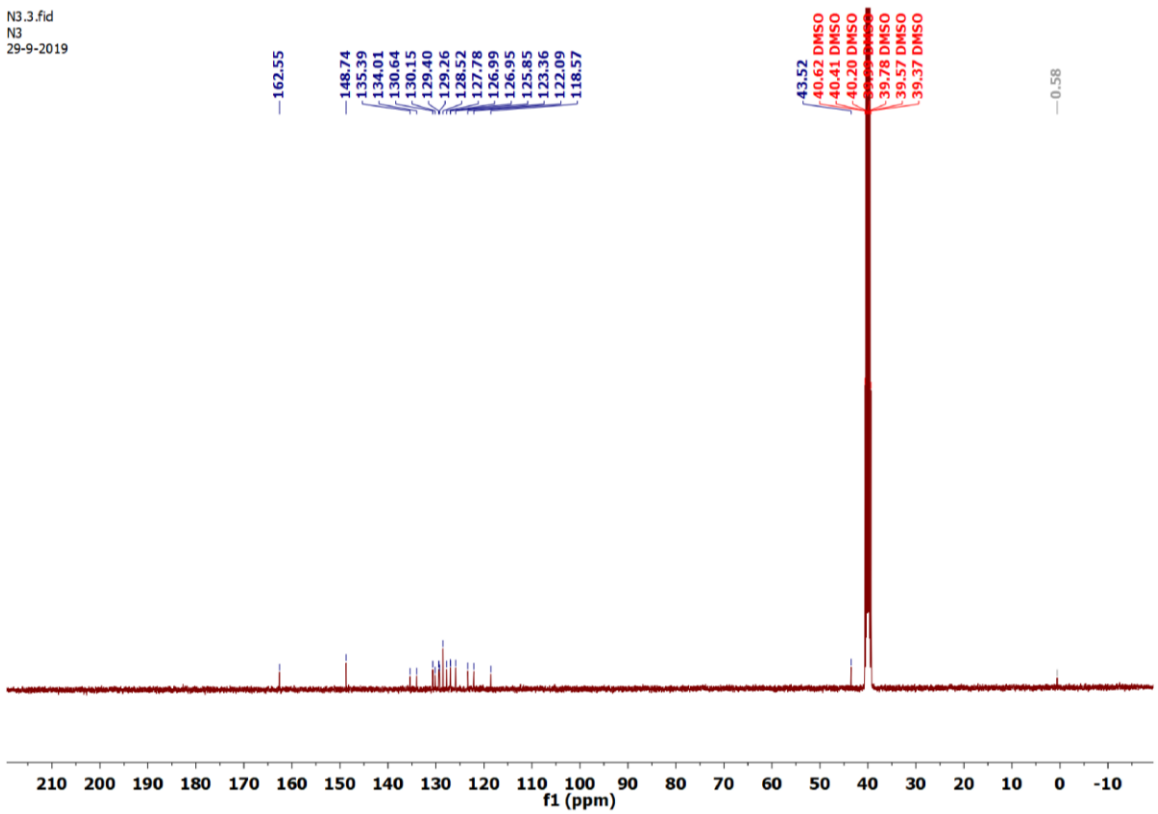

Fig. S-13: ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **7c**.

3. Detaild NMR Results for Titrations of Compounds 7a-c with TBAF

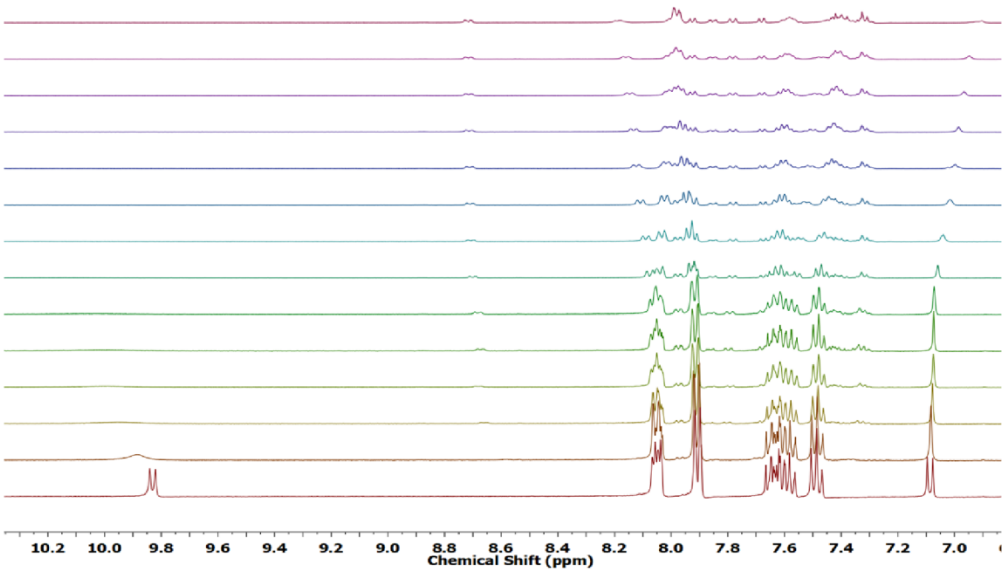

Fig. S-14: ^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 5.2 molar equiv, bottom to top) to **7a** (2.10 x 10^{-2}M) in DMSO-d_6. 0.4 molar equiv of TBAF was added in each step.

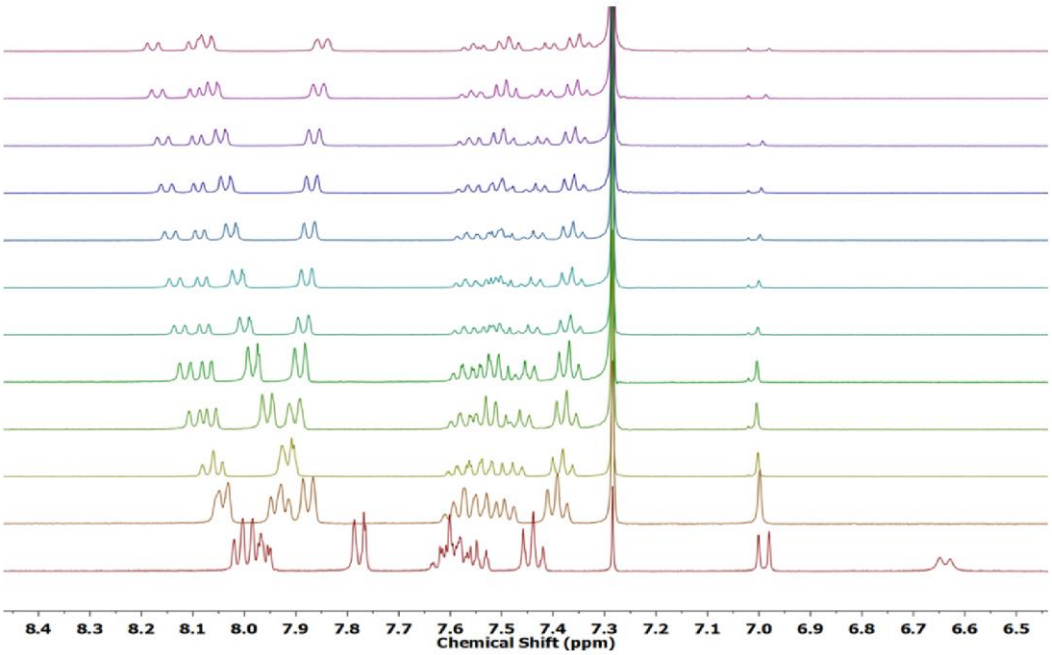

Fig. S-15: ^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 4.4 molar equiv, bottom to top) to **7a** (2.04 x 10^{-2} M) in $CDCl_3$. 0.4 molar equiv of TBAF was added in each step.

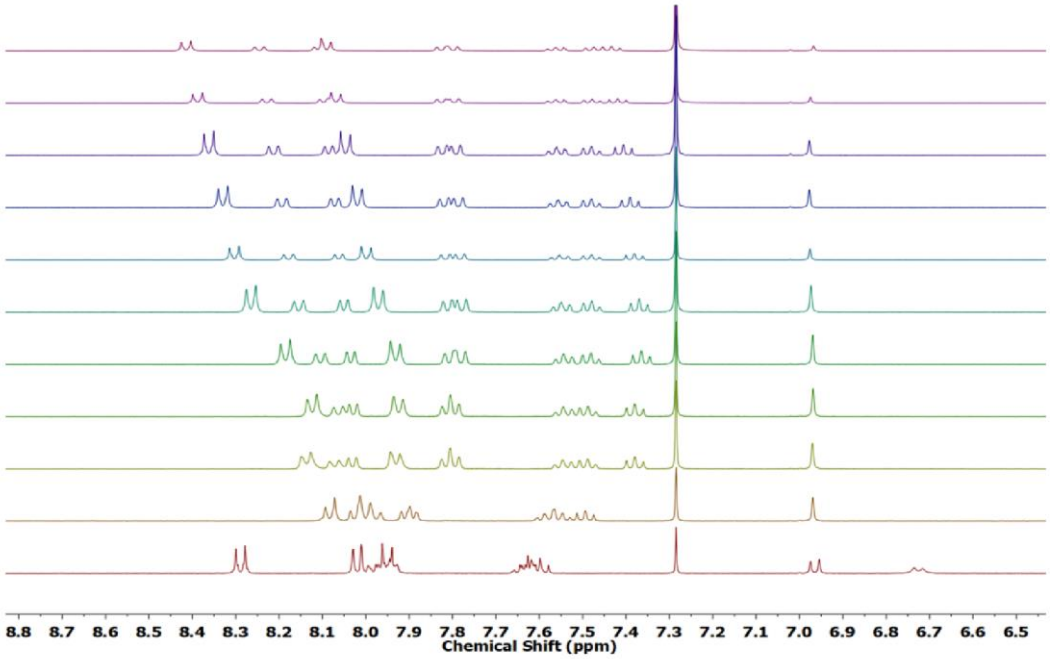

Fig. S-16: ^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 4.0 molar equiv, bottom to top) to **7b** (1.40 x 10^{-2} M) in $CDCl_3$. 0.4 molar equiv of TBAF was added in each step.

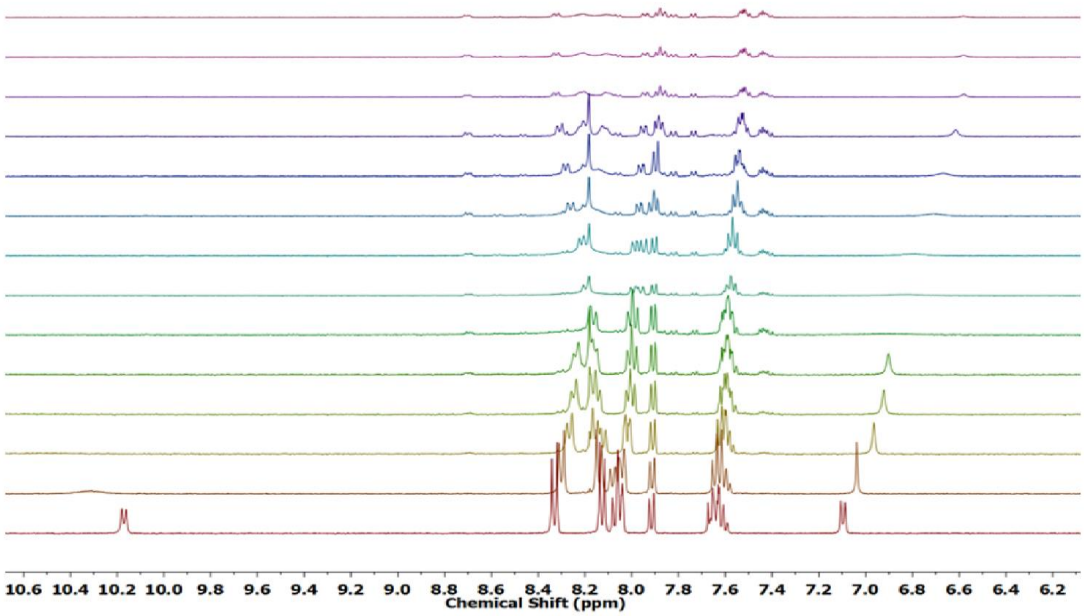

Fig. S-17: ^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 4.4 molar equiv, bottom to top) to **7b** (1.71 x 10^{-2} M) in DMSO-d6. 0.4 molar equiv of TBAF was added in each step.

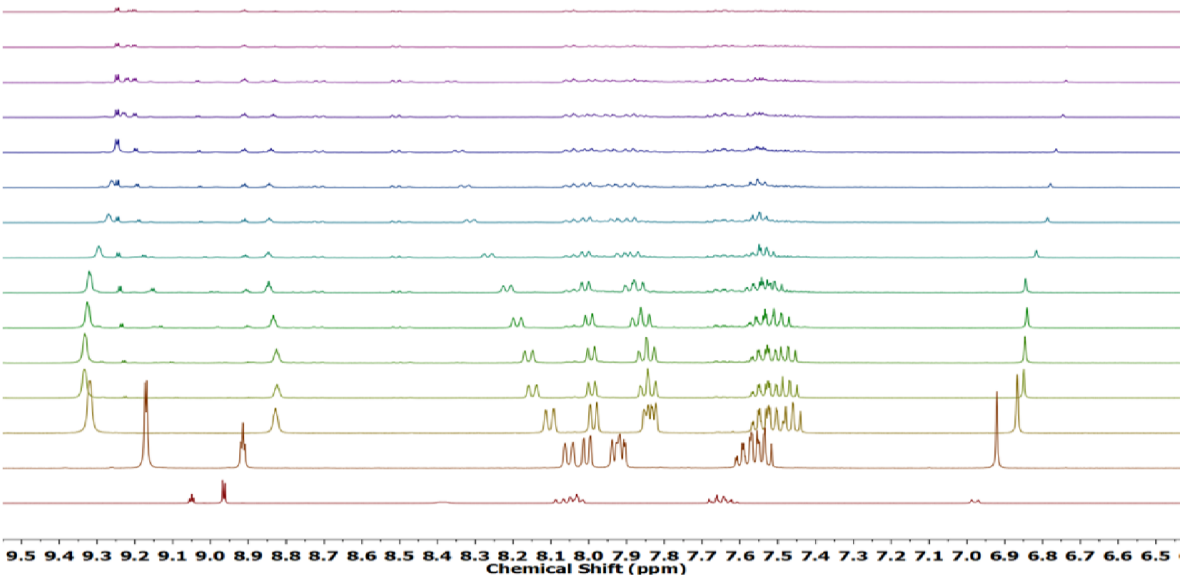

Fig. S-18: ^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 4.0 molar equiv, bottom to top) to **7c** (2.21 x 10^{-2} M) in acetonitrile-d_3. 0.4 molar equiv of TBAF was added in each step.

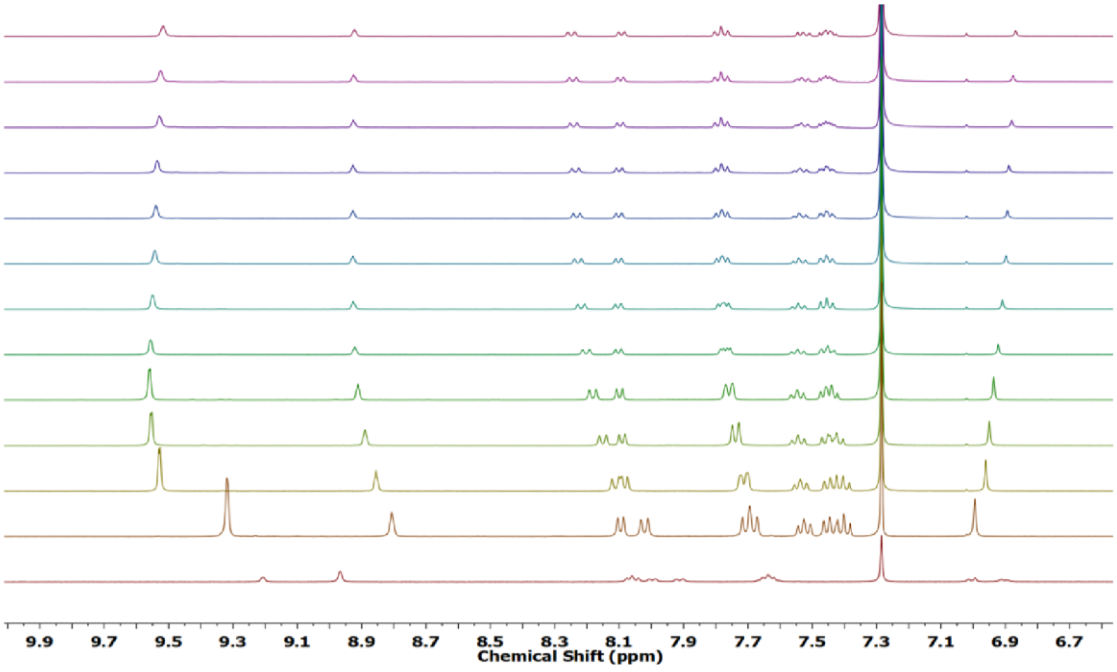

Fig. S-19:^{1}H NMR (400 MHz) spectra monitoring the titration TBAF (0 to 3.6 molar equiv, bottom to top) to **7c** (2.21 x 10^{-2} M) in $CDCl_3$. 0.4 molar equiv of TBAF was added in each step.

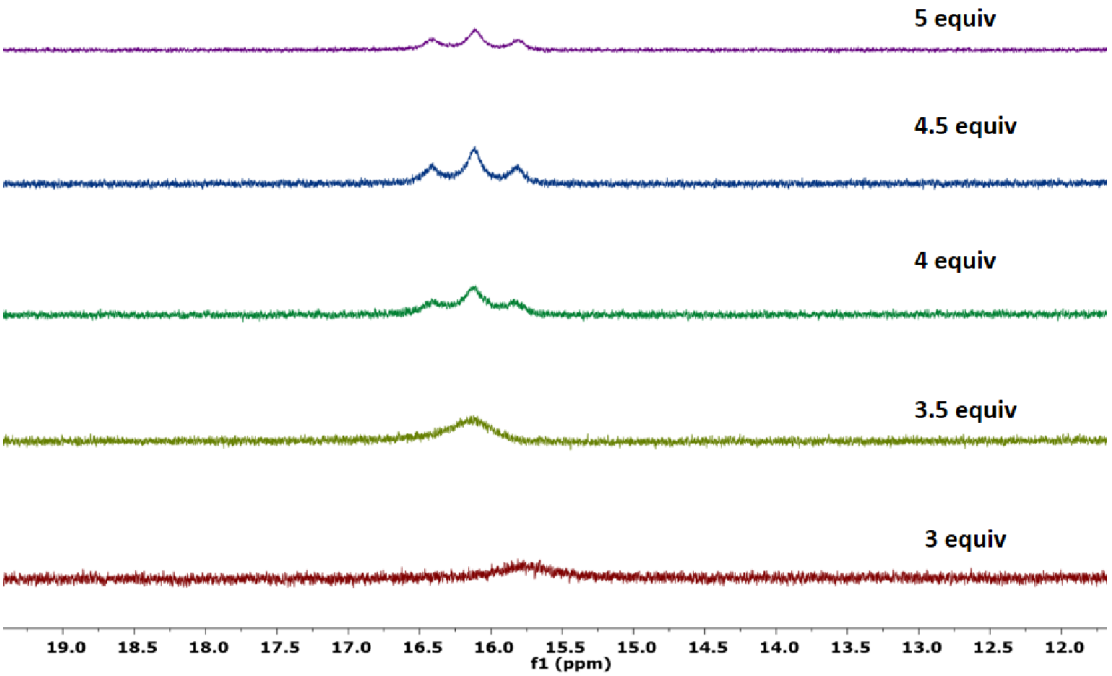

Fig. S-20:Stack plot of ^{1}H NMR (400 MHz) spectra monitoring the titration of TBAF (3 to 5 molar equiv, bottom to top) to **7c** (2.21 $\times 10^{-2}$ M) in DMSO-d_6.

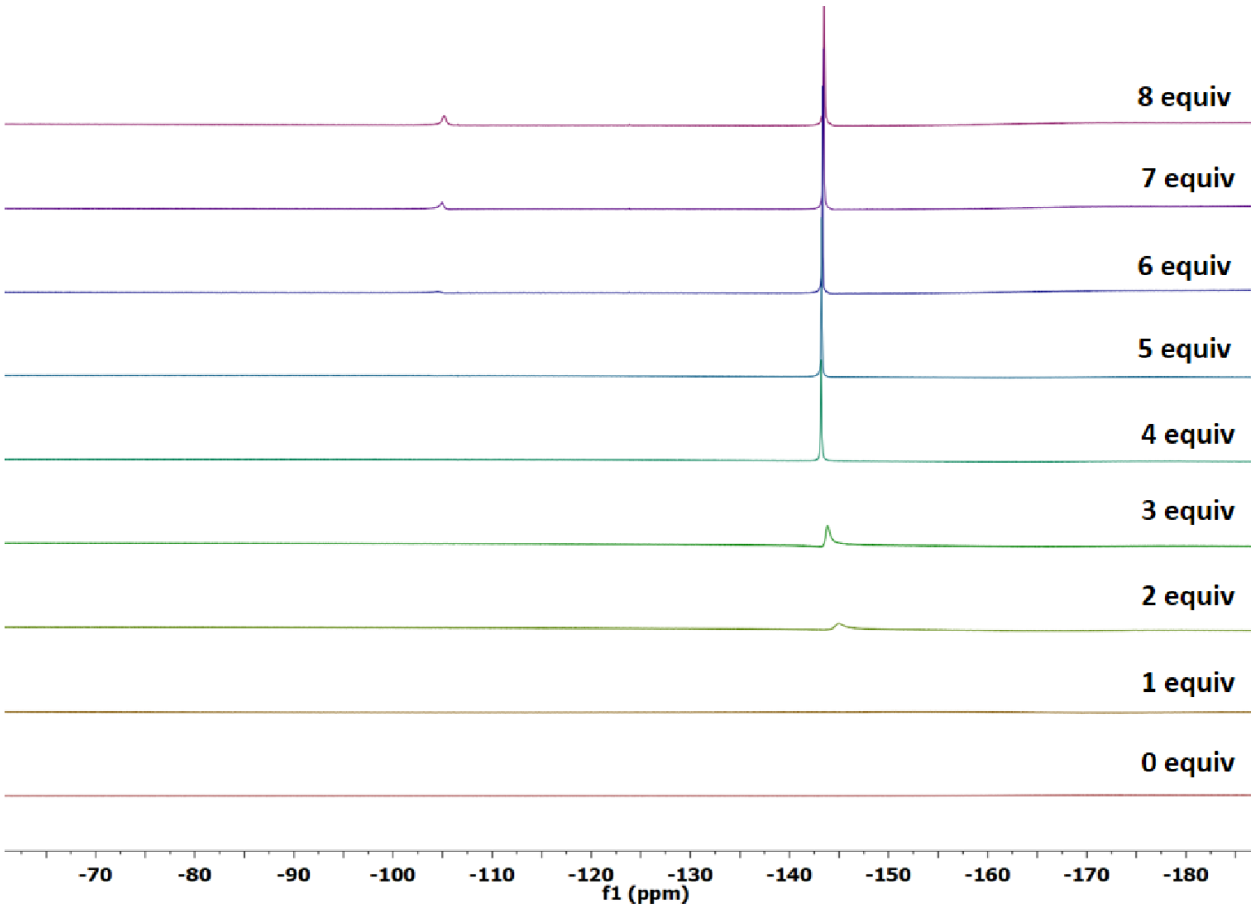

Fig. S-21:Stack plot of ^{19}F NMR (376 MHz) spectra monitoring the titration of TBAF (0 to 8 molar equiv, bottom to top) to **7c** (2.21 $\times 10^{-2}$ M) in DMSO-d_6.

4. UV-Vis Spectral Data for Compounds 7a-c

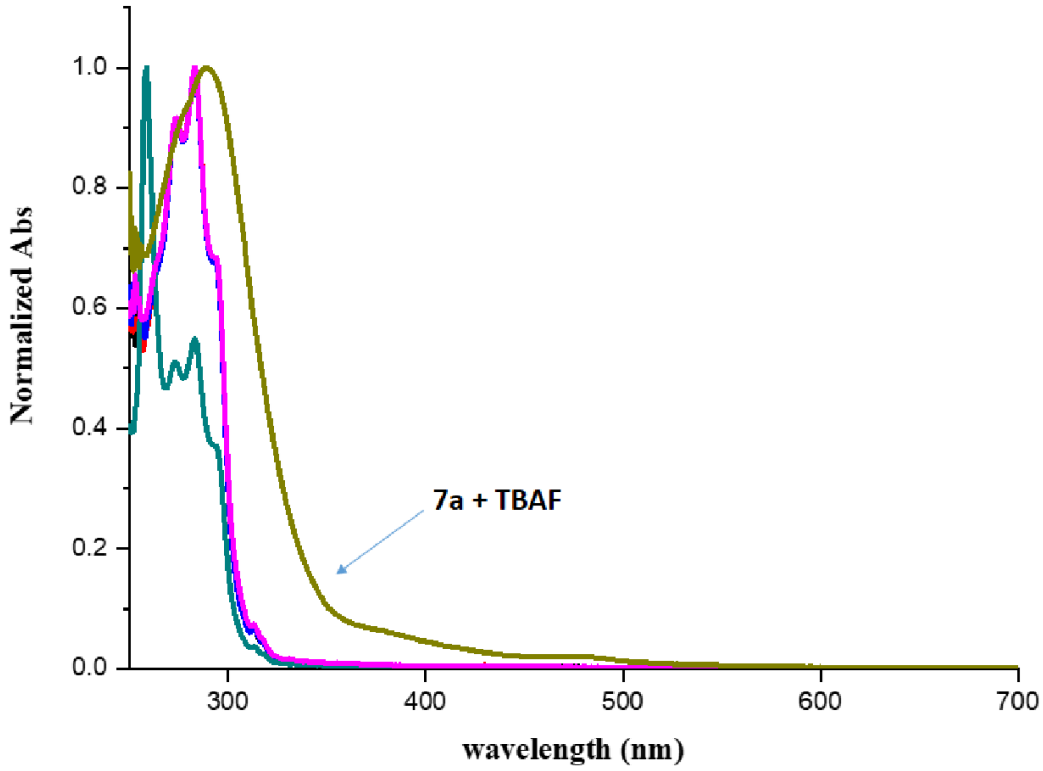

Fig. S-22: Normalized absorption spectra of **7a** (1.3×10^{-5} M) in DMSO upon addition of 50 molar equivalents of tetrabutylammonium salts of F^-, Cl^-, ,Br^-, I^-, and ClO_4^-, respectively.

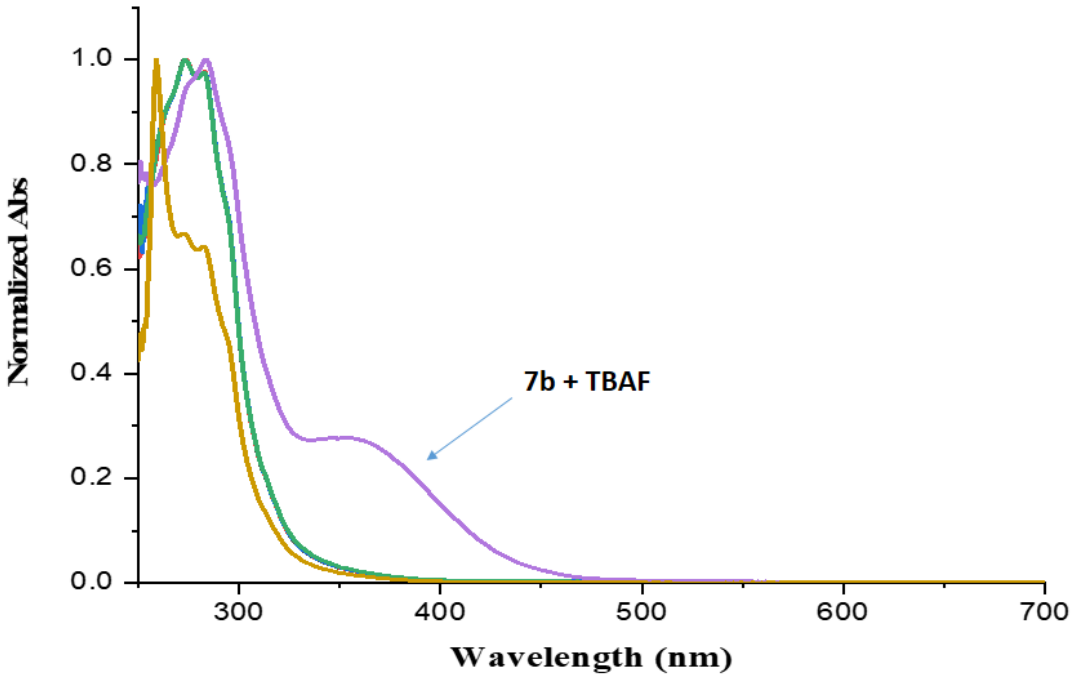

Fig. S-23: Normalized absorption spectra of **7b** (1.3×10^{-5} M) in DMSO upon addition of 50 molar equivalents of tetrabutylammonium salts of F^-, Cl^-, ,Br^-, I^-, and ClO_4^-, respectively.

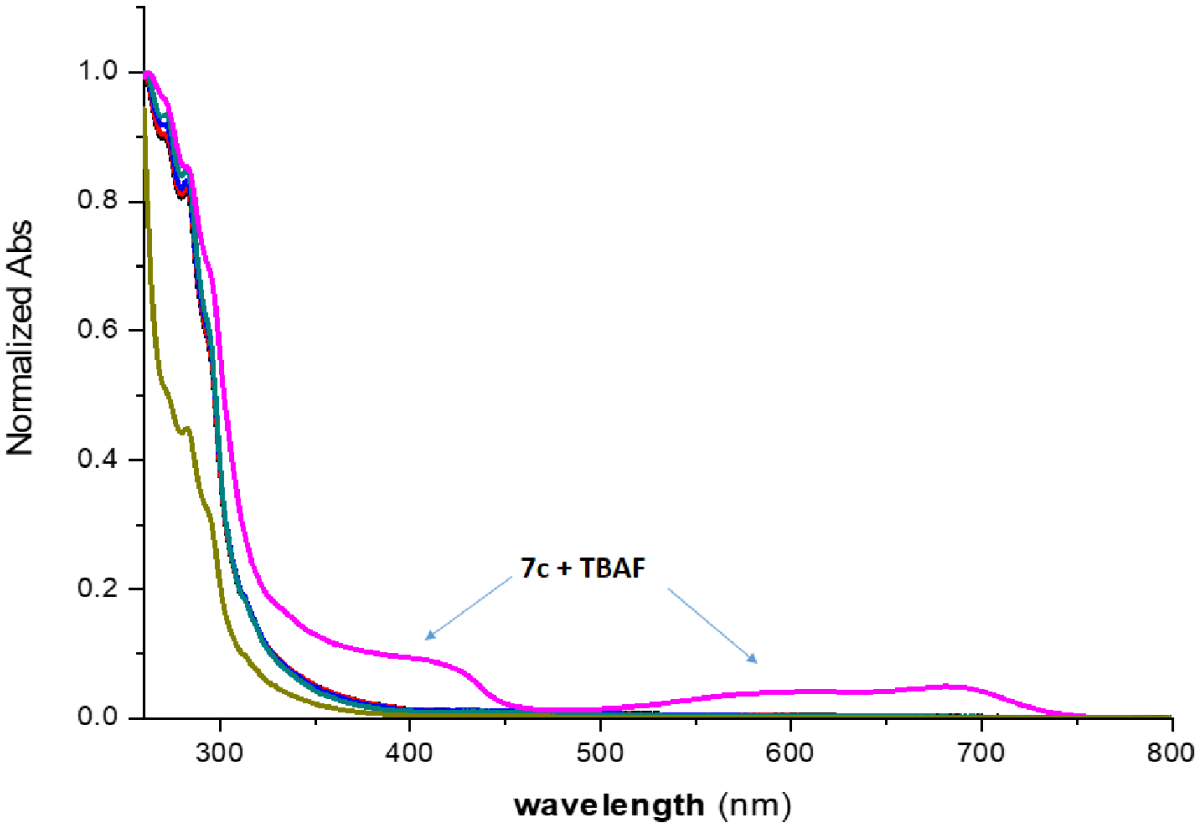

Fig. S-24: Normalized absorption spectra of **7c** (1.3×10^{-5} M) in DMSO upon addition of upon addition of 50 molar equivalents of tetrabutylammonium salts of F^-, Cl^-, ,Br^-, I^-, and ClO_4^-, respectively.

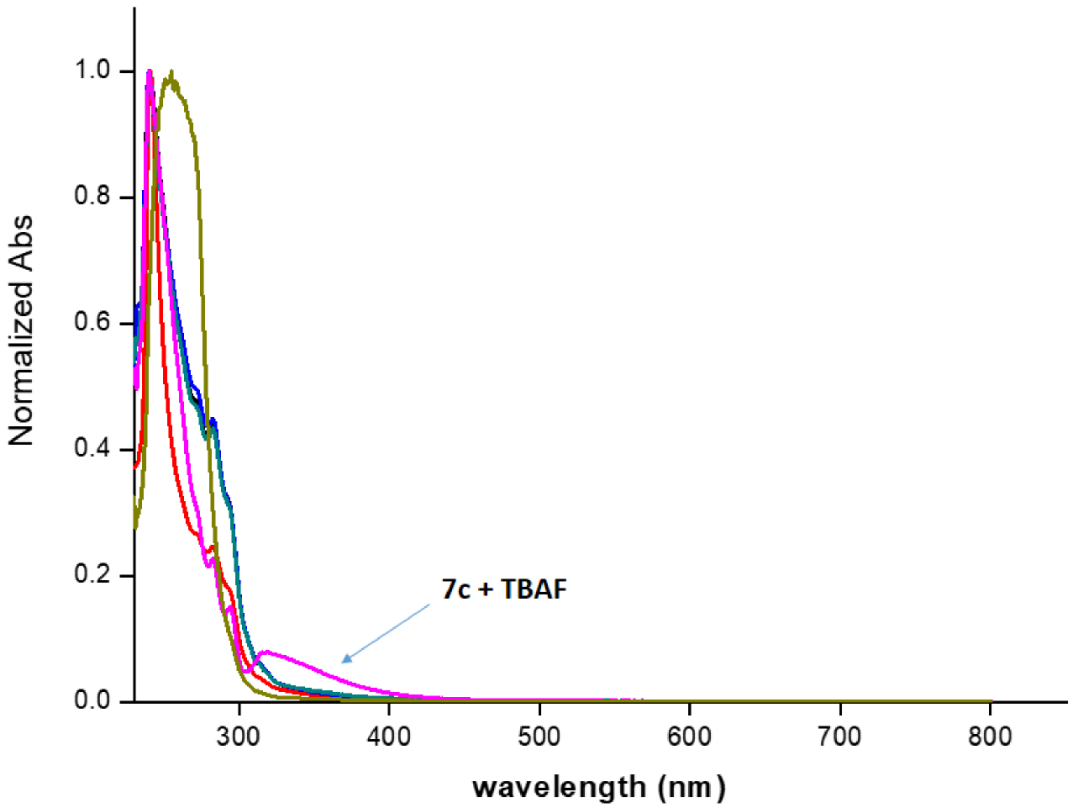

Fig. S-25: Normalized absorption spectra of **7c** (1.3×10^{-5} M) in $CHCl_3$ upon addition of upon addition of 50 molar equivalents of tetrabutylammonium salts of F^- , Cl^- , ,Br^- , I^- , and ClO_4^-, respectively.

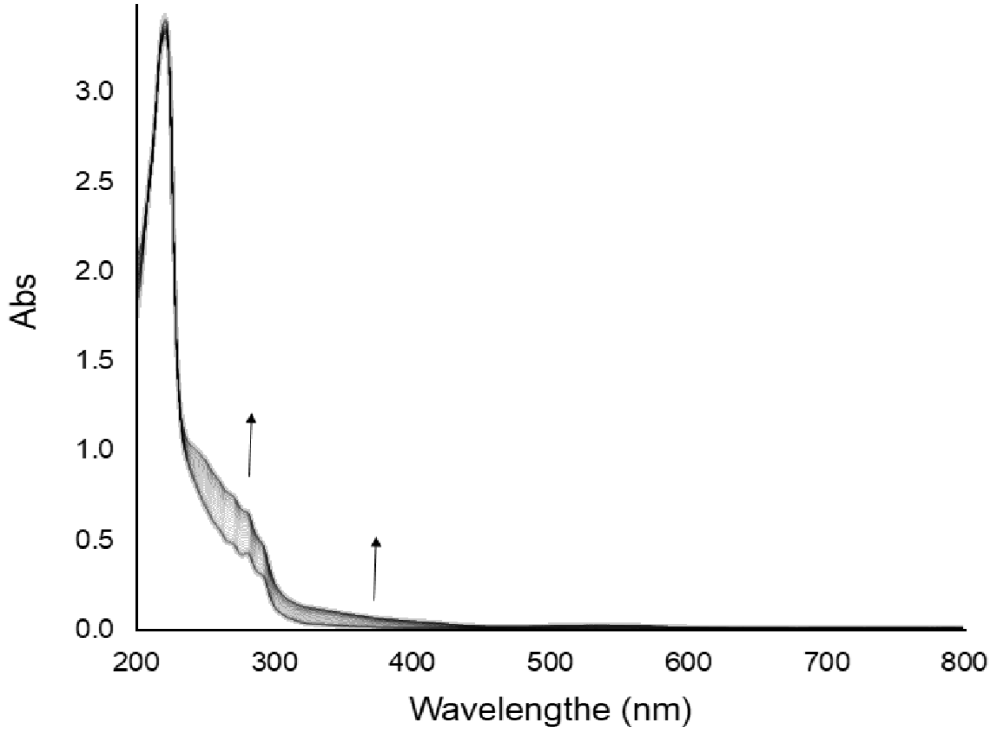

Fig. S-26: UV-Vis absorption spectra monitoring the titration of TBAF (0 to 12 molar equivalents) to **7c** (3.9×10^{-6} M) in CH_3CN.

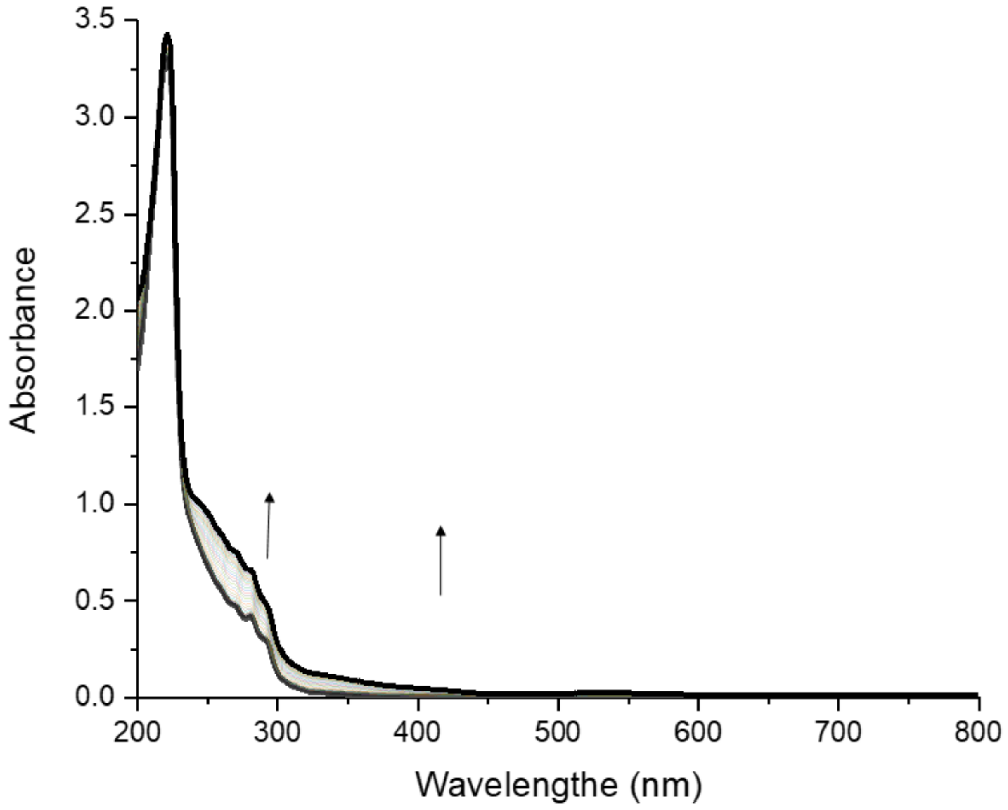

Fig. S-27: UV-Vis absorption spectra monitoring the titration of TBAF (0 to 12 molar equivalents) to **7c** (3.9×10^{-6} M) in $CHCl_3$.

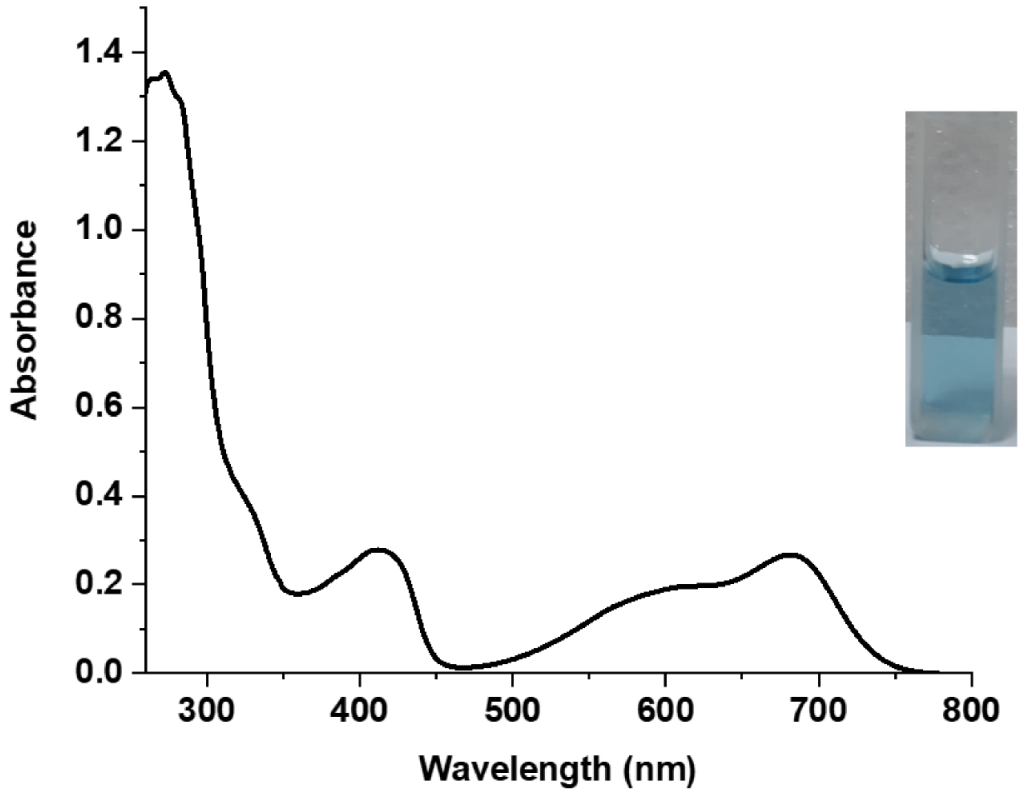

Fig. S-28: Absorption spectra of **7c** (8.2×10^{-5} M) in DMSO upon addition of a mixture of anions (F^-, Cl^-, ,Br^-, I^-, and ClO_4^-).

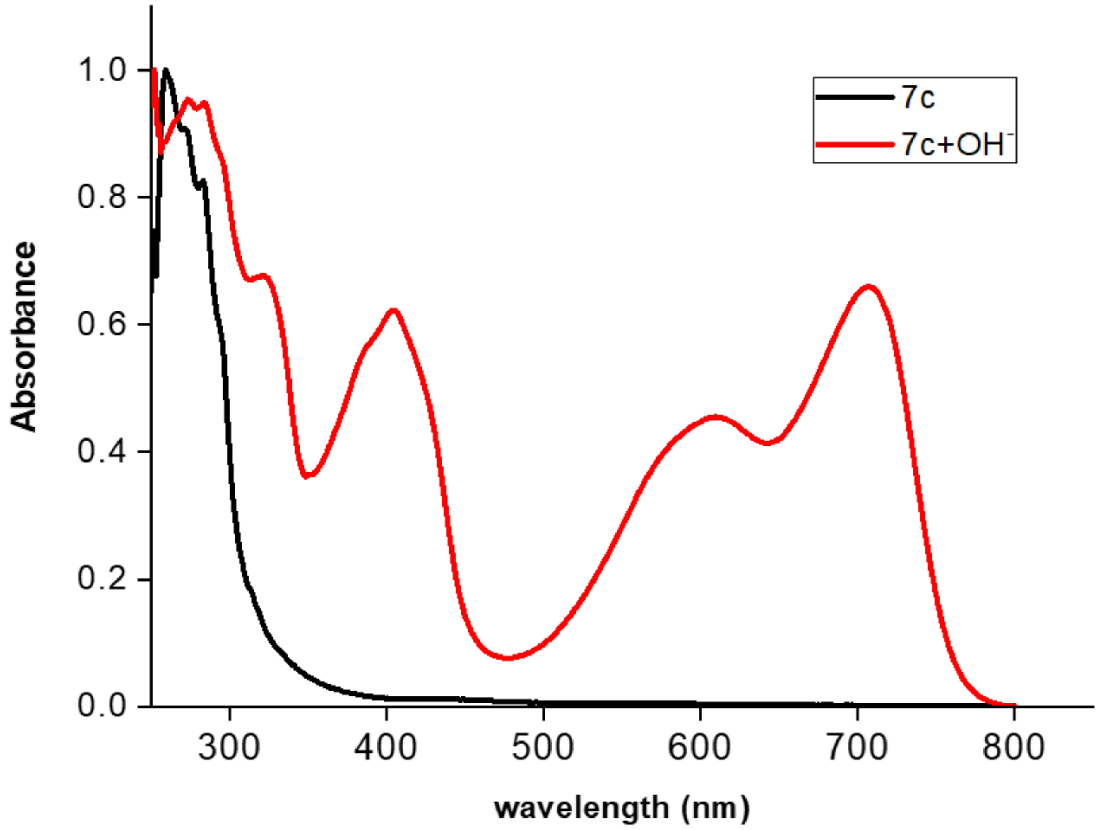

Fig. S-29: UV-Vis absorption spectra of **7c** (6.3×10^{-5} M) in DMSO upon addition 50 molar equivalents of OH^- anion (KOH).

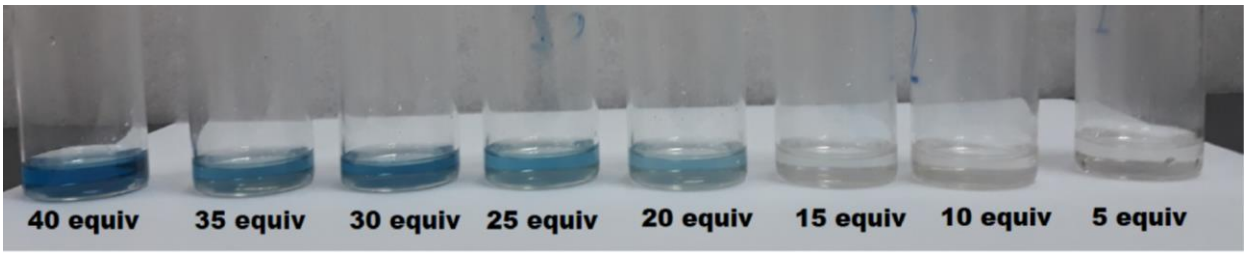

Fig. S-30: Photograph of **7c** (8.2×10^{-5} M) in DMSO upon addition of different molar equivalents of TBAF. Visual LoD is determined to be 1.6×10^{-3} M.

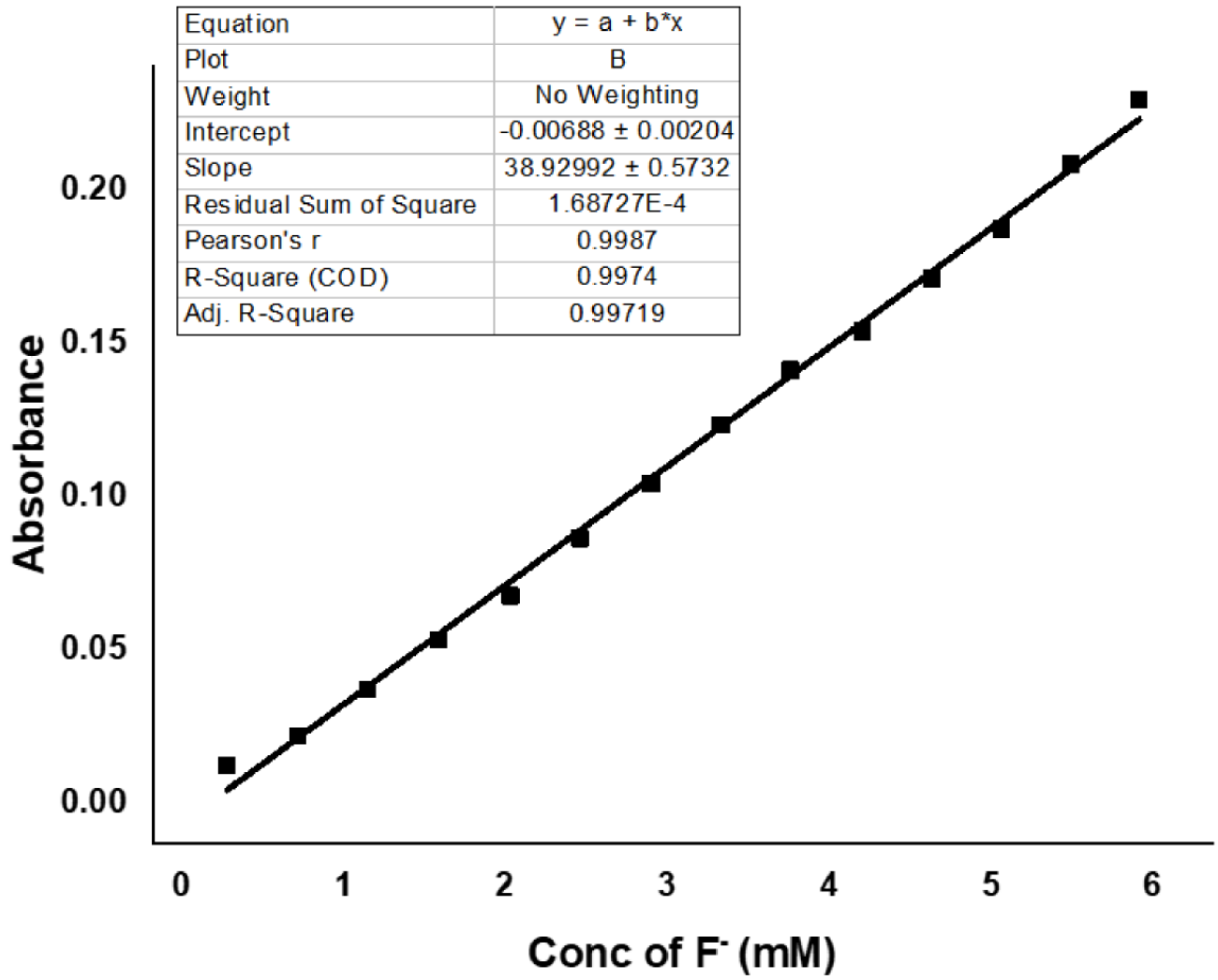

Fig. S-31: Standard calibration curve demonstrating the absorbance increment of **7c** (8.2×10^{-5} M) at 680 nm as a function of the concentration of fluoride anion in DMSO.

The limit of detection (LoD) of compound **7c** to fluoride anion was determined using the (3σ/m) equation. Where σ is defined as the standard deviation of blank samples (number of samples is 20) and m is the slope of the calibration curve. According to the linear plot in Fig. S-31 (R_2 = 0.9974, m = 38.93), the (LoD) of **7c** was determined to be 0.177 mM.

5. Detailed Results of DFT and TD-DFT Calculations

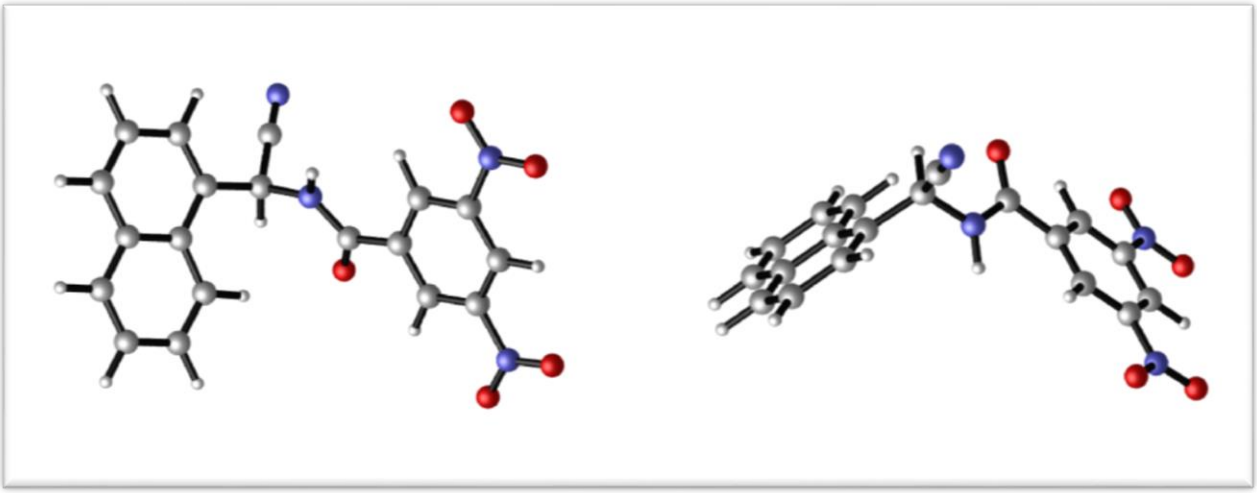

Fig. S-32: Optimized structure of compound **7c** viewed from two different perspectives. Calculations done in the gas phase at the B3LYP/6-31+G(d, p) level of theory.

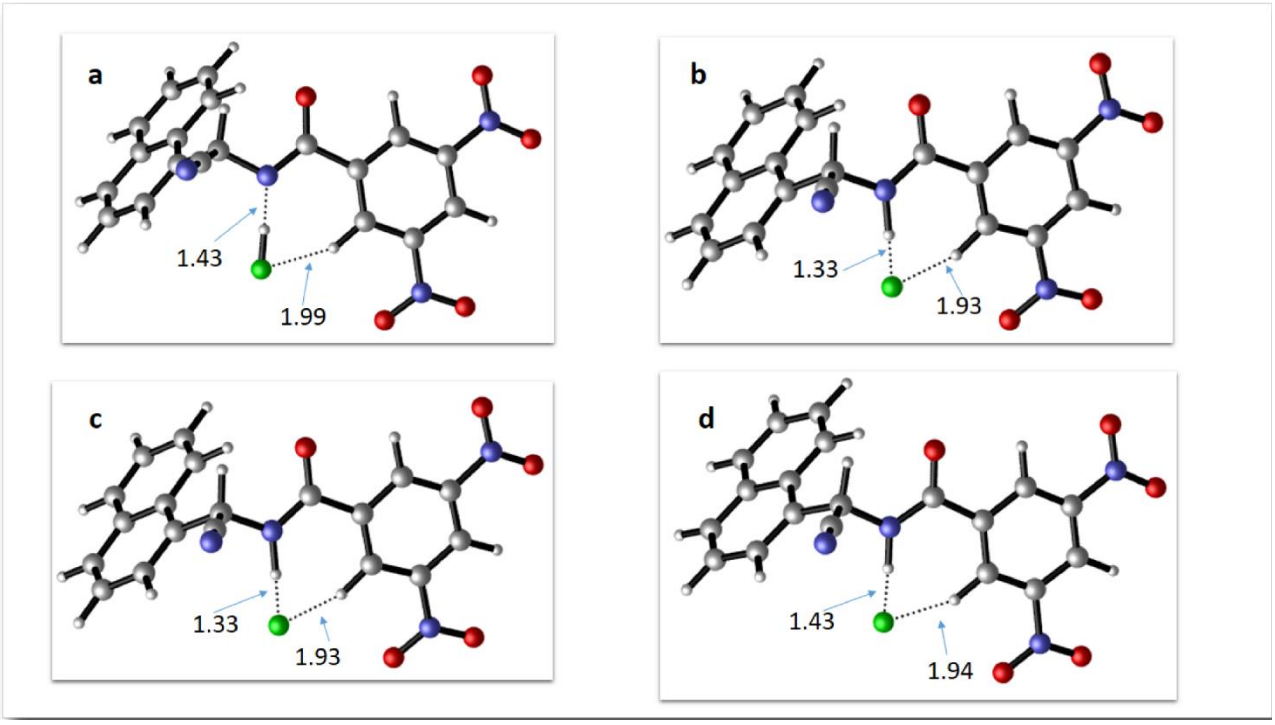

Fig. S-33: Optimized structures of compounds [**7c** + F]$^-$. Calculations done (a) in the gas phase, (b) in $CHCl_3$ (c) in CH_3CN, and (d) in DMSO at the B3LYP/6-31+G(d, p) level of theory.

Cartesian coordinates of optimized **7c** in DMSO

E(RB3LYP) = - 1326.2765 Hartrees; dipole Moment = 7.619254 Debye; basis set = 6-31+G(d, p)

O	0.14947	0.73051	2.34440
O	2.96686	-3.27669	-1.55071
O	4.83817	-2.26715	-2.02258
O	5.69563	2.15374	-0.26636
O	4.19567	3.14488	0.96287
N	-2.24852	-2.90219	3.03250
N	-0.71116	-0.75983	0.85491
H	-0.58991	-1.27500	-0.00689
N	3.73223	-2.31414	-1.48382
N	4.59959	2.19398	0.29341
C	-3.14723	-0.68914	0.41596
C	-3.43252	0.58435	-0.18303
C	-2.75916	1.78947	0.16770
H	-1.98024	1.78210	0.92231
C	-3.07885	2.98642	-0.44077
H	-2.55218	3.89172	-0.15426
C	-4.08592	3.04514	-1.43438
H	-4.32639	3.99354	-1.90498
C	-4.75711	1.89799	-1.79884
H	-5.53272	1.93164	-2.55911
C	-4.45359	0.64757	-1.19206
C	-5.14635	-0.53734	-1.56734
H	-5.91659	-0.47333	-2.33097
C	-4.84910	-1.74248	-0.97474
H	-5.37910	-2.64488	-1.26205
C	-3.84347	-1.81415	0.01981
H	-3.62719	-2.77534	0.47567
C	-2.04269	-0.78509	1.46524
H	-2.08407	0.07361	2.14324
C	-2.17383	-1.97972	2.33169
C	0.29611	0.00318	1.35955
C	1.62034	-0.05998	0.64171
C	2.03634	-1.16652	-0.10539
H	1.42798	-2.05568	-0.21248
C	3.29369	-1.14056	-0.70838
C	4.15552	-0.05567	-0.60305
H	5.12565	-0.05423	-1.08009
C	3.71224	1.02537	0.15256
C	2.47209	1.04206	0.78273
H	2.16438	1.89340	1.37577

Cartesian coordinates of optimized 1:1 complex of **7c** and fluoride anion in DMSO

E(RB3LYP) = -1426.2945 Hartrees; dipole moment = 7. 11.153395 Debye; basis set = 6-31+G(d, p).

O	0.15631	1.42588	1.90993
O	2.73914	-3.21254	-1.58927
O	4.71631	-2.39144	-1.97778
O	5.98269	1.88205	-0.16349
O	4.55234	3.04001	0.99936
N	-2.20919	-1.87967	3.70434
N	-0.69338	-0.48502	0.98638
H	-0.58592	-1.41247	0.42374
N	3.58789	-2.32736	-1.48311
N	4.87209	2.04495	0.34655
C	-3.15943	-0.38347	0.63929
C	-3.41552	0.69849	-0.26972
C	-2.65076	1.90068	-0.29615
H	-1.82178	2.03503	0.39003
C	-2.94318	2.91146	-1.18957
H	-2.34549	3.81823	-1.18881
C	-4.01340	2.77778	-2.10735
H	-4.23137	3.58066	-2.80516
C	-4.77439	1.62879	-2.10921
H	-5.59945	1.51588	-2.80749
C	-4.50179	0.56720	-1.20173
C	-5.29014	-0.61729	-1.20088
H	-6.10871	-0.70276	-1.91037
C	-5.02233	-1.63529	-0.31551
H	-5.62483	-2.53826	-0.31474
C	-3.95229	-1.51324	0.60448
H	-3.75954	-2.33124	1.29151
C	-1.99393	-0.26636	1.62256
H	-1.97514	0.73975	2.05488
C	-2.13474	-1.18077	2.77939
C	0.29488	0.40416	1.21158
C	1.63868	0.14906	0.55635
C	1.95472	-1.00385	-0.17761
H	1.22045	-1.79759	-0.32989
C	3.23794	-1.11741	-0.71772
C	4.21754	-0.14152	-0.56950
H	5.20180	-0.25566	-1.00090
C	3.86716	0.98637	0.16378
C	2.60510	1.14664	0.72905
H	2.36094	2.03227	1.30017
F	-0.51021	-2.66383	-0.25793

Cartesian coordinates of optimized deprotonated **7c** in DMSO

E(RB3LYP) = -1325.8028 Hartrees; dipole moment = 8.106137 Debye; basis set = 6-31+G(d, p).

O	0.33677	-2.56141	0.54329
O	2.17288	3.49898	0.50902
O	4.24848	3.34770	-0.12671
O	6.17857	-0.98204	-1.06578
O	4.96934	-2.77870	-0.85365
N	-2.78734	-0.20891	3.68218
N	-0.59836	-0.47875	1.07126
N	3.15842	2.84519	0.16001
N	5.12015	-1.55620	-0.79545
C	-2.91599	-1.08259	0.28958
C	-3.42245	0.16401	-0.21199
C	-2.98883	1.43461	0.26661
H	-2.20885	1.47757	1.01674
C	-3.52172	2.60562	-0.23275
H	-3.17318	3.56120	0.14839
C	-4.51417	2.57357	-1.24370
H	-4.92463	3.50229	-1.62913
C	-4.95045	1.36314	-1.73759
H	-5.70777	1.32692	-2.51651
C	-4.42429	0.13624	-1.24303
C	-4.87559	-1.11334	-1.75297
H	-5.62966	-1.11862	-2.53560
C	-4.36574	-2.29342	-1.26195
H	-4.70976	-3.24672	-1.65197
C	-3.38927	-2.27096	-0.23559
H	-3.00521	-3.21231	0.14721
C	-1.85226	-1.15496	1.39498
H	-1.67669	-2.22354	1.58794
C	-2.38097	-0.60863	2.66791
C	0.36178	-1.29884	0.67236
C	1.66894	-0.59681	0.33082
C	1.80488	0.79463	0.40319
H	0.96110	1.39777	0.70891
C	3.02754	1.38315	0.08089
C	4.13838	0.64275	-0.31604
H	5.07810	1.11551	-0.56261
C	3.97298	-0.73645	-0.37988
C	2.76627	-1.36581	-0.06766
H	2.66385	-2.44115	-0.12781

Table S-1: TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for compound **7c** in DMSO

No.	Wavelength (nm)	*f*	Symmetry	Major contribs	Minor contribs
1	501.2905552	0.0006	Singlet-A	HOMO->LUMO (100%)	
2	461.3880359	0.0003	Singlet-A	HOMO->L+1 (100%)	
3	386.7737491	0.0001	Singlet-A	H-1->LUMO (100%)	
4	362.7814636	0.0002	Singlet-A	H-1->L+1 (100%)	
5	331.65042	0.0011	Singlet-A	H-8->LUMO (32%), H-7->L+1 (32%), H-2->LUMO (18%)	H-7->LUMO (4%), H-3->LUMO (6%)
6	330.2634267	0	Singlet-A	H-8->L+1 (37%), H-7->LUMO (46%)	H-8->LUMO (7%), H-7->L+1 (2%)
7	325.640051	0.0073	Singlet-A	HOMO->L+2 (93%)	H-2->LUMO (3%)
8	323.5664518	0.0057	Singlet-A	H-8->LUMO (12%), H-7->L+1 (10%), H-2->LUMO (60%)	H-4->LUMO (2%), H-3->LUMO (7%), HOMO->L+2 (5%)
9	312.3578289	0.0144	Singlet-A	H-3->LUMO (83%), H-2->LUMO (13%)	
10	304.8092069	0.0047	Singlet-A	H-3->L+1 (14%), H-2->L+1 (74%)	
11	296.5419589	0.0062	Singlet-A	H-5->LUMO (29%), H-4->LUMO (14%), H-3->L+1 (26%), H-2->L+1 (11%)	H-6->L+1 (9%)
12	293.3981566	0.1513	Singlet-A	HOMO->L+3 (94%)	H-1->L+4 (3%)
13	291.1178779	0.0097	Singlet-A	H-5->LUMO (16%), H-4->LUMO (13%), H-3->L+1 (40%)	H-14->L+1 (2%), H-10->LUMO (6%), H-6->L+1 (7%), H-2->L+1 (9%)
14	285.6449557	0.0031	Singlet-A	H-14->L+1 (12%), H-10->LUMO (34%), H-10->L+1 (14%), H-3->L+1 (11%)	H-15->L+1 (6%), H-14->LUMO (4%), H-11->LUMO (4%), H-8->L+1 (2%)
15	283.7881229	0.0033	Singlet-A	H-15->LUMO (10%), H-14->LUMO (19%), H-10->L+1 (24%)	H-15->L+1 (2%), H-14->L+1 (4%), H-11->L+1 (4%), H-10->LUMO (7%), H-7->L+1 (2%), H-5->L+1 (2%), H-4->LUMO (9%), H-3->L+1 (5%)
16	282.0258246	0.0019	Singlet-A	H-1->L+3 (47%), HOMO->L+4 (44%)	H-1->L+2 (8%)
17	277.8855437	0.0022	Singlet-A	H-5->LUMO (30%), H-4->LUMO (53%)	H-10->L+1 (3%), H-6->L+1 (2%), H-2->LUMO (3%)
18	271.9488342	0.0112	Singlet-A	H-5->L+1 (35%), H-4->L+1 (43%)	H-6->LUMO (7%), H-3->L+2 (3%), H-2->L+2 (2%), H-1->L+2 (3%)
19	270.8793625	0.0091	Singlet-A	H-1->L+2 (88%)	H-1->L+3 (5%), HOMO->L+4 (2%)
20	265.5362653	0.1174	Singlet-A	H-6->LUMO (38%), H-5->L+1 (10%), H-4->L+1 (36%)	H-6->L+1 (5%), H-5->LUMO (4%)

Table S-2: TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for 1:1 complex of **7c** and fluoride anion in DMSO

No.	Wavelength (nm)	*f*	Symmetry	Major contribs	Minor contribs
1	489.0509349	0.0002	Singlet-A	HOMO->LUMO (99%)	
2	461.5597983	0.0005	Singlet-A	HOMO->L+1 (99%)	
3	378.196605	0.0024	Singlet-A	H-1->LUMO (92%)	H-2->LUMO (7%)
4	361.5226506	0.0085	Singlet-A	H-2->LUMO (88%)	H-3->LUMO (2%), H-1->LUMO (7%)
5	361.1330334	0.0005	Singlet-A	H-1->L+1 (97%)	
6	350.3466982	0.0029	Singlet-A	H-3->LUMO (91%)	H-2->LUMO (2%)
7	341.7613788	0.0026	Singlet-A	H-2->L+1 (91%)	H-3->L+1 (3%)
8	334.5228206	0	Singlet-A	H-10->LUMO (15%), H-10->L+1 (15%), H-3->L+1 (48%)	H-11->LUMO (2%), H-11->L+1 (8%), H-3->LUMO (2%), H-2->L+1 (5%)
9	328.4523498	0.0002	Singlet-A	H-11->LUMO (55%), H-11->L+1 (14%), H-10->L+1 (23%)	H-3->LUMO (3%)
10	325.3580524	0.0006	Singlet-A	H-10->LUMO (21%), H-10->L+1 (18%), H-3->L+1 (44%)	H-11->LUMO (3%), H-11->L+1 (9%)
11	314.249995	0.023	Singlet-A	HOMO->L+2 (96%)	
12	311.377249	0	Singlet-A	H-5->LUMO (77%), H-5->L+1 (19%)	H-4->LUMO (2%)
13	309.0410853	0.0094	Singlet-A	H-7->LUMO (27%), H-6->LUMO (14%), H-4->LUMO (37%)	H-9->L+1 (6%), H-8->L+1 (2%), H-6->L+1 (3%), H-4->L+1 (4%)
14	305.7789553	0.0026	Singlet-A	H-7->LUMO (17%), H-6->LUMO (19%), H-4->LUMO (38%)	H-9->L+1 (5%), H-8->LUMO (6%), H-6->L+1 (3%), H-4->L+1 (7%)
15	297.6882831	0.0318	Singlet-A	H-7->LUMO (37%), H-6->LUMO (42%), H-6->L+1 (10%)	H-9->L+1 (3%), H-4->L+1 (3%)
16	293.8222931	0.0021	Singlet-A	H-5->LUMO (12%), H-5->L+1 (52%), H-4->L+1 (27%)	H-4->LUMO (4%)
17	293.1692157	0.0025	Singlet-A	H-5->L+1 (26%), H-4->LUMO (10%), H-4->L+1 (43%)	H-8->L+1 (4%), H-5->LUMO (8%)
18	292.2156851	0.1391	Singlet-A	HOMO->L+3 (91%)	H-1->L+4 (3%)
19	288.120917	0.0062	Singlet-A	H-7->L+1 (25%), H-6->L+1 (51%)	H-17->L+1 (3%), H-13->LUMO (4%), H-6->LUMO (9%)
20	284.4913908	0.0006	Singlet-A	H-17->LUMO (26%), H-17->L+1 (10%), H-13->LUMO (26%), H-13->L+1 (16%)	H-18->LUMO (2%), H-10->LUMO (3%), H-7->L+1 (4%)

Table S-3: TD-DFT calculated electronic transitions, oscillator strength (*f*), and MO composition for deprotonated **7c** in DMSO

No.	Wavelength (nm)	*f*	Symmetry	Major contribs	Minor contribs
1	566.6812606	0.0277	Singlet-A	HOMO->LUMO (91%)	H-1->LUMO (8%)
2	525.2232187	0.0062	Singlet-A	HOMO->L+1 (94%)	H-1->L+1 (6%)
3	498.7296581	0.0007	Singlet-A	H-1->LUMO (87%)	H-1->L+1 (3%), HOMO->LUMO (8%)
4	480.9690163	0	Singlet-A	H-2->LUMO (98%)	
5	471.100361	0.0001	Singlet-A	H-1->L+1 (90%)	H-1->LUMO (3%), HOMO->L+1 (6%)
6	444.0217491	0	Singlet-A	H-2->L+1 (99%)	
7	379.4698773	0.0002	Singlet-A	H-3->LUMO (89%)	H-4->LUMO (8%), H-3->L+1 (3%)
8	364.3165051	0.0002	Singlet-A	H-4->LUMO (60%), H-3->L+1 (37%)	
9	363.1746478	0.0002	Singlet-A	H-4->LUMO (29%), H-3->L+1 (58%)	H-4->L+1 (3%), H-3->LUMO (9%)
10	344.3048959	0.0001	Singlet-A	H-4->L+1 (89%)	H-9->L+1 (3%), H-8->LUMO (3%), H-3->L+1 (2%)
11	329.0800324	0.0001	Singlet-A	H-9->LUMO (31%), H-8->LUMO (19%), H-8->L+1 (37%)	H-9->L+1 (8%)
12	327.8097219	0	Singlet-A	H-9->LUMO (14%), H-9->L+1 (35%), H-8->LUMO (30%), H-8->L+1 (12%)	H-4->L+1 (5%)
13	323.1532124	0.0327	Singlet-A	H-5->LUMO (45%), HOMO->L+2 (41%)	H-7->L+1 (5%), H-1->L+2 (5%)
14	322.0954278	0.0355	Singlet-A	H-5->LUMO (39%), HOMO->L+2 (46%)	H-7->L+1 (5%), H-1->L+2 (7%)
15	308.4797796	0.0122	Singlet-A	H-5->L+1 (81%), HOMO->L+3 (12%)	H-6->L+1 (2%)
16	302.1278188	0.1401	Singlet-A	H-5->L+1 (13%), H-2->L+3 (18%), H-1->L+2 (15%), HOMO->L+3 (44%)	H-2->L+2 (4%), HOMO->L+2 (2%)
17	297.9386577	0.0726	Singlet-A	H-2->L+3 (68%), H-1->L+2 (11%)	H-2->L+2 (3%), H-1->L+3 (4%), HOMO->L+2 (2%), HOMO->L+3 (7%)
18	292.1812533	0.0528	Singlet-A	H-1->L+2 (50%), HOMO->L+3 (30%)	H-3->L+4 (2%), H-2->L+2 (3%), HOMO->L+2 (7%)
19	289.0343925	0.0019	Singlet-A	H-6->LUMO (86%)	H-6->L+1 (4%), H-5->LUMO (4%), H-1->L+3 (3%)
20	286.0667567	0.0068	Singlet-A	H-1->L+3 (81%)	H-6->LUMO (3%), H-2->L+2 (3%), H-1->L+2 (3%), HOMO->L+3 (3%)

6. Mass Spectrometric Analysis of 7c and Fluoride Anion

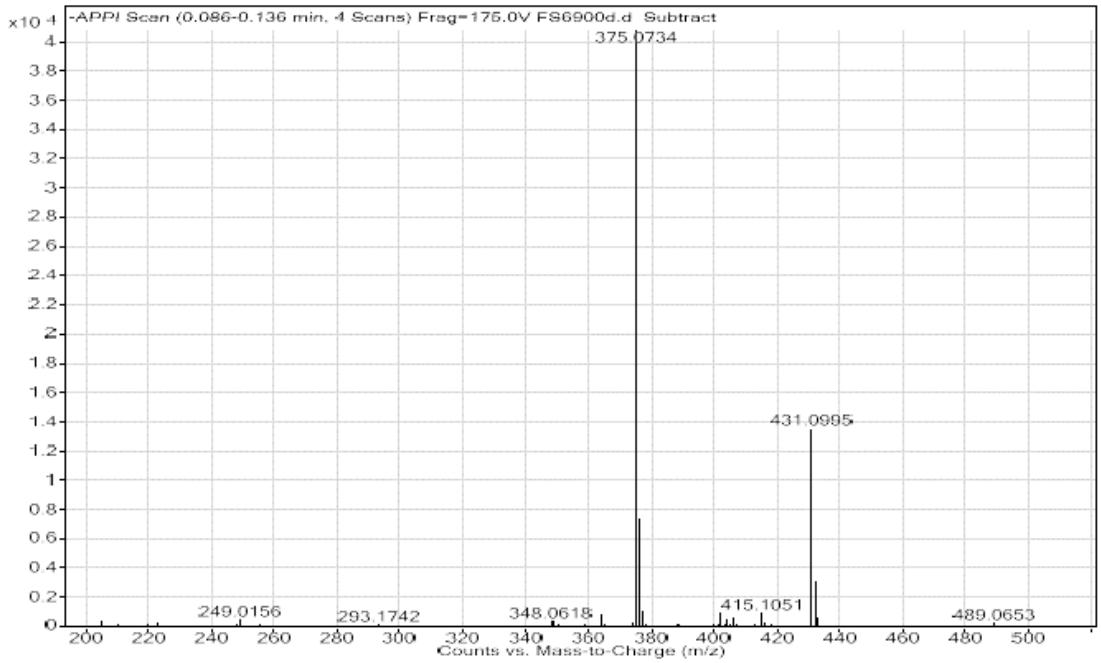

Fig. S-34: High-resolution mass spectrum (APPI-TOF, negative mode) of the mixture of **7c** and TBAF. Sample was prepared by mixing **7c** and TBAF (1:1 molar ratio) in acetone. The peak at *m/z* 375.0734 matches the $[M - H]^-$ ion, while the peak at *m/z* 431.0995 matches the $[M + F + (H_2O)_2]^-$ ion.