Supplementary Information *for*

Combined Photophysical, NMR and Theoretical (DFT) Study on the Interaction of a Multi Component System in Absence and Presence of Different Biologically and Environmentally Important ions

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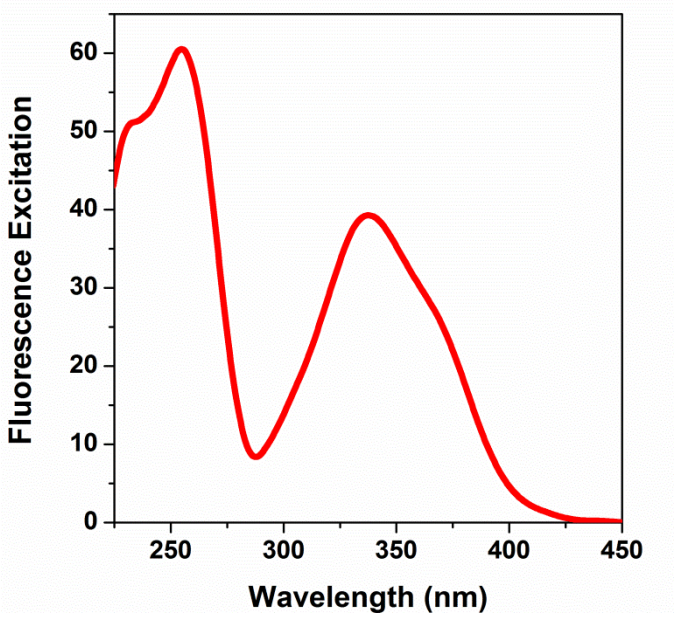

Figure S1. Fluorescence Excitation Spectra of DANSn2, in Acetonitrile, at $\lambda_{emi.}$=538 nm

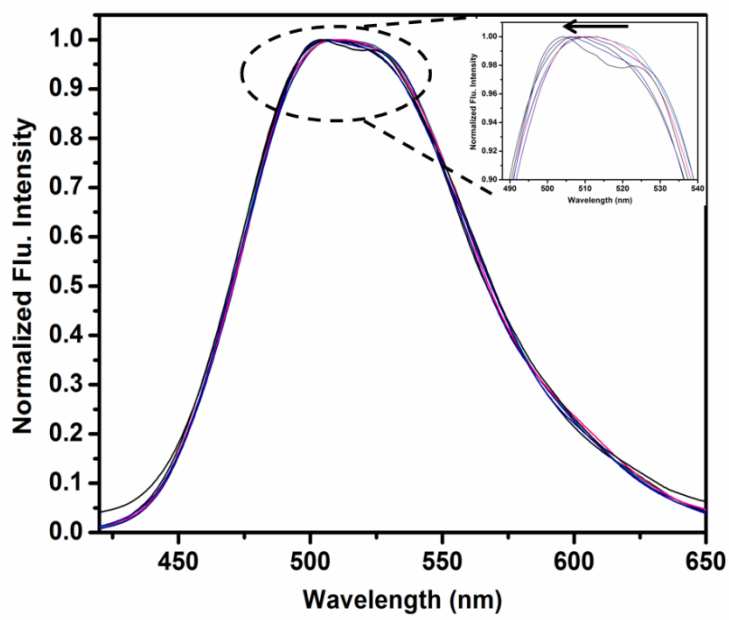

Figure S2. Normalized fluorescence emission spectra of DANSn2 upon increasing addition of Fluoride. Inset shows the small change in the position of emission maxima, and the arrow depicts the increasing fluoride concentration as well as the blue shift.

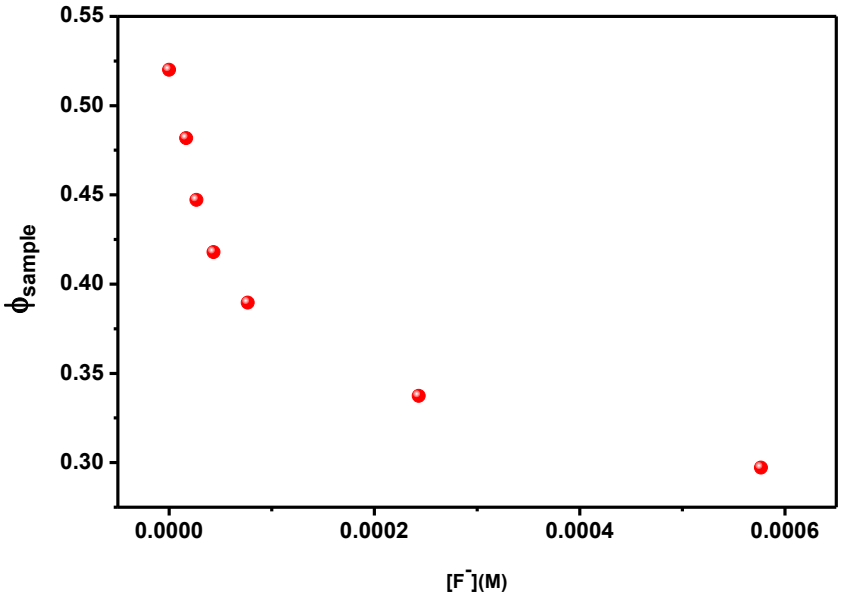

Figure S3. Change of quantum yield of DANSn2 with the concentration of fluoride ion.

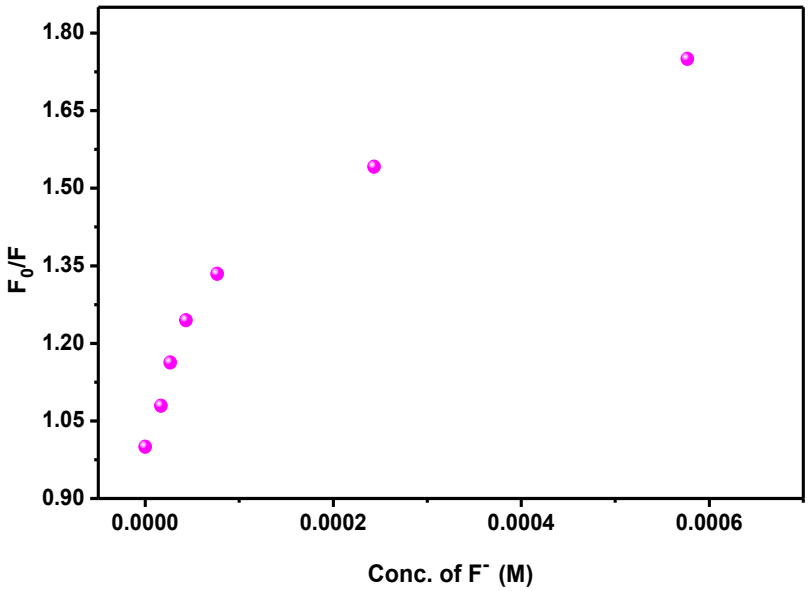

Figure S4. Variation of Fo/F of DANSn2 with the concentration of fluoride ion. F and F_0 are fluorescence intensities of DANSn2 with and without addition of fluoride ion.

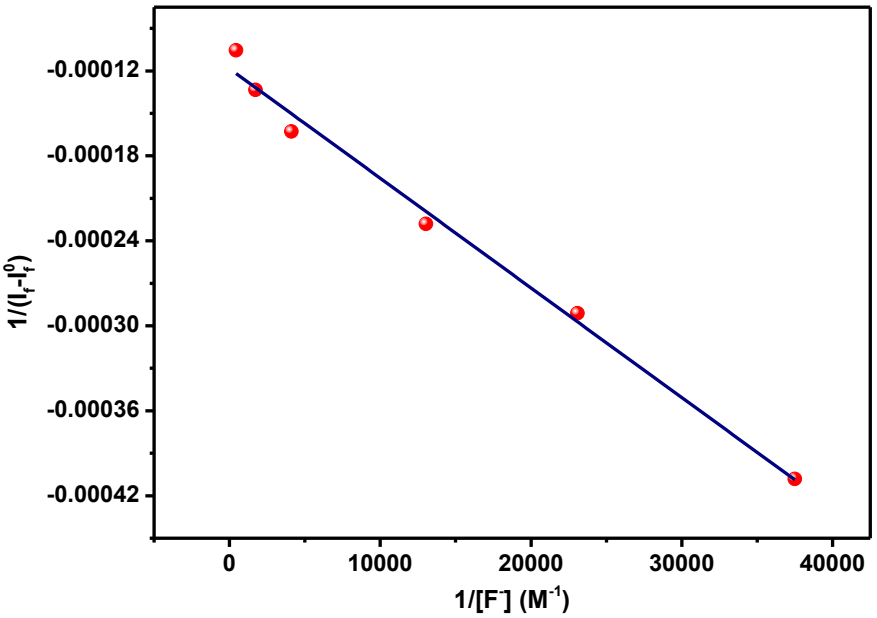

Figure S5. Benesi-Hildebrand plot for determination of binding constant of **DANSn2** (1.0×10^{-5} M) with fluoride ion from steady state emission data.

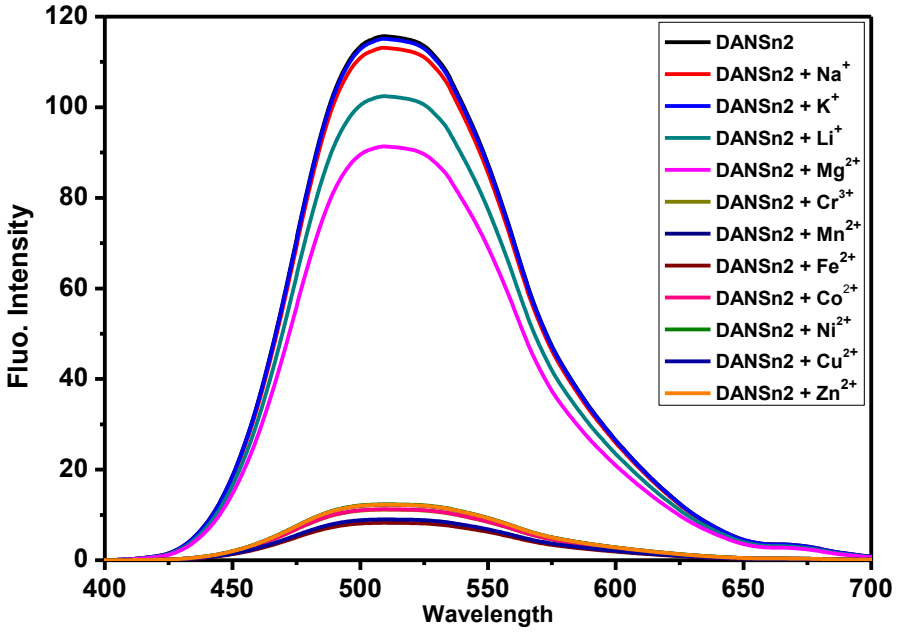

Figure S6. Fluorescence response of **DANSn2** in absence and presence of different metal ions. $\lambda_{exc.}$=445 nm. Concentration of probe ~ 1.0×10^{-5} M and metal ions ~ 1.0×10^{-3}M.

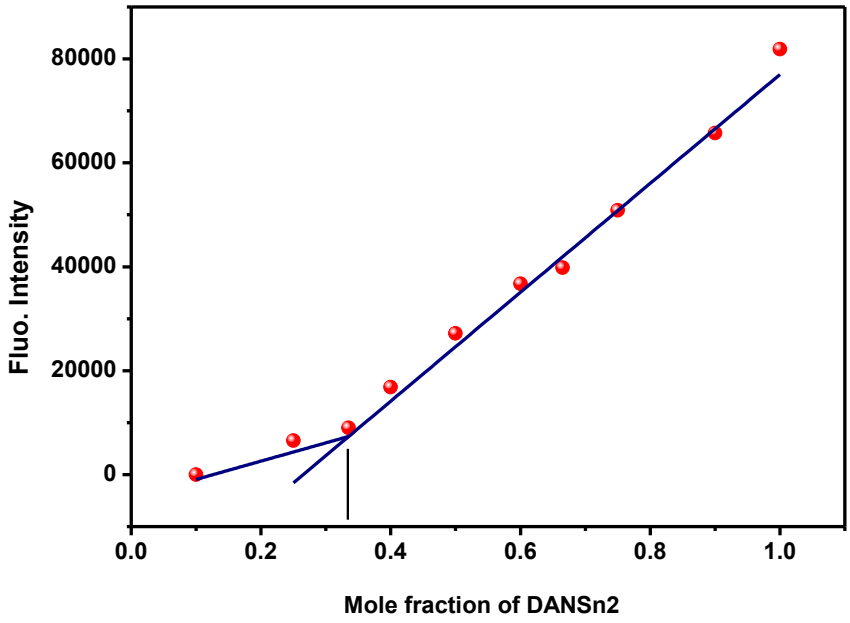

Figure S7. Jobs plot for the complexation of the DANSn2 with Zn^{2+} ions in ACN. $\lambda_{exc.}$ = 338 nm.

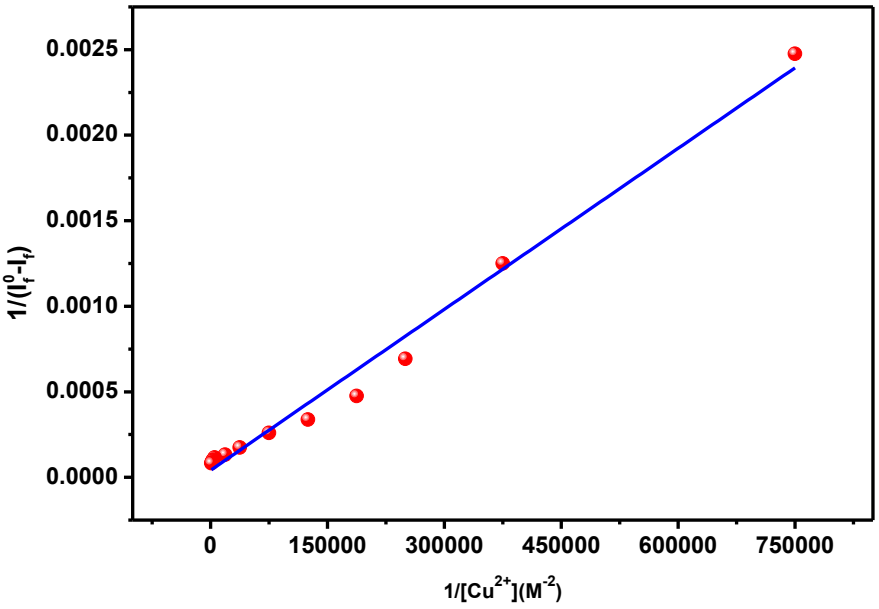

Figure S8. Benesi-Hildebrand plot for determination of binding constant of **DANSn2** (1.0×10^{-5} M) with copper ion from steady state emission data.

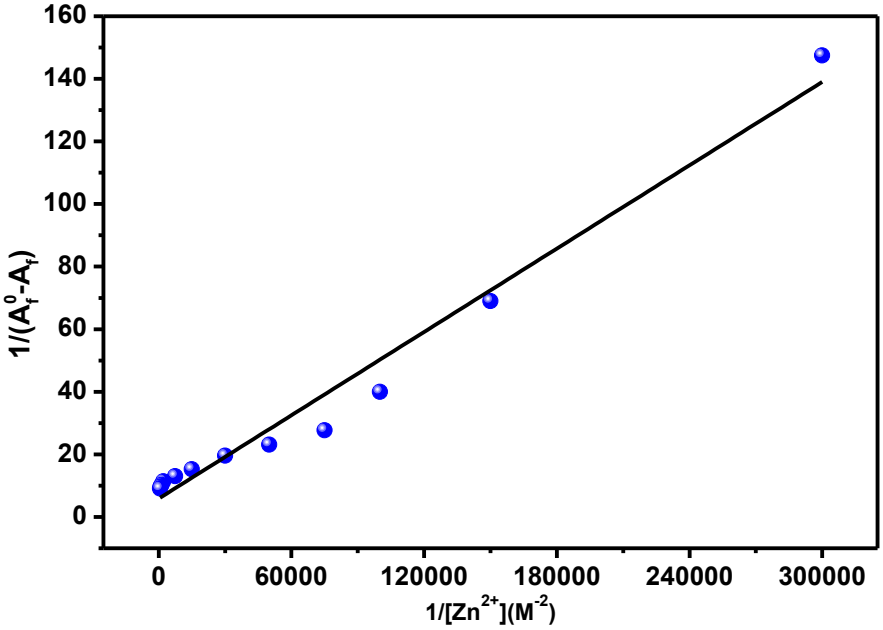

Figure S9. Benesi-Hildebrand plot for determination of binding constant of **DANSn2** (1.0×10^{-5} M) with copper ion from steady state absorption data.

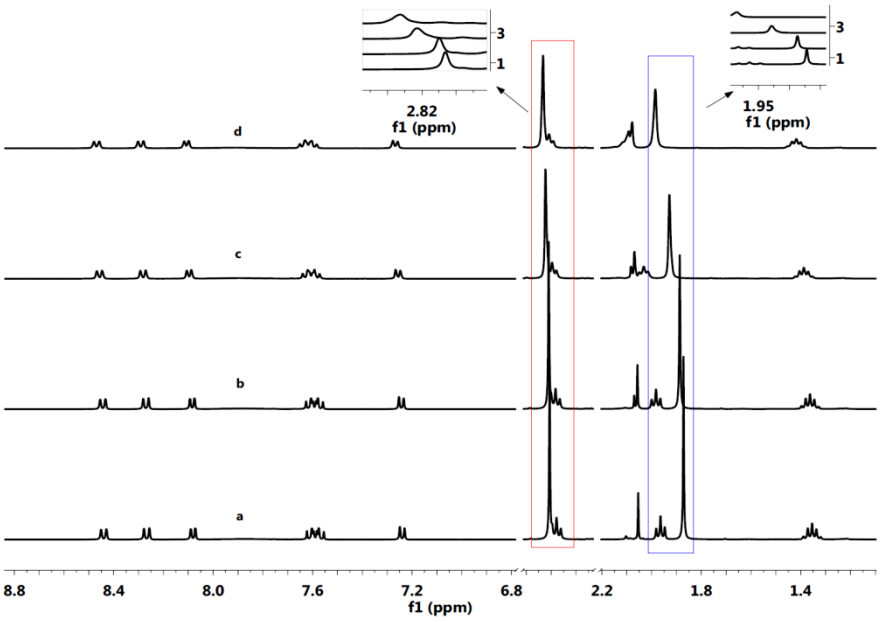

Figure S10. Zoomed ^{1}H NMR spectra of DANSn2 in DMSO-d_6 in presence of (a) 0 eq., (b) 0.2 eq., (c) 0.5 eq., (d) 1.12 eq. of Zinc(II) perchlorate.

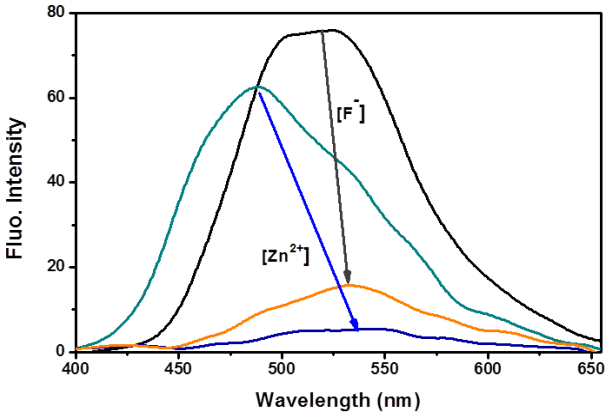

Figure S11. Change in emission profile of DANSn2 in Acetonitrile, upon addition of Zinc salt in presence of fluoride salt to evaluate the cooperative effect in ion binding.

Table S1. Binding Constants of DANSn2 with Zn^{2+} in the presence of F^{-}.

Complexes	**Binding Constant (10^{-4})**
DANSn2 + Zn^{2+}	0.652 M^{-2}
DANSn2 + Zn^{2+} (in presence of F^{-})	0.061 M^{-2}

Table S2. Cartesian coordinates of the optimized structure of DANSn2.

Center Number	Atomic Number	Coordinates(Angstroms)		
		X	Y	Z
1	16	2.144270	-1.603074	-0.702735
2	8	2.898375	-2.64063	-0.01398
3	8	2.1534	-1.50579	-2.15398
4	7	-4.07678	0.051844	0.385017
5	7	2.681125	-0.15059	-0.11566
6	1	2.118141	0.628387	-0.48394
7	7	1.542065	2.487055	0.112497
8	6	-3.95088	0.679565	1.700044
9	1	-3.06505	0.309882	2.218832
10	1	-4.8332	0.440206	2.300819
11	1	-3.87001	1.776664	1.613934
12	6	-2.86858	0.050085	-0.35691
13	6	-1.83048	-0.8575	0.050983
14	6	-0.56562	-0.82472	-0.60918
15	6	0.44625	-1.71481	-0.12333
16	6	2.81186	-0.05502	1.345929
17	1	3.627733	-0.71359	1.651417
18	1	1.89485	-0.3954	1.855635
19	6	3.097889	1.388655	1.747705
20	1	3.337253	1.402728	2.81657
21	1	3.990338	1.745378	1.222315
22	6	1.90809	2.321993	1.522197
23	1	1.0377	1.89551	2.036884
24	1	2.10645	3.307941	1.984576
25	6	0.197372	3.035943	-0.00022
26	1	-0.52701	2.336873	0.430284
27	1	-0.05589	3.172701	-1.05434
28	1	0.105824	4.011088	0.512477
29	6	2.49831	3.329897	-0.59554
30	1	2.551973	4.344937	-0.1615
31	1	2.200939	3.413645	-1.64407
32	1	3.495689	2.884892	-0.56625
33	6	-2.06854	-1.82541	1.064755
34	1	-3.06419	-1.88653	1.491194
35	6	-1.08394	-2.69189	1.464118
36	1	-1.2841	-3.4396	2.224396
37	6	0.202927	-2.61346	0.885059
38	1	1.007104	-3.26283	1.215556
39	6	-2.66299	0.858394	-1.45445
40	1	-3.44492	1.52803	-1.79532
41	6	-1.4287	0.835869	-2.1415
42	1	-1.29837	1.473993	-3.0108
43	6	-0.38907	0.046835	-1.72183
44	1	0.544952	0.040941	-2.27008
45	6	-5.24998	0.548661	-0.31257
46	1	-5.23397	1.642471	-0.46045
47	1	-6.13528	0.304259	0.280607
48	1	-5.33793	0.061189	-1.28587

Table S3. Cartesian coordinates of the optimized structure of the DANSn2···Cu^{2+} complex.

Center Number	Atomic Number	Coordinates(Angstroms)		
		X	Y	Z
1	16	1.435488	0.383797	-0.692482
2	8	1.220706	0.848090	-2.047125
3	8	1.790950	1.421625	0.361323
4	7	-5.003300	0.364000	0.642356
5	7	2.591624	-0.686600	-0.430413
6	6	-4.988250	0.067546	2.128038
7	1	-4.097470	-0.482435	2.416484
8	1	-5.881130	-0.504508	2.383620
9	1	-5.009940	1.022101	2.662997
10	6	-3.765170	0.832793	0.136230
11	6	-2.573570	-0.009300	0.202594
12	6	-1.319270	0.544531	-0.211434
13	6	-0.157200	-0.274253	-0.138808
14	6	3.260894	-1.374108	-1.558280
15	1	3.325898	-0.717989	-2.434014
16	1	2.672499	-2.255589	-1.835852
17	6	4.650752	-1.830137	-1.112581
18	1	4.566533	-2.557154	-0.299112
19	1	5.093267	-2.373278	-1.953489
20	6	-2.607330	-1.356547	0.599908
21	1	-3.539060	-1.834103	0.896906
22	6	-1.451010	-2.133035	0.653529
23	1	-1.511490	-3.168227	0.974858
24	6	-0.213810	-1.586648	0.298770
25	1	0.693422	-2.181317	0.350474
26	6	-3.676800	2.119612	-0.439177
27	1	-4.552330	2.750719	-0.522355
28	6	-2.457110	2.632826	-0.834411
29	1	-2.398280	3.644265	-1.225119
30	6	-1.275890	1.871714	-0.710598
31	1	-0.338120	2.316147	-1.028296
32	6	-6.195430	1.231924	0.364821
33	1	-6.125190	2.180986	0.906348
34	1	-7.081930	0.70855	0.730009
35	1	-6.299820	1.417022	-0.706324
36	6	5.631500	-0.708652	-0.759449
37	1	6.653786	-1.108062	-0.765650
38	1	5.588417	0.083135	-1.516690
39	7	5.436125	-0.052385	0.576659
40	6	6.376764	1.100131	0.698855
41	1	6.242390	1.588958	1.667003
42	1	7.410406	0.740945	0.633234
43	1	6.202978	1.815112	-0.109142
44	6	5.672723	-1.004430	1.696011
45	1	6.670791	-1.446106	1.596837
46	1	5.620023	-0.468374	2.646056
47	1	4.925577	-1.798721	1.687434
48	29	3.615309	0.659351	0.659997
49	29	-5.564770	-1.341746	-0.459804

Table S4. Cartesian coordinates of the optimized structure of the DANSn2⋯ F^- complex.

Center Number	Atomic Number	Coordinates(Angstroms)		
		X	Y	Z
1	16	0.886431	1.258176	1.125757
2	8	1.468032	2.570826	0.78898
3	8	0.717318	0.921313	2.542834
4	7	-5.11765	-0.61949	-0.77733
5	7	1.611705	0.061748	0.391692
6	1	1.597671	-1.27192	0.85182
7	7	5.74106	-0.51759	-0.57348
8	6	-4.97363	-0.72594	-2.22568
9	1	-4.154	-0.09354	-2.57113
10	1	-5.90029	-0.39697	-2.70938
11	1	-4.76304	-1.76459	-2.53771
12	6	-3.87316	-0.75527	-0.0865
13	6	-2.9724	0.361311	-0.10279
14	6	-1.68957	0.236604	0.511004
15	6	-0.79744	1.353783	0.439309
16	6	2.006558	0.26899	-0.99408
17	1	1.478409	1.1185	-1.45042
18	1	1.720165	-0.62963	-1.56124
19	6	3.515993	0.492563	-1.13607
20	1	3.744355	0.662361	-2.19747
21	1	3.794541	1.392432	-0.57588
22	6	4.289684	-0.70232	-0.59363
23	1	3.956146	-0.88199	0.432887
24	1	4.025485	-1.6111	-1.17652
25	6	6.372803	-1.60714	0.145552
26	1	5.964617	-1.66562	1.157793
27	1	7.452415	-1.43345	0.21282
28	1	6.209021	-2.58739	-0.34623
29	6	6.29676	-0.41154	-1.90712
30	1	6.073351	-1.30568	-2.52618
31	1	7.384789	-0.30261	-1.84495
32	1	5.898488	0.46724	-2.41928
33	6	-3.34568	1.596764	-0.69948
34	1	-4.3489	1.695861	-1.10122
35	6	-2.46724	2.649366	-0.73663
36	1	-2.76492	3.592071	-1.18764
37	6	-1.17311	2.520447	-0.17849
38	1	-0.46204	3.339523	-0.21068
39	6	-3.51422	-1.90623	0.577732
40	1	-4.18878	-2.75649	0.602515
41	6	-2.25572	-2.00626	1.21729
42	1	-1.98796	-2.92624	1.727566
43	6	-1.35319	-0.97599	1.178138
44	1	-0.39035	-1.08493	1.660296
45	6	-6.19143	-1.4708	-0.30686
46	1	-6.05302	-2.53543	-0.5713
47	1	-7.13011	-1.13578	-0.76082
48	1	-6.27844	-1.39031	0.779336
49	9	1.617869	-2.28279	1.084434

Fluorescence Microscopy Studies.

Fluorescence microscopy studies have been performed to evaluate the utility of the present DANSn2 system as an imaging probe in live cells. Fluorescence images were taken after incubation with increasing concentration of DANSn2 (0 to 40 μM) to the tetrahymena cells for 2 h. It can be seen that the fluorescence images display blue emission due to presence of a slightly acidic medium inside the cell. The results shows that DANSn2 is cell-permeable and may be used for live cell imaging studies.

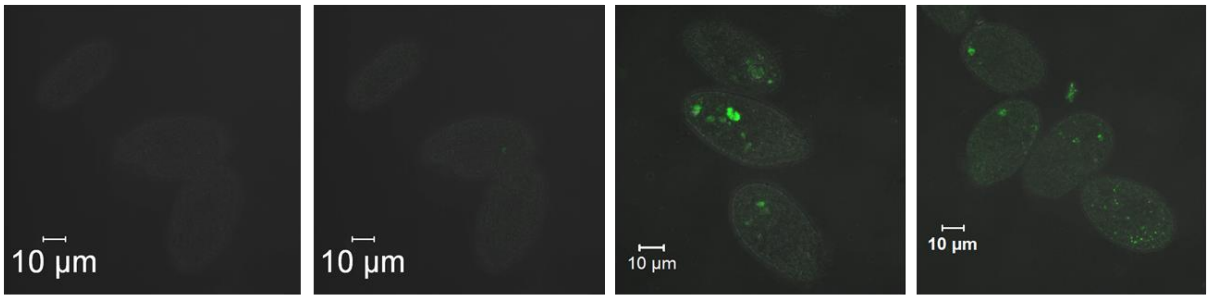

Figure S12. Fluorescence microscopy images of Tetrahymena cells (1) DIC image (2) after incubation with 0μM DNASn2 (3) 10μM DNASn2 (4) 10 μM DANSn2^{+}10μM Cu2^{+}, for 2 hours.

We have also carried out the toxicity studies on the present system by employing the same cells used for imaging(Figure S11). The growth curve of tetrahymena cell was found to be similar in the presence or absence of DANSn2. Hence, DANSn2 is non-toxic under the present experimental condition.

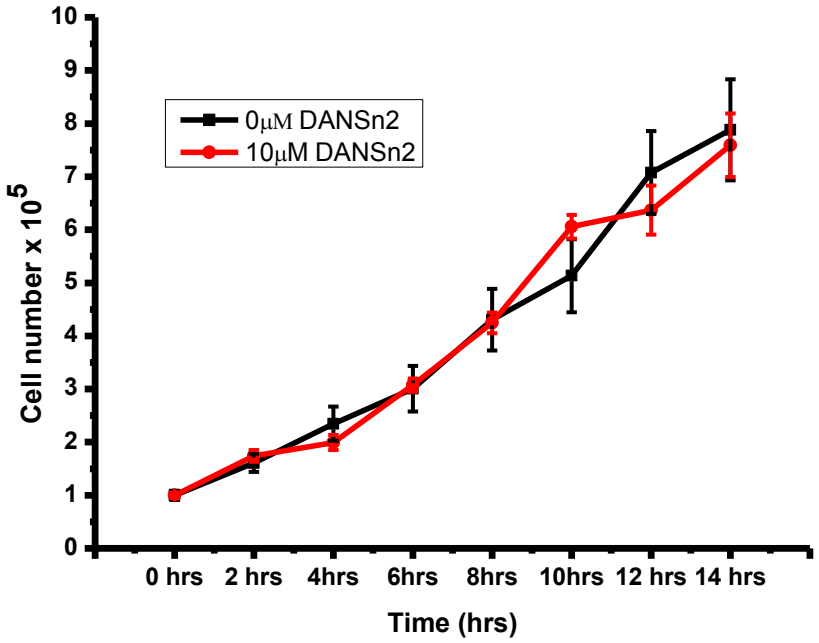

Figure S13. Growth curve of Tetrahymena: Tetrahymena cells were grown in presence of 0 μM DANSn2 and 10 μM DANSn2. DANSn2 was added when cells density reached 1×10^5 /ml. The cell numbers were counted every 2 hours and the numbers of cells were plotted against time in hours.