Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Electronic Supplementary Information

Antipyrine based fluorescence "turn-on" dual sensor for Zn^{2+} and Al^{3+} and its' selective "turn-off" fluorescence sensing towards 2,4,6-trinitrophenol (TNP) in aggregated state

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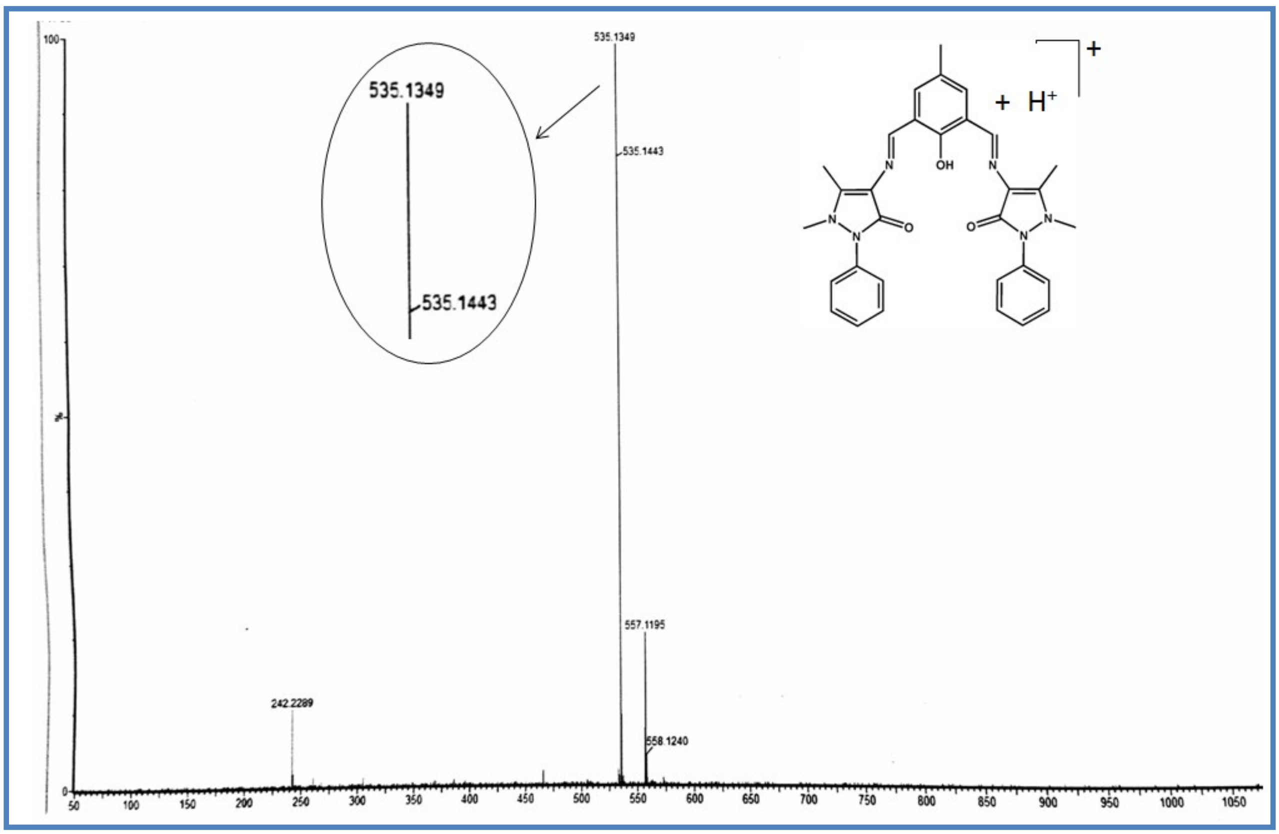


Fig. S1: Mass spectrum of DFCAP in methanol.

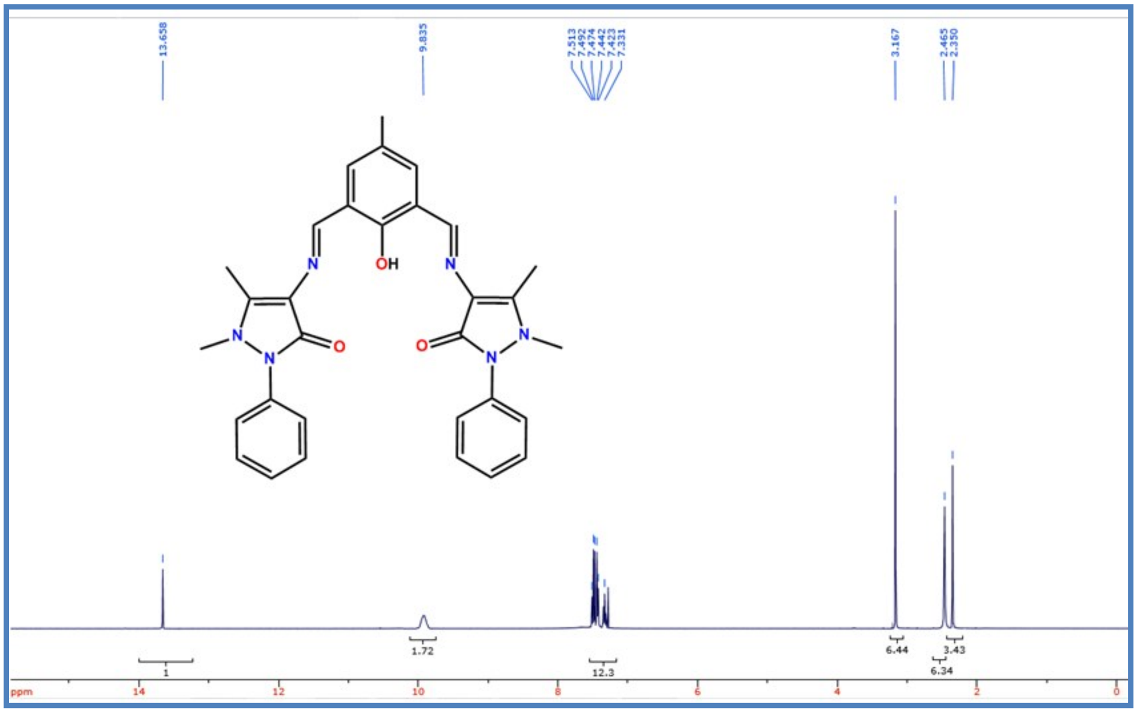


Fig. S2: ^{1}H NMR spectrum of DFCAP in $CDCl_3$.

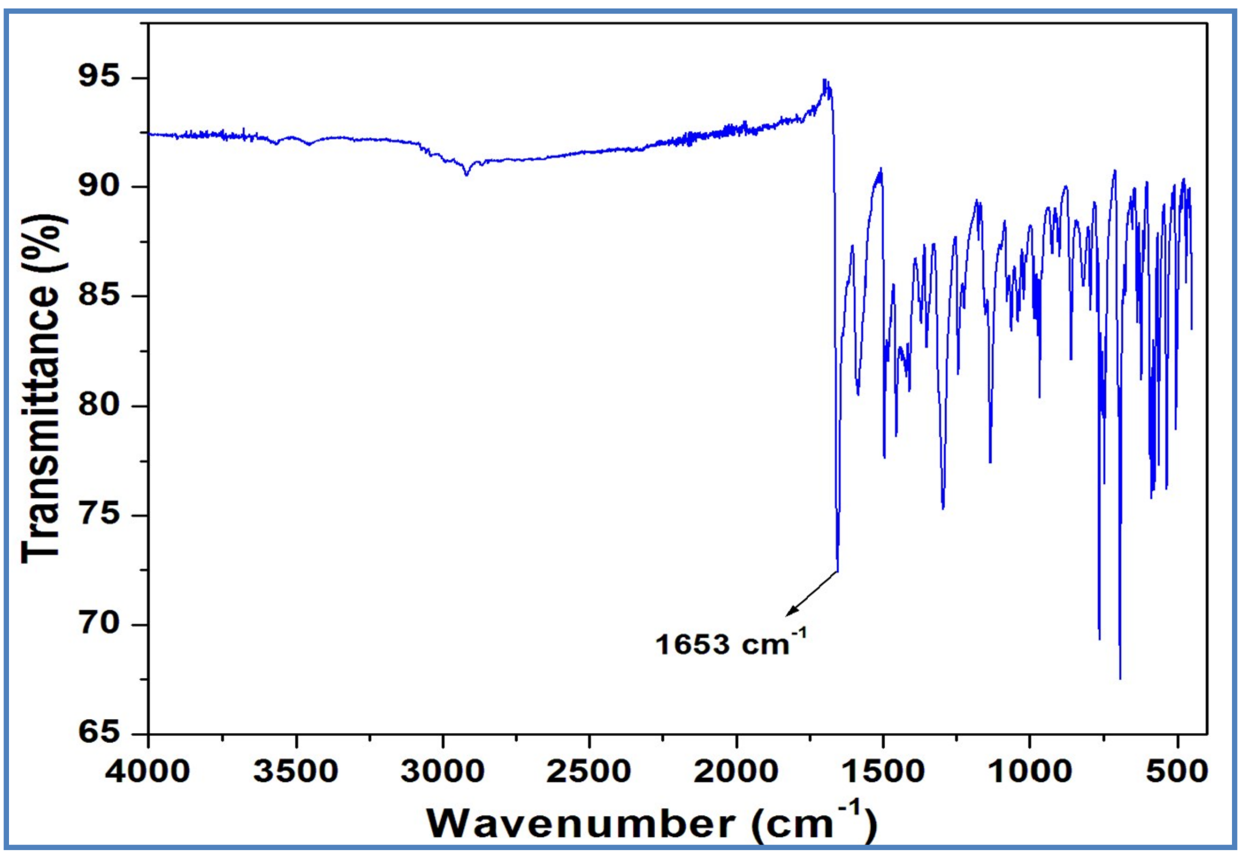


Fig. S3: FT-IR spectrum of DFCAP showing sharp peak at 1653 cm-1 for C=N bond.

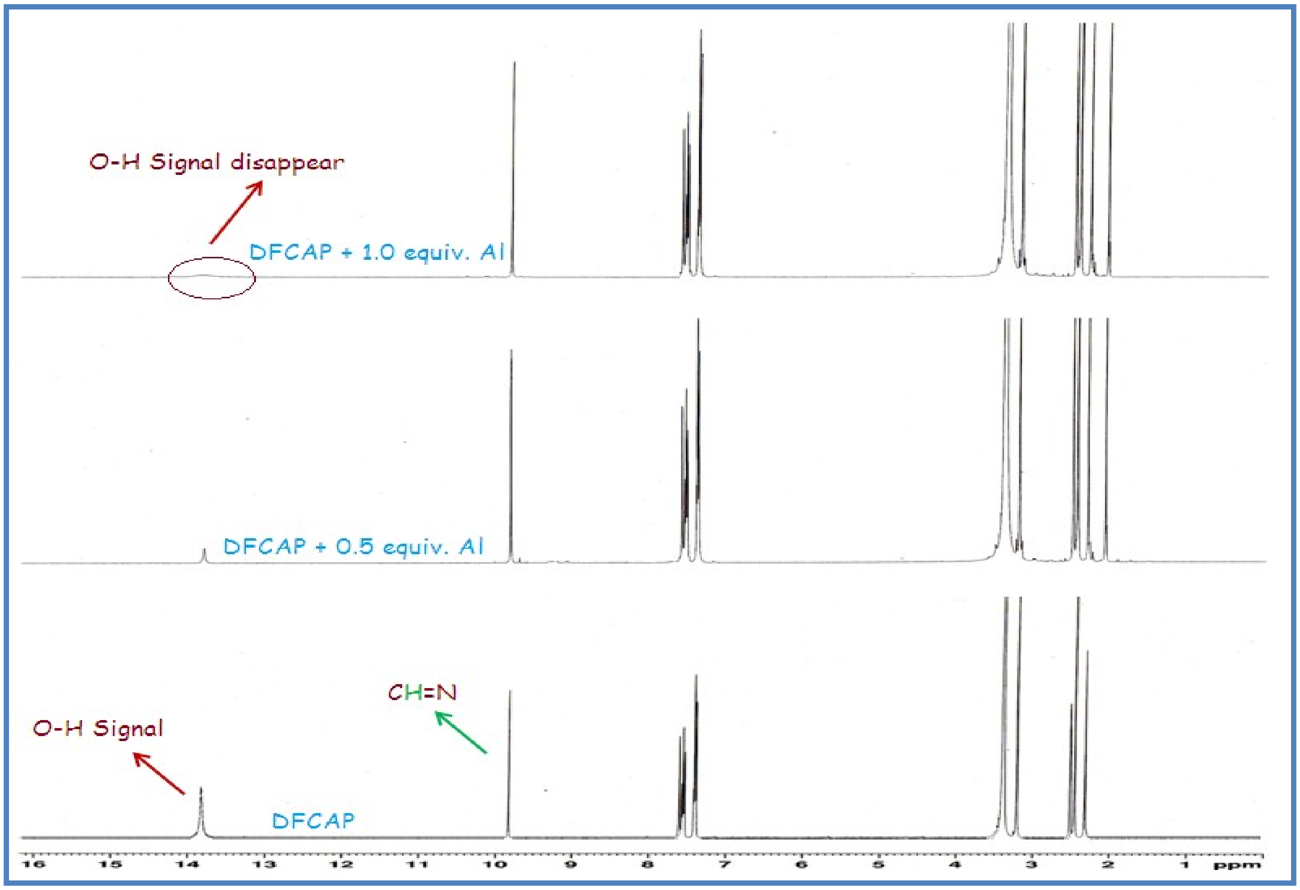


Fig. S4: NMR spectral changes of DFCAP in DMSO-d_6 titrated with 0.5 equiv. and 1.0 equiv. of Al^{3+} in DMSO-d_6.

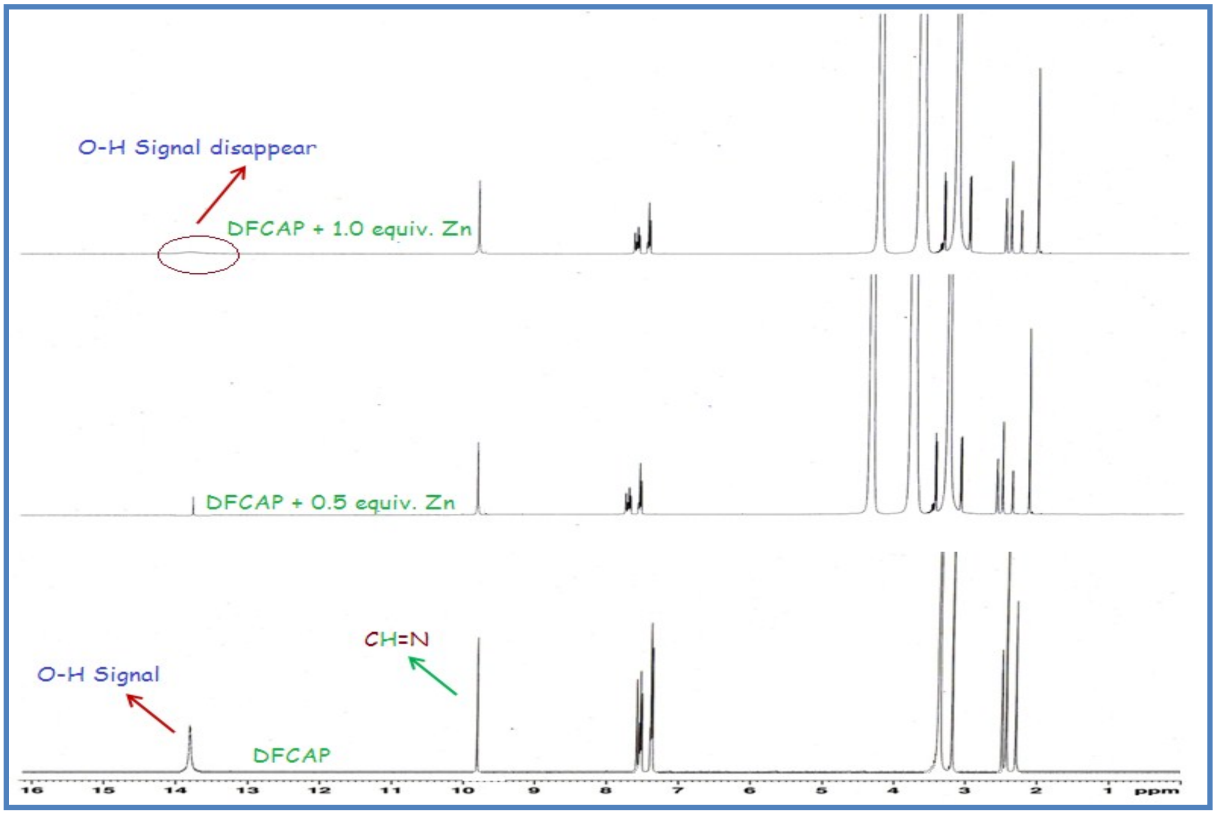


Fig. S5: NMR spectral changes of DFCAP in DMSO-d_6 titrated with 0.5 equiv. and 1.0 equiv. of Zn^{2+} in DMSO-d_6.

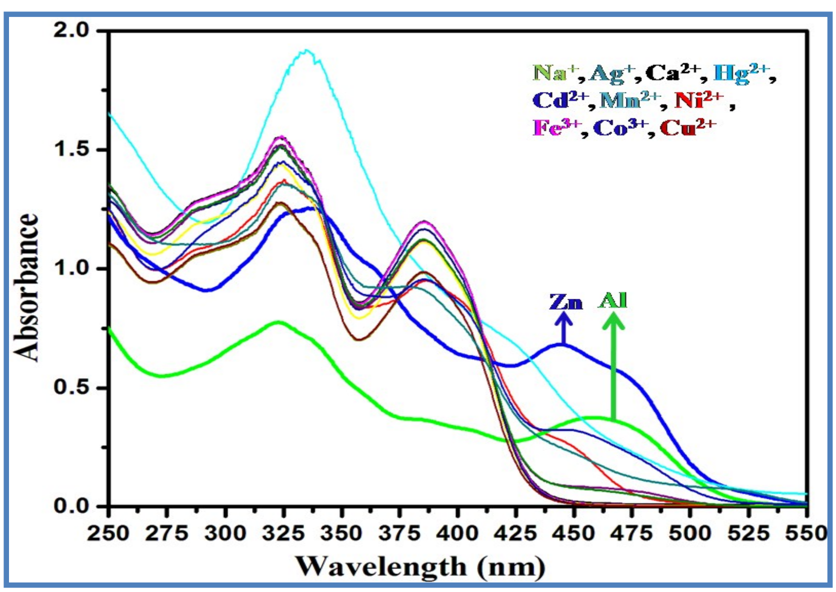


Fig. S6: Absorption spectra of DFCAP (40 μM) in the presence of different metal ions (100 μM).

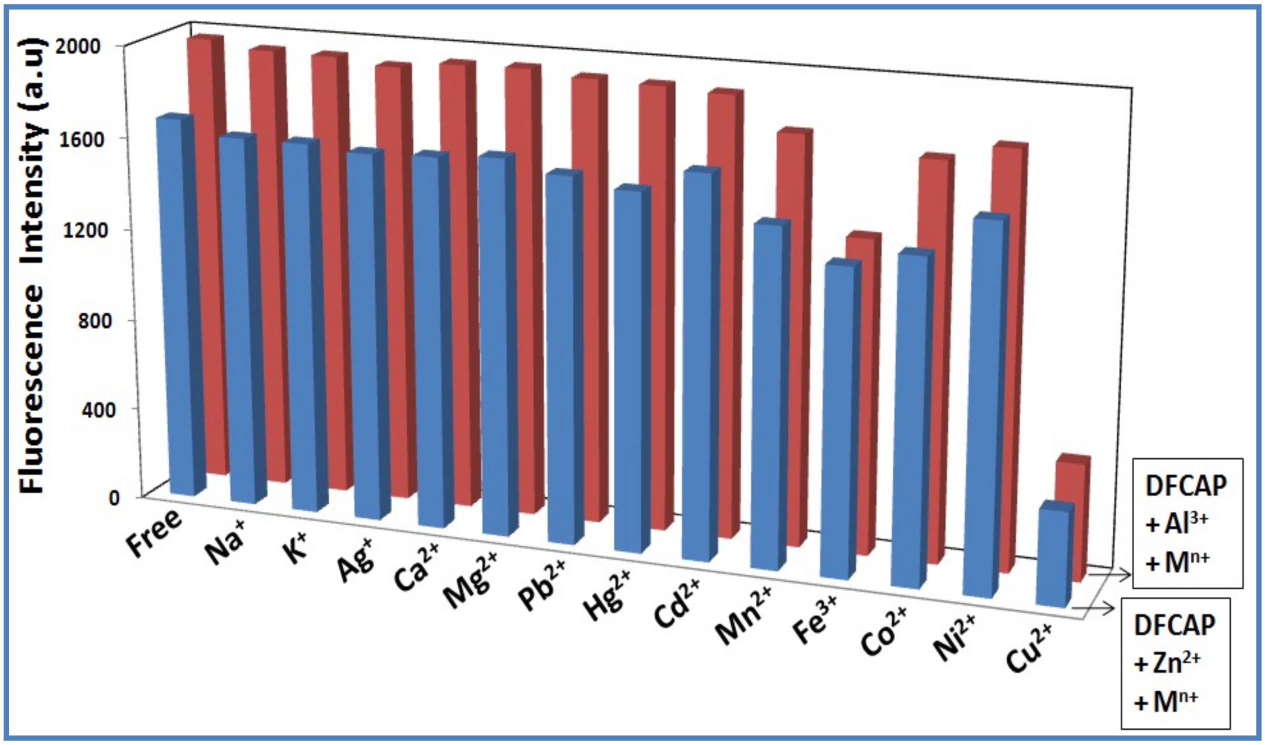


Fig. S7: Fluorescence intensity of DFCAP (40 μM) in the presence of a mixture of metal ions, including Zn^{2+} and Al^{3+} in methanol at room temperature (excitation: 390 nm).

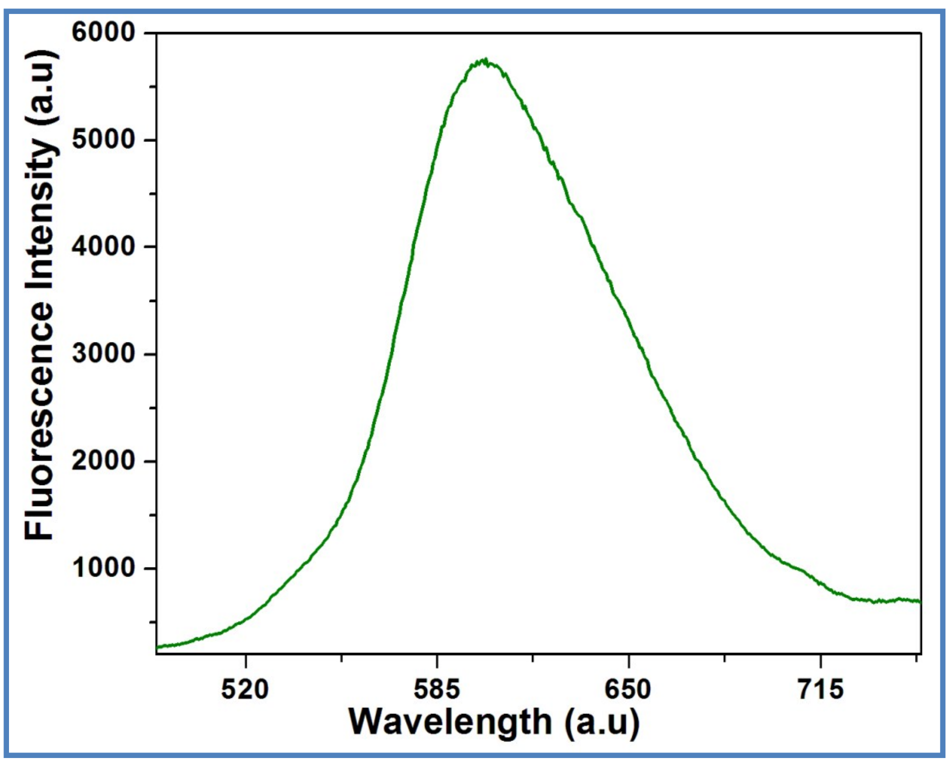


Fig. S8: Solid state emission of DFCAP.

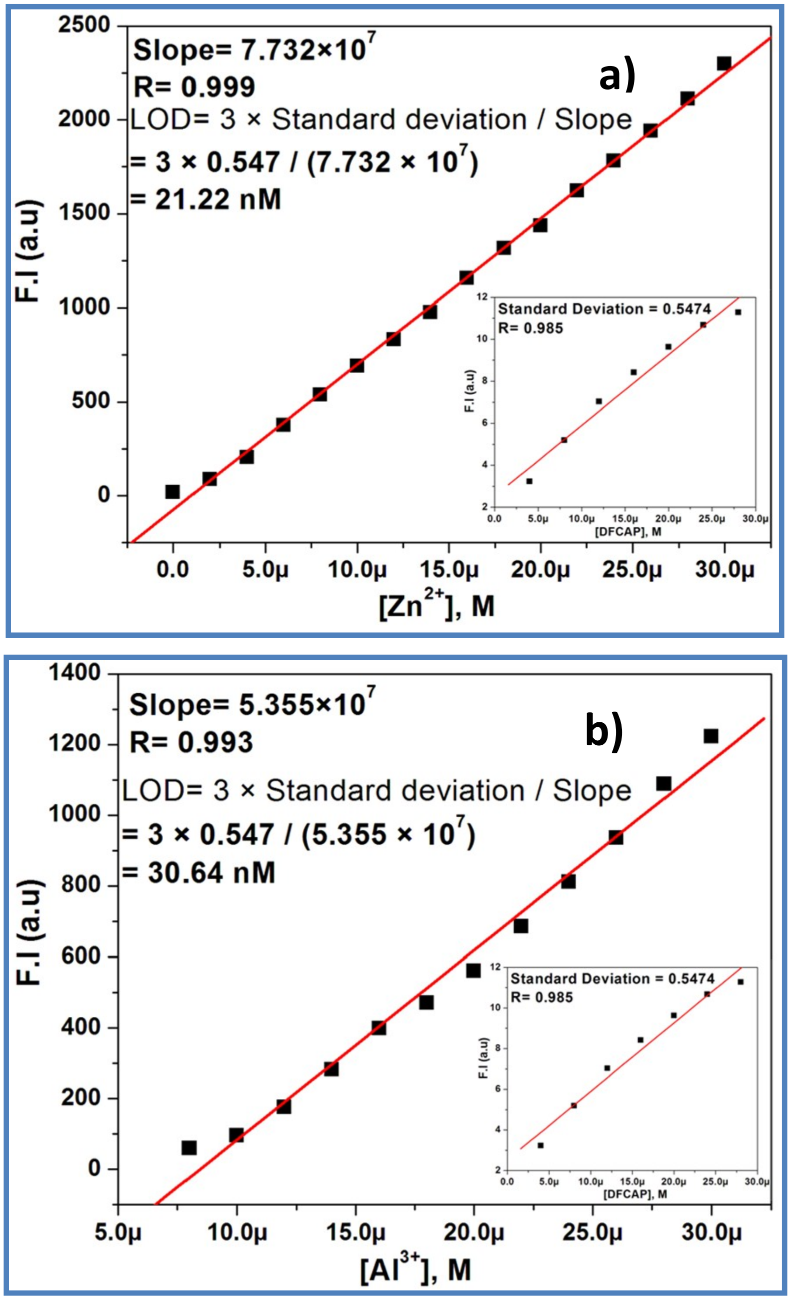


Fig. S9: (a) Calculation of the detection limit (LOD) of DFCAP for Zn^{2+} and (b) LOD of DFCAP for Al^{3+}.

(The detection limit DL of DFCAP for Zn^{2+} and Al^{3+} was determined from 3σ method by following equation: DL = K* Sb1/S. Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the calibration curve obtained from Linear dynamic plot of F.I. *vs* [Zn^{2+} or Al^{3+}])

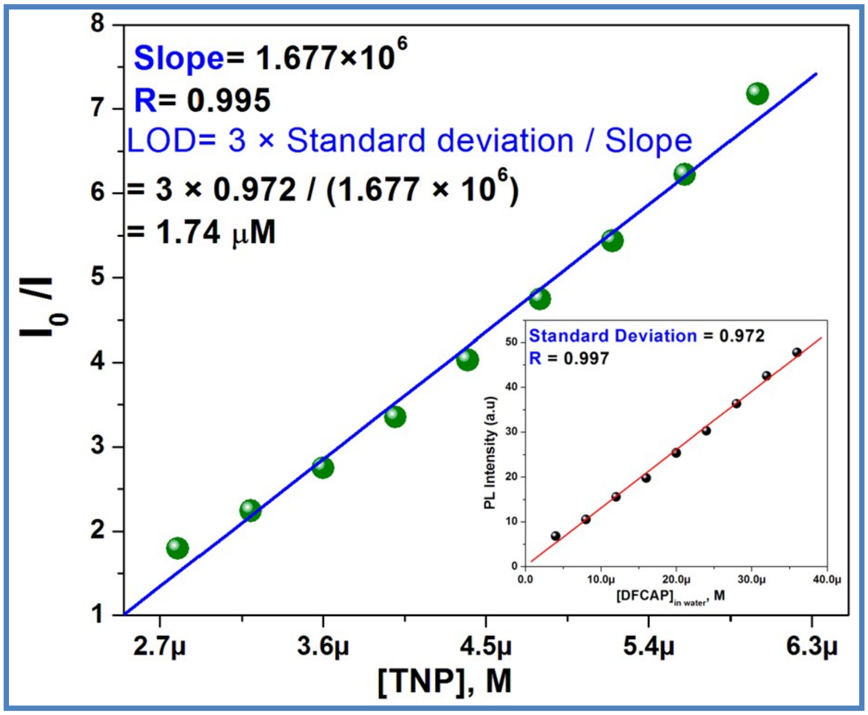


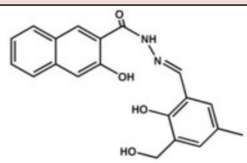
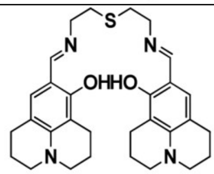
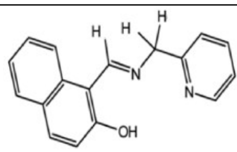
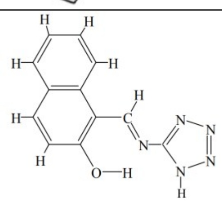
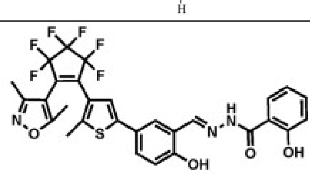
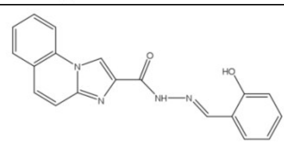
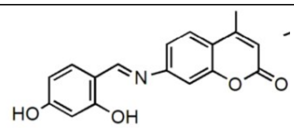
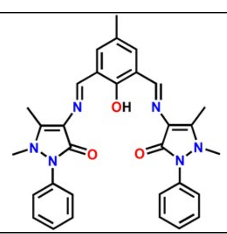
Fig. S10: Calculation of the detection limit (LOD) of DFCAP with TNP.

(The detection limit DL of DFCAP for Zn^{2+} and Al^{3+} was determined from 3σ method by following equation: DL = K* Sb1/S. Where K = 2 or 3 (we take 3 in this case); Sb1 is the standard deviation of the blank solution; S is the slope of the To obtain the slope, the fluorescence emission intensity at 538 nm was plotted against the concentration of TNP.)

Table S1: Real samples study

Samples	**Concentration of Al^{+3}**			**Concentration of Zn^{+2}**		
	Spiked (μM)	**Found (μM)**	**Actual Conc. Of Al^{3+} in sample water (ppb)**	**Spiked (μM)**	**Found (μM)**	**Actual Conc. Of Zn^{2+} in sample water (ppb)**
Sample - 1	20	25	135	20	22	111
Sample - 2	20	26	173	20	24	307
Sample - 3	20	27	181	20	26	418

Table S2: Comparison study

Sl. No.	Probe	No. of steps for synthesis	Excitation/ Emission (nm)	LOD (Al^{3+}, Zn^{2+})	DFT study	AIE property	Nitro Aromatic sensing	Ref.
1		2	398/ 498 (Al^{3+}), 486 (Zn^{2+})	0.92 nM, 3.1 nM	yes	na	na	1
2		1	355/ 418 (Al^{3+}), 445 (Zn^{2+})	1.34 µM, 1.59 µM	na	na	na	2
3		1	370/ 432 (Al^{3+}), 446 (Zn^{2+})	0.648 µM, 1.96 µM	na	na	na	3
4		1	420/ 470 (Al^{3+}), 483 (Zn^{2+})	5.86 µM, 1.81 µM	yes	na	na	4
5		1	372/ 512 (Al^{3+}), 556 (Zn^{2+})	83.10 nm, 0.33 µM	na	na	na	5
6		5	305, 315 (Al^{3+}, Zn^{2+}) / 450 (Al^{3+}), 489 (Zn^{2+})	17.3 µM, 0.636 nM	yes	na	na	6
7		4	357,405 (Al^{3+}, Zn^{2+}) / 427 (Al^{3+}), 496 (Zn^{2+})	3.7 µM, 3.86 µM	na	na	na	7
8		2	390/ 480 (Al^{3+}), 508 (Zn^{2+})	30.64 nM, 21.22 nM	yes	yes	yes	Present work

References:

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