Single step fluorescent recognition of As^{3+}, Nd^{3+} and Br^- consuming pyrene-allied calix[4]arene : Their application to real samples, computational modelling and paper based device

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INDEX

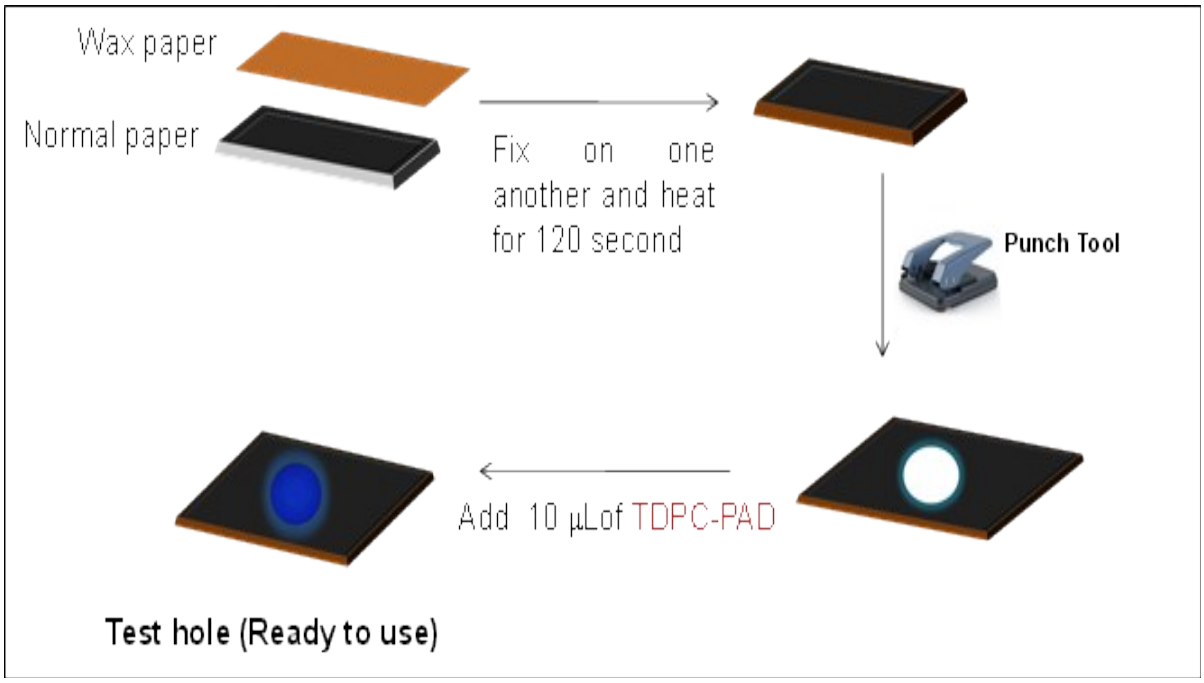

Figure S1: Fabrication of paper based wax printed test panel for the detection of ions

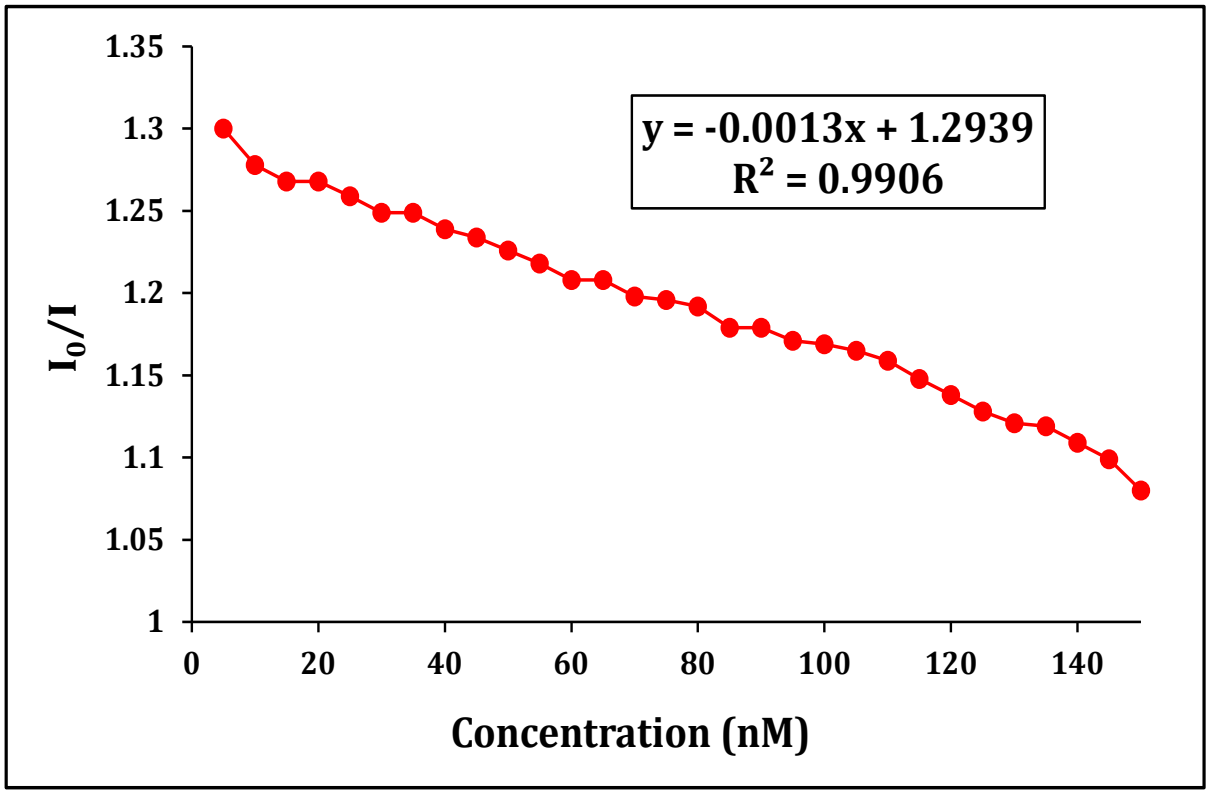

Figure S2: Linearity plots of TDPC (1×10^{-8} M) with As^{3+} (0-150 nM)

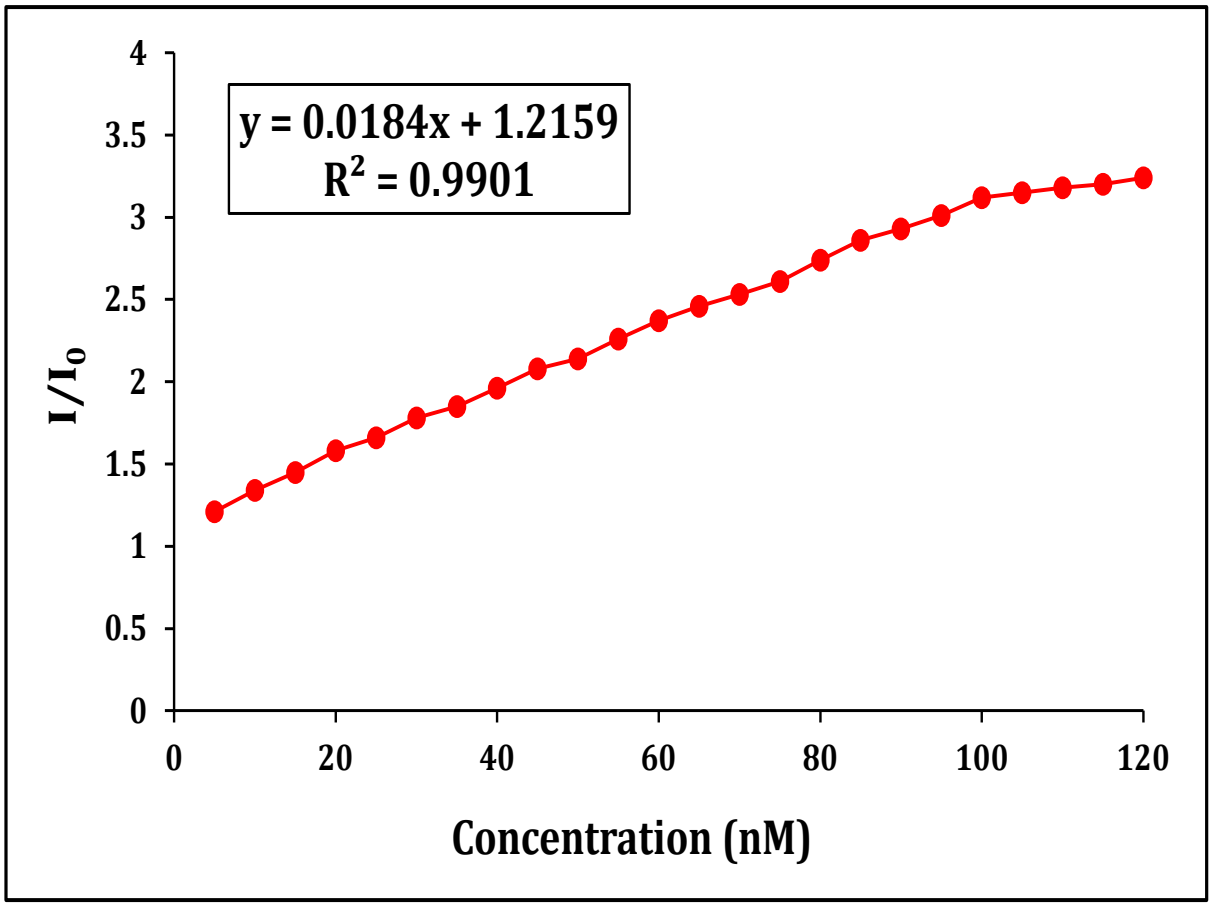

Figure S3: Linearity plots of TDPC (1×10^{-8} M) with Nd^{3+} (0-120 nM)

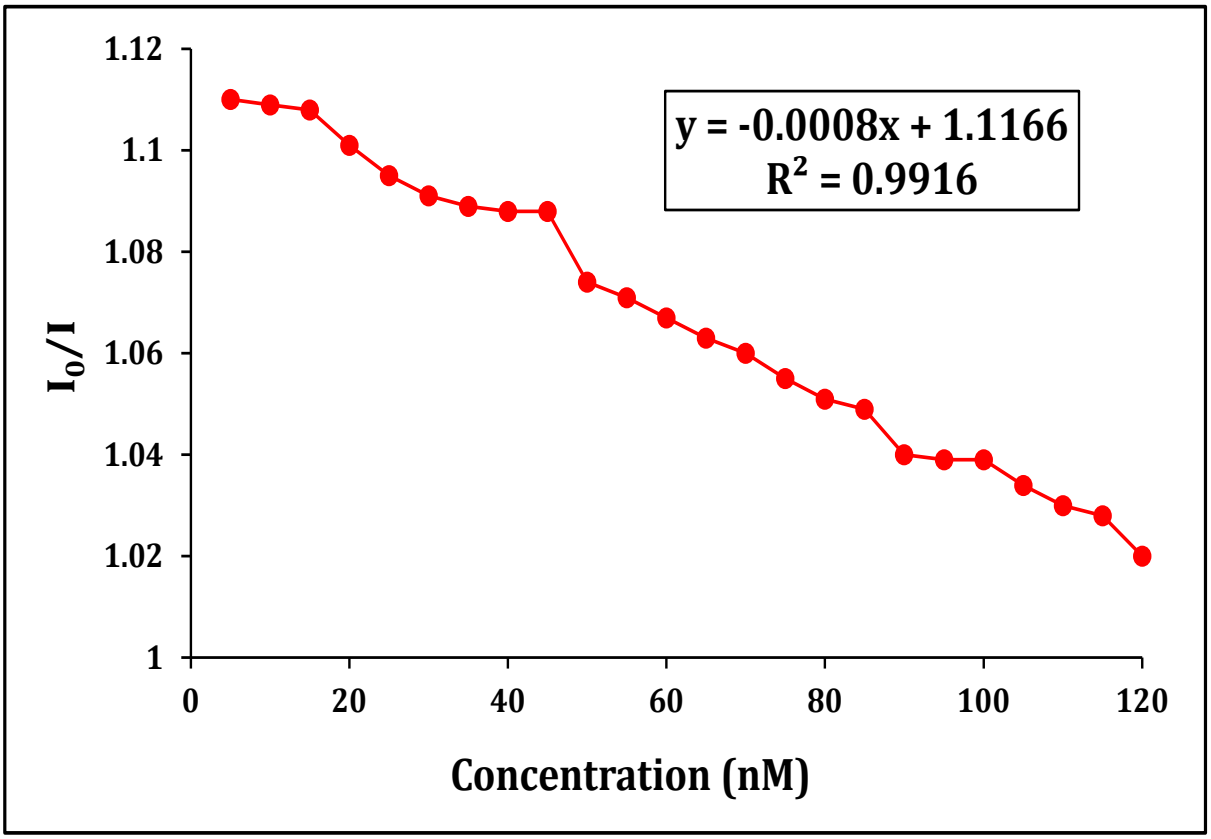

Figure S4: Linearity plots of TDPC (1×10^{-8} M) with Br^- (0-120 nM)

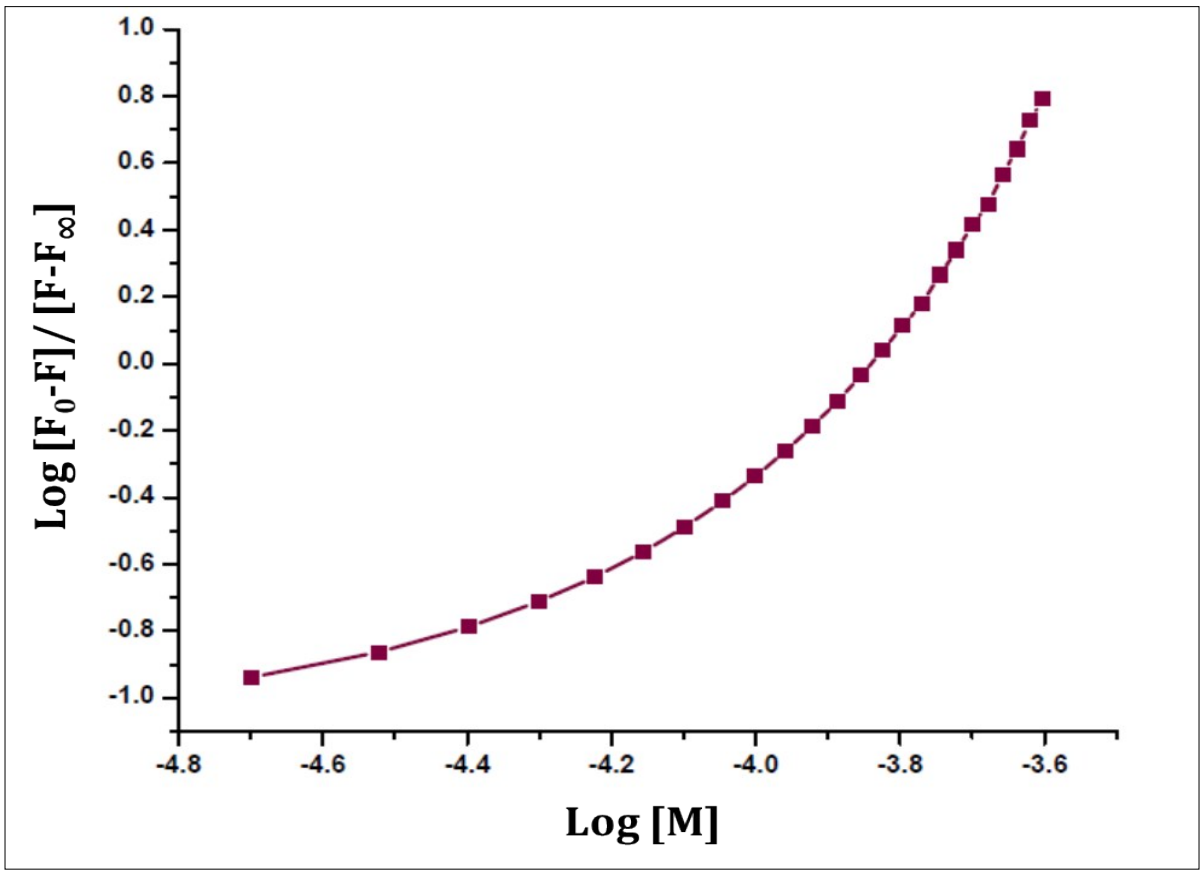

Figure S5: Binding constant plot for As^{3+} with TDPC ligand from emission titration.

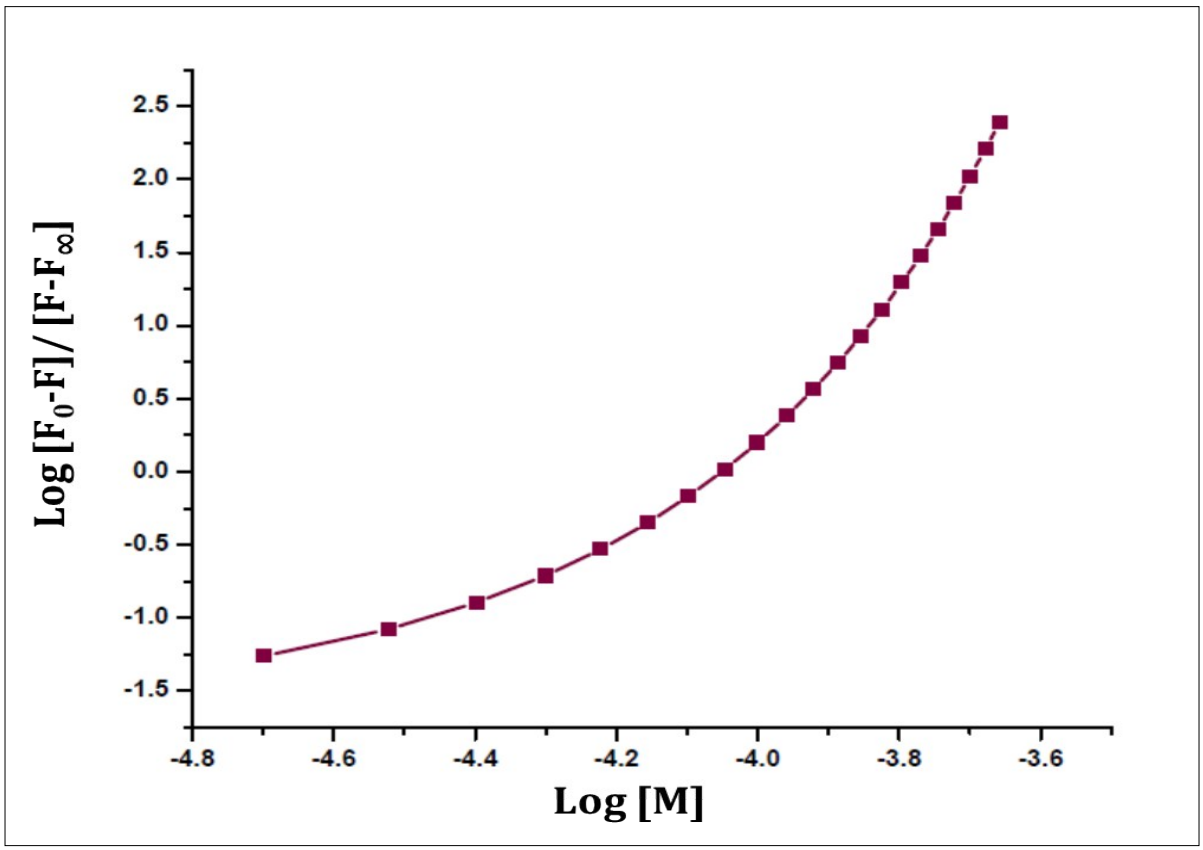

Figure S6: Binding constant plot for Nd^{3+} with TDPC ligand from emission titration.

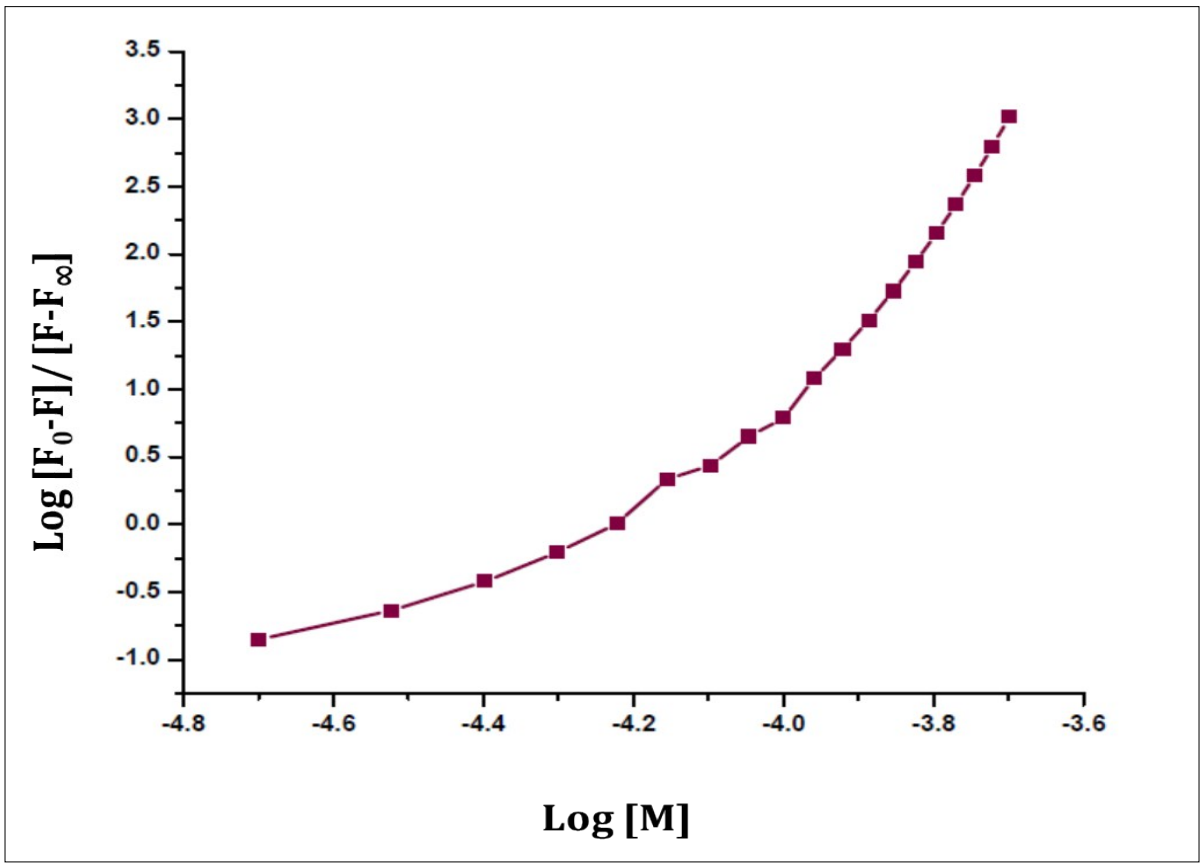

Figure S7: Binding constant plot for Br^- with TDPC ligand from emission titration.

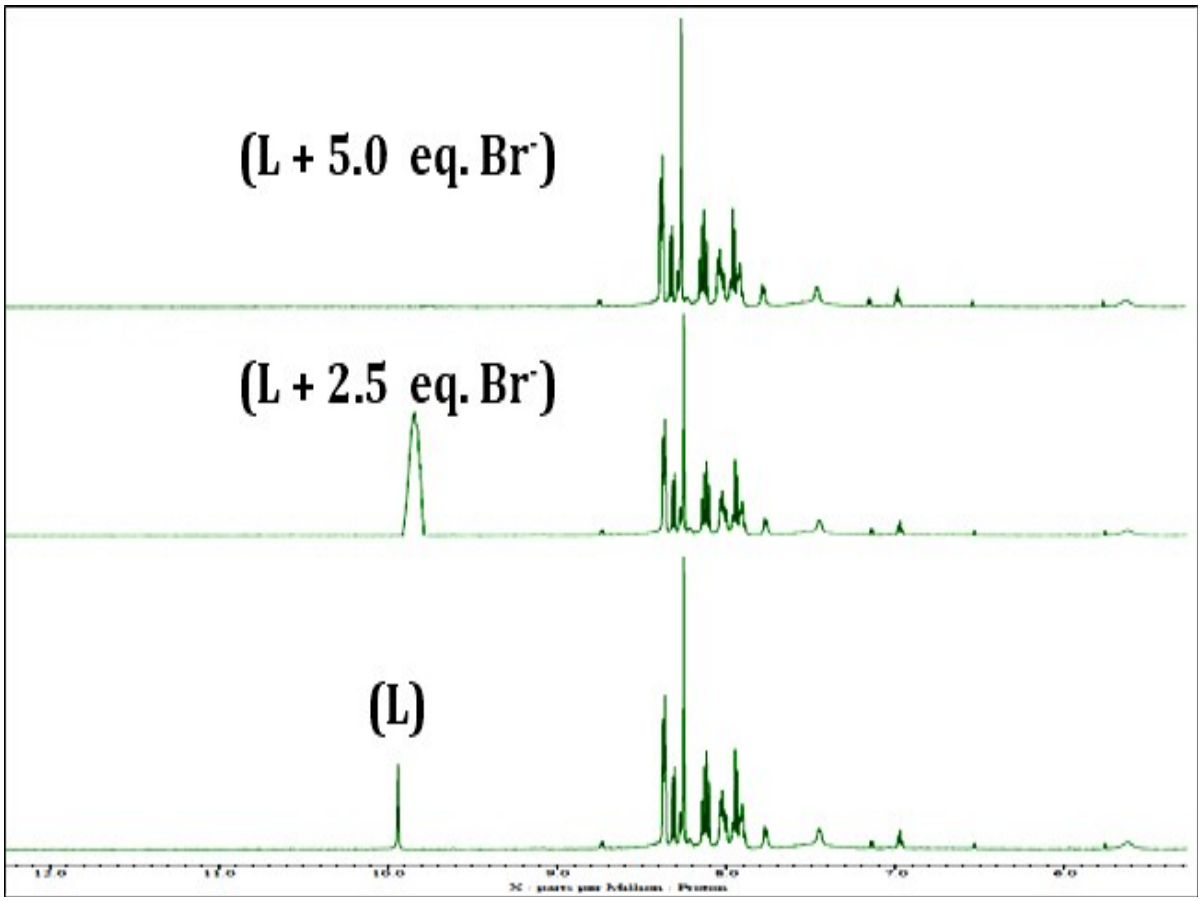

Figure S8: Selected portion of the ^{1}H NMR spectra for TDPC ligand and recorded in DMSO-d6 upon addition of 2.5 and 5 equivalent amount of Br^{-}.

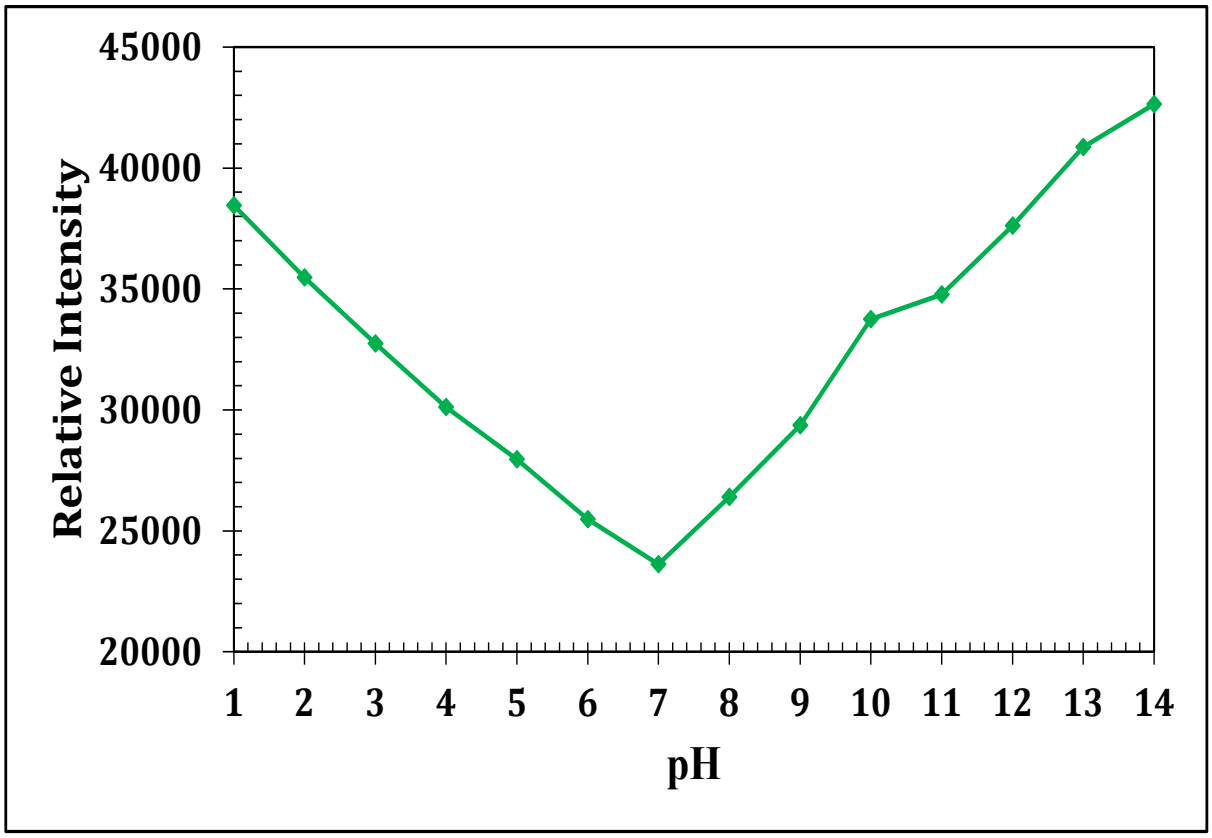

Figure S9: Shows the effect of fluorescence intensities of TDPC with As^{3+} complex by varying pH.

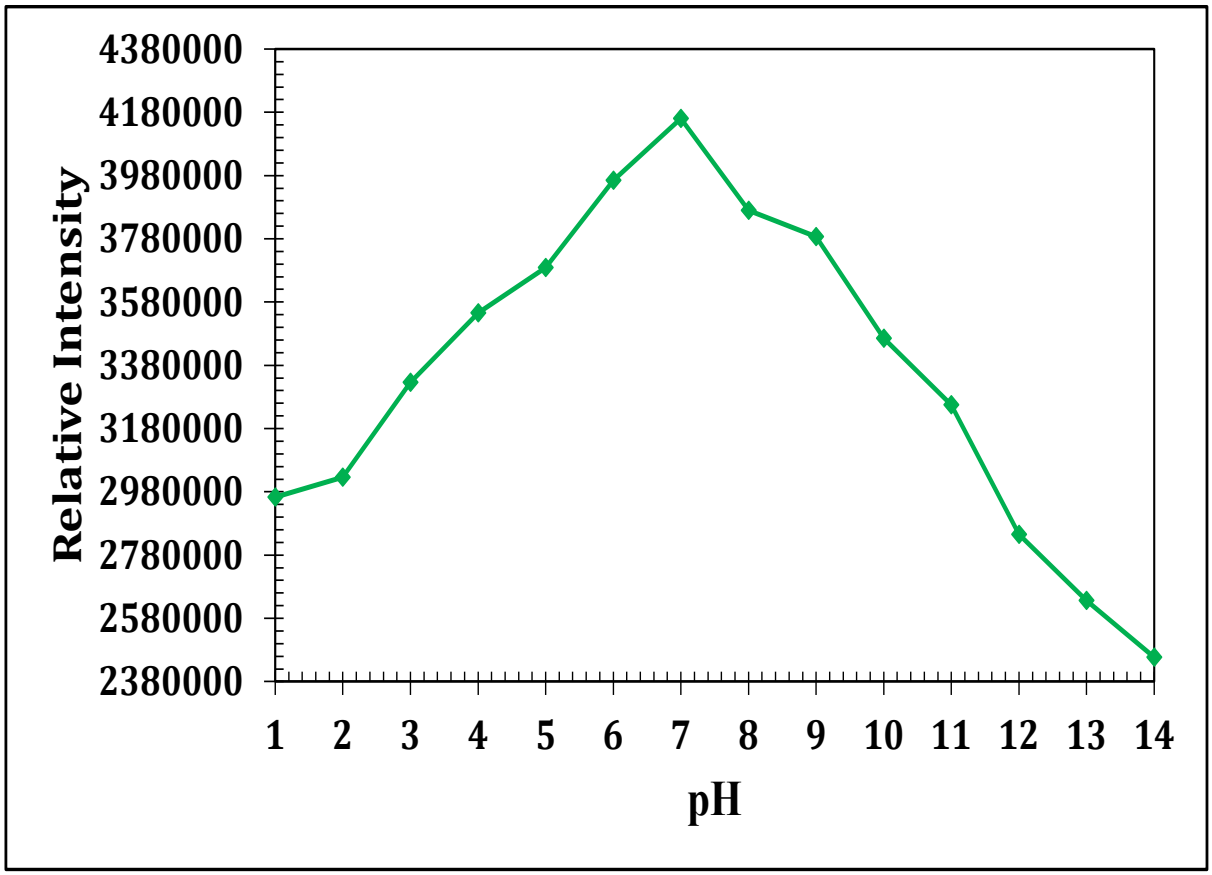

Figure S10: Shows the effect of fluorescence intensities of TDPC with Nd^{3+} complex by varying pH.

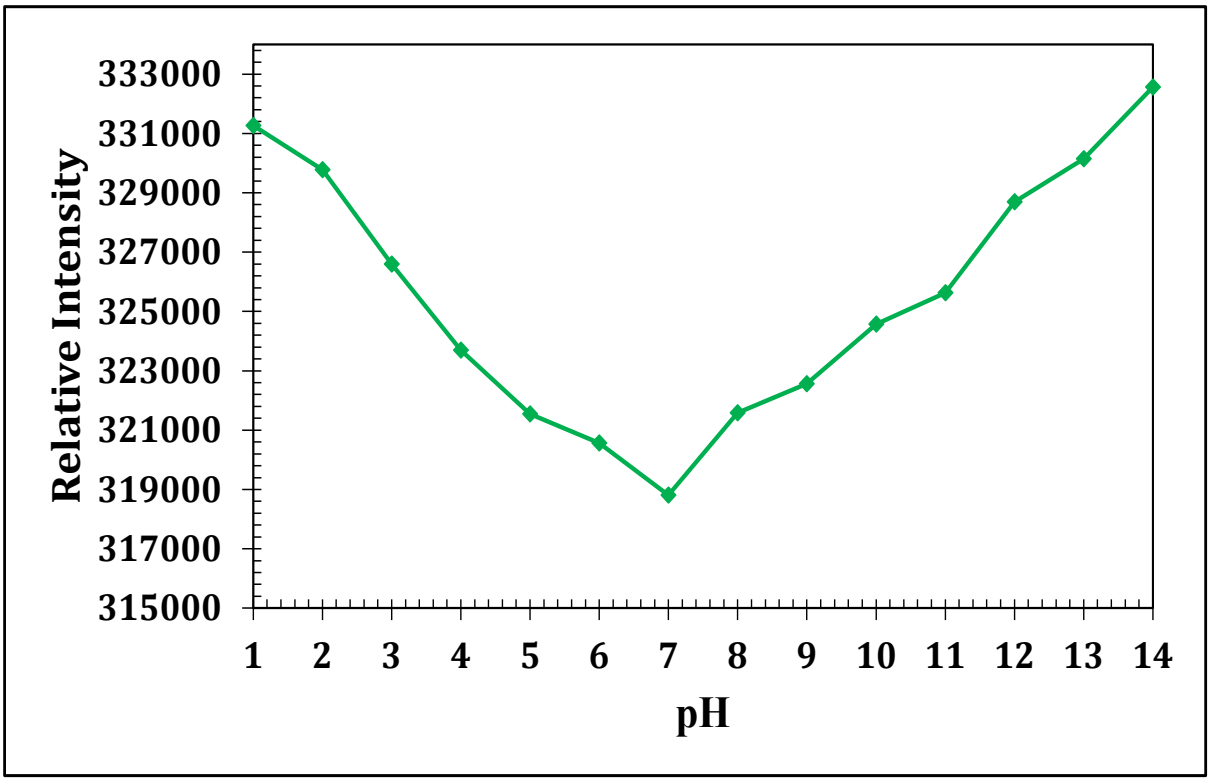

Figure S11: Shows the effect of fluorescence intensities of TDPC with and Br^- complex by varying pH.

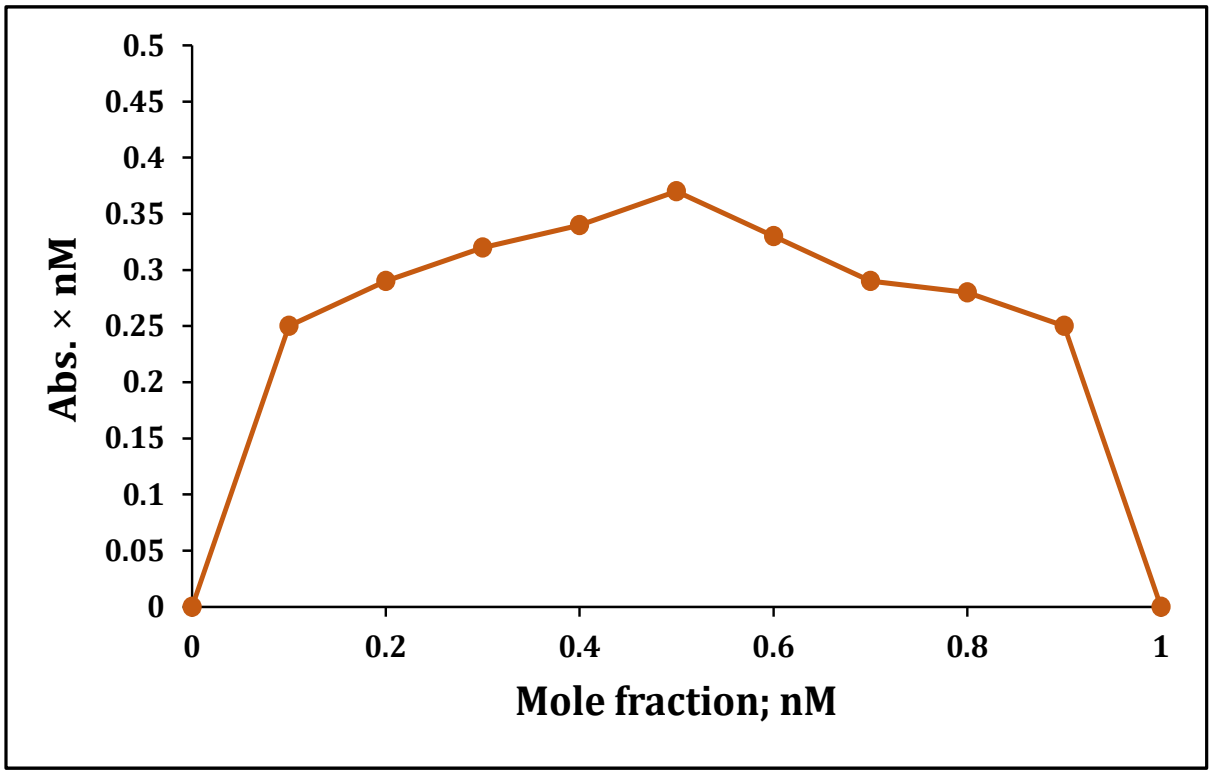

Figure S12: Job's plot obtained from the absorption titration of TDPC with As^{3+}.

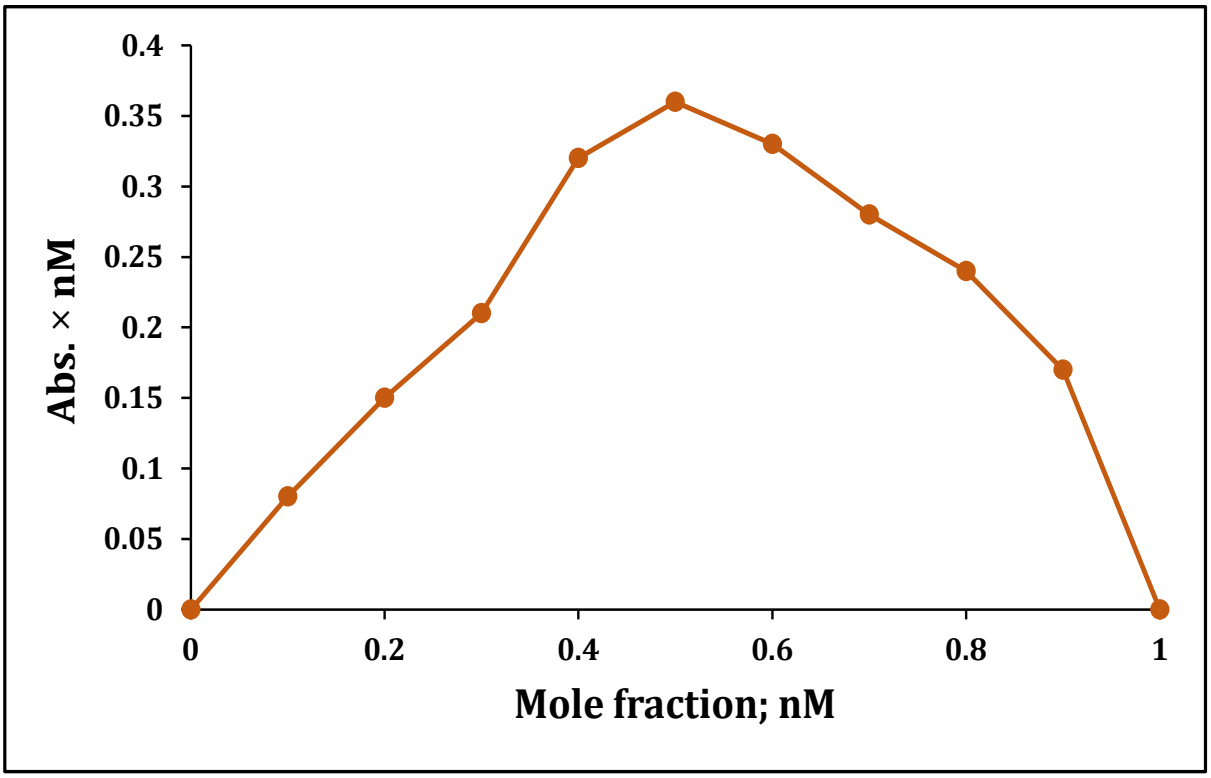

Figure S13: Job's plot obtained from the absorption titration of TDPC with Nd^{3+}.

Figure S14: Job's plot obtained from the absorption titration of TDPC with Br^-.

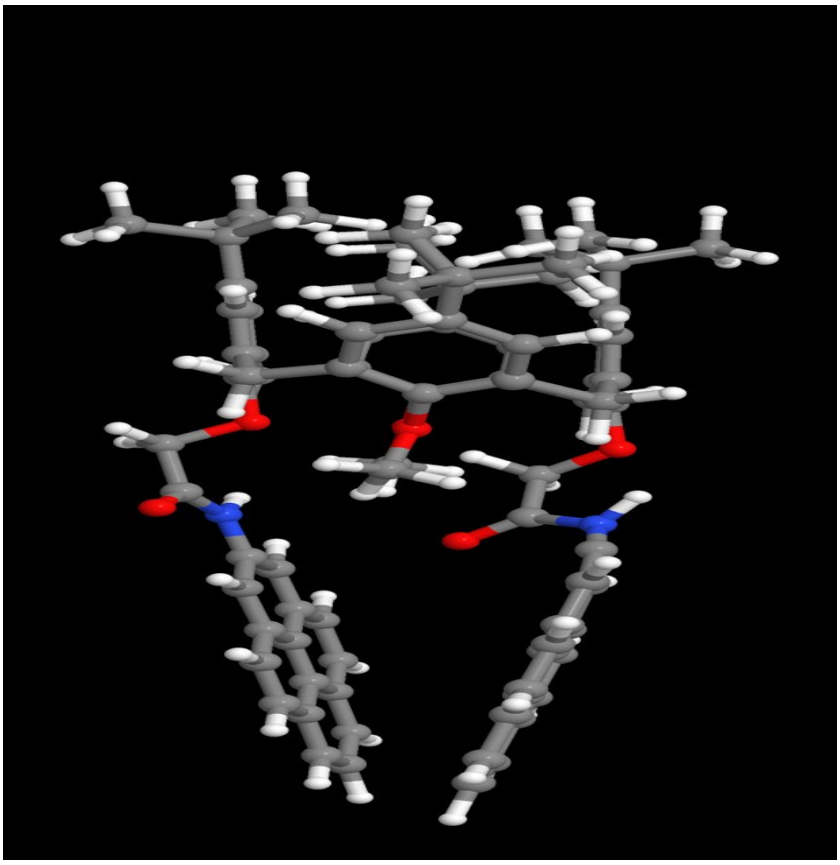

Figure S15: Optimized geometry of TDPC molecule.

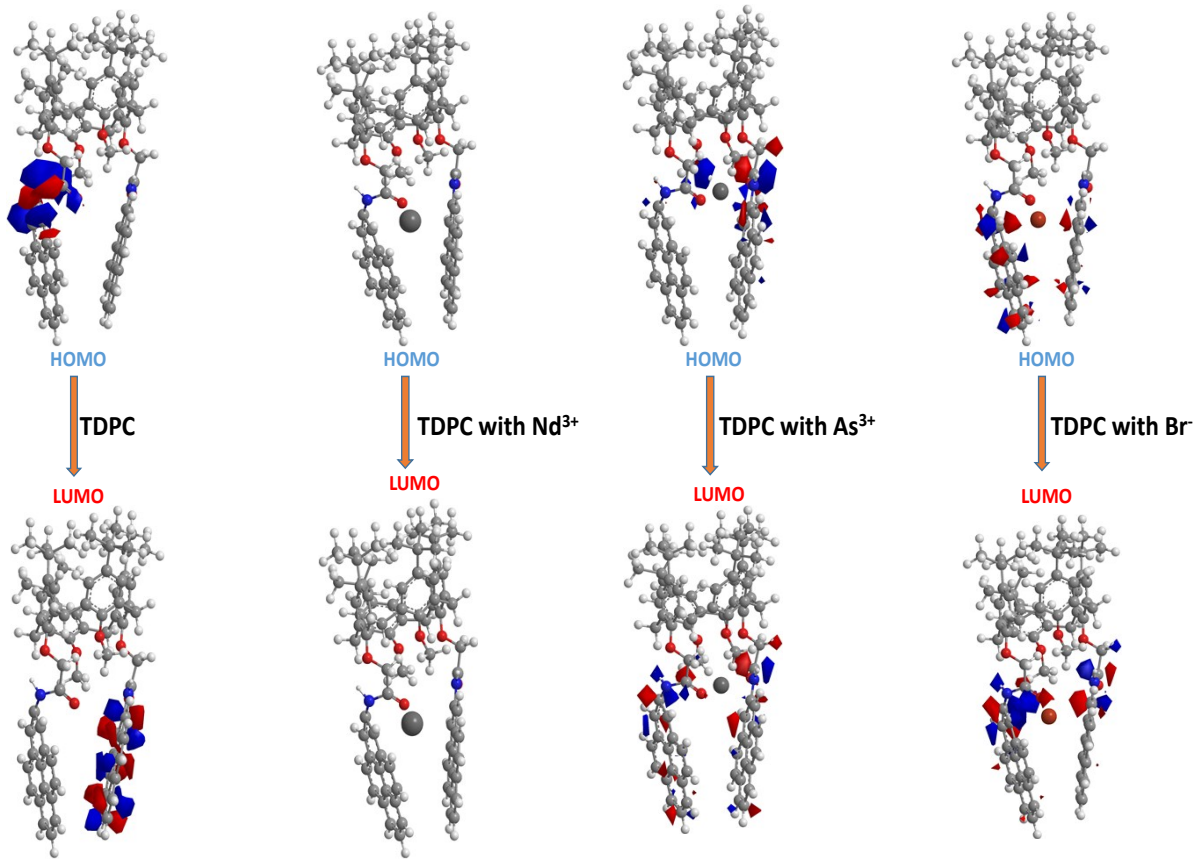

Figure S16: HOMO- LUMO orbital analysis of free ligand TDPC with Nd^{3+}, As^{3+} and Br^{-} complexes.

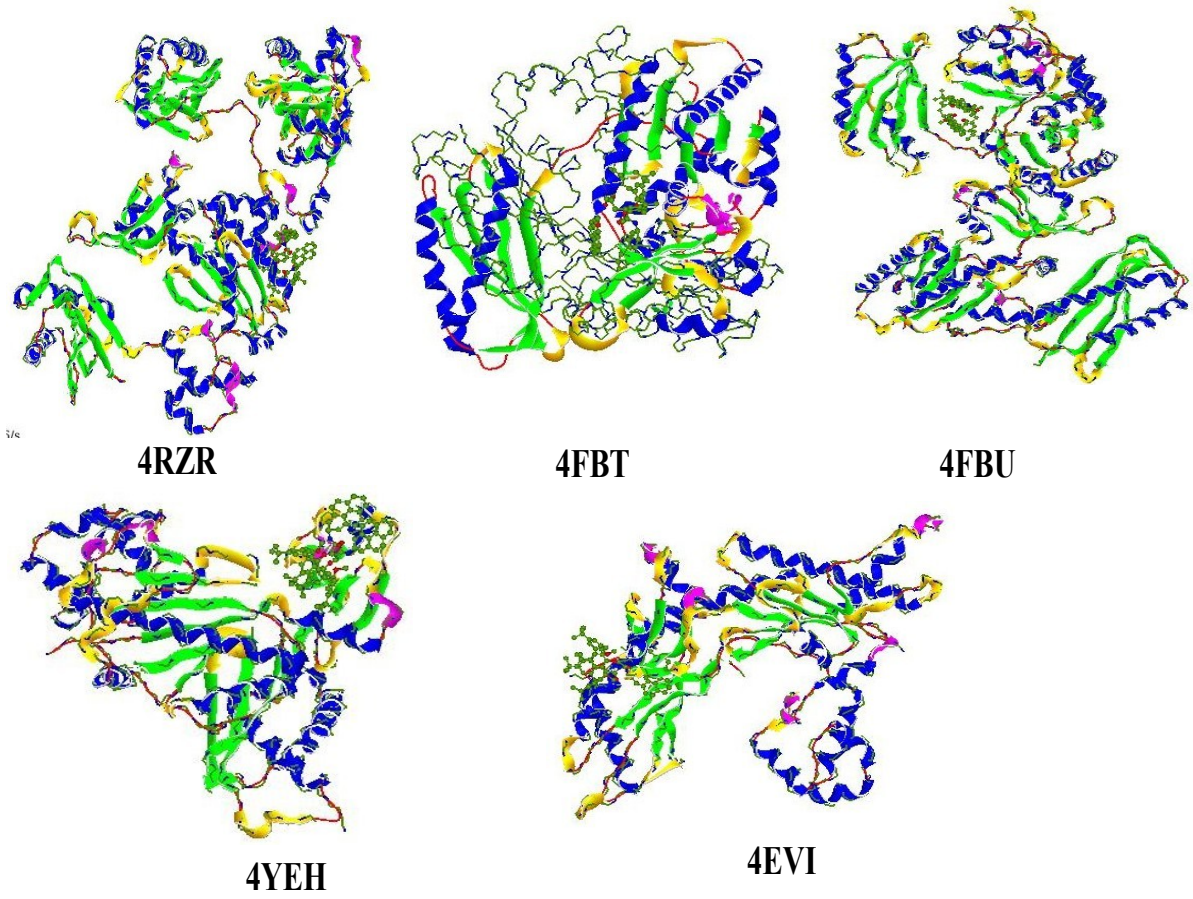

Figure S17: Molecular docking interaction between the title molecule TDPC and 4RZR, 4FBT, 4FBU, 4EYH and 4EVI; Molecule TDPC is shown by solid surface form and protein receptors are shown by ribbon form

Method	Recognized ion	Linear Range	Limit of Detection	Ref
PVC membrane	Nd^{3+}	1.0×10^{-2} - 1×10^{-6} M	6.2×10^{-7}M	44
Selective PVC membrane	Nd^{3+}	5.0×10^{-7} - 1.0×10^{-2}M	1.0×10^{-7}M	45
PVC membrane	Nd^{3+}	5.0×10^{-6} - 1.0×10^{-2} M	4.8×10^{-6} M	46
Colorimetric sensor	As^{3+}	5.0- 100 ppb	7.2 ppb	47
Nanoporous gold microelectrode (Anodic stripping voltammetry)	As^{3+}	10-200 µg L^{-1} - 2-30 µg L^{-1}	0.62 µg L^{-1}	48
Colorimetric Detection	As^{3+}		54 nM	49
Selective polymeric membrane electrode	Br^-	2.2×10^{-6} - 1.0×10^{-1}M	1.4×10^{-6} M	50
Potentiometric ion selective electrode	Br^-	10^{-5} – 10^{-2} M	7.8×10^{-6} M	51
Electrochemical sensors	Br^-	10-1000 µM	1.56 µM	52

Table S1: Comparison of proposed TDPC fluorescence sensor with various previously reported determination methods for Nd^{3+}, As^{3+} and Br^-.

Molecule	HOMO	LUMO	Energy Gap
TDPC	-6.895	-4.760	-2.135
TDPC with Nd^{3+}	-7.373	-7.373	0.001
TDPC with As^{3+}	-2.071	-1.267	-0.804
TDPC with Br^{-}	-4.281	-1.565	-2.716

Table S2: HOMO, LUMO and energy gap values of free TDPC and TDPC with Nd^{3+}, As^{3+} and Br^{-} complexes

Different receptors	E VALUE (Kcal/mol)
4RZR	-485.77
4FBT	-500.94
4FBU	-441.09
4EYH	-414.11
4EVI	-404.40

Table S3: Energy value docking results of different receptors with ligand molecules using hex software