Supporting Material

for

Turn-on detection of Al^{3+} and Zn^{2+} ions by NSN donors probe: Reversibility, logic gates and DFT calculations

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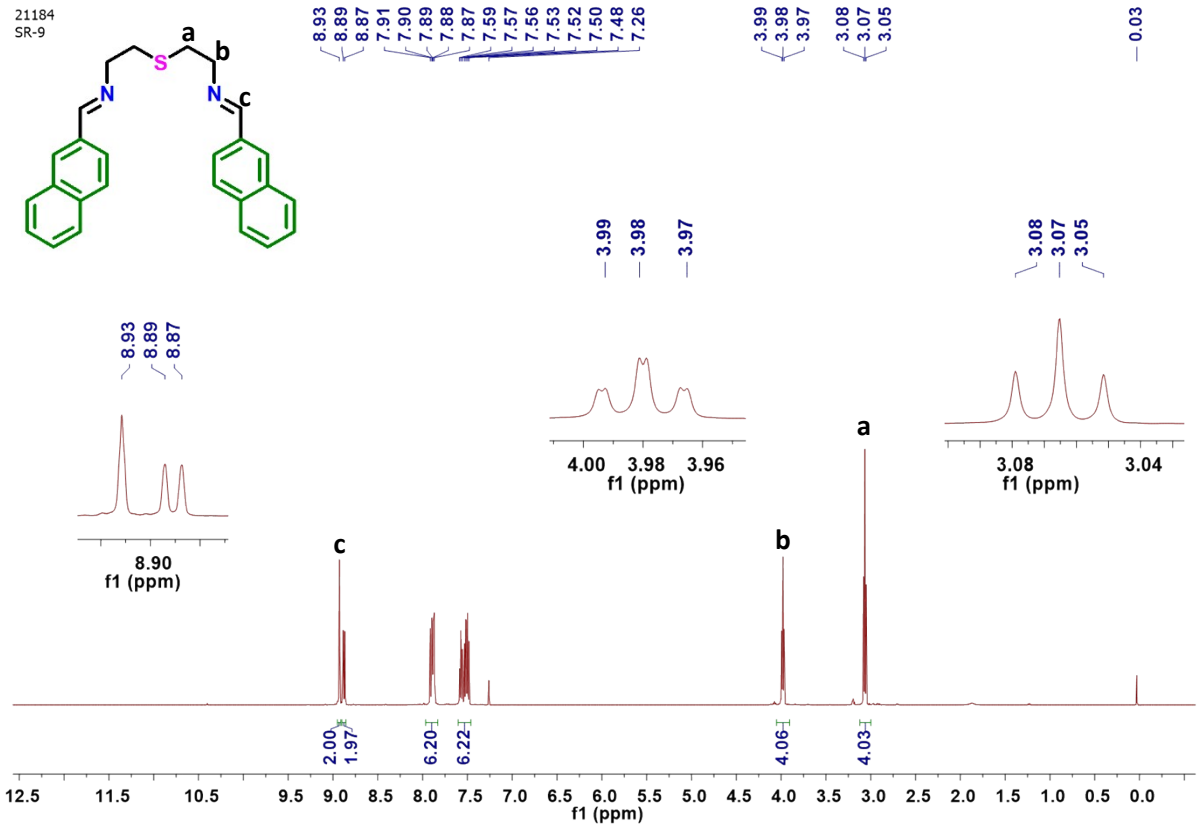

Fig. S1. ^{1}H NMR spectrum of **NpSb** in $CDCl_3$ at room temperature. ^{1}H NMR ($CDCl_3$, 500 MHz, TMS), δ (ppm): 8.93 (s, 2H, -C<u>H</u>=N-), 8.89 (m, 2H), 7.89 (m, 6H), 7.59-7.48 (m, 6H), 3.98 (t, 4H, -C<u>H</u>$_2$-N-), 3.07 (t, 4H, -C<u>H</u>$_2$-S<).

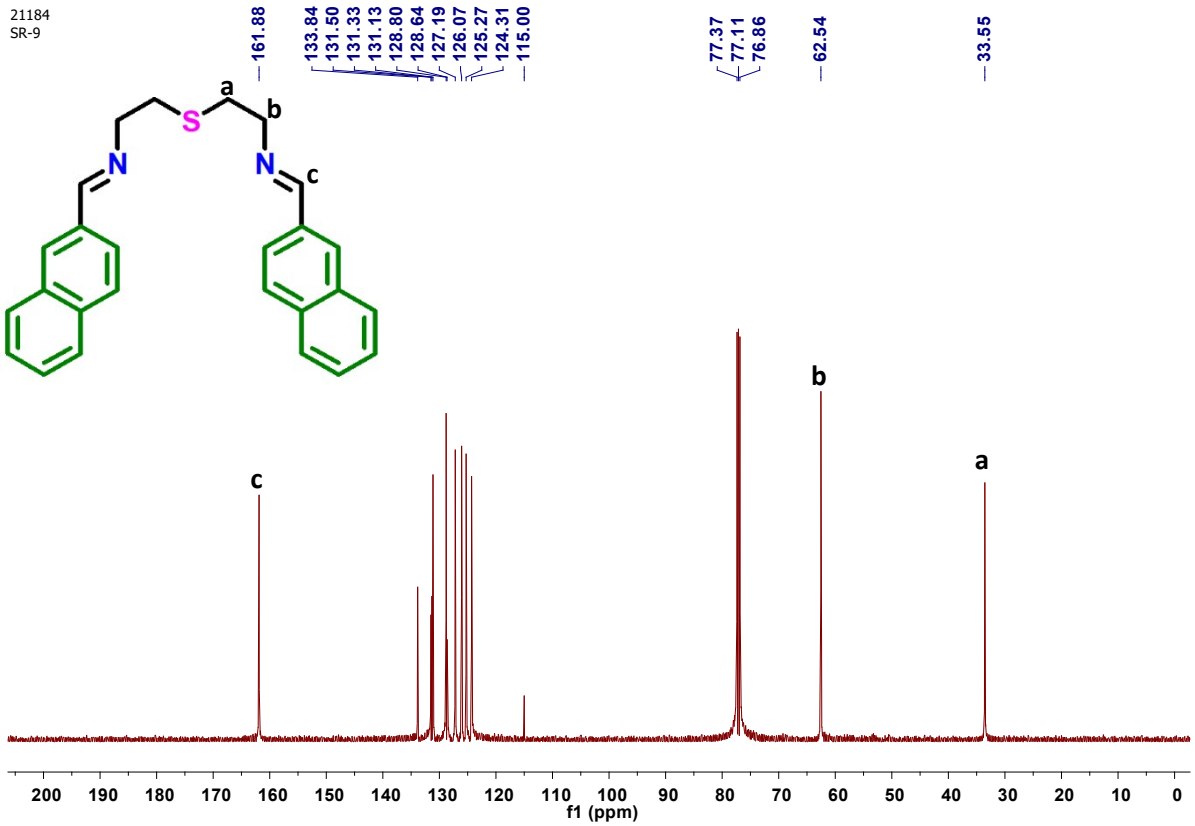

Fig. S2. ^{13}C NMR spectrum of **NpSb** in $CDCl_3$ at room temperature. ^{13}C NMR ($CDCl_3$, 500 MHz), δ (ppm): 161.88, 133.84, 131.50, 131.33, 131.13, 128.80, 128.64, 127.19, 126.07, 125.47, 124.31, 115.00, 62.54, 33.55.

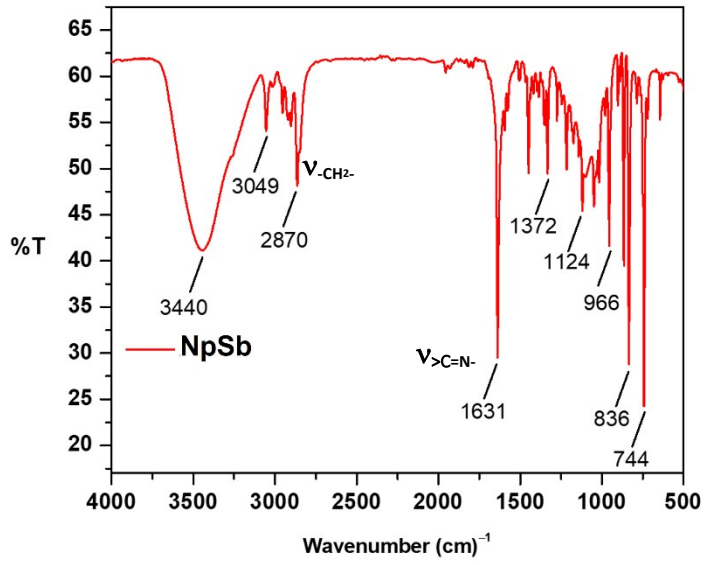

Fig. S3. FT-IR spectrum of **NpSb**. IR data (KBr disk, cm^{-1}): 3440, 3049, 2870 ,1631 ($\nu_{C=N}$), 1372, 1124, 966, 836, 744.

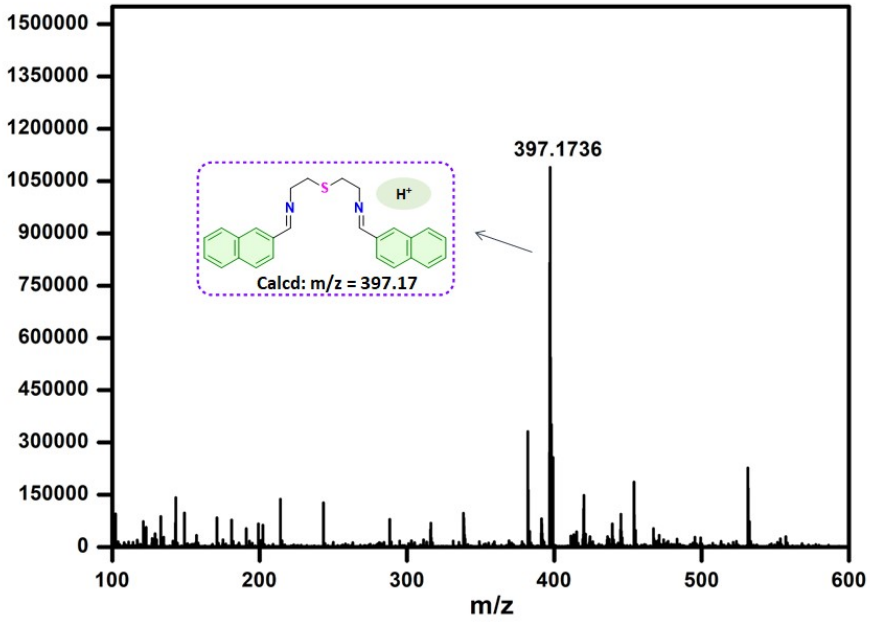

Fig. S4. ESI-MS analysis of probe **NpSb** in methanol at room temperature.

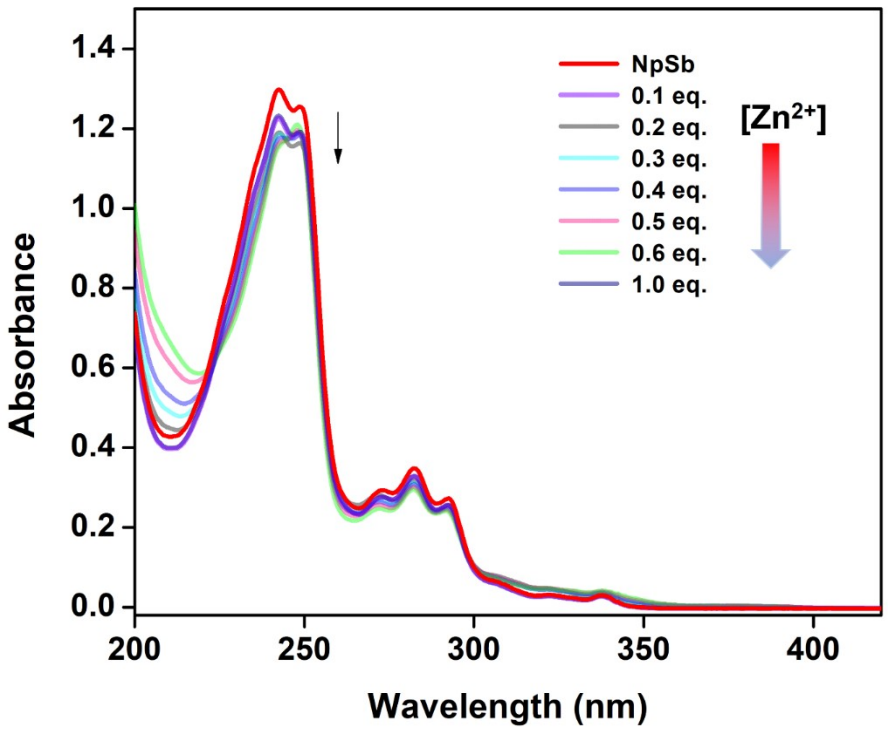

Fig. S5. UV-Vis spectral changes for **NpSb** (1.0 x 10^{-5} M) in CH_3CN-H_2O (4:1, v/v) after successive addition of Zn^{2+} ions (0-1.0 equiv.).

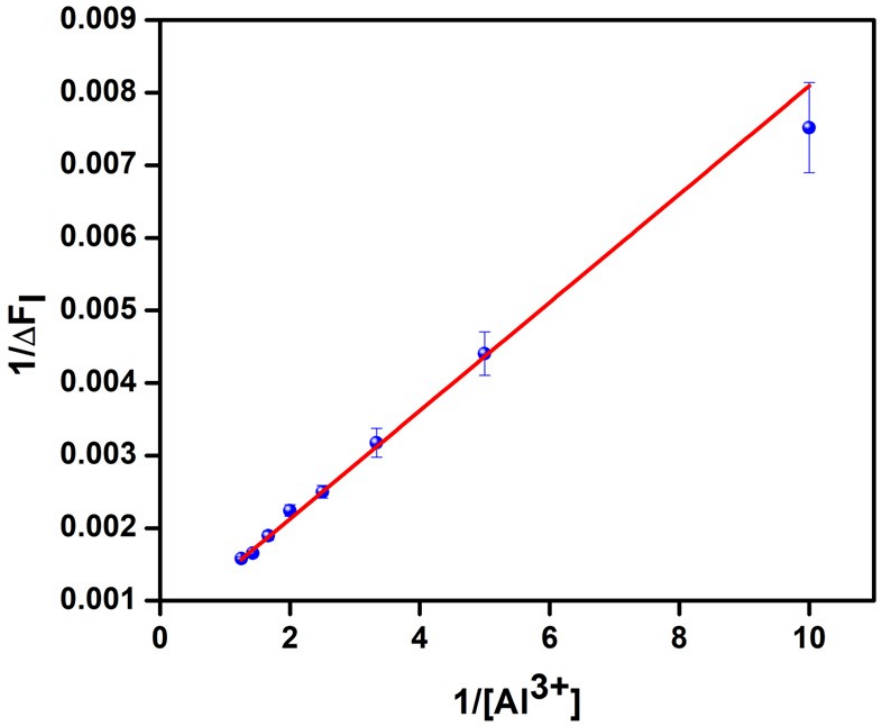

Fig. S6. Determination of binding constant of **NpSb** for Al^{3+} by employing Benesi-Hildebrand plots from fluorescence spectroscopy.

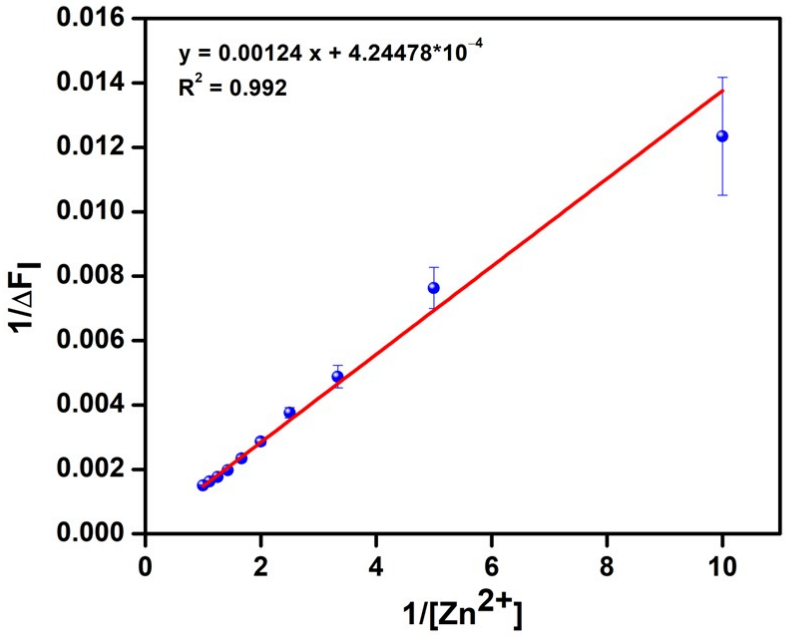

Fig. S7. Determination of binding constant of **NpSb** for Zn^{2+} by employing Benesi-Hildebrand plots from fluorescence spectroscopy.

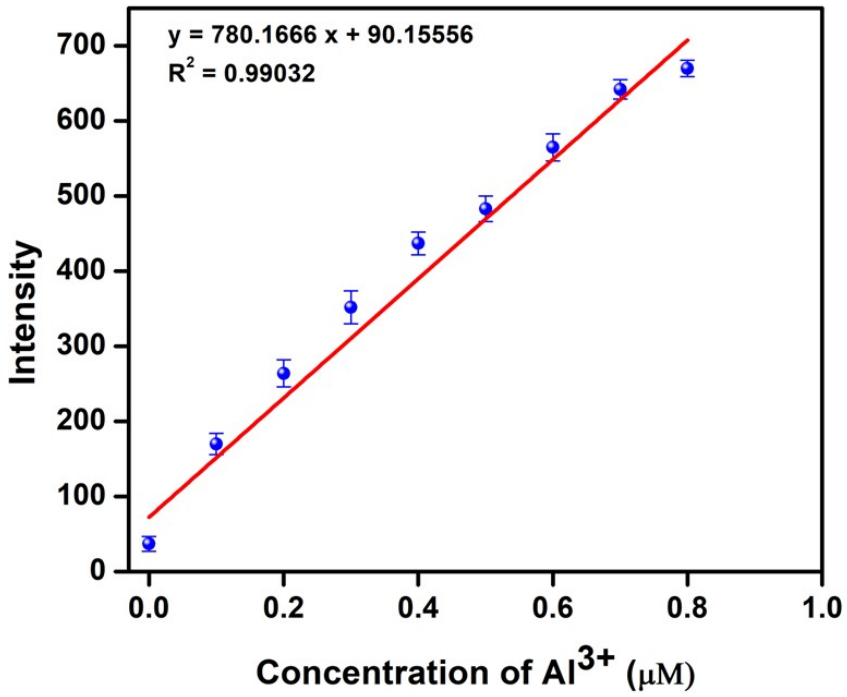

Fig. S8. Linear curves of the emission intensity of **NpSb** with Al^{3+} for the determination of LoD in CH_3CN-H_2O (4:1, v/v).

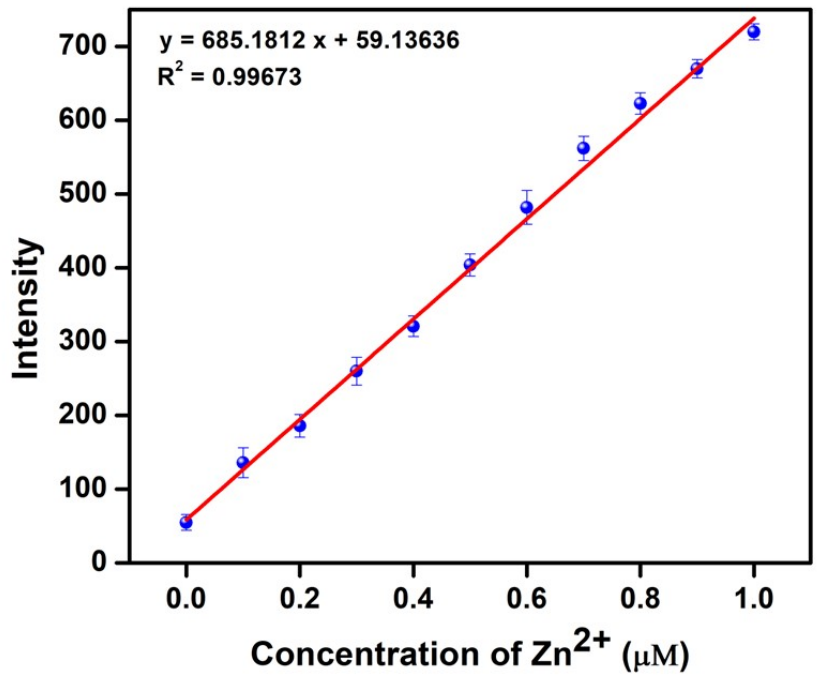

Fig. S9. Linear curves of the emission intensity of **NpSb** with Zn^{2+} for the determination of LoD in CH_3CN-H_2O (4:1, v/v).

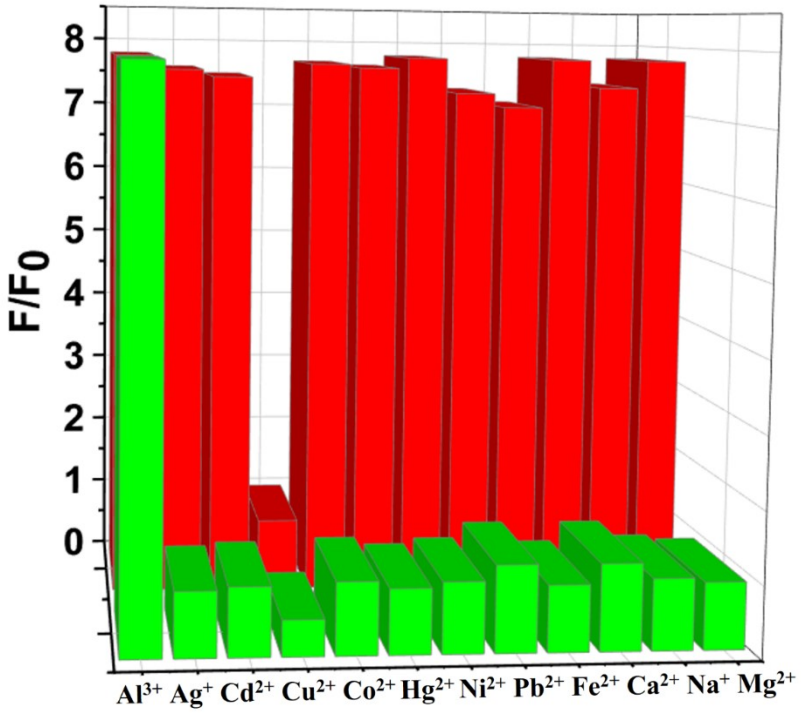

Fig. S10. Relative fluorescence Intensity of **NpSb** with Al^{3+} in the presence of 10 equiv of other cations in CH_3CN-H_2O (4:1, v/v).

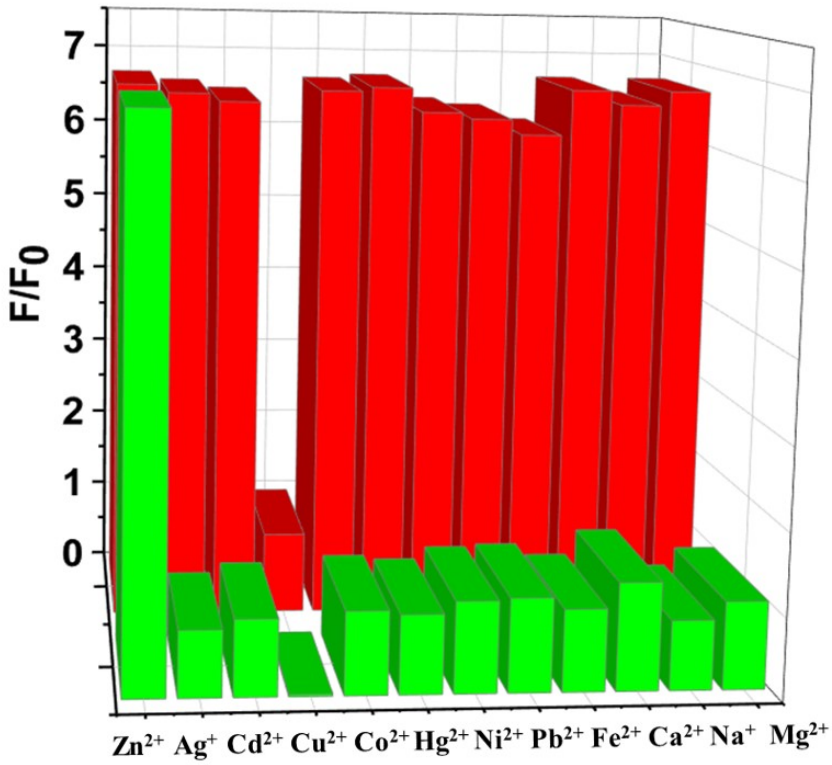

Fig. S11. Relative fluorescence intensity of **NpSb** with Zn^{2+} in the presence of 10 equiv of other cations in CH_3CN-H_2O (4:1, v/v) solution.

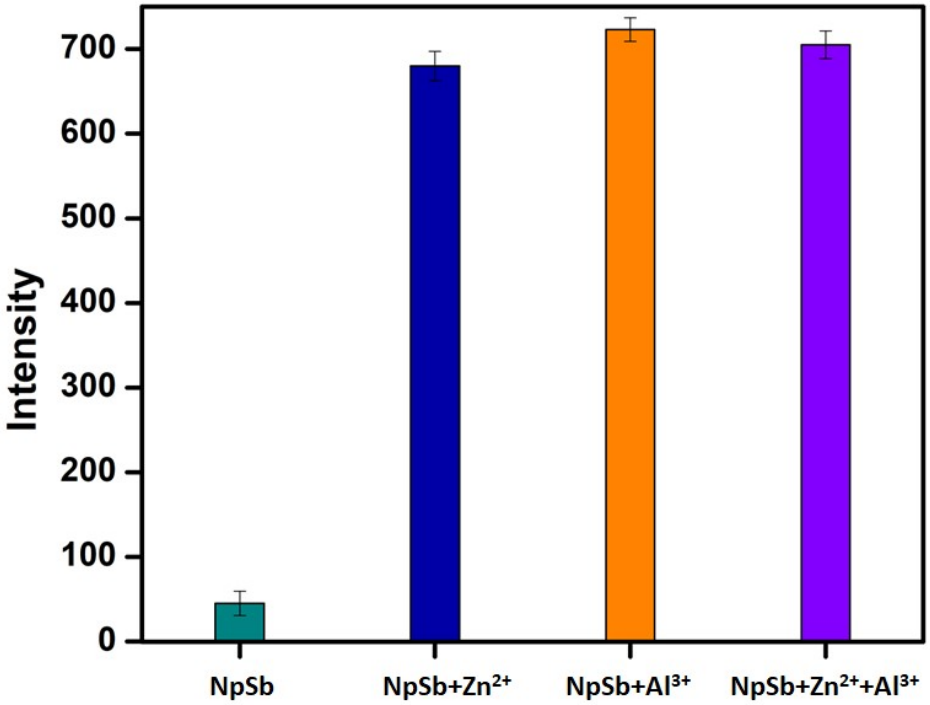

Fig. S12. Fluorescence Intensity of **NpSb** with Al^{3+} and Zn^{2+} in CH_3CN-H_2O (4:1, v/v) solution.

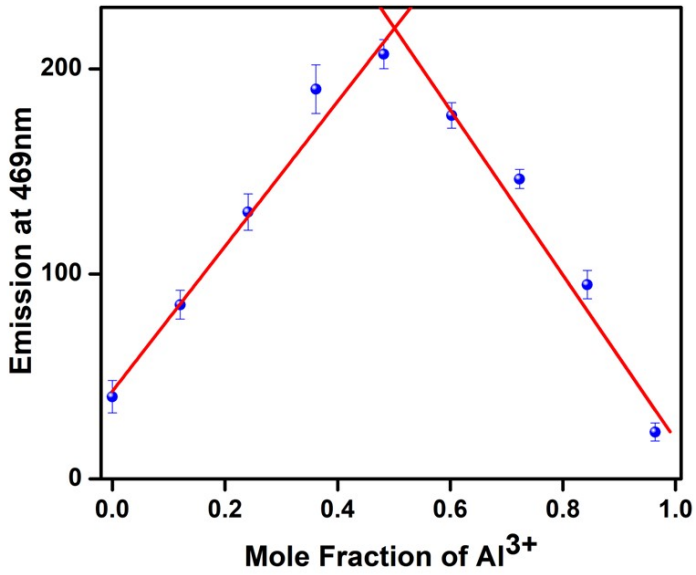

Fig. S13. Job's Plot analyses for **NpSb** *vs*. Al^{3+}

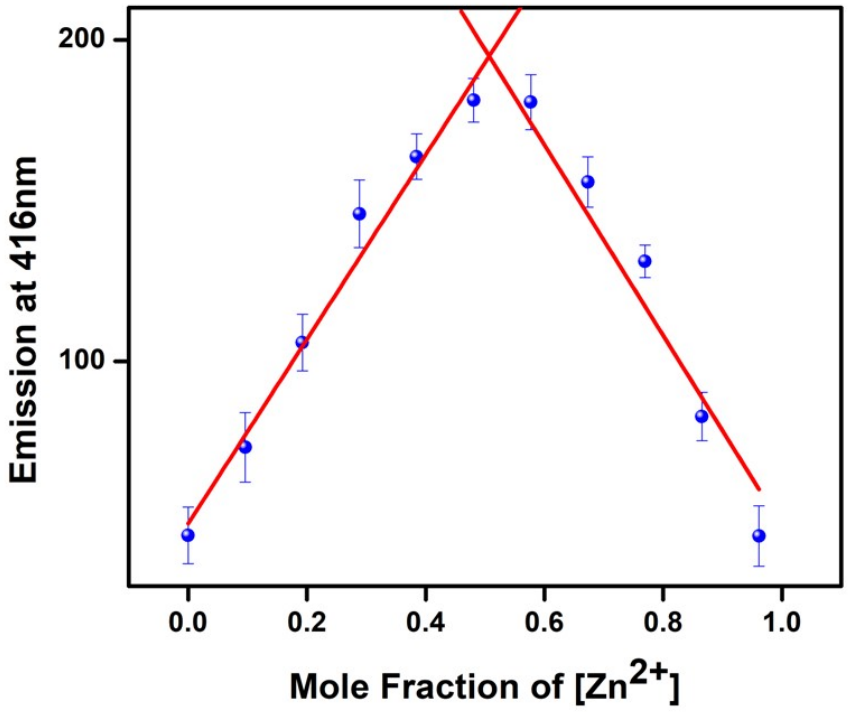

Fig. S14. Job's Plot analyses for **NpSb** *vs*. Zn^{2+}

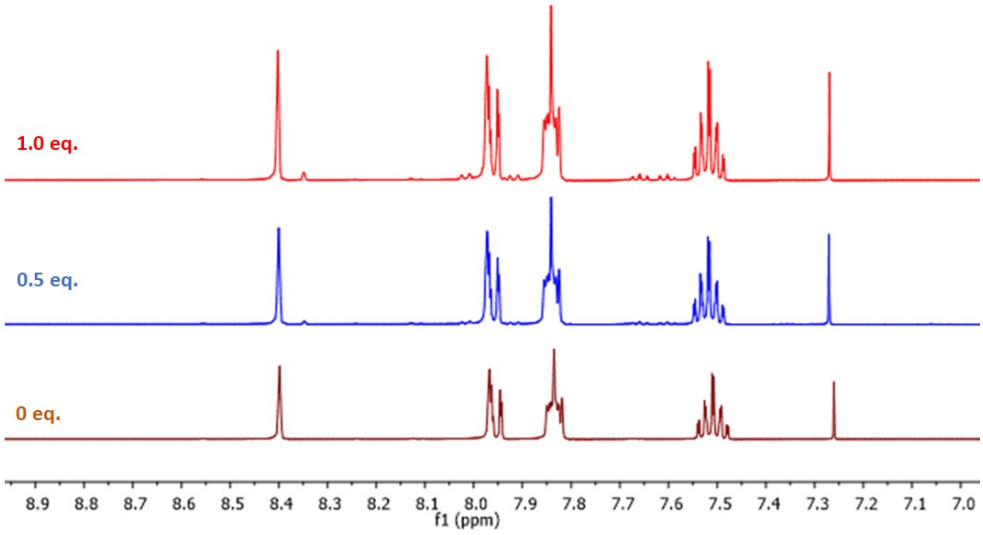

Fig. S15.^{1}H NMR spectra of **NpSb** when treated with Zn^{2+} ions.

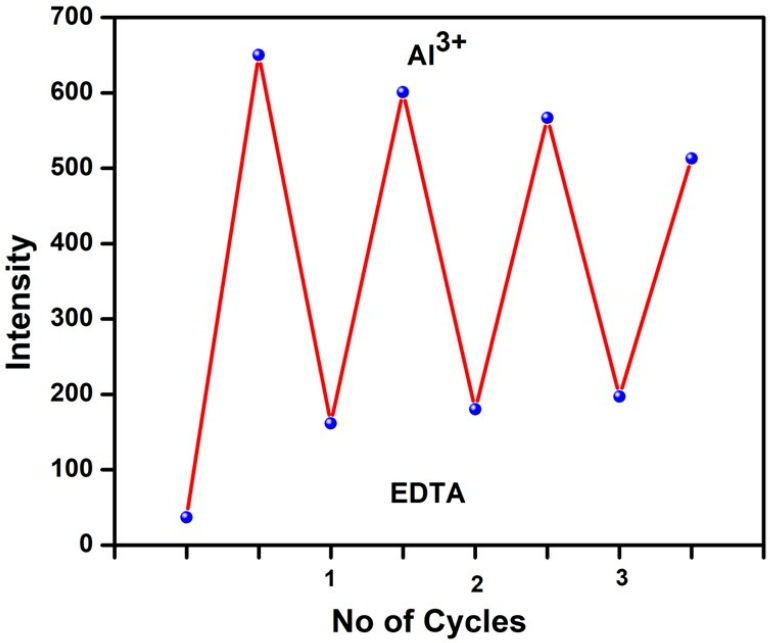

Fig. S16. Emission intensity of **NpSb** after the alternate addition of Al^{3+} and EDTA.

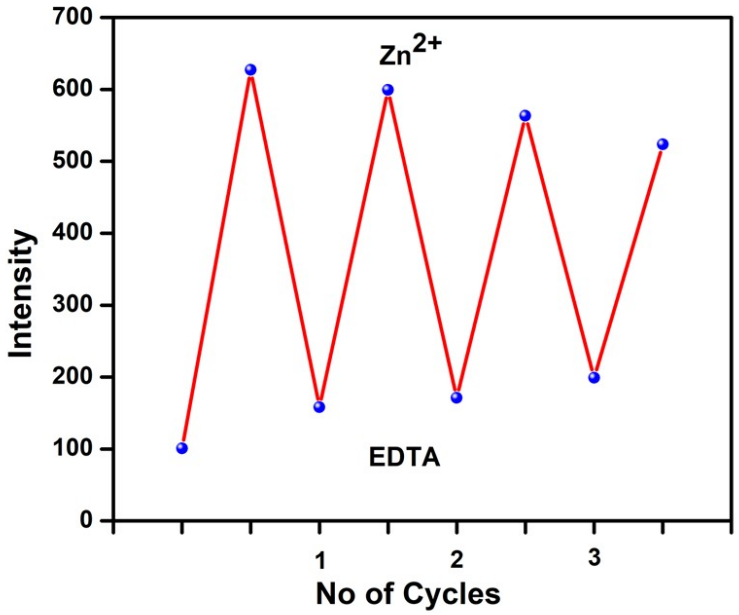

Fig. S17. Emission intensity of **NpSb** after the alternate addition of Zn^{2+} and EDTA.

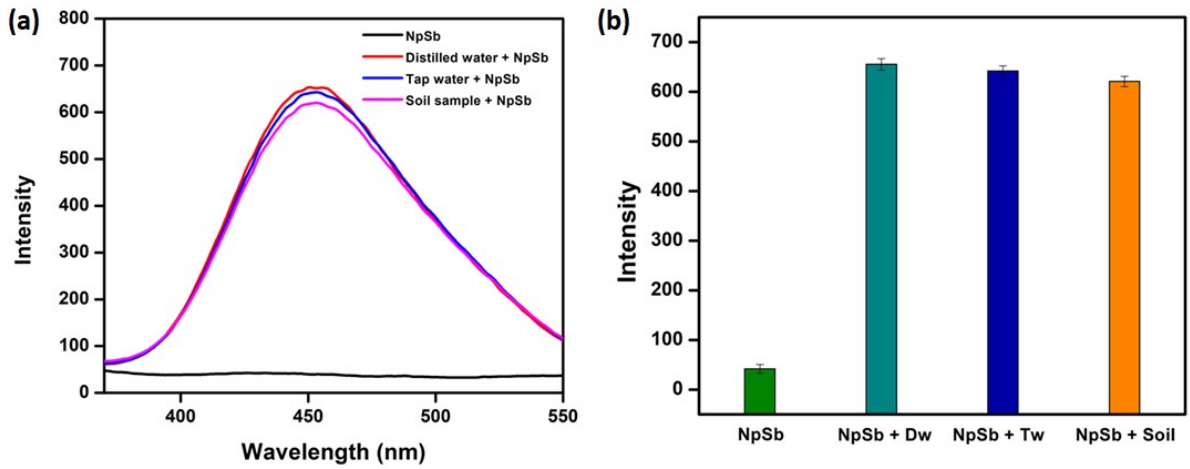

Fig. S18. Interaction of probe **NpSb** with real samples (distilled water, tap water and soil sample) spiked with 2.0 equiv of Al^{3+} ions. (Dw = distilled water; Tw = tap water).

Calculation of Quantum Yield.

The fluorescence quantum yield (Φ) was calculated via integration of the area under fluorescence curve using equation.

$$\Phi_{sample} = \Phi_{ref} \times \frac{OD_{ref} \times A_{sample} \times \zeta_{sample}}{OD_{sample} \times A_{ref} \times \zeta_{ref}}$$

Where, OD = Optical density,

ζ = Refractive indices of solvent

A= Area under the curve

The standard use for the calculation was anthracene (0.27 in ethanol) with excitation at 340nm.

Table S1. Crystallographic data for **NpSb**.

Formula	$C_{26}H_{24}N_2S$
Formula weight ($gmol^{-1}$)	396.53
Space group (hall)	-P 2yn
Temperature/K	150(2)
λ (Å) (Cu-Kα)	1.54184
Crystal system	monoclinic
a (Å)	5.7751(6)
b (Å)	46.275(3)
c (Å)	7.7780(8)
α(˚)	90
β (˚)	90.655(10)
γ (˚)	90
V ($Å^3$)	2078.5(3)
Z	4
ρ_{calc}(gcm^{-3})	1.267
Crystal size (mm)	0.18 × 0.15 × 0.10
F(000)	840
Index ranges	-7 <*h*<7
	-56 <*k*< 56
	-9<*l*< 9
Reflns/ para/ restraints.	3889/263/407
GOF on F^2	1.119
*R*1[a] [$I > 2\sigma(I)$]	0.1178
*R*1[all data]	0.1694
*wR*2[b] [$I > 2\sigma(I)$]	0.3025
*wR*2 [all data]	0.3474

[a]R1= Σ||Fo|-|Fc||/Σ|Fo|; [b]wR2=|Σw(|Fo|^2- |Fc|^2)|/Σ|w(Fo)^2|$^{1/2}$

Table S2. Selected bond lengths [Å] and angles [°] in the single crystals of **NpSb**.

Bond Length (Å)		**Bond Angle (°)**	
S(1)–C(13)	1.784(10)	C(13)–S(1)–C(14)	101.7(5)
S(1) –C(14)	1.803(9)	C(12)–C(13)–S(1)	112.6(7)
C(13)–C(12)	1.510(13)	C(15)–C(14)–S(1)	112.6(6)
C(14)–C(15)	1.510(13)	C(15)–N(2)–C(16)	116.1(8)
C(12)–N(1)	1.477(12)	C(11)–N(1)–C(12)	116.0(10)
C(15)–N(2)	1.478(11)		
C(11)–N(1)	1.263(12)		
C(16)–N(2)	1.257(11)		

Table S3. Detection of Al^{3+} in real samples.

Tap water	**Al^{3+} added (µM)**	**Al^{3+} calculated (µM)**	**% Recovery**
	0.3	0.28	93.3
	0.8	0.77	96.2
Distilled water			
	0.3	0.29	96.6
	0.8	0.83	103.7
Soil sample			
	0.3	0.31	103.3
	0.8	0.81	98.7