Supporting information

A novel Zn^{2+} and HSO_4^- selective fluorescent "turn-on" chemosensor based on isonicotiamide: INHIBIT type's logic gate and application in cancer cell imaging

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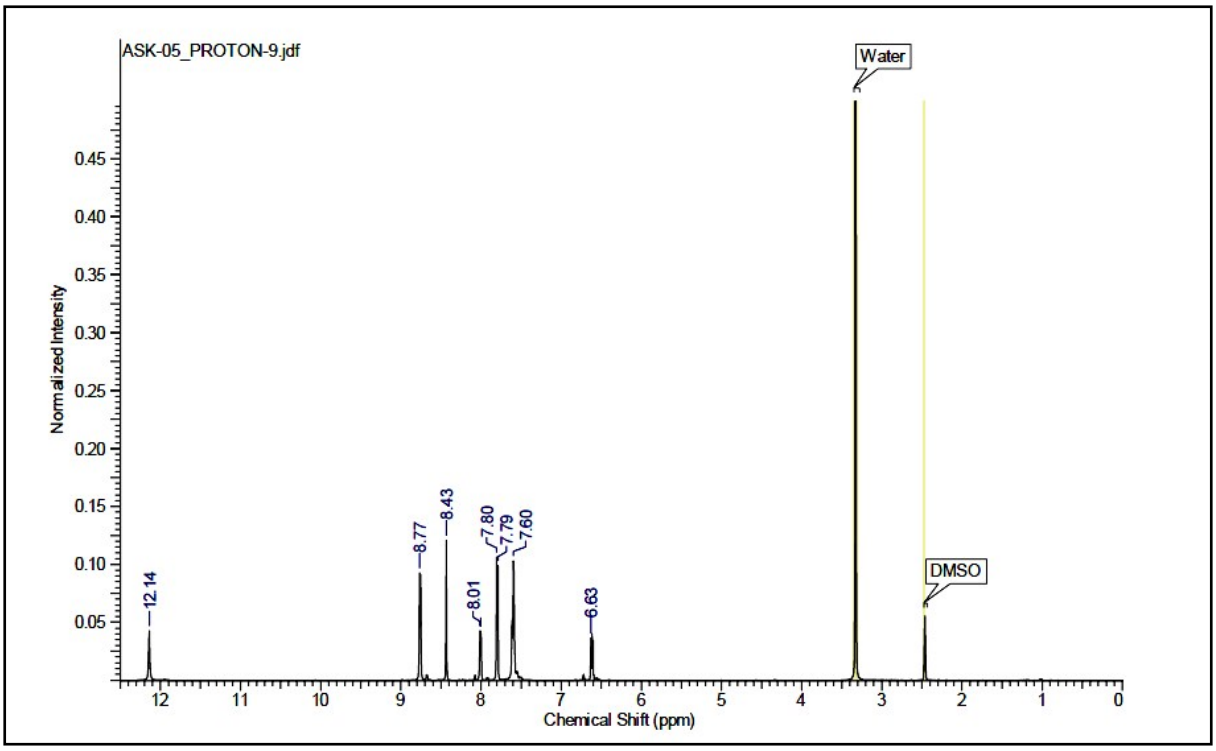

Figure S1. ^{1}H-NMR of receptor **1.**

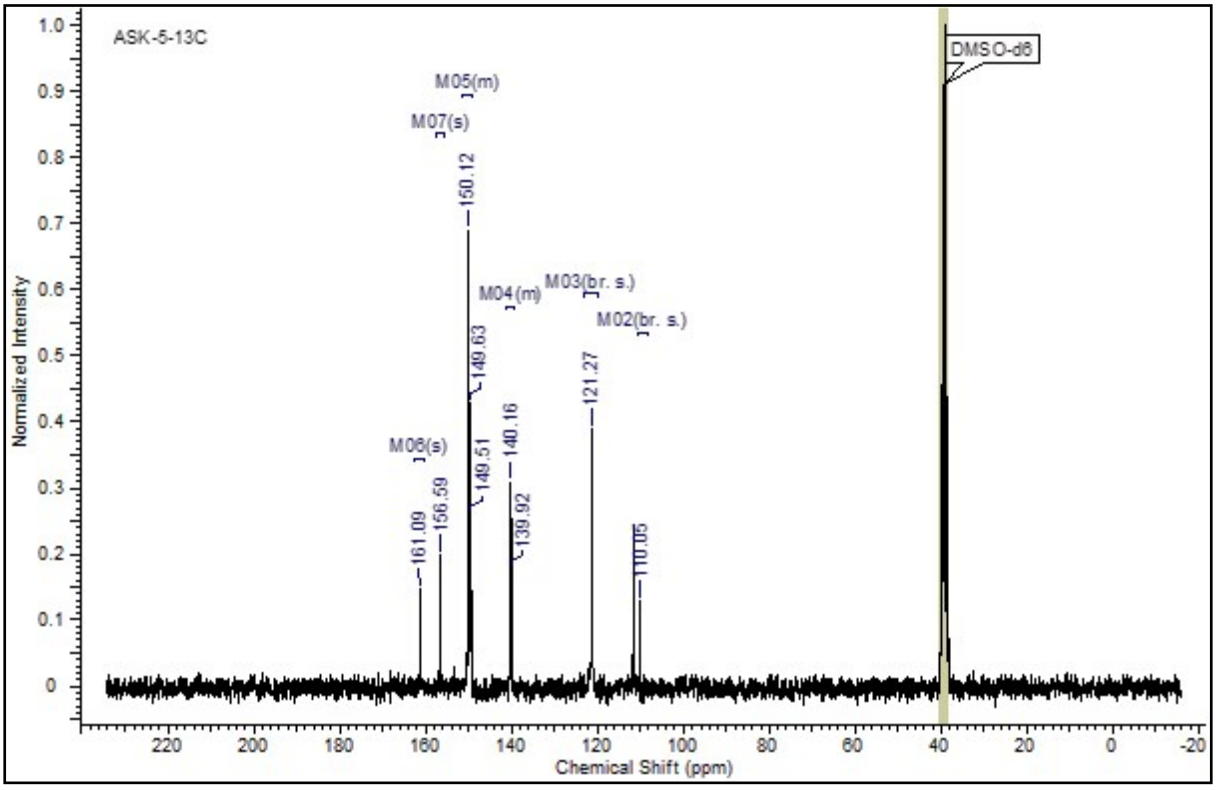

Figure S2. ^{13}C-NMR of receptor **1**

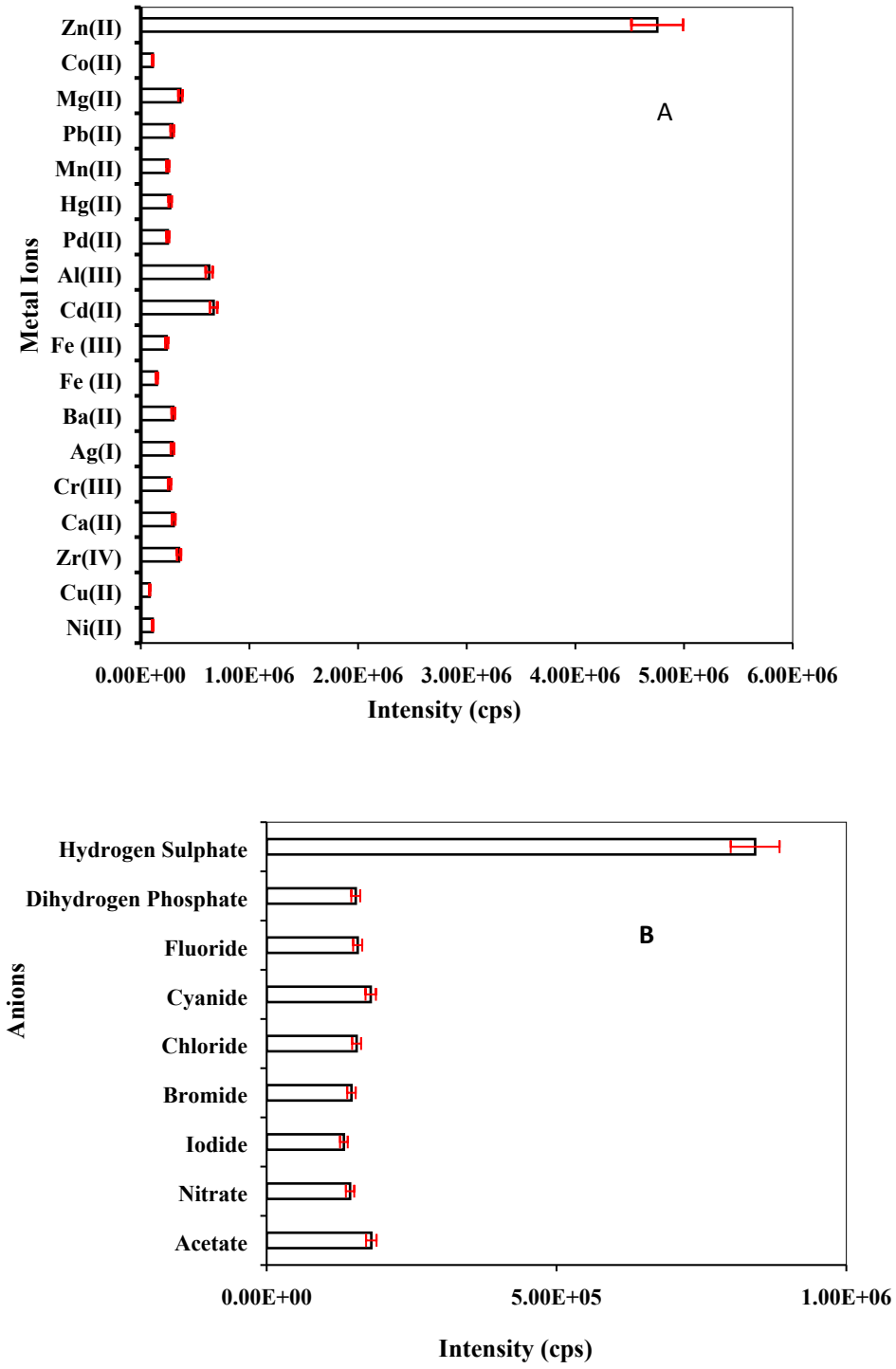

Figure S3. Fluorescence spectrometric response of receptor **1** (0.1 mM) upon addition of 100 µL of respective (A) cation and (B) anions salts.

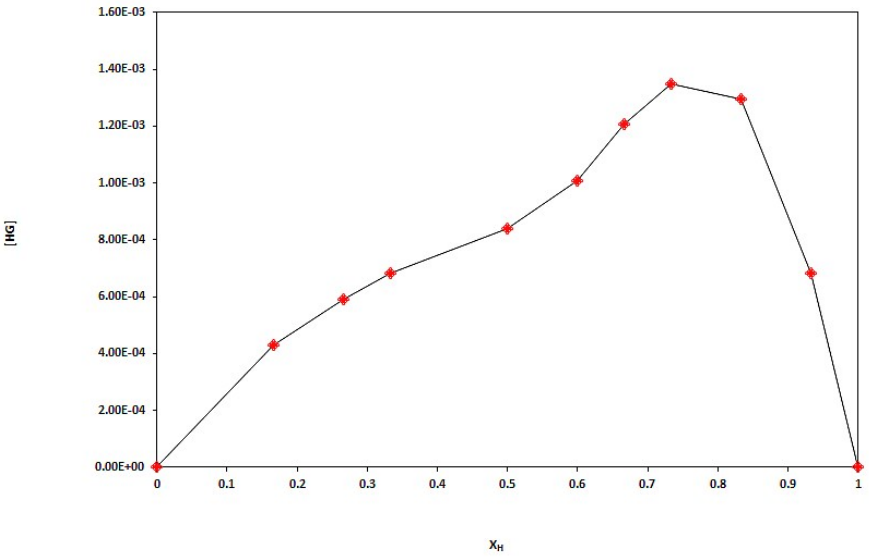

Figure S4. Job's plot representing the stoichiometry of complex **1**.Zn^{2+} (host : guest; 2:1).

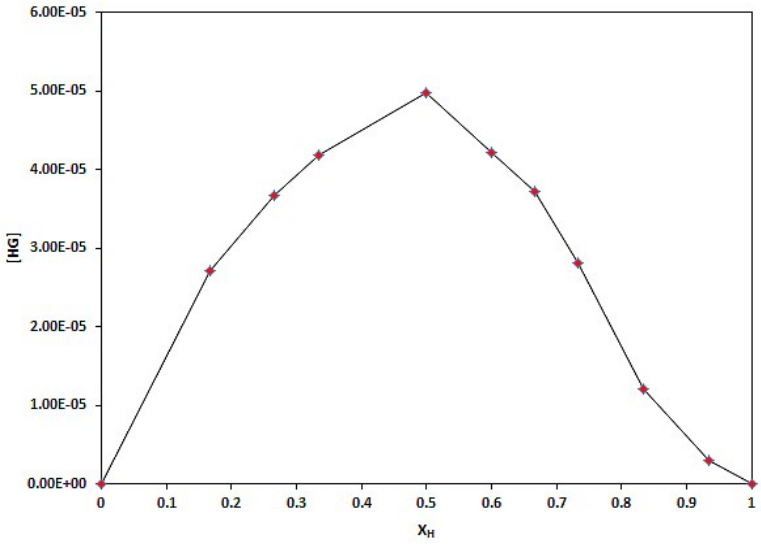

Figure S5. Job's plot representing the stoichiometry of complex **1**.HSO_4^- (host: guest; 1:1).

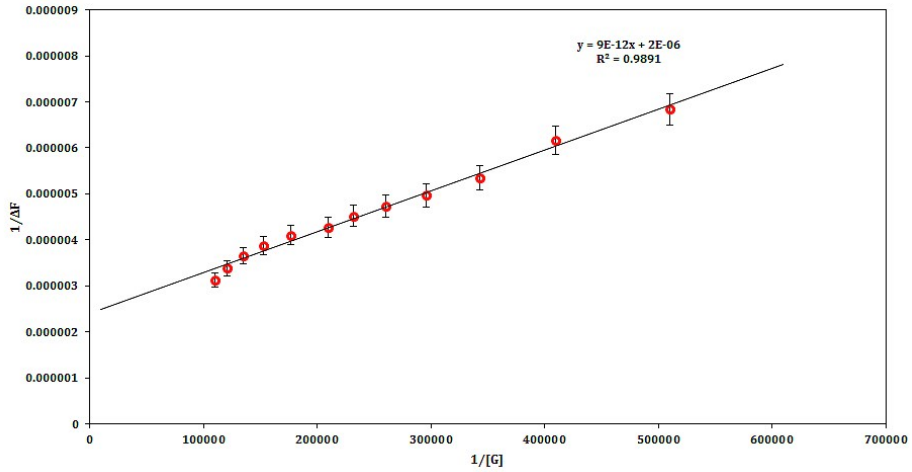

Figure S6. Benesi-Hildebrand plot for receptor **1** of **Zn^{2+},** ($1/\Delta F$) vs $1/[G]$, $K_a = 2.46 \times 10^5$ M^{-1}.

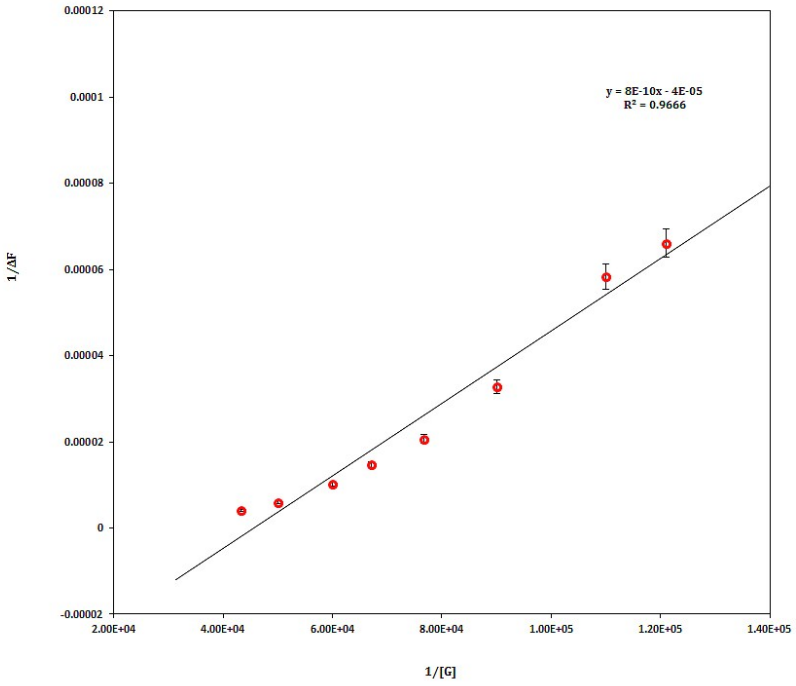

Figure S7. Benesi-Hildebrand plot for receptor **1** of **HSO_4^-,** ($1/\Delta F$) vs $1/[G]$, $K_a = 5.00 \times 10^4$ M^{-1}.

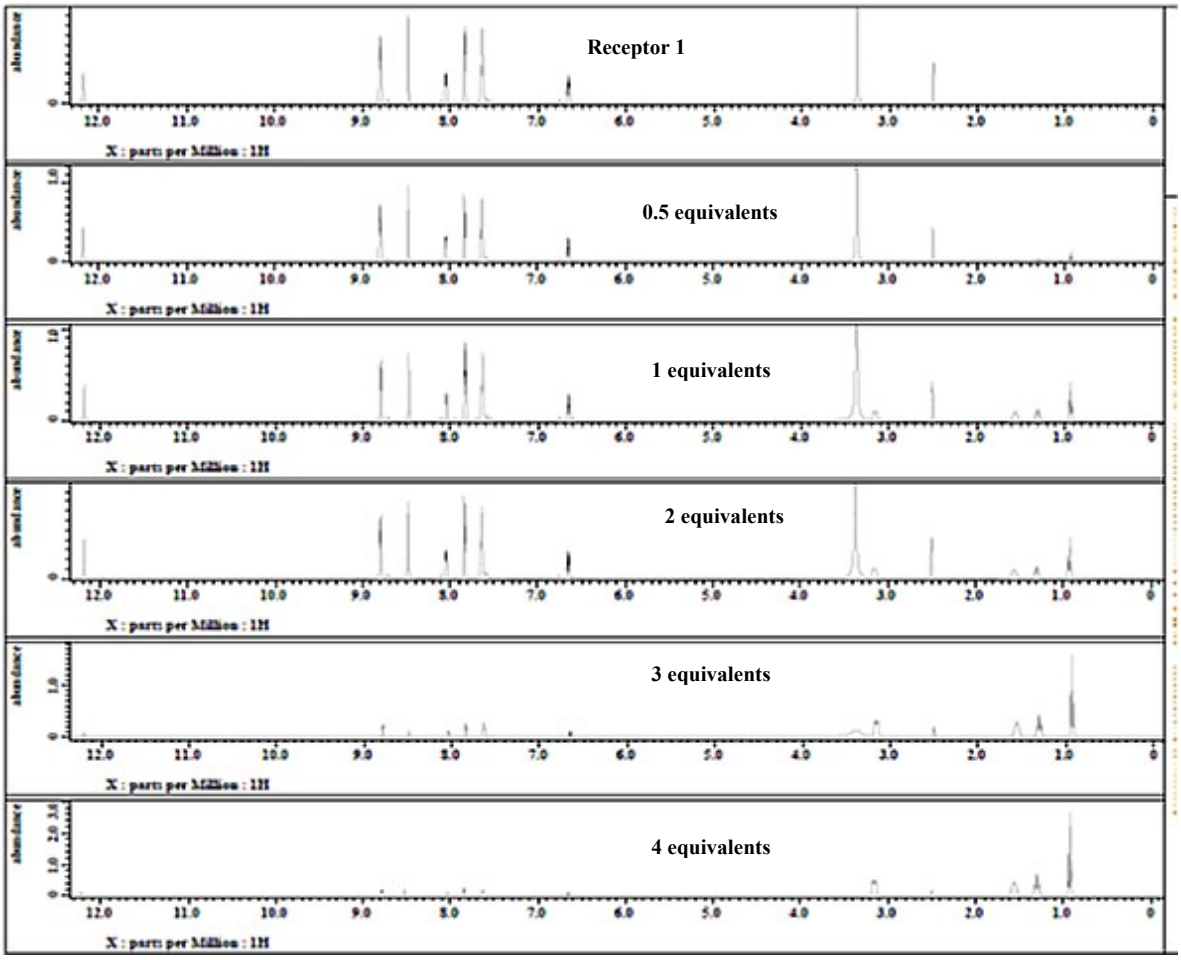

Figure S8. ^{1}H-NMR titration of receptor **1** with HSO_4^- in DMSO-d_6.

Table S1. X-ray crystallographic data for receptor **1.**

Empirical formula	$C_{12}H_{11}N_5O$
mol. wt	241.26
Crystal System	Tetragonal
a(Å)	13.2948(5)
b(Å)	13.2948(5)
c(Å)	25.8974(11)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
V(A^3)	4577.4(3)
Z	16
T/K	296(2)
λ	0.71073
ρ_{calcd}(gm/cm^3)	1.400
μ(mm^{-1})	0.096
goodness for fit	1.032
θ range (deg)	1.72-28.69
total no of reflns	11470
no of unique reflns	2959
no. of obsd data (I > 2σ(I))	2483
R_{int}	0.0142
R1 ($F^2>2\sigma(F^2)$), wR2 (F^2)[a]	0.0379, 0.1160

Table S2. Selected bond lengths (A˚) and bond angles (˚) with in parenthesis of receptor **1.**

Parameters	Experimental	B3LYP/6-31G(d,p)
Bond lengths		
O(1)-C(7)	1.224(1)	1.220
N(1)-C(1)	1.338(1)	1.351
C(1)-C(5)	1.430(1)	1.437
C(5)-C(6)	1.456(1)	1.448
N(3)-C(6)	1.279(2)	1.290
N(3)-N(4)	1.384(1)	1.361
C(7)-C(8)	1.504(1)	1.504
N(2)-C(1)	1.351(1)	1.350
Bond angles		
C(9)-C(8)-C(7)	124.2(1)	124.44
C(10)-C(9)-C(8)	118.6(1)	118.70
O(1)-C(7)-C(8)	120.0(1)	122.27
N(4)-C(7)-C(8)	116.0(1)	114.58
C(7)-N(4)-N(3)	118.2(1)	119.51
C(6)-N(3)-N(4)	115.5(1)	118.09
N(3)-C(6)-C(5)	122.9(1)	122.67
N(1)-C(1)-C(5)	122.2(1)	121.89

Table S3: Comparison of proposed sensor with various sensors of Zn^{2+} and HSO_4^- ions

S.No	Authors	Solvent Used	Ions detected	Detection Limit	Ref. No.
1	A. Mallick *et al*	Acetonitrile- Water (5:1)	F^- ions & HSO_4^-	-	23
2	A. Wu *et al*	Methanol	HSO_4^-	1.39 μM	24
3	A. Kuwar *et al*	Water	HSO_4^-	0.25 μM	25
4	N. Kaur *et al*	Water	HSO_4^-	37 μM	26
5	N. Kaur *et al*	Water	HSO_4^-	1.12 μM	27
6.	N. Singh *et al*	Water	F^- ions & HSO_4^-	4.84 pM & 5.67 nM	28
7.	Río et al	Water	HSO_4^-	1.42 mM	29
8.	Melchert et al	Water	HSO_4^-	150 μM	30
9.	Othman et al	Water	HSO_4^-	-	31
10.	Lv et al	Ethanol: water	Zn^{2+}	1.8 mM	32
11.	Gupta et al	Methanol : water	Zn^{2+}	0.2 μM	33
12	Cassella et al	water	Zn^{2+}	-	34
13	Li et al	Water	Zn^{2+}	25 nM	35
14	Weng et al	Water	Zn^{2+}	75 nM	36
15	Su et al	Water	Zn^{2+}	1.87 μM	37
16	Jakubaa et al	Water	Zn^{2+}	1.7 nM	38
17.	Andrade et al	water	HSO_4^-	60 nM	39
17.	**Kuwar et al**	**Acetonitrile- Water (1:1)**	**Zn^{2+} & HSO_4^-**	**3.81 nM and 0.95 nM**	**Proposed Sensor**