Supporting Information

ESIPT- based fluorescent probe for the detection of multianalyte and a facile approach to discriminate arsenate and PPi in water

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Experimental procedure

The stock of **HJ-DNP** was prepared at 0.01 M concentration in DMSO solvent. The stocks of anions and metal ions were prepared at 0.01 M in water. The UV-Vis studies were performed with 12.5 µL of stock in 2.5 mL of total volume (0.05 mM). The fluorescence studies were performed with 25 µL of stock and diluted to a total volume of 2.5 mL (0.1 mM). These emission studies were recorded while the excitation wavelength being 365nm, slit width 20/20.

UV-Vis and fluorescence spectral studies with water

The aggregation studies were recorded in DMSO with the increase in percentage of water. The UV-Vis studies and fluorescence studies were performed by adding different fractions of DMSO-water from 2% of DMSO, 10%, 20% and so on to 100% of DMSO. The fractions were decided with total volume of the solvent mixture.

UV-Vis and fluorescence spectral studies with metals

Binding behavior of receptor **HJ-DNP** with different metal ions such as Ni^{2+}, Ag^{+}, Fe^{+2}, Fe^{3+}, Cr^{3+}, Cd^{2+}, Cu^{2+}, Mn^{2+}, Na^{+}, Mg^{2+}, Ca^{2+}, Co^{2+}, Hg^{2+} was studied. The stock of metal ions and **HJ-DNP** were prepared of 0.01 M concentration in water and DMSO respectively. The UV-Vis spectrum was recorded with **HJ-DNP** (0.05 M) and 10 equivalents (0.5 mM) of each metal ions, diluted to 2.5 mL in DMSO-water (80:20) mixture. For emission spectrum, receptor **HJ-DNP** (0.1 mM) and 5 equivalents (0.5 mM) of each metal ions were added and diluted to a total volume of 2.5ml of DMSO-water (80:20) mixture.

UV-Vis and fluorescence spectral studies with oxy-anions

Receptor **HJ-DNP** was checked with various anions and oxy-metals ions such as Cl^{-}, I^{-}, Br^{-}, CH_3COO^{-}, PO_4^{-}, NO_3^{-}, F^{-}, OH^{-}, PPi , HSO_4^{-} and arsenate. The stock of anions and probe were prepared of 0.01 M concentration in water and DMSO respectively. The UV-Vis spectra were recorded with 12.5µL (0.05 mM) of stock and 10 equivalents (0.5 mM) of each anion, made up to 2.5mL in DMSO-water (80:20) mixture. For emission spectrum, the spectra were recorded by diluting 25µL (100µM) of stock and 5 equivalents (500µM) of each anion, to 2.5 mL of DMSO-water (80:20) mixture excited at 365nm.

Life time experiments

Fluorescence lifetime measurements were studied for solutions of ligand **HJ-DNP** (100 µM), ligand with chromium (100 µM), arsenate (1 mM) and pyrophosphate (9.45 mM) in DMSO-water (80:20) while monitoring the emission at 505 nm using 360 nm LED as excitation source. Average fluorescence lifetimes, τ_{av}, were obtained by global fitting the decay traces to tri-exponential decay functions. Quantum yield values were estimated measured using the relative method and quinine sulphate in methanol as the reference standard.

Arsenate detection in real water samples

The recovery experiments with arsenate ion were carried out by using natural water samples (ground water, pond water, and tap water) as well as the water sample collected after washing rice. The arsenate stocks were prepared separately in different water samples mentioned above. All the samples were spiked with known concentrations of arsenate (0.0 to 1 mM). For the studies, a stock solution of **HJ-DNP** (0.1 mM) was taken and different concentration of arsenate in water samples was added for each experiment. The experiments were performed three times and the average value was calculated for further calculations.

The % recovery was calculated by using the known formula,

$$\text{Recovery \%} = \frac{Calculated\ \ arsenate}{Arsenate\ added} \times 100$$

Linear regression equations were used to calculate the concentration of arsenate and response of **HJ-DNP** in the presence of spiked arsenate.

Chromium detection in real life samples

Tomatoes (500 g) collected from the local super market and washed thoroughly before using them for analysis. 25g of washed tomatoes were grinded using mortar and pestle. The extract was filtered and centrifuged to get the clear orange color tomato extract obtained. This clear solution was further diluted to 15 mL with distilled water and spiked with different amounts (5, 10, 15, 20, 25 µM) of Cr^{3+} ion. Tomatoes extract spiked with Cr^{3+} ion further used for the emission titration with probe **HJ-DNP** (0.1 mM) in DMSO-water (80:20) solution.

Preparation of sodium alginate beads

1g of sodium alginate was dissolved in 100 mL of deionized water and the solution was stirred vigorously for 3-4 hours to form a homogenous solution of alginate. The hydrogel beads were prepared by adding 0.1 mL of alginate to a solution of calcium chloride (0.5g in 50 mL). The clear hydrogel beads were collected and the excess of solution was wiped. The beads were collected in a tight container and were used immediately. These beads were immersed in a solution of **HJ-DNP** (0.1 M) for 2 hours, washed with water and used for further studies.

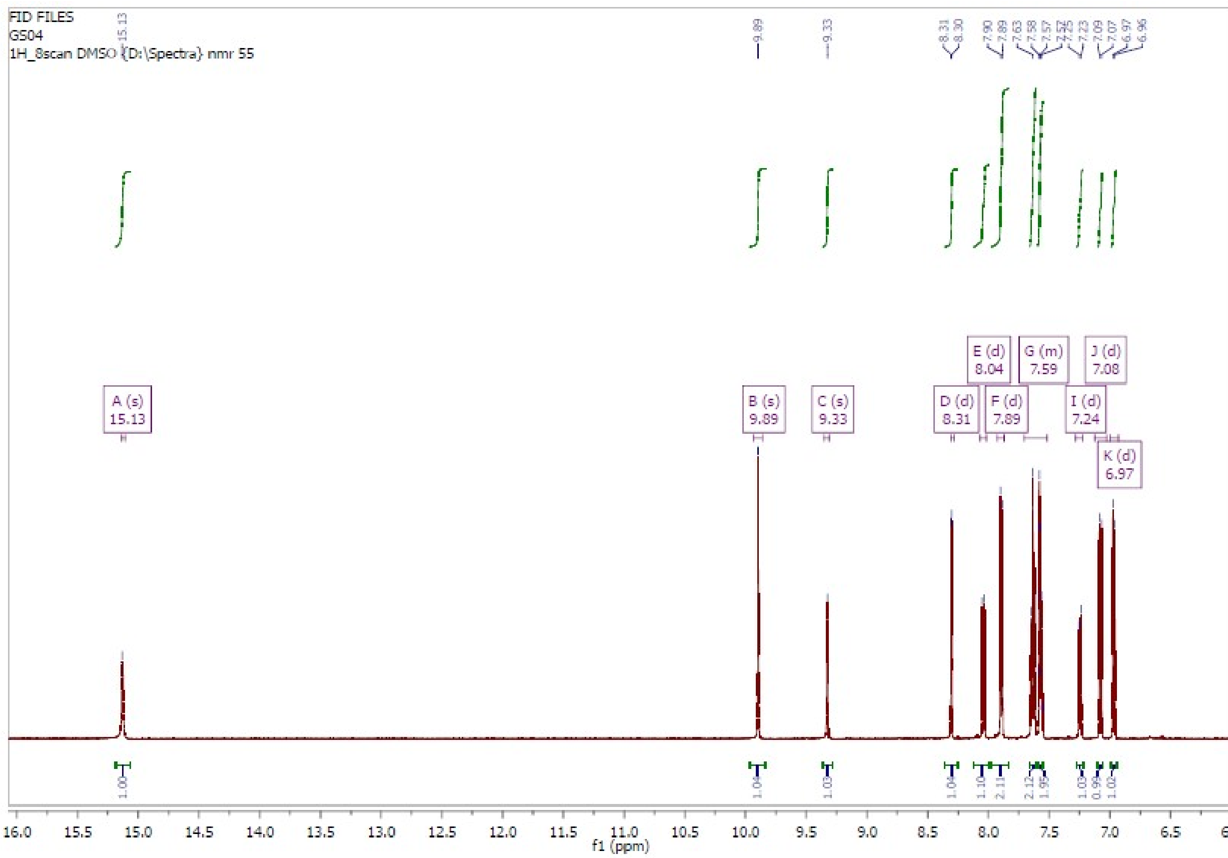


Fig. S1. ^{1}H-NMR spectrum of Receptor **HJ-DNP** in DMSO-d_6

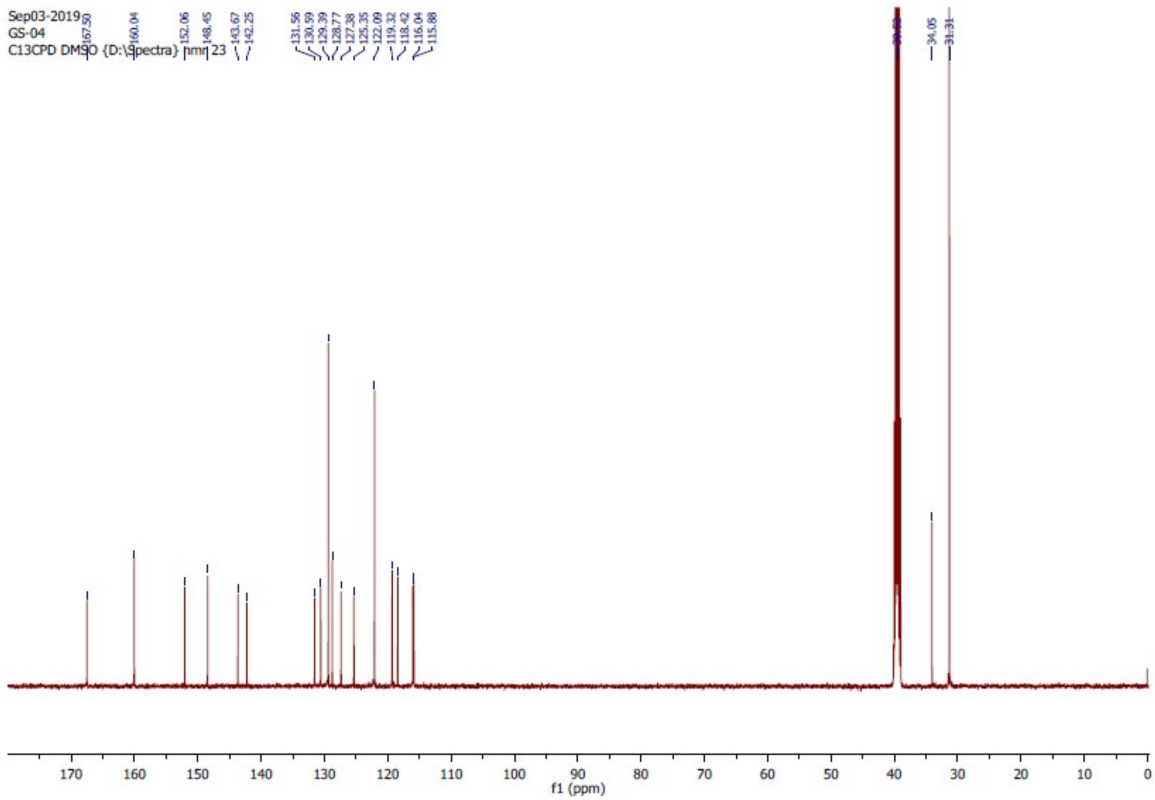


Fig. S2. ^{13}C-NMR spectrum of Receptor **HJ-DNP** in DMSO-d_6

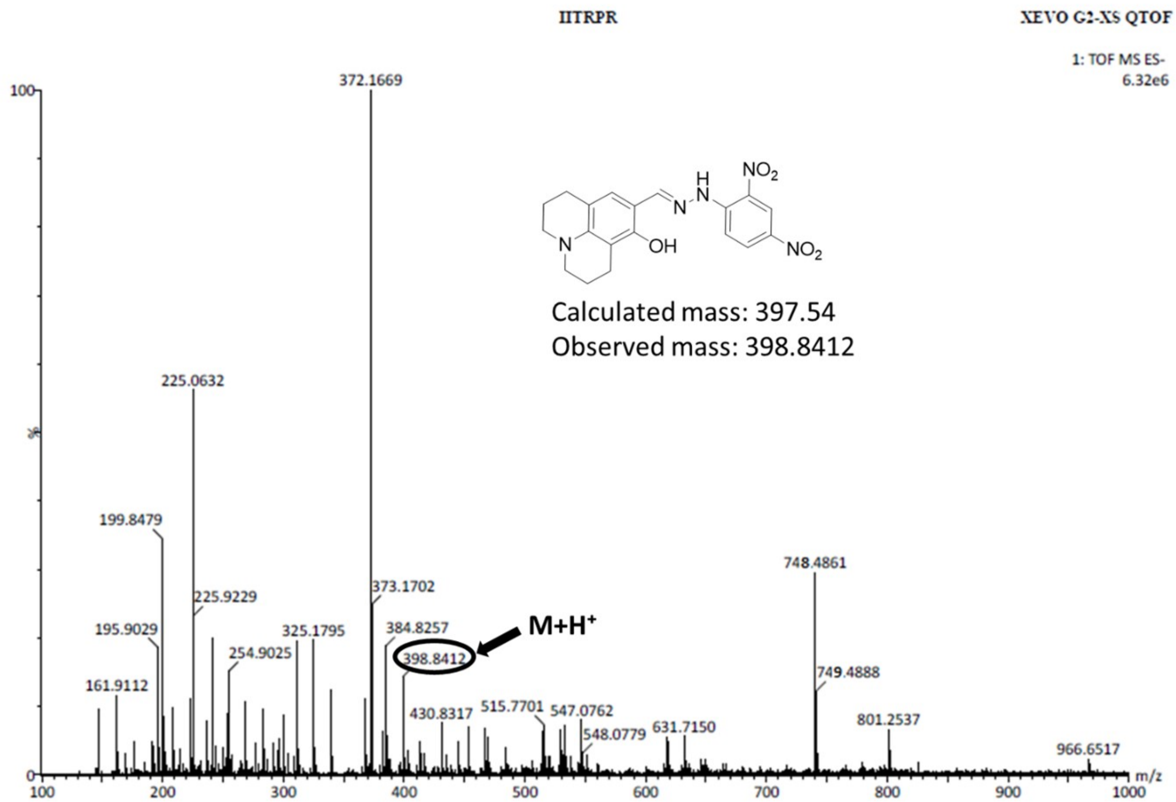


Fig. S3. ESI- Mass spectrum of Receptor **HJ-DNP**

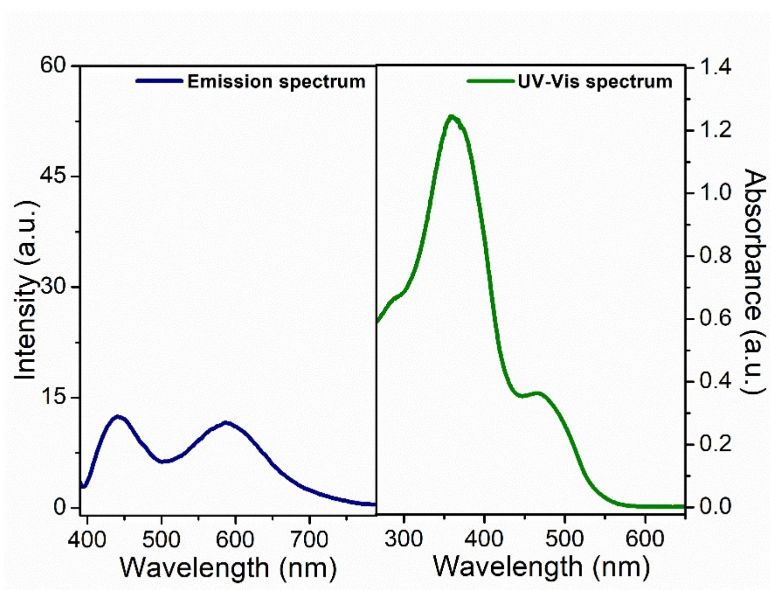
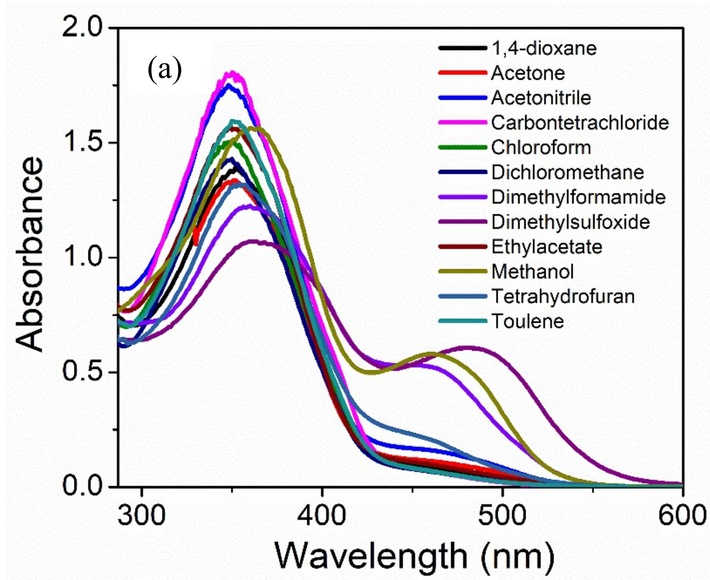


Fig. S4. The UV-Vis absorbance and Emission spectra of **HJ-DNP** in DMSO.



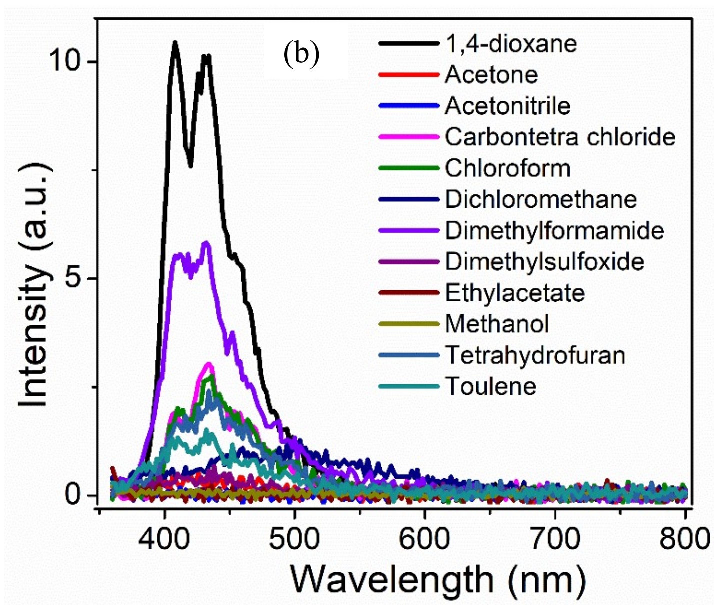


Fig. S5. (a) Absorption spectra and (b) Emission spectra of receptor **HJ-DNP** in solvents: 1,4-dioxane, acetone, acetonitrile, carbon tetrachloride, chloroform, dichloromethane, dimethylformamide, dimethyl sulfoxide, ethyl acetate, methanol, tetrahydrofuran, toluene.

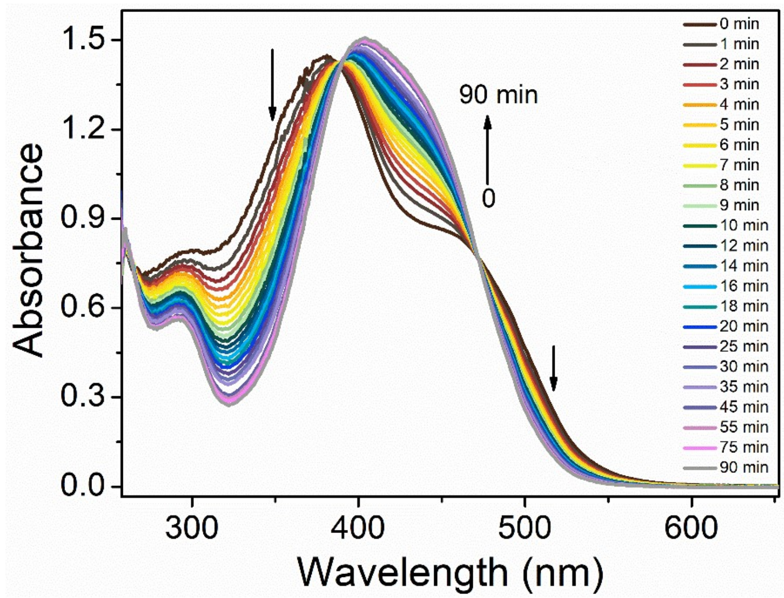


Fig. S6: The absorption spectra of probe **HJ-DNP** with the irradiation of strong UV light for 90 min.

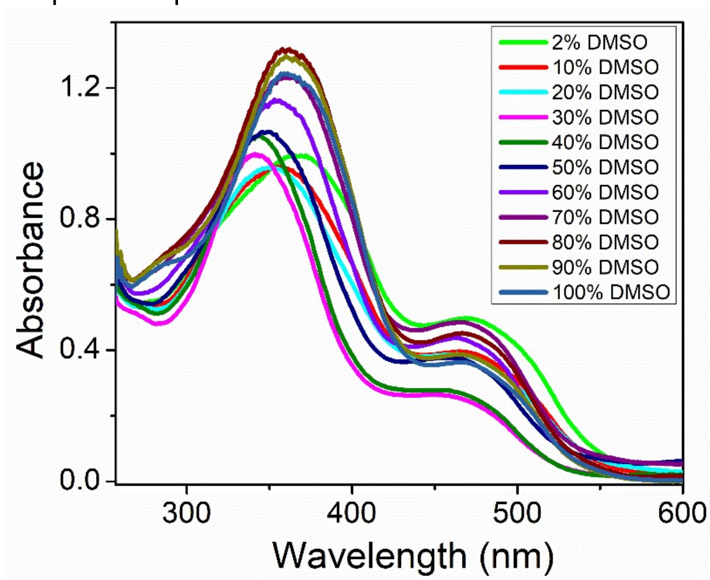
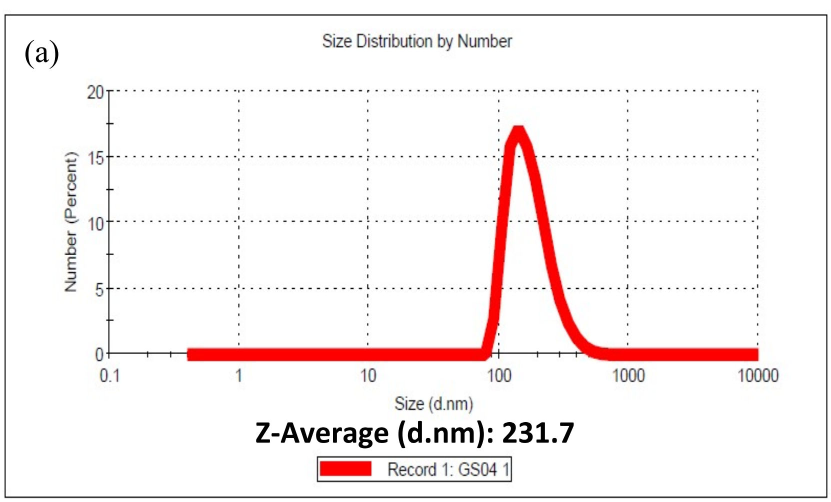


Fig. S7. Absorption spectra of probe **HJ-DNP** with different amounts of water in DMSO.



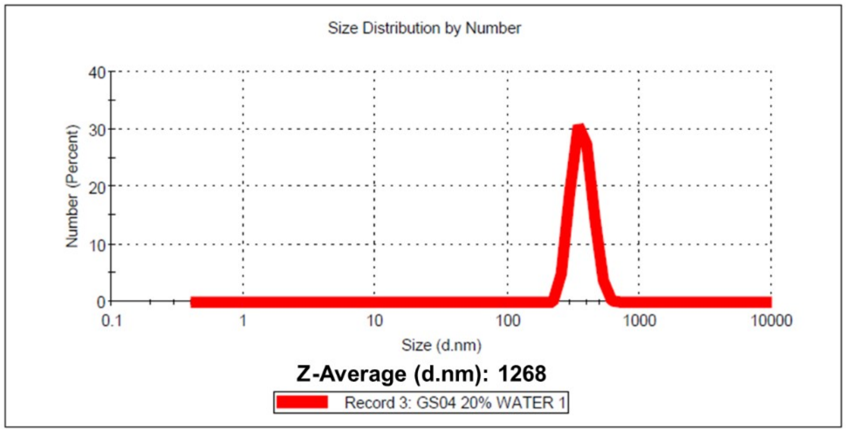


Fig. S8. The DLS studies of receptor **HJ-DNP** in (a) DMSO (b) DMSO: water (80:20) mixture

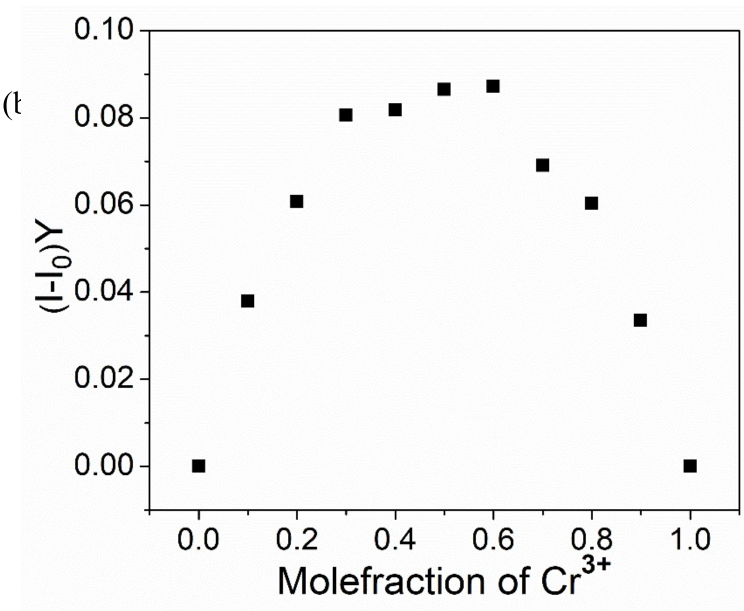


Fig. S9. Job's plot for the binding of probe **HJ-DNP** with Cr^{3+}

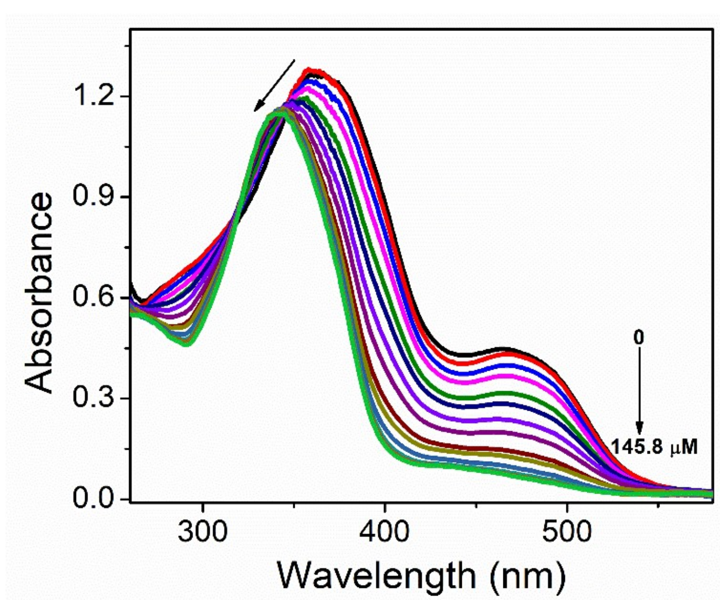


Fig. S10. UV-Vis absorption spectra of receptor **HJ-DNP** with Cr^{3+} in DMSO-water (80:20) mixture.

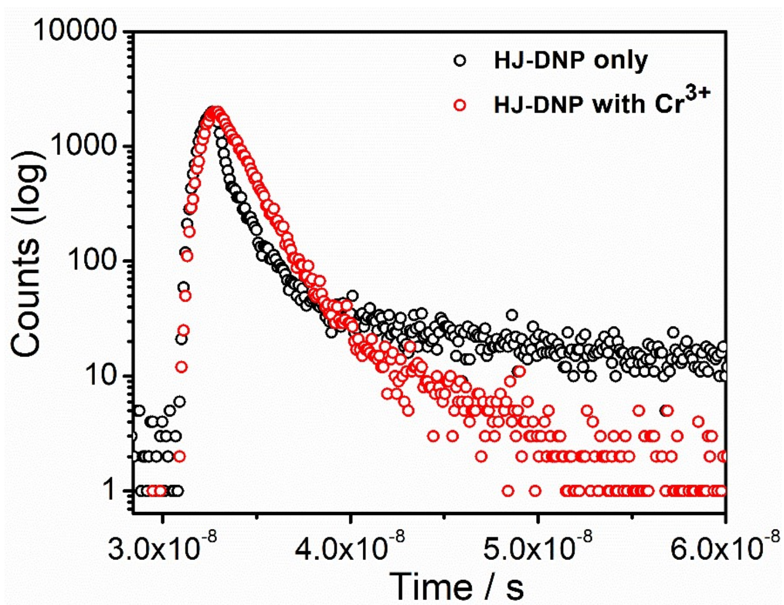


Fig. S11. Lifetime measurement spectra of receptor **HJ-DNP** with Cr^{3+} in DMSO-water (80:20) mixture (λ_{ex} = 360 nm, monitored at 505 nm).

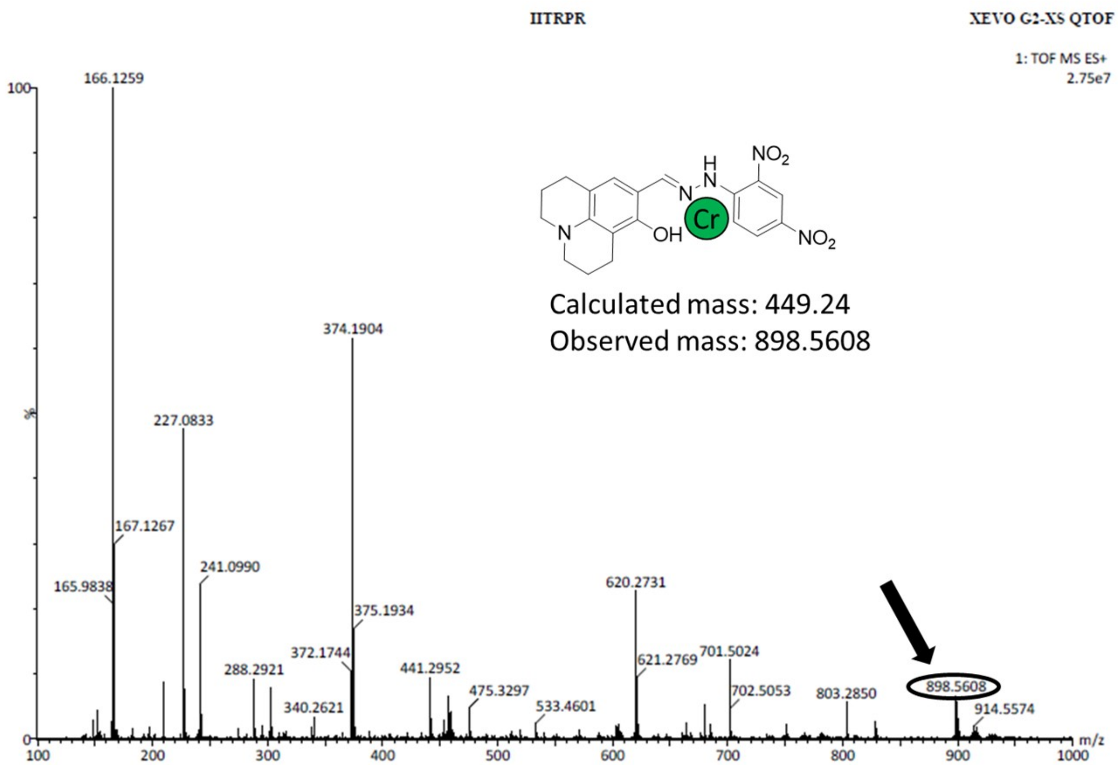


Fig. S12: ESI-MS of **HJ-DNP** with analyte Cr^{3+}

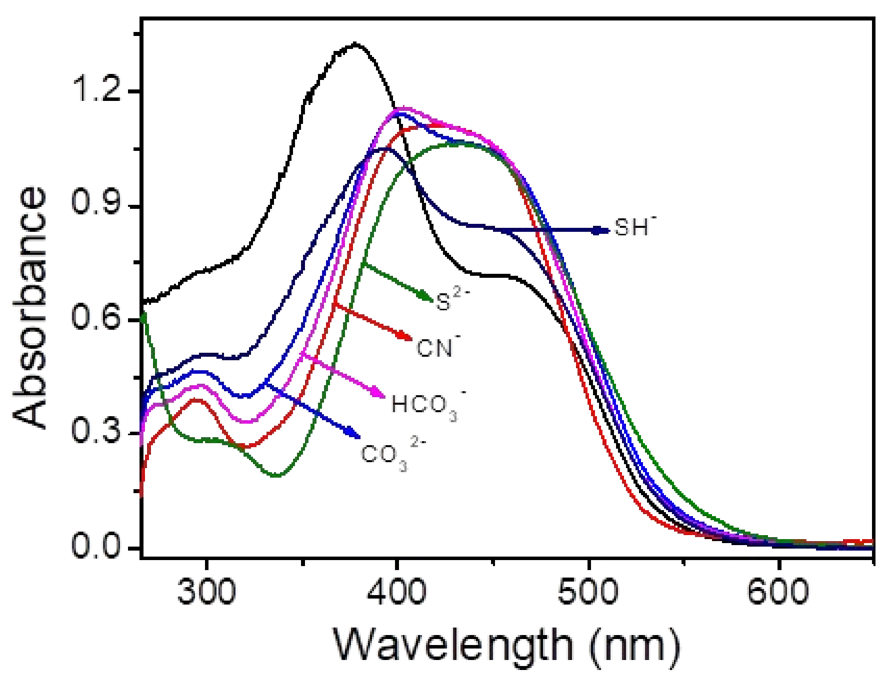


Fig. S13: The UV absorption spectra of **HJ-DNP** (0.05 mM) with anions such as S^{2-}, HS^-, CN^-, CO_3^{2-} and HCO_3^- (0.35 mM)

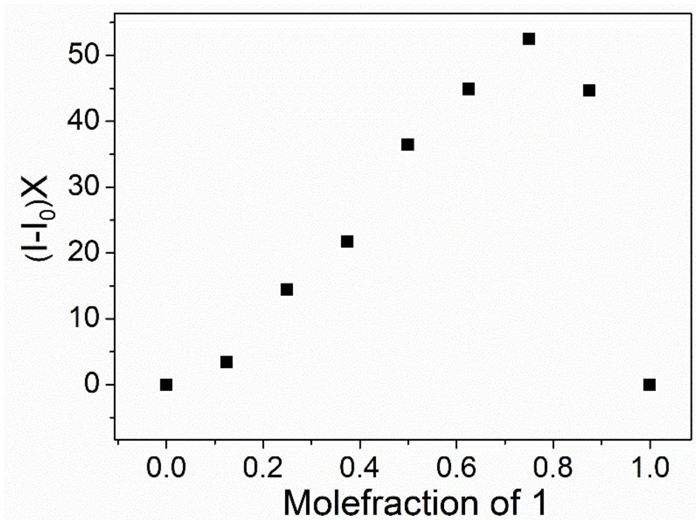


Fig. S14. Job's plot of probe **HJ-DNP** with $HAsO_4^{2-}$

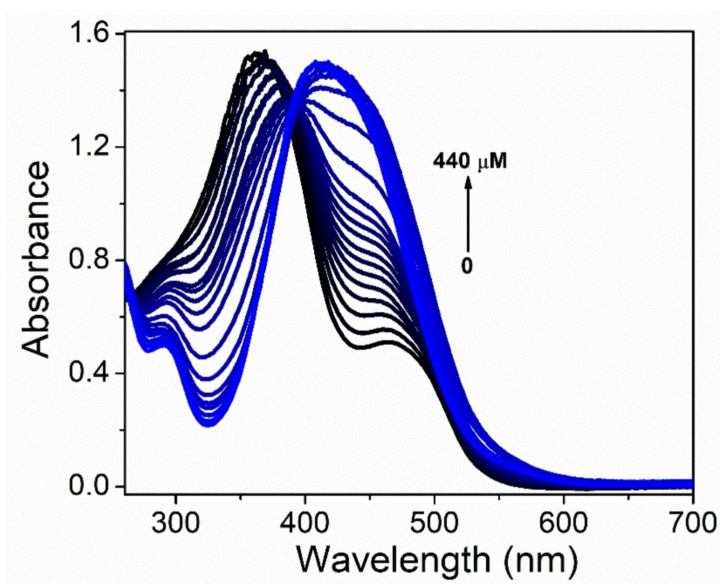


Fig. S15. UV-Vis absorption spectra of receptor **HJ-DNP** with $HAsO_4^{2-}$ in DMSO-water (80:20) mixture.

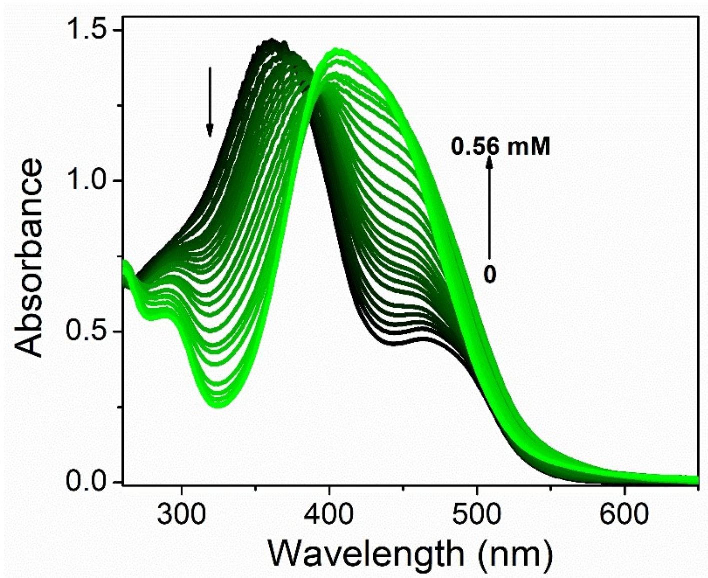


Fig. S16. UV-Vis absorption spectra of receptor **HJ-DNP** with $P_2O_7^{4-}$ in DMSO-water (80:20) mixture.

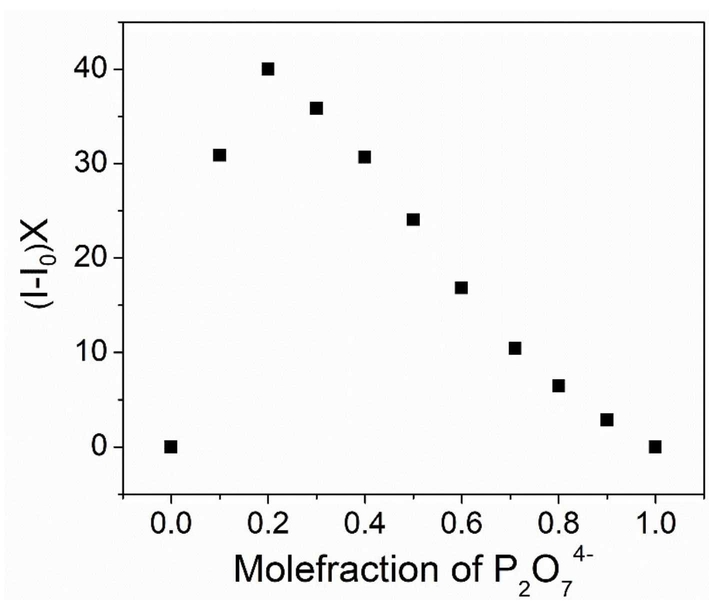


Fig. S17. Job's plot of probe **HJ-DNP** with $P_2O_7^{4-}$

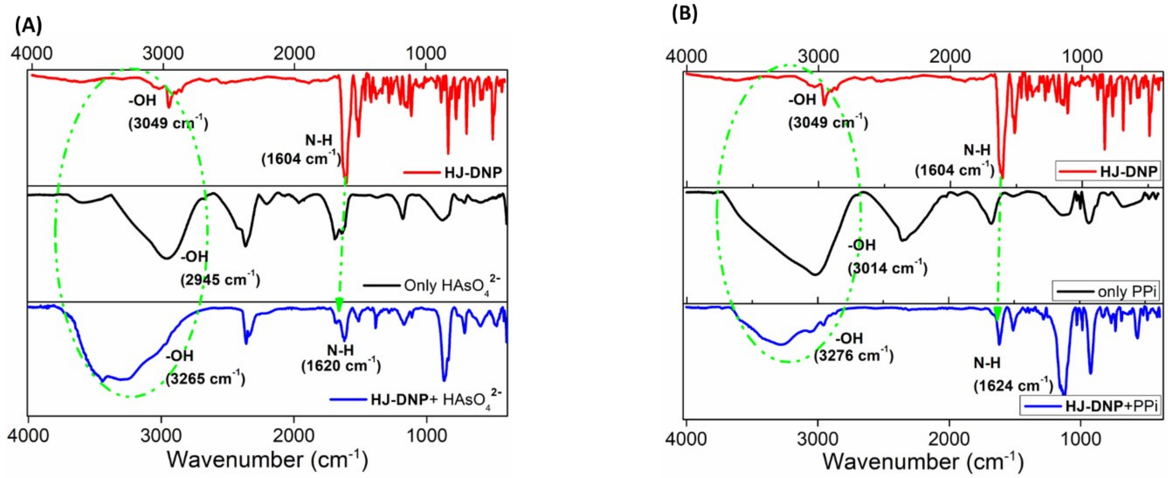


Fig. S18: FTIR spectrum of receptor **HJ-DNP** with oxy-anions $HAsO_4^{2-}$ (arsenate) and PPi (pyrophosphate) by KBr method.

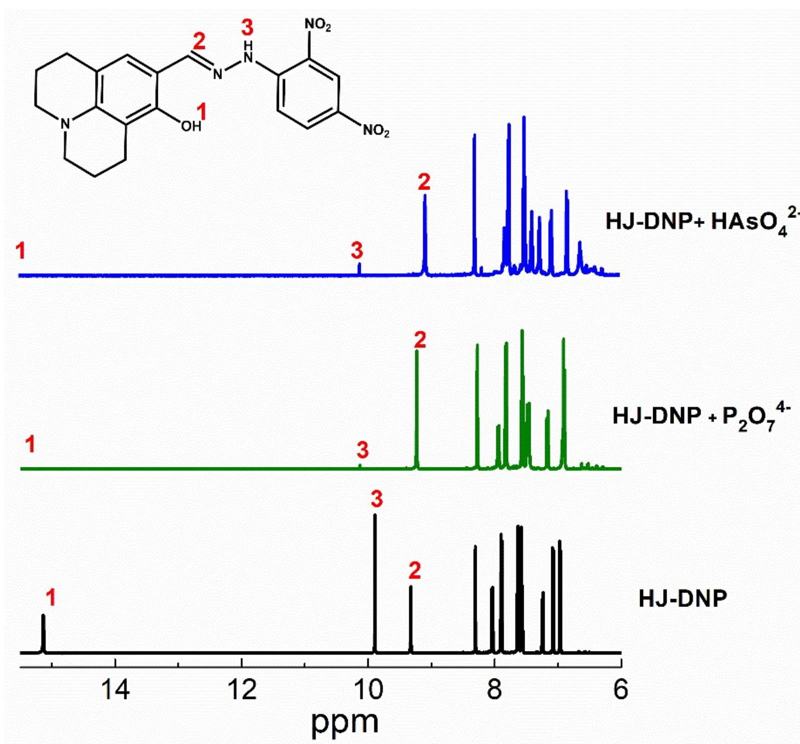


Fig. S19: ¹H-NMR spectra of receptor **HJ-DNP** with oxy-anions $HAsO_4^{2-}$ (arsenate) and $P_2O_7^{4-}$ (pyrophosphate) in DMSO-d_6.

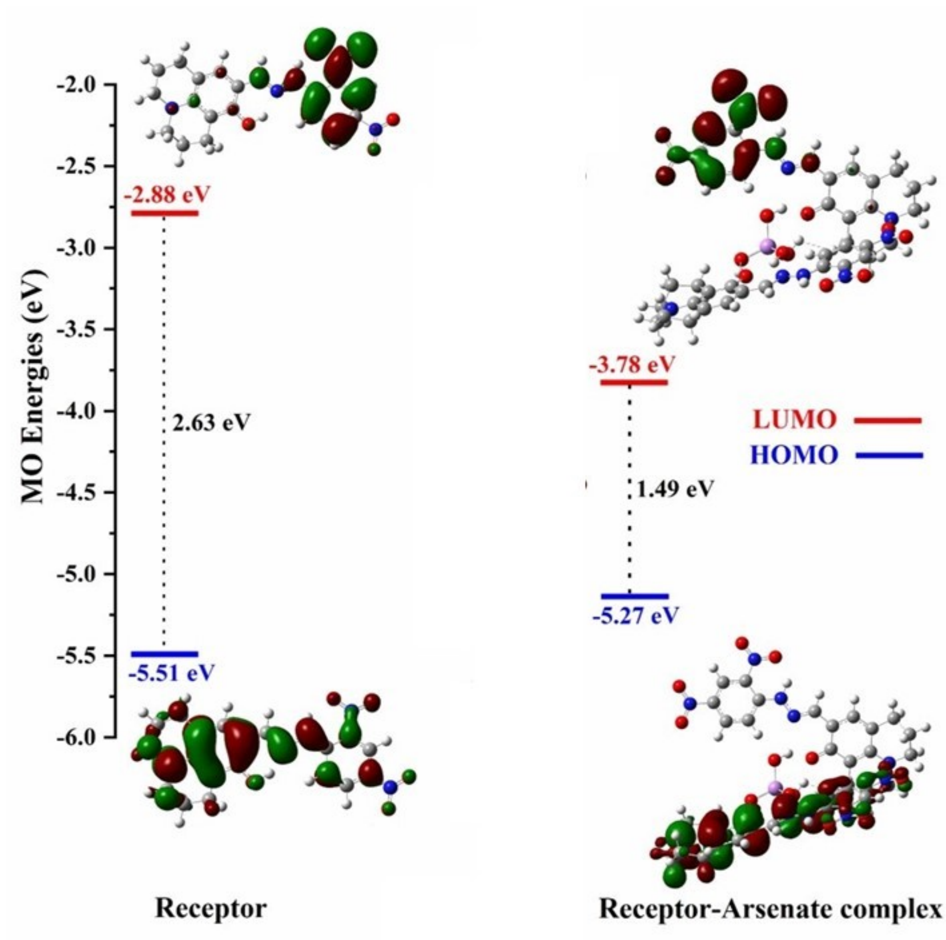
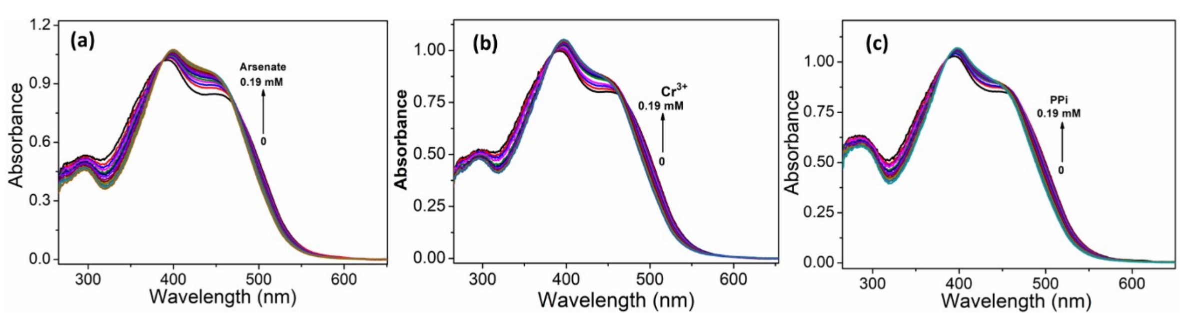


Fig. S20: HOMO-LUMO energy levels of receptor **HJ-DNP** and **HJ-DNP** with arsenate



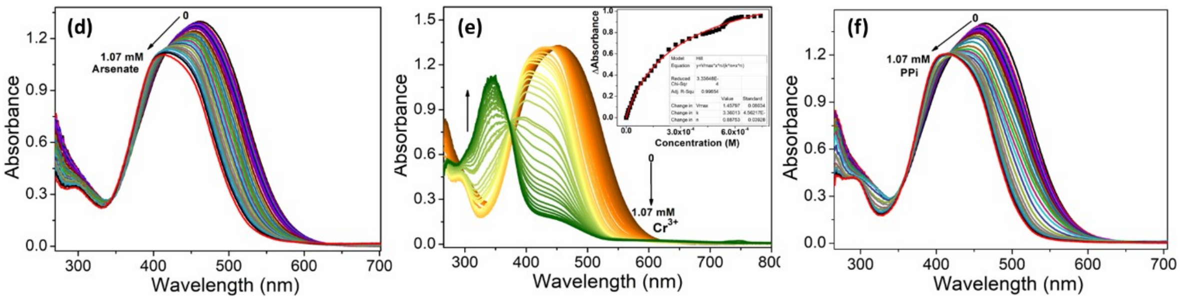


Fig. S21: The wavelength vs absorbance spectra of probe **HJ-DNP** (0.1 mM) with (a) Arsenate (0-0.19 mM) (b) Cr^{3+} (0-0.19 mM) (c) PPi (0-0.19 mM) at pH 5 and (d) Arsenate (0-1.07 mM) (e) Cr^{3+} (0-1.07 mM) (f) PPi (0-1.07 mM) at pH 9.

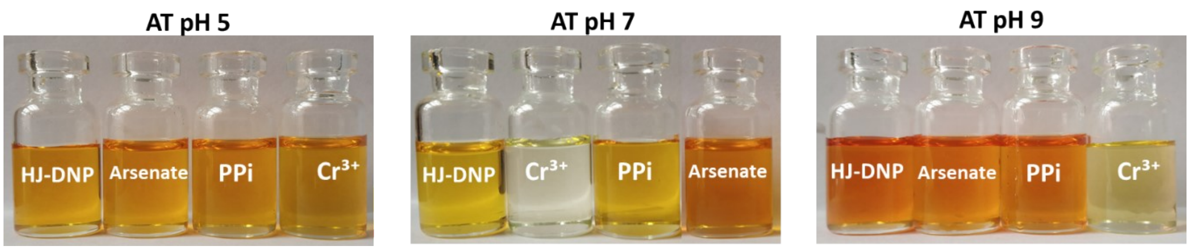


Fig S22: The photographic image of probe **HJ-DNP** (0.05 mM) with analytes pyrophosphate (PPi) (0.56 mM), arsenate (0.44 mM), and Cr^{3+} (0.14 mM) at different pH.

Table S1. Binding constant and Limit of detection of the analytes in DMSO-water (80:20) mixture

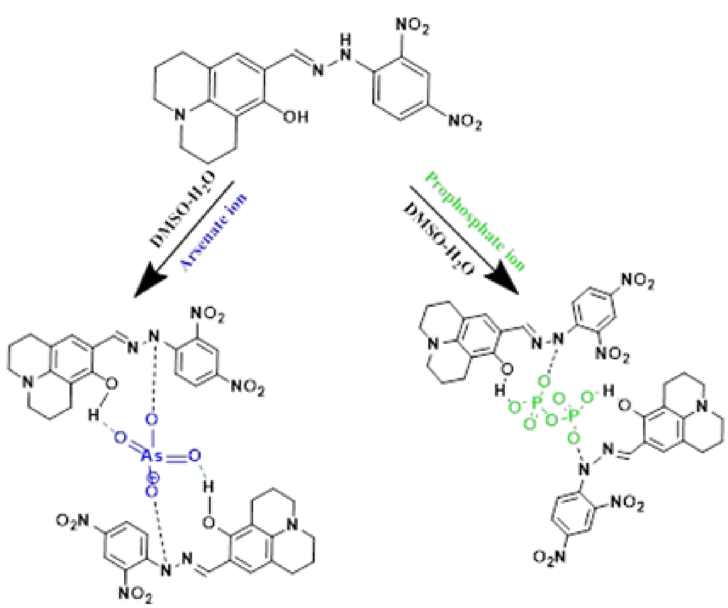
Analyte	**Solvent**	**Binding constant (M^{-1})**	**Limit of detection (M)**
Cr^{3+}	DMSO-water	1.55×10^4	2.46×10^{-6}
$HAsO_4^{-2}$	DMSO-water	1.66×10^4	5.54×10^{-6}
$P_2O_7^{4-}$	DMSO-water	8.77×10^2	1.92×10^{-4}

Table S2: Lifetime measurements of probe with analytes: $HAsO_4^{2-}$, $P_2O_7^{4-}$ and Cr^{3+} monitored at 505nm using 360nm LED as excitation source

Sample	Time (ns)	Relative Amplitude	Avg. lifetime
Probe (Chi sq. 1.114)	T_1= 0.255 ± 0.061	19.82%	0.828 ± 3.11
	T_2= 1.310 ± 0.111	54.41%	
	T_3= 15.917 ± 3.11	25.77%	
Probe+ $HAsO_4^{2-}$ (Chi sq. 1.214)	T_1= 1.279 ± 0.088	63.16%	1.776 ± 0.42
	T_2= 5.316 ± 0.417	36.84%	
Probe+ $P_2O_7^{4-}$ (Chi sq. 1.223)	T_1= 4.184 ± 1.804	46.16%	3.245 ± 2.92
	T_2= 11.991 ± 2.296	32.22%	
	T_3= 1.265 ± 0.165	21.62%	
Probe+ Cr^{3+} (Chi sq. 0.97)	T_1= 0.49 ± 0.64	19.58%	2.071 ± 0.09
	T_2= 1.08 ± 0.13	73.98%	
	T_3= 4.031 ± 0.66	6.44%	

Table S3: The comparative table of LODs of probe **HJ-DNP** with the analytes $HAsO_4^{2-}$, $P_2O_7^{4-}$ and Cr^{3+} at different pH.

Analyte	LOD (M)		
	pH 5.0	pH 7.0	pH 9.0
Cr^{3+}	ND	9.36 x 10^{-7} (4.34 x 10^{4})	1.60 x 10^{-6} (2.97 x 10^{5})
$HAsO_4^{-2}$	ND	2.12 x 10^{-6} (7.35 x 10^{3})	ND
$P_2O_7^{4-}$	ND	1.07 x 10^{-6} (8.69 x 10^{2})	ND
ND= Not determined, Binding constant values are presented in parenthesis			



Scheme S1: The proposed mechanism of probe **HJ-DNP** with arsenate and PPi in DMSO-water (80:20) mixture.

Optimized coordinates of Receptor-Enol form at B3LYP/6-311G(d,p) level of theory.

6	-4.493126000	-0.122244000	0.065423000
6	-5.307504000	2.268043000	0.470157000
7	-5.806090000	-0.552590000	0.042705000
6	-6.631795000	1.763765000	-0.100616000
6	-6.894879000	0.350200000	0.404525000
6	-2.880241000	1.666461000	0.224415000
6	-1.805355000	0.772024000	0.059617000
6	-3.438751000	-1.050255000	-0.115776000
6	-2.118910000	-0.602674000	-0.107483000
6	-3.707135000	-2.524845000	-0.321949000
6	-6.110133000	-1.979744000	0.096185000
6	-5.144551000	-2.772495000	-0.775967000
8	-1.148109000	-1.526434000	-0.280434000
6	-0.459565000	1.266563000	0.068999000
7	0.579299000	0.493423000	-0.026661000
7	1.797169000	1.111368000	-0.046885000
6	2.955915000	0.416058000	0.017950000
6	4.237683000	1.043870000	-0.094769000
6	2.947009000	-0.992809000	0.210759000
6	5.412478000	0.298867000	-0.033721000
6	4.110627000	-1.717451000	0.269647000
6	5.347172000	-1.066531000	0.142154000
7	4.391107000	2.480359000	-0.281026000
8	5.514831000	2.941458000	-0.403499000
8	3.366161000	3.182448000	-0.306811000
7	6.587006000	-1.843573000	0.205852000
8	6.484338000	-3.055864000	0.363397000
8	7.647659000	-1.239941000	0.098033000
1	-0.331221000	2.349970000	0.159927000
1	-5.429684000	2.450880000	1.545888000

1	-5.035840000	3.228395000	0.023060000
1	-7.458373000	2.416651000	0.192215000
1	-6.591459000	1.751744000	-1.194491000
1	-7.812943000	-0.047710000	-0.036239000
1	-7.043124000	0.364799000	1.496868000
1	-2.656583000	2.721997000	0.353074000
1	-2.996750000	-2.923253000	-1.049326000
1	-3.512153000	-3.068584000	0.611330000
1	-6.069358000	-2.346838000	1.134581000
1	-7.138290000	-2.111744000	-0.250589000
1	-5.270240000	-2.458300000	-1.817011000
1	-5.389330000	-3.836690000	-0.723156000
1	1.875004000	2.123257000	-0.143162000
1	1.993731000	-1.484386000	0.329903000
1	6.365137000	0.798341000	-0.126060000
1	4.093766000	-2.787962000	0.420070000
1	-0.285944000	-1.059781000	-0.289586000

Optimized coordinates of Receptor-Keto form at B3LYP/6-311G(d,p) level of theory.

6	-4.424065000	0.059739000	0.032931000
6	-5.102598000	-1.695127000	1.791914000
7	-5.740755000	0.469199000	-0.003710000
6	-6.285949000	-0.769491000	2.061422000
6	-6.795084000	-0.220379000	0.736098000
6	-2.741223000	-1.368511000	1.042559000
6	-1.725988000	-0.778528000	0.228598000
6	-3.469059000	0.660333000	-0.789544000
6	-2.093928000	0.274504000	-0.727238000
6	-3.827706000	1.764482000	-1.754717000
6	-6.194728000	1.371110000	-1.061774000
6	-5.144670000	2.432934000	-1.367246000
8	-1.216205000	0.821502000	-1.459390000
6	-0.414854000	-1.197019000	0.324352000
7	0.566107000	-0.664713000	-0.426294000
7	1.829697000	-1.218784000	-0.434889000
6	2.922255000	-0.460526000	-0.135796000
6	4.258645000	-0.922685000	-0.324053000
6	2.762796000	0.841102000	0.402279000
6	5.351510000	-0.130002000	0.015072000
6	3.846296000	1.619667000	0.735484000
6	5.142045000	1.126691000	0.541991000

7	4.558940000	-2.237382000	-0.889997000
8	5.726750000	-2.564275000	-1.016807000
8	3.610001000	-2.962993000	-1.218731000
7	6.298196000	1.958669000	0.899703000
8	6.068473000	3.069490000	1.363106000
8	7.414694000	1.492477000	0.714940000
1	-0.116697000	-1.979991000	1.015906000
1	-5.468212000	-2.582359000	1.256665000
1	-4.663514000	-2.055195000	2.726100000
1	-7.094338000	-1.302147000	2.569754000
1	-5.978879000	0.061048000	2.705332000
1	-7.601081000	0.498955000	0.905465000
1	-7.220133000	-1.039665000	0.133091000
1	-2.454630000	-2.154921000	1.736469000
1	-3.008835000	2.486810000	-1.782082000
1	-3.895746000	1.363052000	-2.774511000
1	-6.429419000	0.799618000	-1.973410000
1	-7.125621000	1.834013000	-0.724007000
1	-5.003529000	3.055566000	-0.477736000
1	-5.506807000	3.084064000	-2.167684000
1	1.988428000	-2.080757000	-0.946953000
1	1.758964000	1.216780000	0.541053000
1	6.352074000	-0.505644000	-0.138410000
1	3.715274000	2.611198000	1.146190000
1	0.227423000	0.037692000	-1.125139000

Optimized coordinates of Keto-Enol transition state at B3LYP/6-311G(d,p) level of theory.

6	-4.394941000	0.097130000	-0.011095000
6	-5.321155000	-1.937670000	1.258502000
7	-5.679176000	0.594796000	-0.078261000
6	-6.487019000	-1.016497000	1.608530000
6	-6.832720000	-0.168745000	0.391954000
6	-2.882410000	-1.616781000	0.795395000
6	-1.775692000	-0.933137000	0.224508000
6	-3.330440000	0.799849000	-0.595189000
6	-2.003284000	0.312822000	-0.492644000
6	-3.541043000	2.105317000	-1.324857000
6	-5.981123000	1.729795000	-0.949621000
6	-4.858969000	2.760588000	-0.918448000
8	-1.013446000	0.951573000	-1.014901000

6	-0.475908000	-1.426065000	0.320991000
7	0.526681000	-0.753743000	-0.237557000
7	1.796825000	-1.286714000	-0.277689000
6	2.885617000	-0.508815000	-0.050135000
6	4.220075000	-0.964912000	-0.278065000
6	2.732409000	0.812796000	0.444977000
6	5.315647000	-0.146597000	-0.018003000
6	3.819447000	1.614061000	0.698493000
6	5.113188000	1.127959000	0.467086000
7	4.509325000	-2.295490000	-0.801809000
8	5.672884000	-2.614024000	-0.982812000
8	3.553867000	-3.049847000	-1.043569000
7	6.271646000	1.985360000	0.740857000
8	6.048357000	3.112315000	1.168463000
8	7.385969000	1.524777000	0.527658000
1	-0.252168000	-2.359130000	0.833674000
1	-5.666501000	-2.676891000	0.522837000
1	-4.992243000	-2.502827000	2.134722000
1	-7.365476000	-1.591928000	1.912999000
1	-6.214655000	-0.360832000	2.441920000
1	-7.621974000	0.547033000	0.637666000
1	-7.224721000	-0.813017000	-0.411986000
1	-2.700565000	-2.550452000	1.321664000
1	-2.693259000	2.763711000	-1.123289000
1	-3.526624000	1.933364000	-2.409172000
1	-6.147074000	1.383939000	-1.981968000
1	-6.919680000	2.170539000	-0.603685000
1	-4.780827000	3.166967000	0.095196000
1	-5.107318000	3.590800000	-1.585311000
1	1.952606000	-2.179252000	-0.738177000
1	1.731992000	1.184532000	0.616123000
1	6.313473000	-0.516806000	-0.199761000
1	3.694492000	2.619162000	1.076704000
1	0.109384000	0.152366000	-0.767715000

Optimized coordinates of Receptor-Cr(III) at B3LYP/LANL2DZ level of theory.

6	-3.848827000	1.130030000	1.189006000
6	-4.500917000	0.387275000	0.147759000
6	-4.648018000	2.087225000	2.065308000
7	-5.874584000	0.565633000	-0.103345000
6	-5.923484000	2.572448000	1.351910000

6	-6.703428000	1.361179000	0.817940000
6	-2.488451000	0.963084000	1.404052000
6	-1.658354000	0.059011000	0.663797000
6	-3.728772000	-0.511508000	-0.636026000
6	-2.355800000	-0.655933000	-0.350582000
6	-4.367331000	-1.307481000	-1.775022000
6	-6.575222000	-0.397307000	-0.961219000
6	-5.727667000	-0.716595000	-2.200805000
8	-1.626392000	-1.628011000	-1.147974000
6	-0.269304000	-0.025380000	1.007782000
7	0.610527000	-0.852274000	0.356440000
7	1.926168000	-0.915852000	0.920821000
1	0.110336000	0.585777000	1.821882000
1	-4.934715000	1.581075000	3.000662000
1	-4.020246000	2.939811000	2.352954000
1	-6.558750000	3.140590000	2.043355000
1	-5.662917000	3.232362000	0.513882000
1	-7.593649000	1.694105000	0.268270000
1	-7.054527000	0.746570000	1.668938000
1	-2.013430000	1.541221000	2.195266000
1	-3.719248000	-1.310954000	-2.668873000
1	-4.514029000	-2.358797000	-1.474194000
1	-6.803262000	-1.332606000	-0.414210000
1	-7.532183000	0.045035000	-1.264246000
1	-5.570021000	0.209184000	-2.768105000
1	-6.259070000	-1.424916000	-2.848501000
1	-2.226396000	-2.082977000	-1.774191000
24	0.270924000	-2.010913000	-0.996123000
1	2.093472000	-1.479339000	1.758067000
6	2.979976000	-0.222310000	0.380657000
6	4.330765000	-0.377731000	0.864516000
6	2.773985000	0.682612000	-0.709882000
6	5.401295000	0.316307000	0.266807000
6	3.828334000	1.369137000	-1.292000000
1	1.761136000	0.822457000	-1.068361000
6	5.145866000	1.173758000	-0.799732000
1	6.407910000	0.175770000	0.642490000
1	3.666741000	2.057032000	-2.113759000
7	4.652489000	-1.248136000	1.975530000
8	3.681360000	-1.862674000	2.596681000
8	5.878551000	-1.396109000	2.324725000
7	6.257591000	1.894656000	-1.418722000
8	5.991840000	2.678064000	-2.401328000
8	7.440573000	1.714403000	-0.957735000

Optimized coordinates of Receptor-Arsenate at B3LYP/LANL2DZ level of theory.

6	-6.268306000	0.605106000	0.217039000
6	-5.691350000	-0.241595000	1.266909000
6	-7.669076000	0.322751000	-0.281158000
7	-6.460922000	-1.252822000	1.784350000
6	-7.942652000	-1.191074000	-0.241875000
6	-7.740020000	-1.711251000	1.185381000
6	-5.521529000	1.656283000	-0.270349000
6	-4.200936000	1.954373000	0.192471000
6	-4.384991000	0.014124000	1.756631000
6	-3.616508000	1.096092000	1.242991000
6	-3.751923000	-0.878559000	2.812388000
6	-6.014539000	-1.974590000	2.999039000
6	-4.498965000	-2.216006000	2.961096000
8	-2.405171000	1.333630000	1.691962000
6	-3.570138000	3.085227000	-0.415573000
7	-2.316153000	3.504743000	-0.235958000
7	-2.027182000	4.658219000	-0.921669000
6	-0.769794000	5.231789000	-0.924036000
6	-0.533172000	6.498898000	-1.565167000
6	0.335210000	4.586166000	-0.300050000
6	0.744329000	7.088353000	-1.563470000
6	1.595464000	5.170146000	-0.300814000
6	1.790539000	6.422606000	-0.931322000
7	-1.585900000	7.246240000	-2.247465000
8	-1.313593000	8.380142000	-2.762169000
8	-2.778309000	6.731775000	-2.314576000
7	3.126272000	7.035755000	-0.932284000
8	4.075376000	6.402399000	-0.351427000
8	3.273714000	8.167945000	-1.512130000
1	-4.214721000	3.644411000	-1.107218000
1	-8.405027000	0.841484000	0.355923000
1	-7.793811000	0.720840000	-1.294709000
1	-8.969531000	-1.411467000	-0.556808000
1	-7.259189000	-1.720097000	-0.914972000
1	-7.721579000	-2.807184000	1.181692000
1	-8.568307000	-1.388961000	1.837955000
1	-5.952682000	2.287539000	-1.045434000
1	-2.706430000	-1.076340000	2.551837000
1	-3.723355000	-0.352350000	3.779051000
1	-6.282714000	-1.380140000	3.886970000

1	-6.562093000	-2.920752000	3.048462000
1	-4.274056000	-2.875438000	2.115084000
1	-4.186537000	-2.726224000	3.880046000
1	-1.422039000	0.622355000	2.796761000
1	-2.749099000	5.174578000	-1.445036000
1	0.197921000	3.612376000	0.160154000
1	0.902630000	8.044199000	-2.048404000
1	2.433996000	4.671682000	0.172463000

Optimized coordinates of Receptor-PPi at B3LYP/LANL2DZ level of theory.

6	6.761242000	-2.919340000	-0.456808000
6	6.776122000	-1.779377000	0.418840000
6	8.063881000	-3.556895000	-0.919791000
7	7.988061000	-1.239838000	0.839014000
6	9.214852000	-2.535243000	-0.898116000
6	9.275742000	-1.867459000	0.483787000
6	5.538867000	-3.435816000	-0.860941000
6	4.283428000	-2.911636000	-0.438255000
6	5.539553000	-1.206889000	0.852790000
6	4.326673000	-1.784982000	0.436166000
6	5.519189000	0.015219000	1.764999000
6	8.026791000	-0.198339000	1.883045000
6	6.854746000	0.777800000	1.720159000
8	3.121897000	-1.281300000	0.868356000
6	3.106247000	-3.579773000	-0.936333000
7	1.827845000	-3.296213000	-0.731020000
7	0.986693000	-4.211411000	-1.387065000
6	-0.369763000	-4.159813000	-1.342116000
6	-1.190445000	-5.155340000	-2.006777000
6	-1.057485000	-3.117512000	-0.633742000
6	-2.593626000	-5.107844000	-1.940549000
6	-2.435322000	-3.078449000	-0.574680000
6	-3.210251000	-4.083927000	-1.223342000
7	-0.622547000	-6.253546000	-2.766220000
8	-1.398527000	-7.103774000	-3.326392000
8	0.673761000	-6.347619000	-2.859572000
7	-4.655038000	-4.050846000	-1.136210000
8	-5.200158000	-3.132478000	-0.402942000
8	-5.347595000	-4.923870000	-1.773024000
1	3.348981000	-4.442478000	-1.573901000
1	8.326333000	-4.401301000	-0.262481000
1	7.938059000	-3.973578000	-1.927113000

1	10.174210000	-3.025624000	-1.106771000
1	9.054795000	-1.767718000	-1.666856000
1	10.044185000	-1.083869000	0.493082000
1	9.563358000	-2.615550000	1.244291000
1	5.537346000	-4.295313000	-1.531022000
1	4.711161000	0.701207000	1.483653000
1	5.304596000	-0.289532000	2.801035000
1	7.995768000	-0.656901000	2.887337000
1	8.982486000	0.332914000	1.794722000
1	6.957217000	1.303040000	0.761518000
1	6.886252000	1.530033000	2.517885000
1	3.108934000	-0.479298000	1.492974000
1	1.382924000	-4.990701000	-1.930379000
1	-0.482379000	-2.343794000	-0.139992000
1	-3.178867000	-5.869608000	-2.441943000
1	-2.939012000	-2.278718000	-0.044042000
33	0.675420000	0.496018000	1.803126000
8	2.291464000	0.712500000	2.249454000
8	0.496365000	-0.941222000	0.774961000
1	1.344382000	-1.420822000	0.527649000
8	-0.511516000	0.271302000	3.091309000
8	-0.007060000	1.836451000	0.869591000
1	-1.018576000	1.910131000	0.947037000