

# **Nitrogen-doped Graphene Oxide dots- based “turn-off” H<sub>2</sub>O<sub>2</sub>, Au (III) and “turn off– on” Hg (II) sensors as Logic gates and Molecular Keypad Lock**

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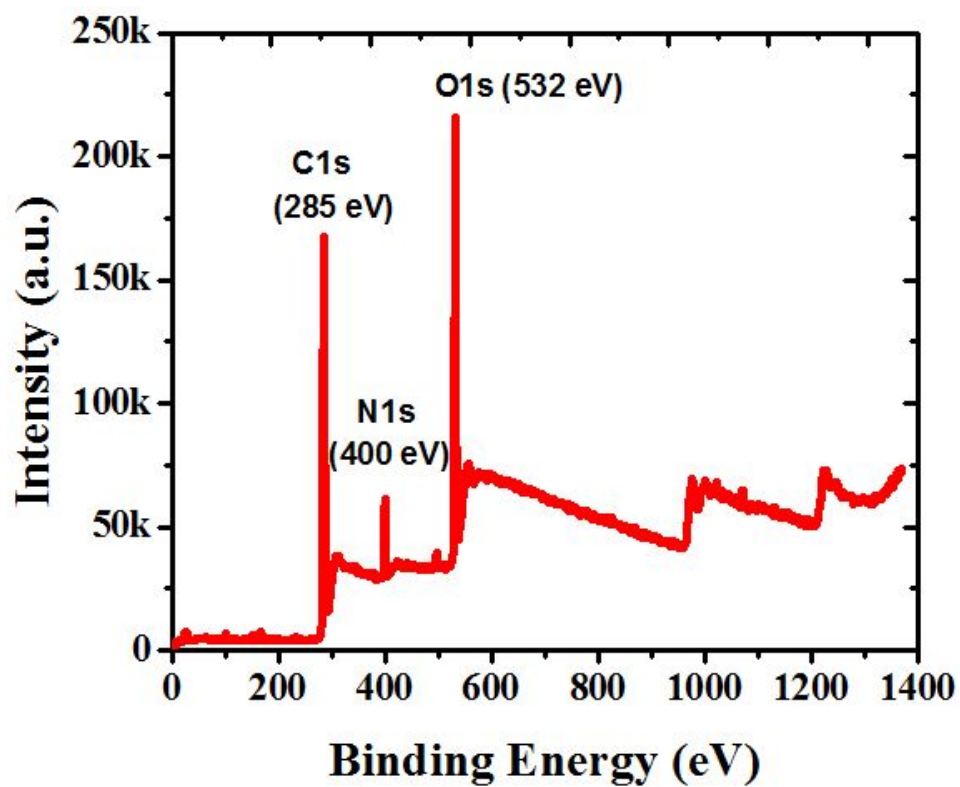


Figure S1. The XPS full survey scan of as-prepared NGODs

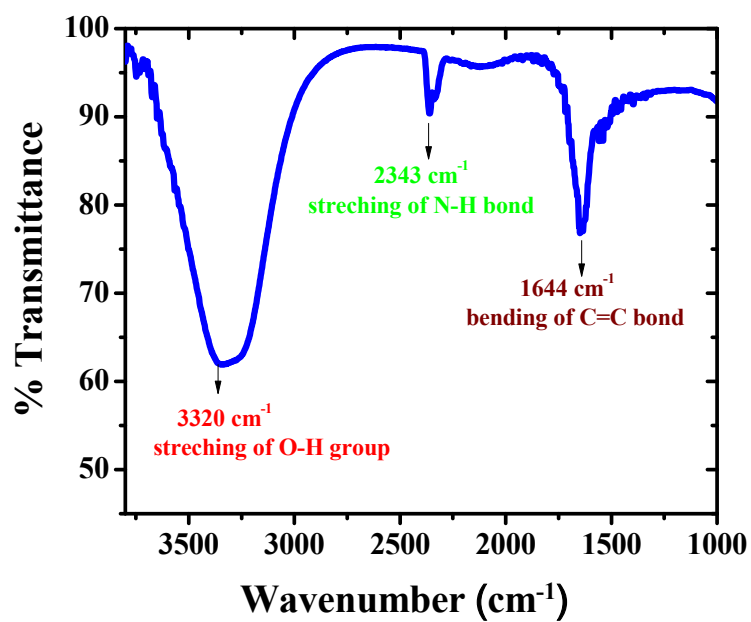
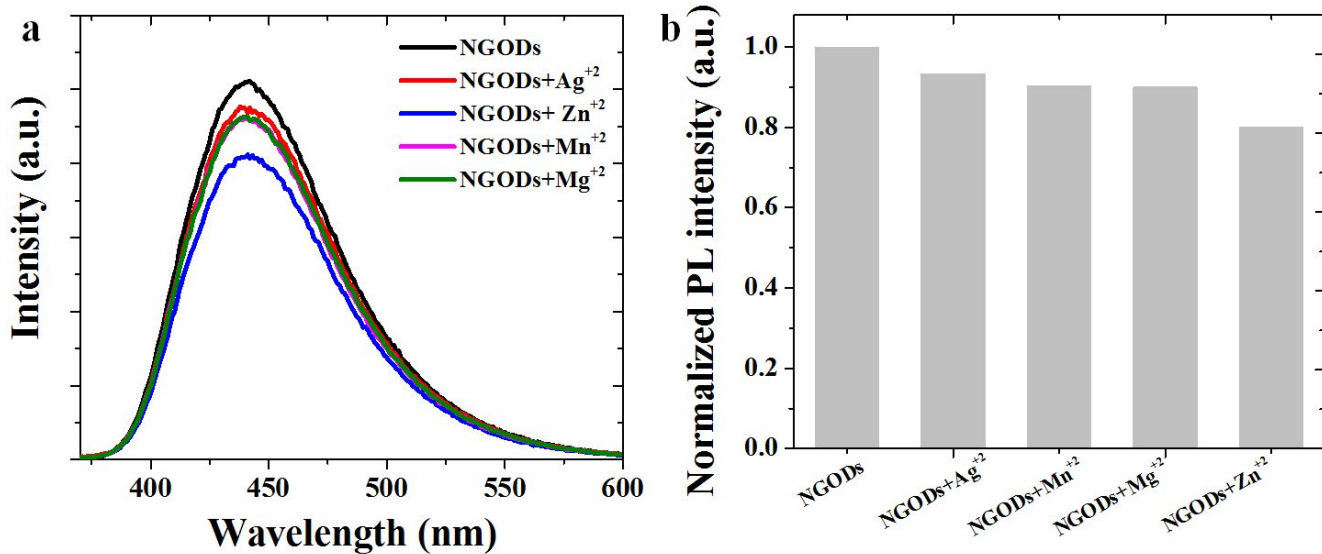
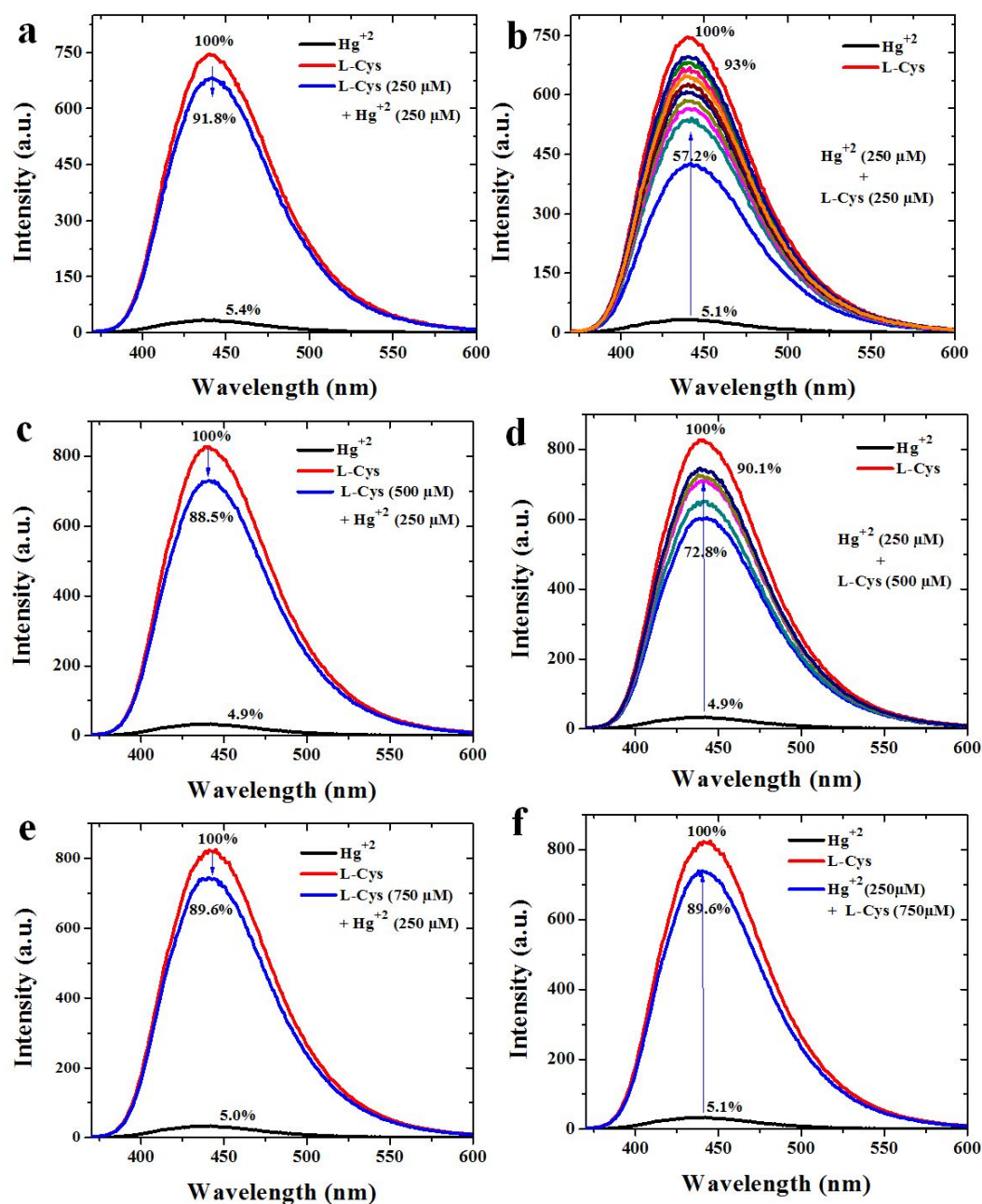


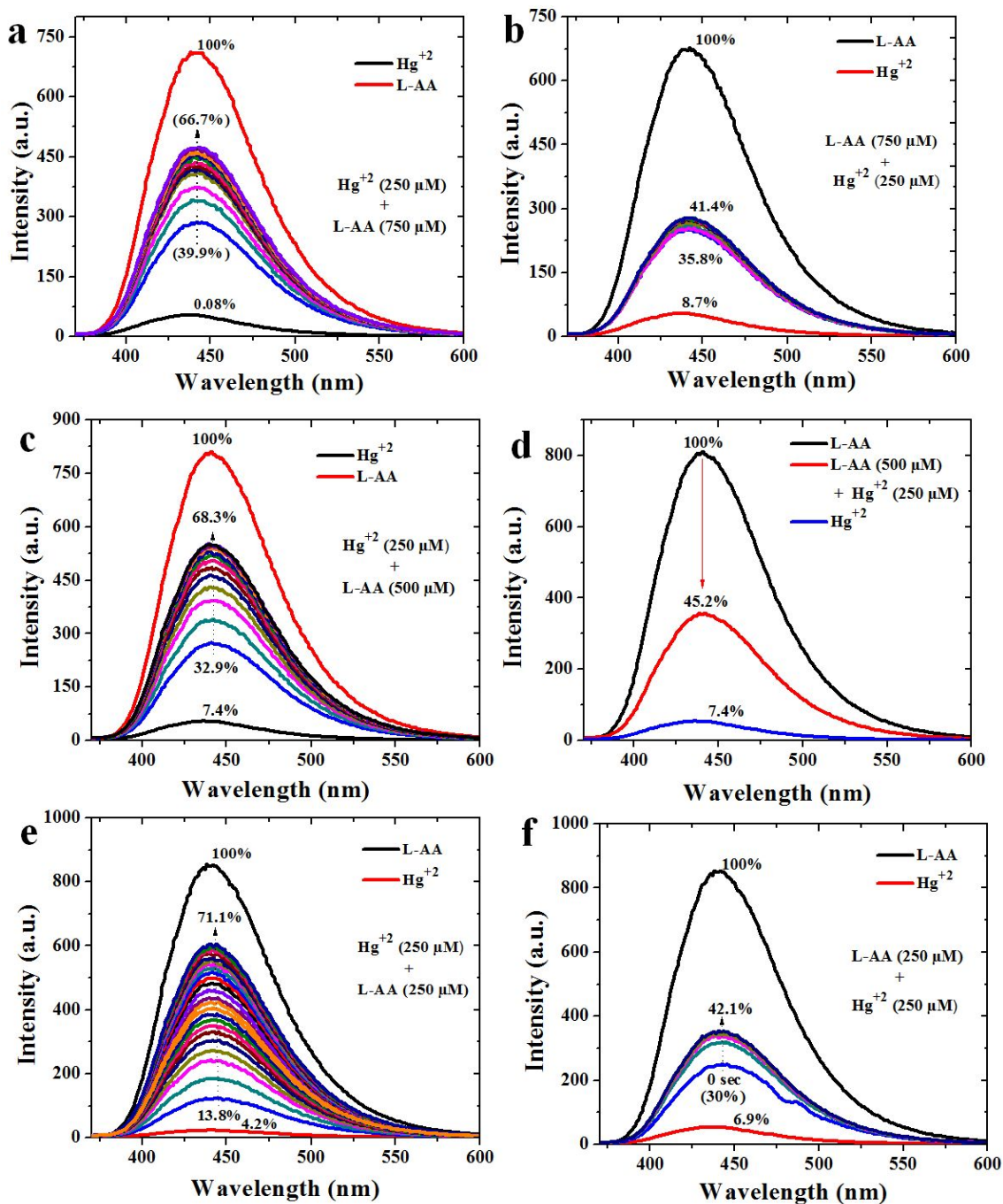
Figure S2. FTIR spectrum of as-prepared NGODs.



**Figure S3.** PL spectroscopy analysis of Ag<sup>+</sup>, Mn<sup>2+</sup>, Mg<sup>2+</sup>, and Zn<sup>2+</sup> using NGODs as probe (a) PL Intensity vs wavelength at  $\lambda_{ex} = 344$  nm for different metal ions at 250  $\mu$ M concentration and (b) Corresponding normalized graph at  $\lambda_{em} = 441$  nm.

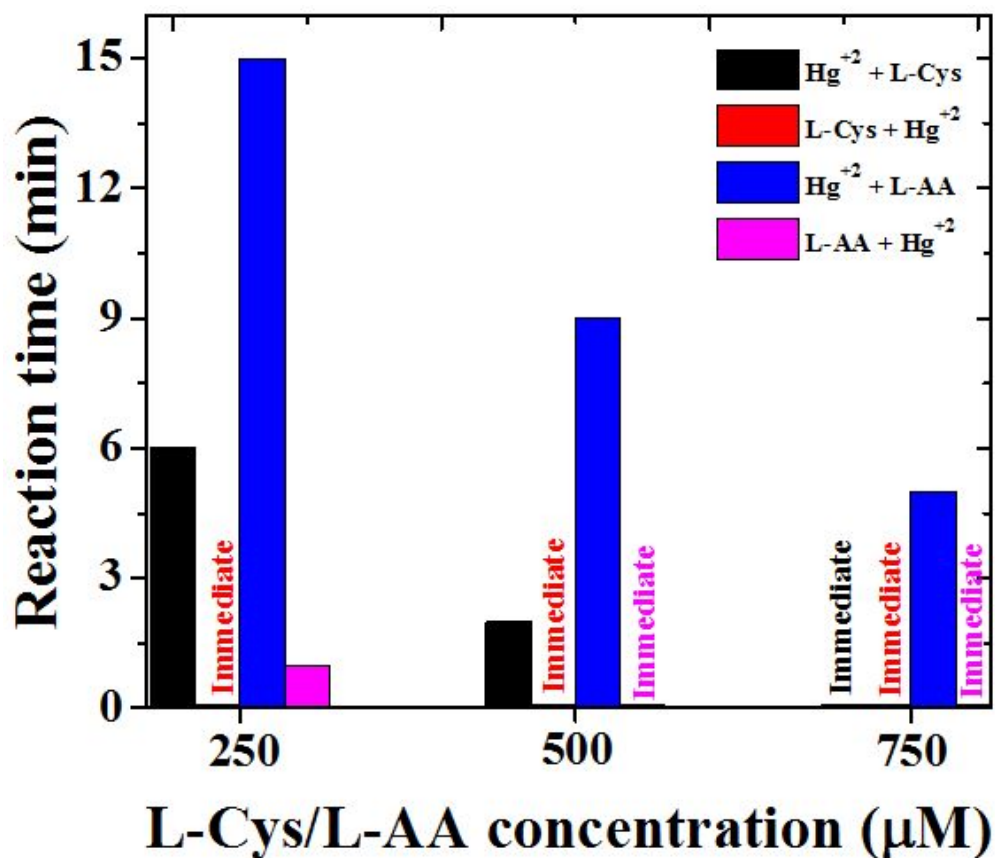


**Figure S4. Effect of variation in the order of addition of L-Cys and Hg<sup>+2</sup>:** Time dependent PL (excitation wavelength = 344nm) response, taken after every 40 ± 10 seconds, at 3 different concentrations of L-Cys in (First Column) NGODs + L-Cys + Hg<sup>+2</sup> (a) 250 μM, (c) 500 μM and (e) 750 μM; (Second Column) NGODs + Hg<sup>+2</sup> + L-Cys (b) 250 μM, (d) 500 μM and (f) 750 μM complexes. The control sample (i.e. as prepared NGODs with L-Cysteine (L-Cys)) is shown for reference as 100% in each set of experiment and the concentration of Hg<sup>+2</sup> is kept fixed/constant at 250 μM.



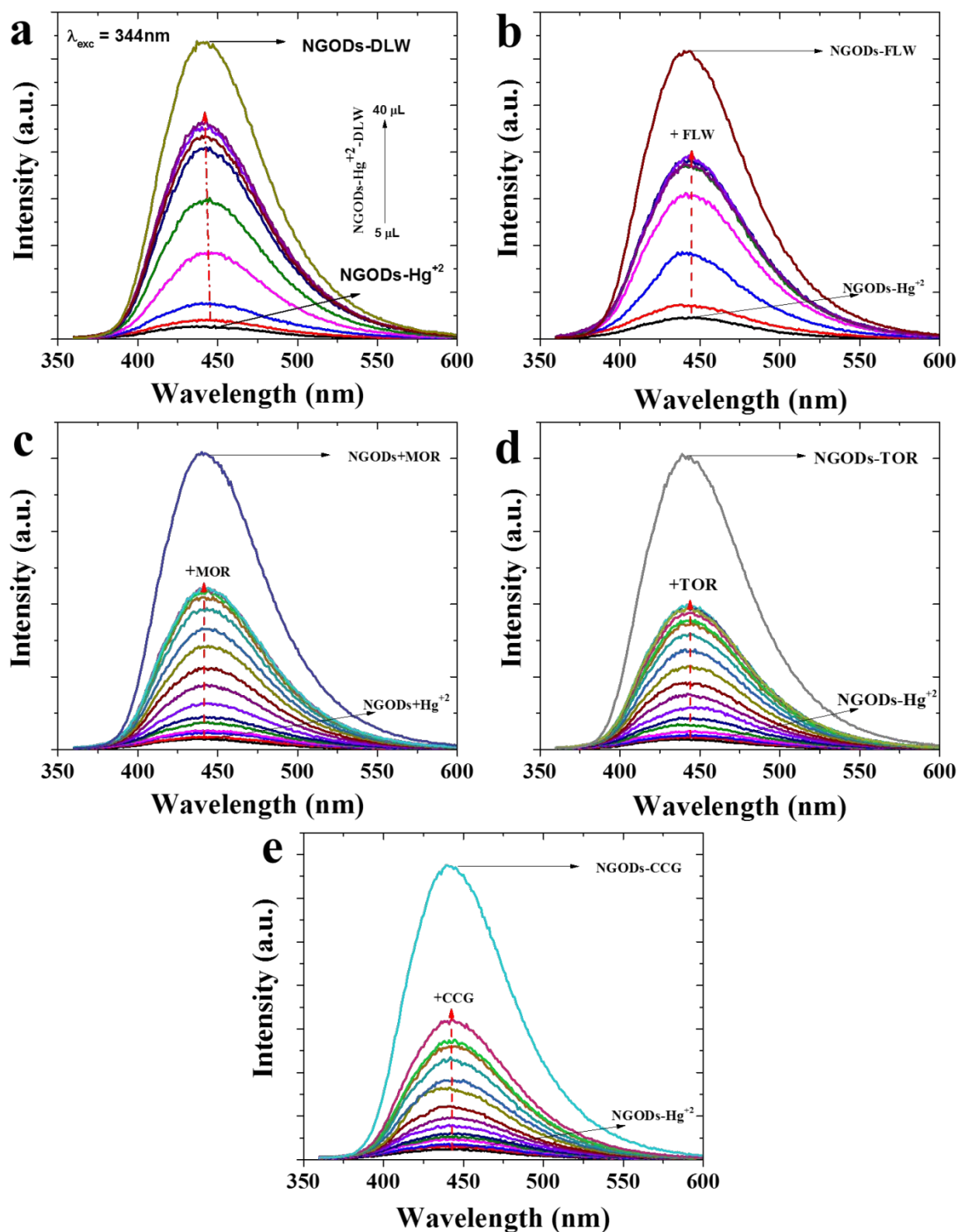
**Figure S5.** Effect of variation in the order of addition of L-AA and  $\text{Hg}^{+2}$ : Time dependent PL (excitation wavelength = 344nm) response, taken after every  $40 \pm 10$  seconds, at 3

different concentrations of L-AA in (First Column) NGODs +  $\text{Hg}^{+2}$  + L-AA (a) 750  $\mu\text{M}$ , (c) 500  $\mu\text{M}$  and (e) 250  $\mu\text{M}$ ; (Second Column) NGODs +L-AA+ $\text{Hg}^{+2}$  (b) 750  $\mu\text{M}$ , (d) 500  $\mu\text{M}$  and (f) 250  $\mu\text{M}$  complexes. The control sample (i.e. as prepared NGODs with L-Ascorbic acid (L-AA)) is shown for reference as 100% in each set of experiment and the concentration of  $\text{Hg}^{+2}$  is kept fixed/constant at 250  $\mu\text{M}$ .



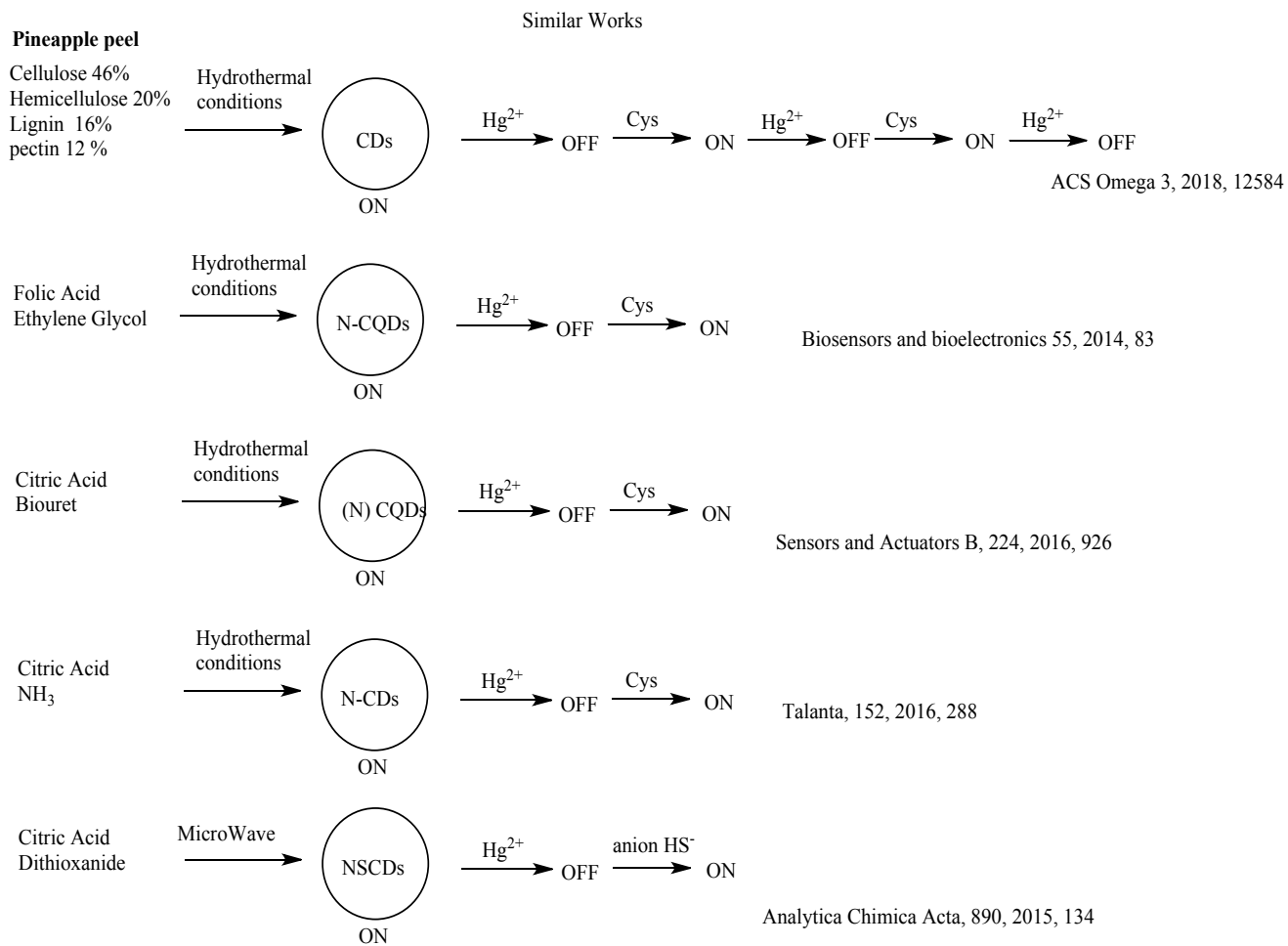
**Figure S6. Data analysis of Figure S3 and Figure S4 representing time taken in PL signal recovery and quenching during  $\text{Hg}^{+2}$  detection:** Reaction time vs concentration of L-Cys and L-AA (color of the word “immediate” represents the solution complex mentioned in the bar graph labels)





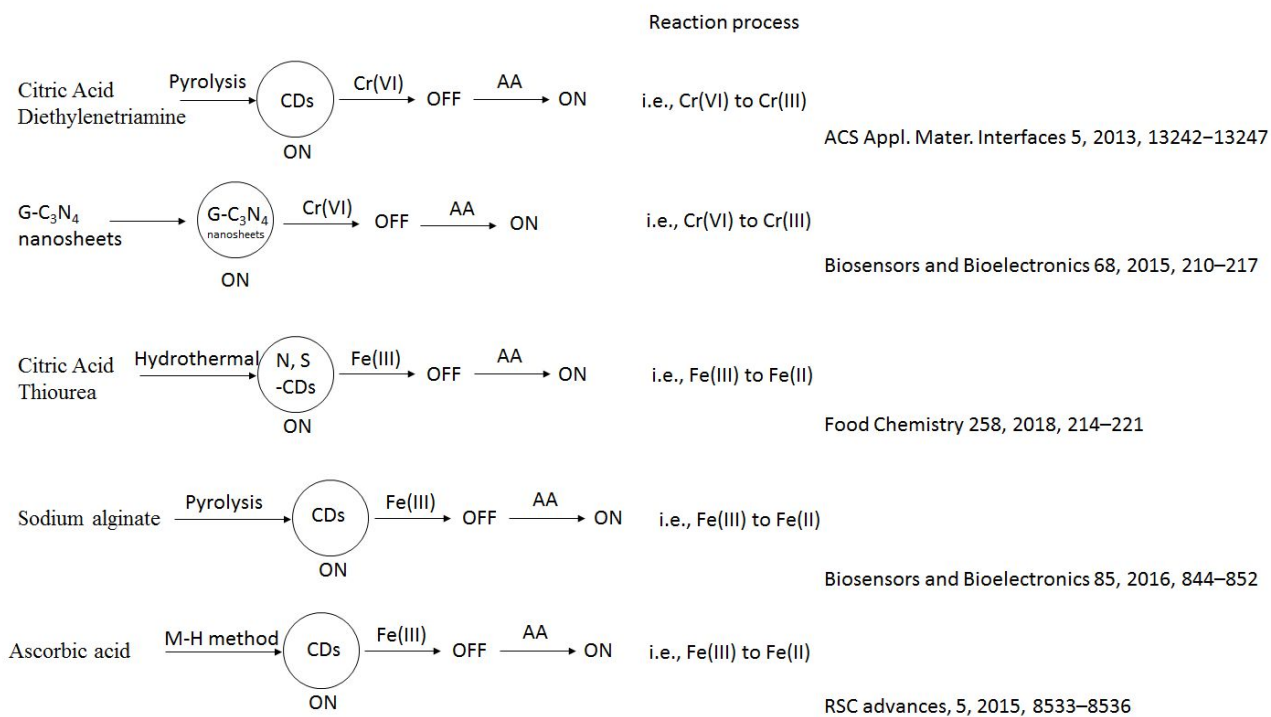
**Figure S7.** PL response of NGODs+Hg<sup>2+</sup> in different dilutions of citrus fruit juice (a) NGODs+Hg<sup>2+</sup> + diluted lemon water (DLW) from Green lemon, (b) NGODs+Hg<sup>2+</sup>+ Fanta lemon water (FLW), (c) NGODs+Hg<sup>2+</sup>+ Mandarina orange (MOR), (d) NGODs+Hg<sup>2+</sup>+Tangerine orange (TOR) and (e) NGODs+Hg<sup>2+</sup>+ Cotton candy grape (CCG).



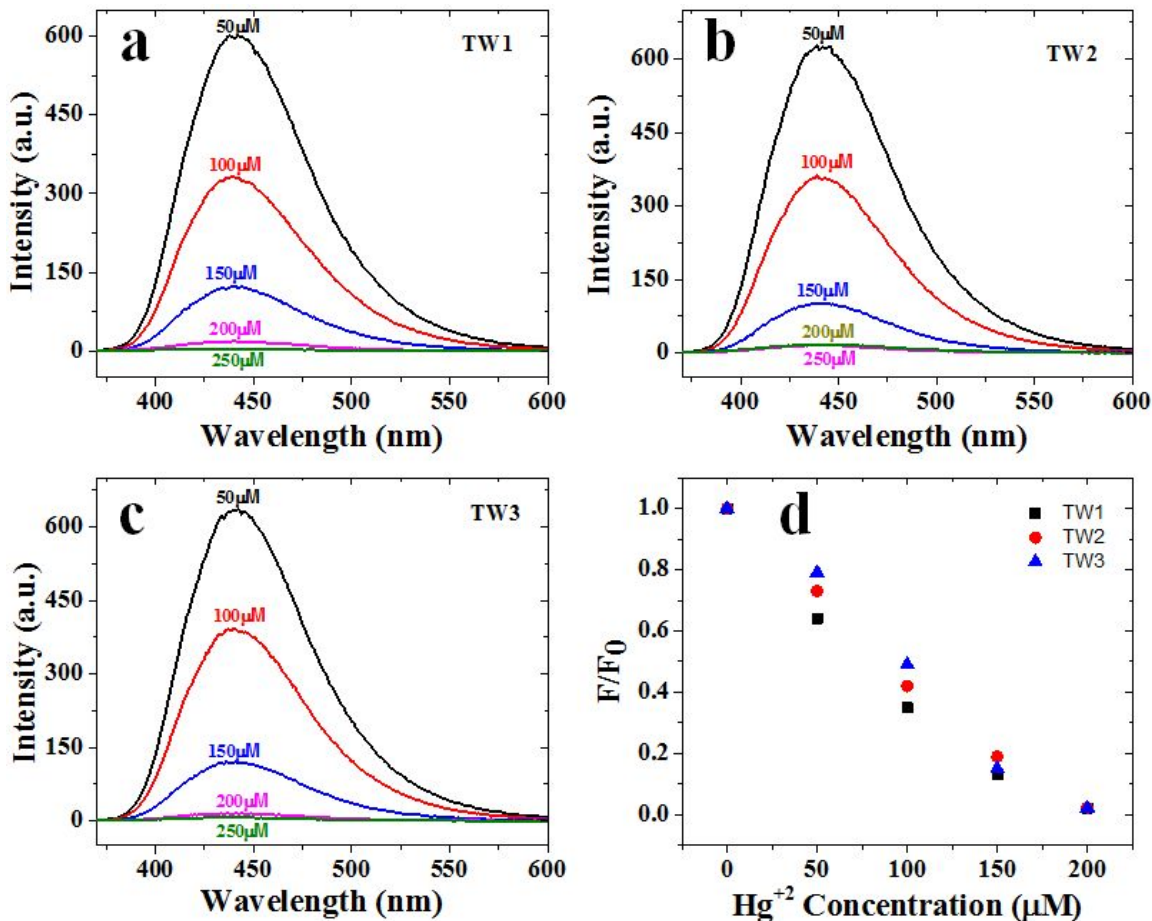


**Figure S8.** Schematically represented outcome of similar works related to PL signal recovery using L-Cystine (Cys) and anion  $HS^-$

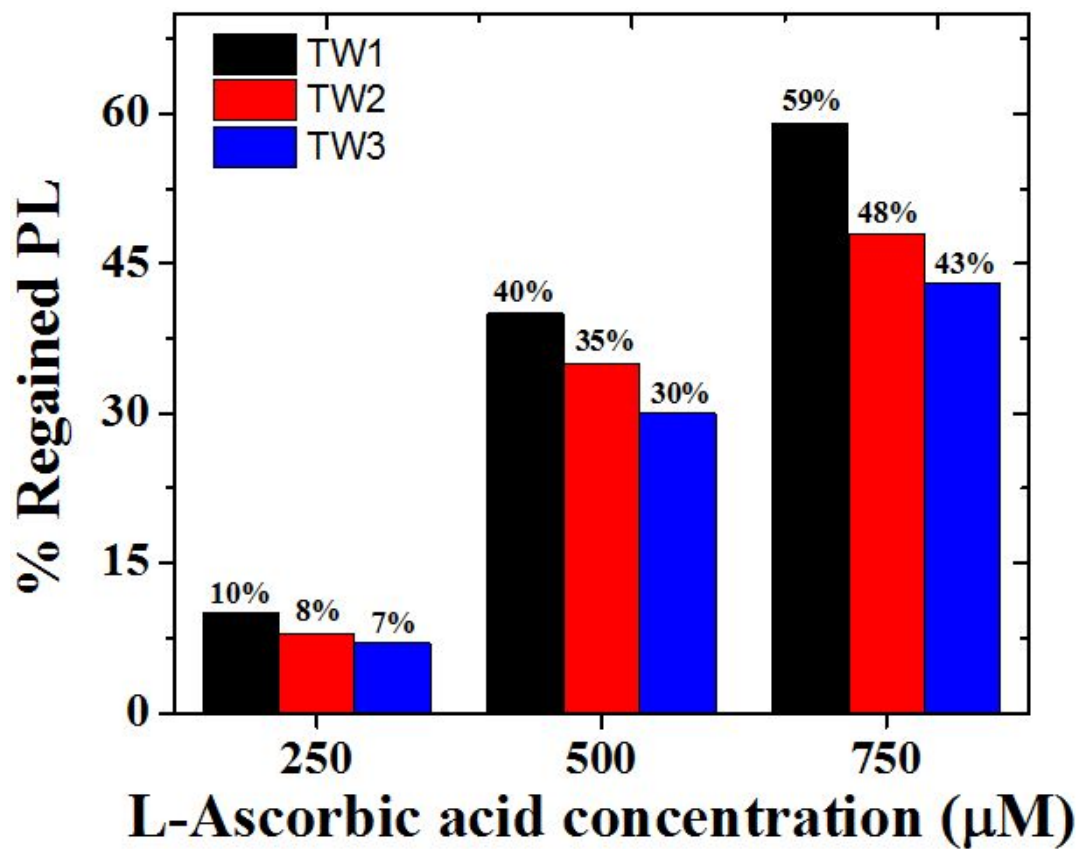
### Similar Works



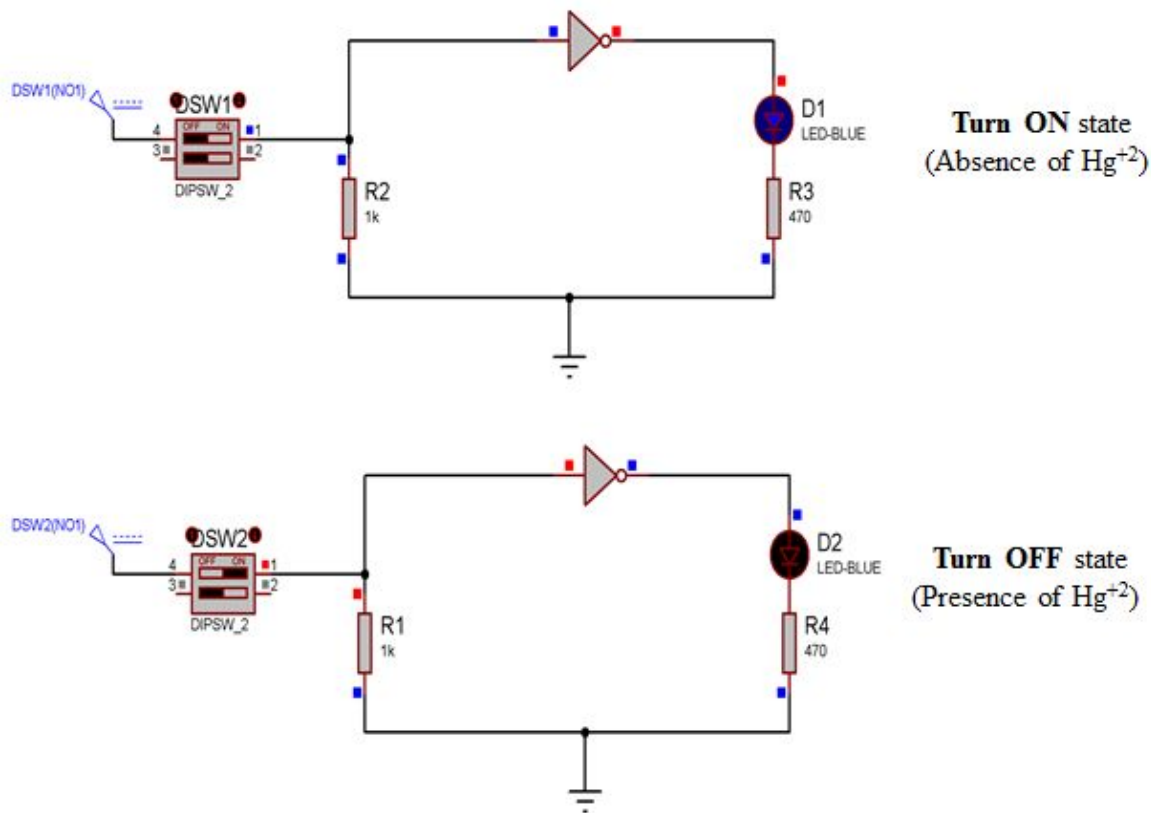
**Figure S9.** Schematically represented outcome of similar works related to PL signal recovery (quenching from Cr<sup>+6</sup> and Fe<sup>+3</sup>) using L-Ascorbic acid



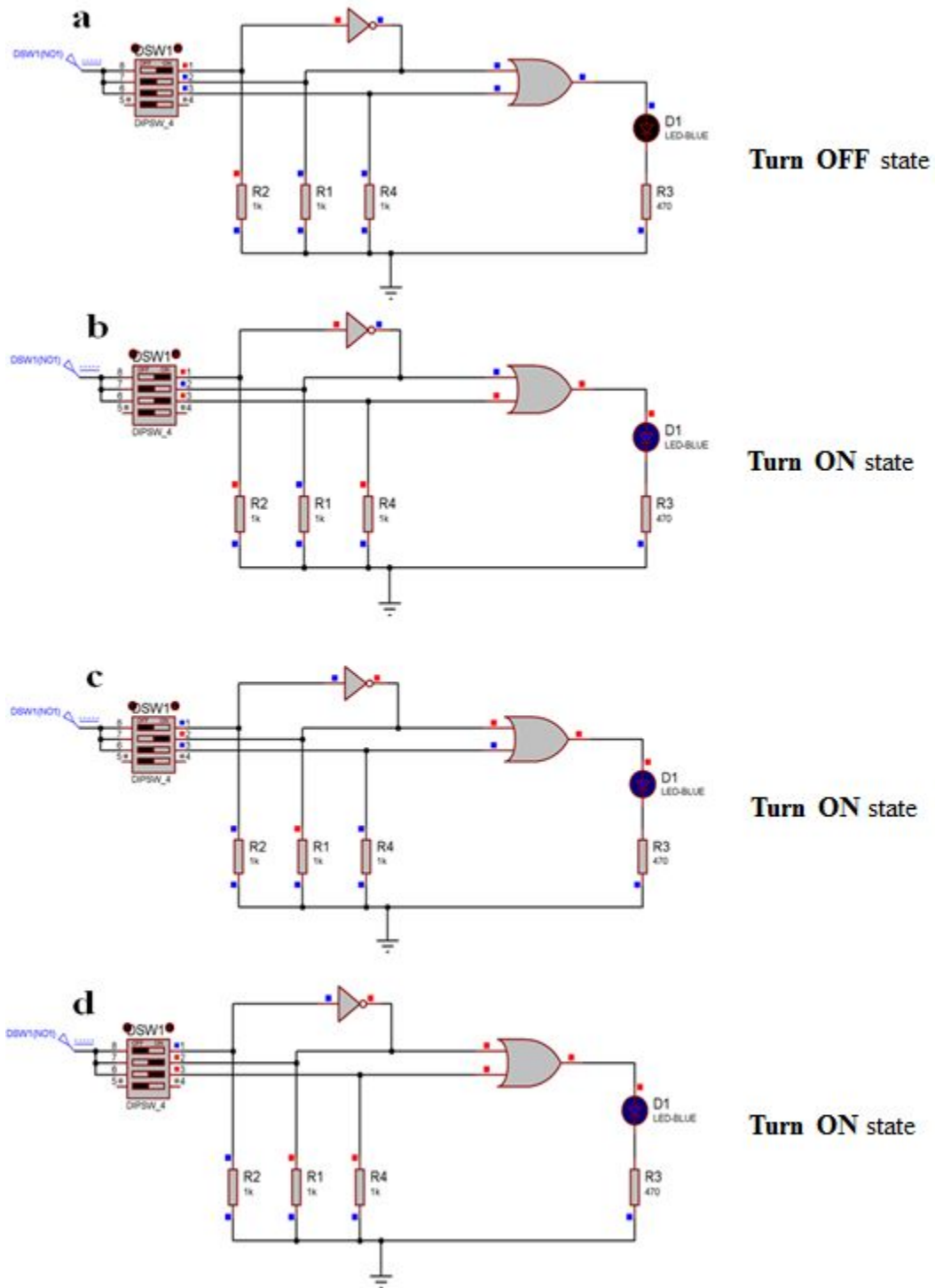
**Figure S10.** Optical response of NGODs from  $\text{Hg}^{2+}$  spiked real tap water collected from three different places (a) TW1 (google map view: 18.94926,-99.2709454), (b) TW2 (18.977705, -99.247733) and (c) TW3 (18.9808869,-99.2401062) and (d)  $F/F_0$  vs  $\text{Hg}^{2+}$  concentration, ( $F$  is PL intensity of NGODs- $\text{Hg}^{2+}$  complex at different concentrations of  $\text{Hg}^{2+}$  and  $F_0$  is NGODs PL intensity (fixed)).



**Figure S11.** Regained PL signal (%) from Hg (II) spiked tap water sample from 3 different locations (TW1, TW2 and TW3) at 3 different concentrations of L-Ascorbic acid.

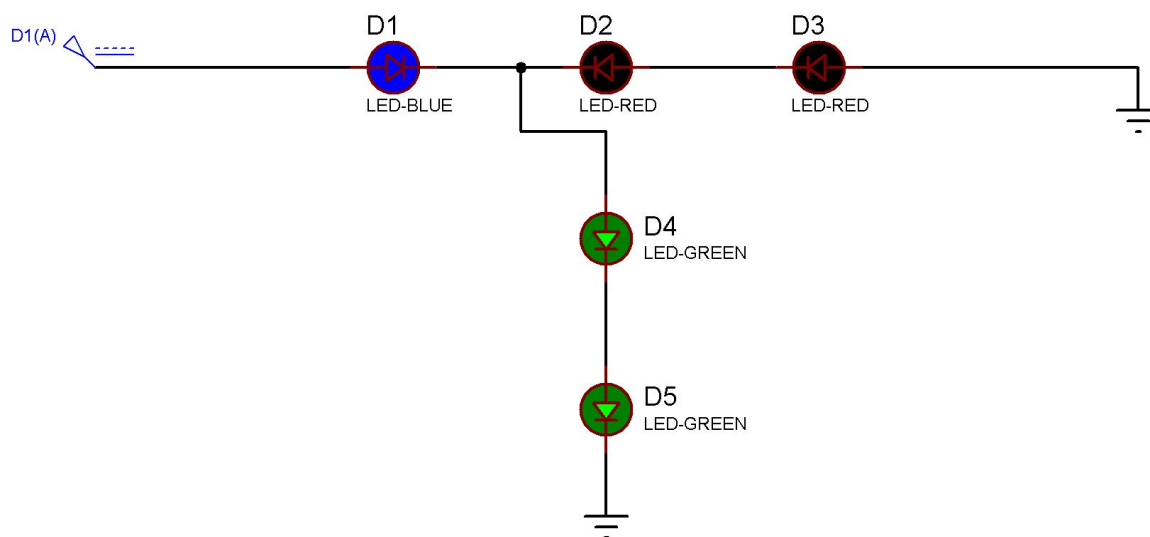


**Figure S12.** NGODs-Hg<sup>2+</sup> complex is representing NOT gate (upper image) operations (where the presence (upper) and absence (lower) of Hg<sup>2+</sup> in NGODs' solution represents OFF (upper) and ON (lower) respectively in the executed circuit; the outputs were found to match with the experimental results). Red dots indicate TURN ON state and blue dots indicate TURN OFF state.



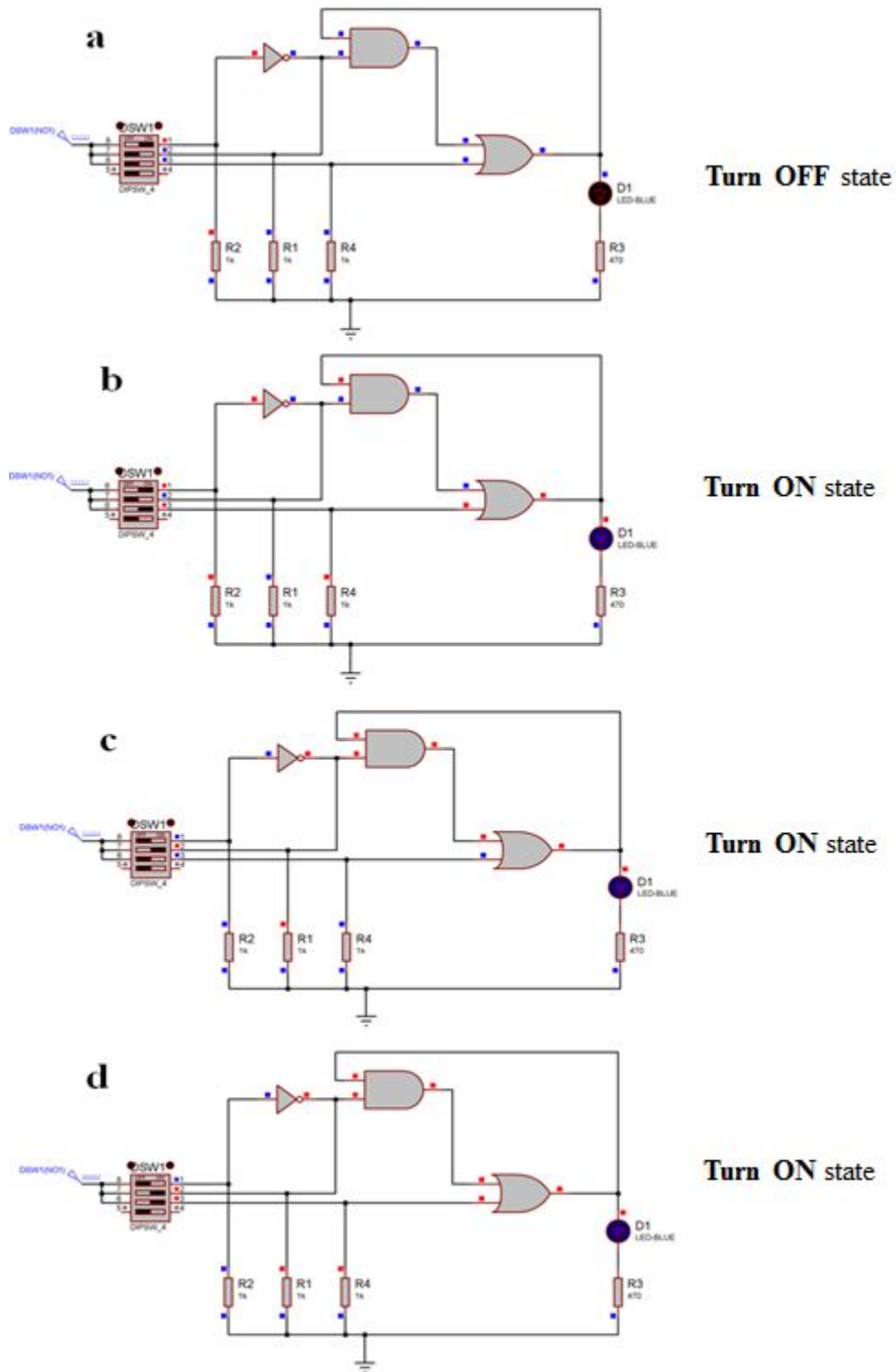
**Figure S13.** Simulations corresponding to figure 8a; (a) Input 1 is 1, input 2 is 0 and input 3 is 0 gives output 0 (turn off state), (b) Input 1 is 0, input 2 is 1 and input 3 is 0 gives output 1 (turn on state) (c) Input 1 is 1, input 2 is 0 and input 3 is 1 gives output 1 (turn on state), and (d) Input 1 is 0, input 2 is 1 and input 3 is 1 gives output 1 (turn on state). Red dots

indicate Turn ON state and blue dots indicates Turn OFF state. (Input 1=  $\text{Hg}^{+2}$ ; Input 2 = Output of Input 1; Input 3= L-Cys/L-AA) ; Red dots indicate TURN ON state and blue dots indicate TURN OFF state.



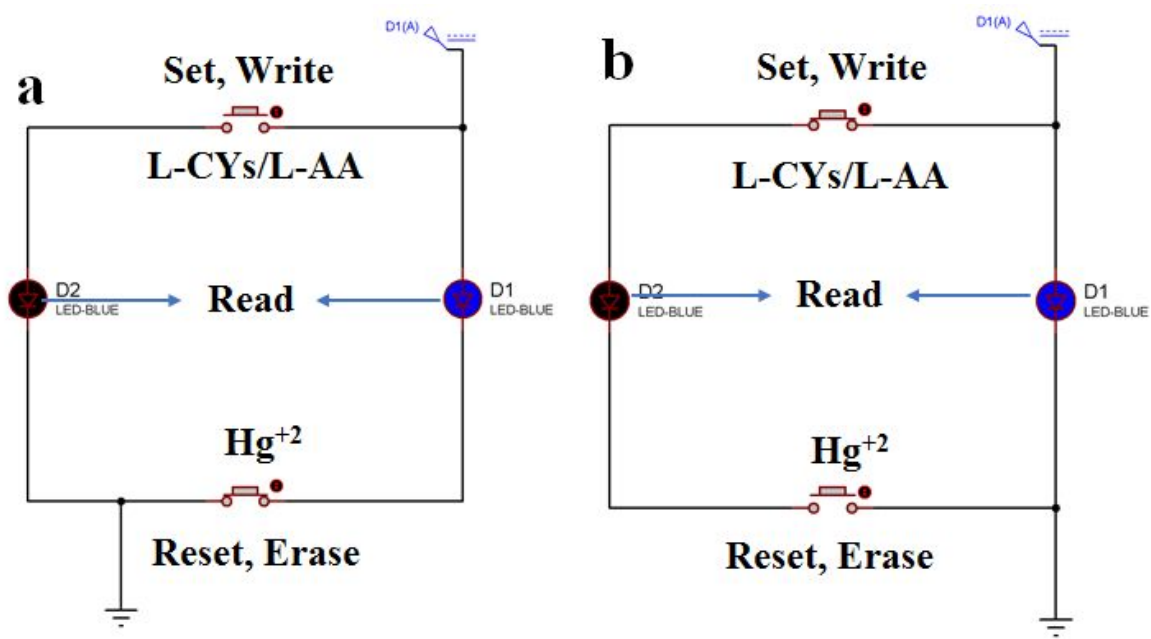
**Figure S14.** Simulations corresponding to figure 8e (D1=L-AA, D2= $\text{Hg}^{+2}$ , D3=OFF, D4=L-AA and D5=ON)





**Figure S15.** Simulations corresponding to figure 9e: (a) Input 1 is 1, input 2 is 0 and input 3 is 0 then the output is 0 (turn off state), (b) Input 1 is 1, input 2 is 0 and input 3 is 1 then the output is 1 (turn on state) (c) Input 1 is 0, input 2 is 1 and input 3 is 0 then the output is 0 (turn on state), and (d) Input 1 is 0, input 2 is 1 and input 3 is 1 then the output is 1 (turn on

state). Red dots indicates Turn ON state and blue dots indicates Turn OFF state. (Input 1=  $\text{Hg}^{+2}$ ; Input 2 = Output of Input 1; Memory element initial = O(OFF); Input 3= L-Cys/L-AA)



**Figure S16.** Simulations corresponding to figure 9f; (a) Reset and (b) Set.