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Deep learning assisted detection of toxic heavy metal ions based on visual fluorescence response from carbon nanoparticles array

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Materials and Reagents

Alizarin red S, cysteine, dithiothreitol, glutamic acid, histidine, lysine, p-phenylenediamine, tryptophan, tyrosine, ceric ammonium nitrate, 2,4-dinitrophenylhydrazine (DNPH), arsenic oxide, cadmium nitrate, mercuric chloride, potassium dichromate, lead nitrate, magnesium chloride, aluminium nitrate, calcium chloride, chromium nitrate, manganese acetate, ferric nitrate, cobalt chloride, nickel acetate, coper sulfate, zinc chloride, and sodium hydroxide were purchased from either Central Drug House (P) Ltd., India or Sisco Research Laboratories Pvt. Ltd., India. Potassium bromide, branched chain polyethylenimine, Ninhydrin, 5,5′-dithio-bis-(2-nitrobenzoic acid) (DTNB), and dialysis membrane (2kDa) were bought from Sigma-Aldrich. Milli-Q ultrapure water was used as a solvent in all experiments unless specified.

Accuracy and f-measure

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

$$Precision = \frac{TP}{TP + FP}$$

$$Recall = \frac{TP}{TP + FN}$$

$$f\_measure = 2\frac{Precision - Recall}{Precision + Recall}$$

A true positive (TP) is an outcome where the model correctly predicts the positive class whereas a true negative (TN) refers to the model correctly predicting the negative class. False-negative (FP) is a test result that wrongly indicates that a particular condition is absent whereas a False-positive (FP) result indicates that a given condition is present when it is not.

Pseudocode for MLP

Algorithm: Multi-layer perception classifier
Input: A set of observation of the form (x_i, y_i), for i =1,...,n
'h' an activation function to apply to the inputs
'w' a random initialization of weights and biases 'b' close to zero
for number of *epochs* ***do***
    for each of (x_i, y_i) **do**
        y'_i =compute h (x_i)
        if $y'_i \neq y_i$ **then**
            Update the parameters using eq. 1 and 2
        end if
    end for
end for

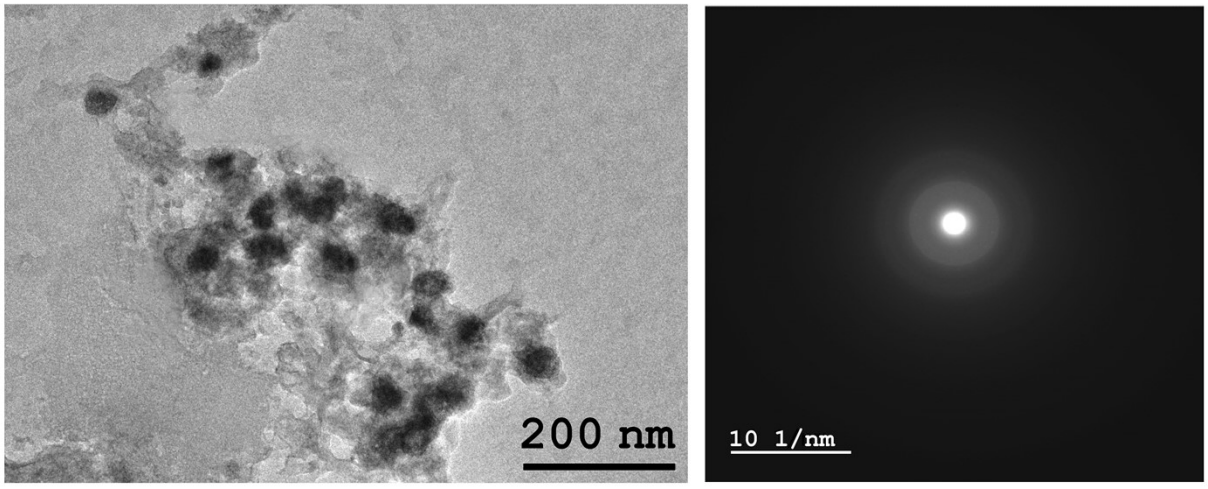

Figure S1. TEM and SAED pattern of $CNP_{ARS\text{-}Cys}$.

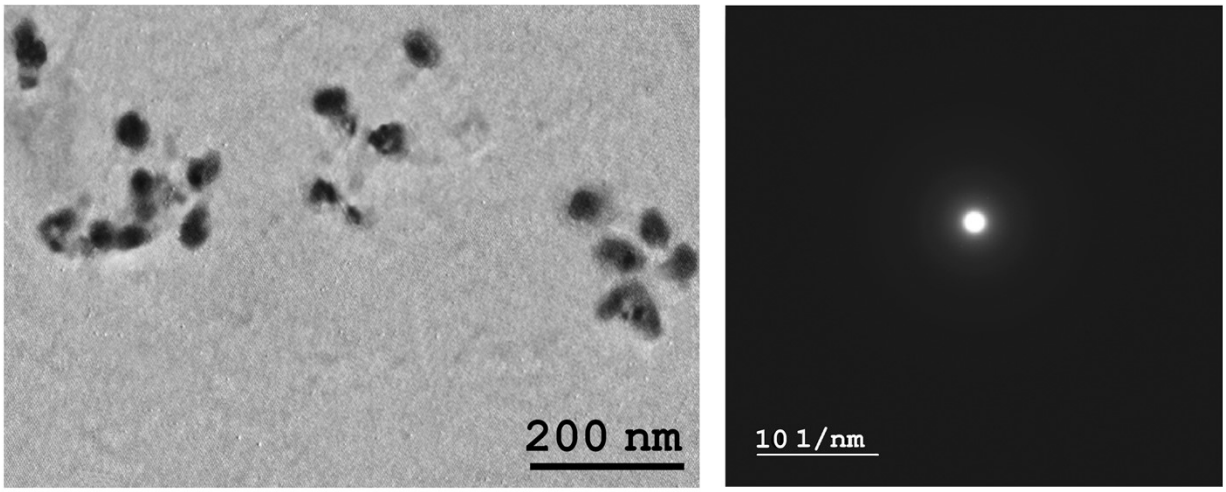

Figure S2. TEM and SAED pattern of $CNP_{ARS\text{-}DTT}$.

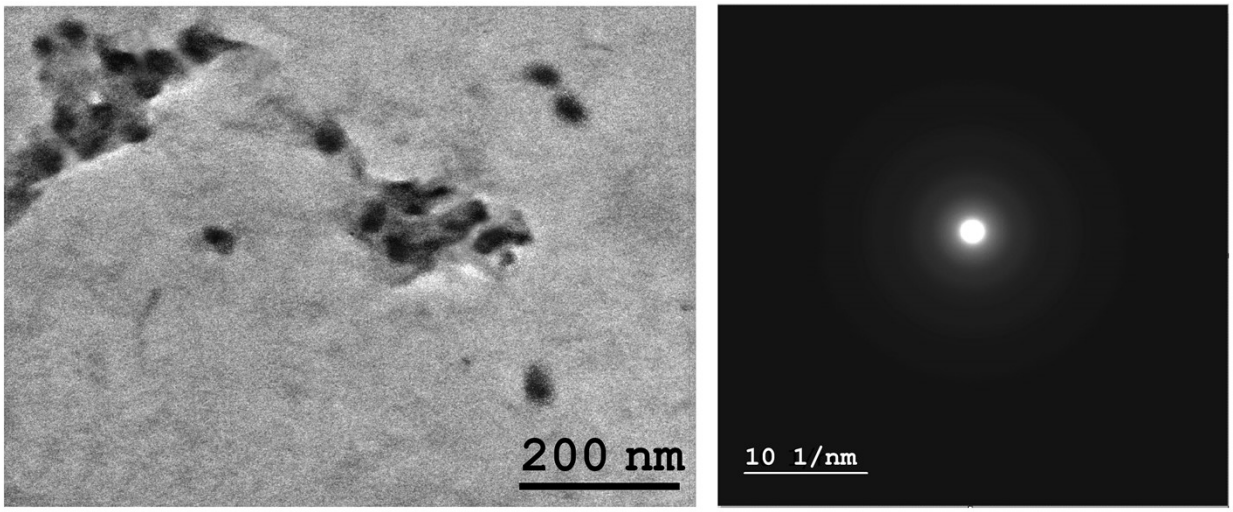

Figure S3. TEM and SAED pattern of $CNP_{ARS\text{-}Glu}$.

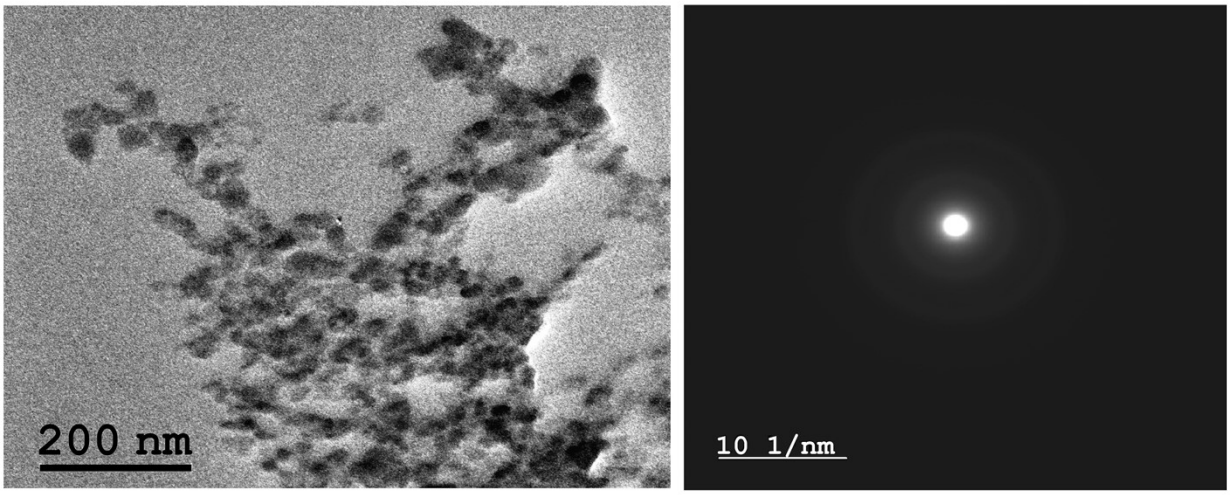

Figure S4. TEM and SAED pattern of $CNP_{ARS\text{-}His}$.

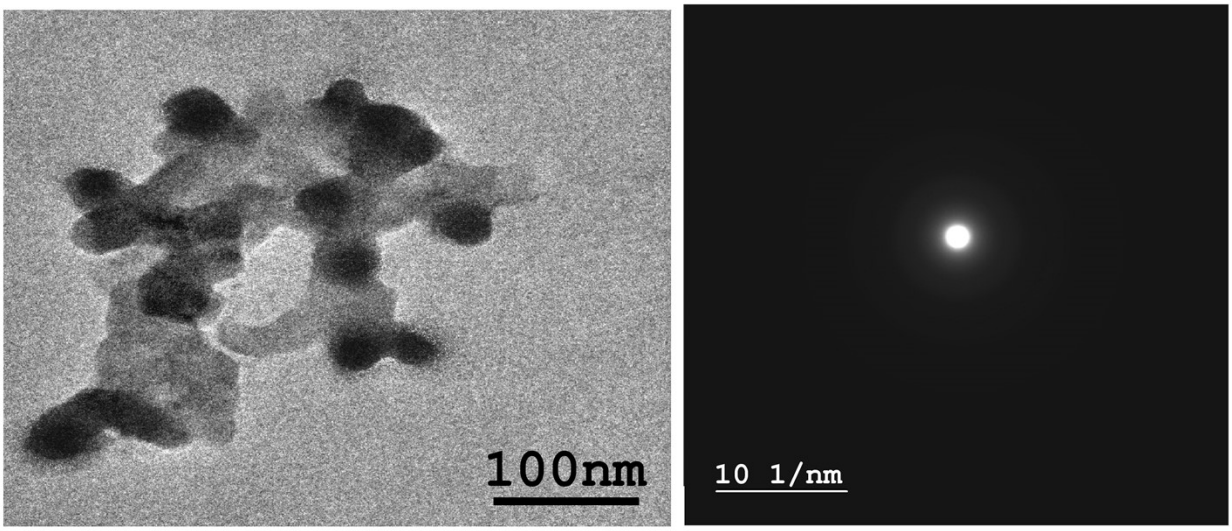

Figure S5. TEM and SAED pattern of $CNP_{ARS\text{-}Lys}$.

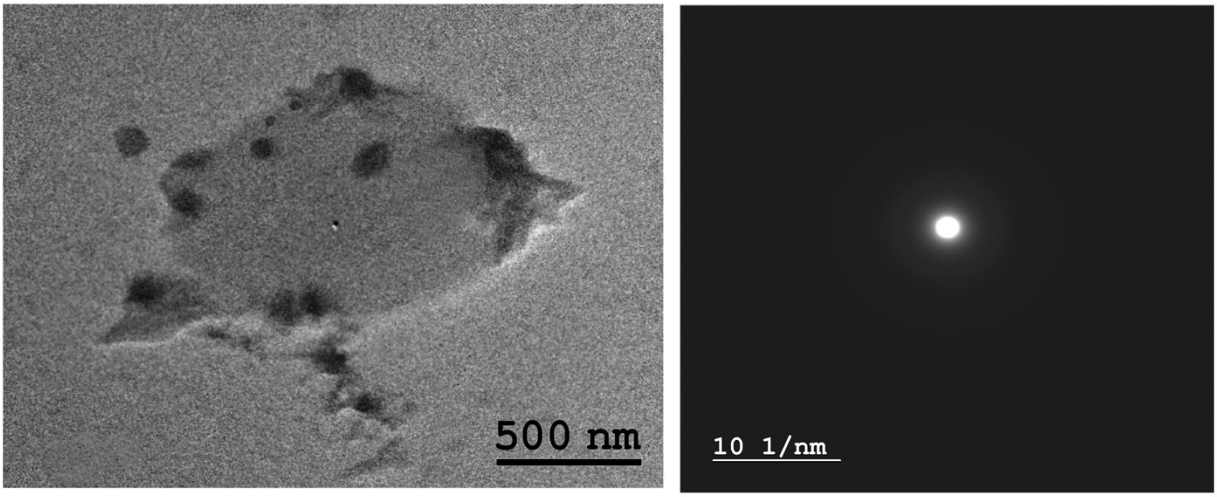

Figure S6. TEM and SAED pattern of $CNP_{ARS\text{-}pPD}$.

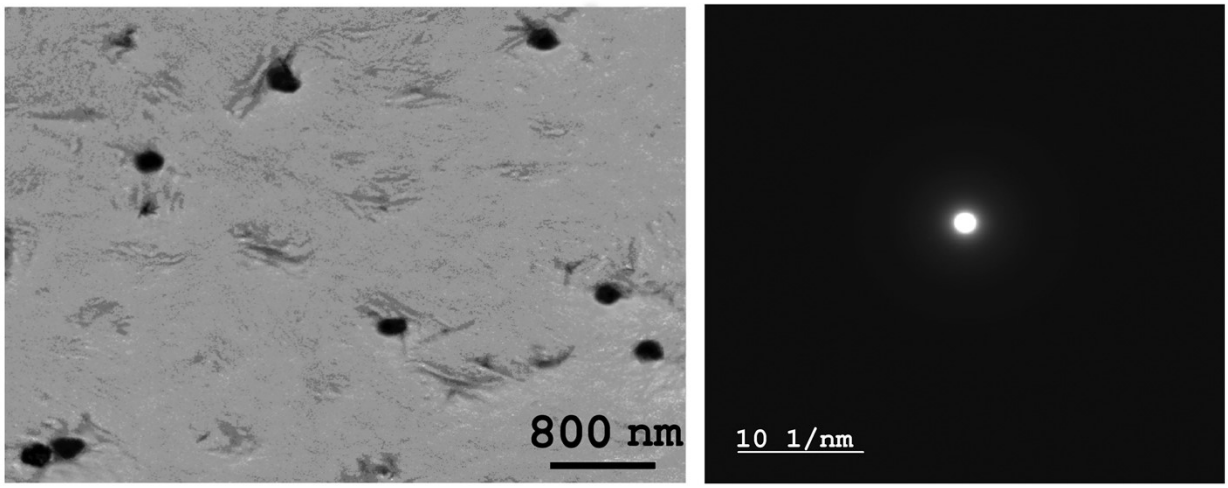

Figure S7. TEM and SAED pattern of $CNP_{ARS\text{-}PEI}$.

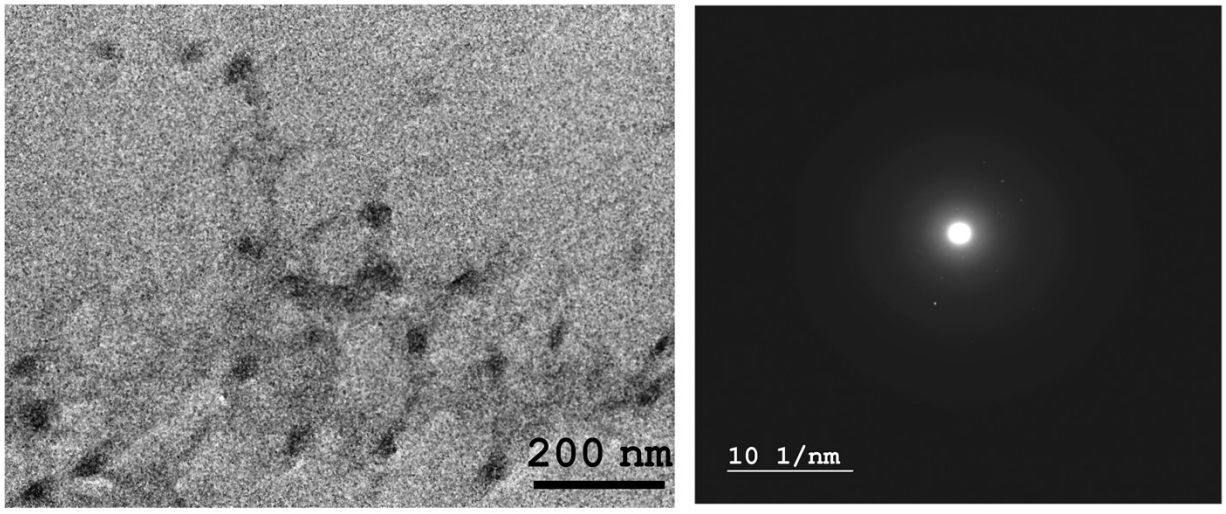

Figure S8. TEM and SAED pattern of $CNP_{ARS\text{-}Trp}$.

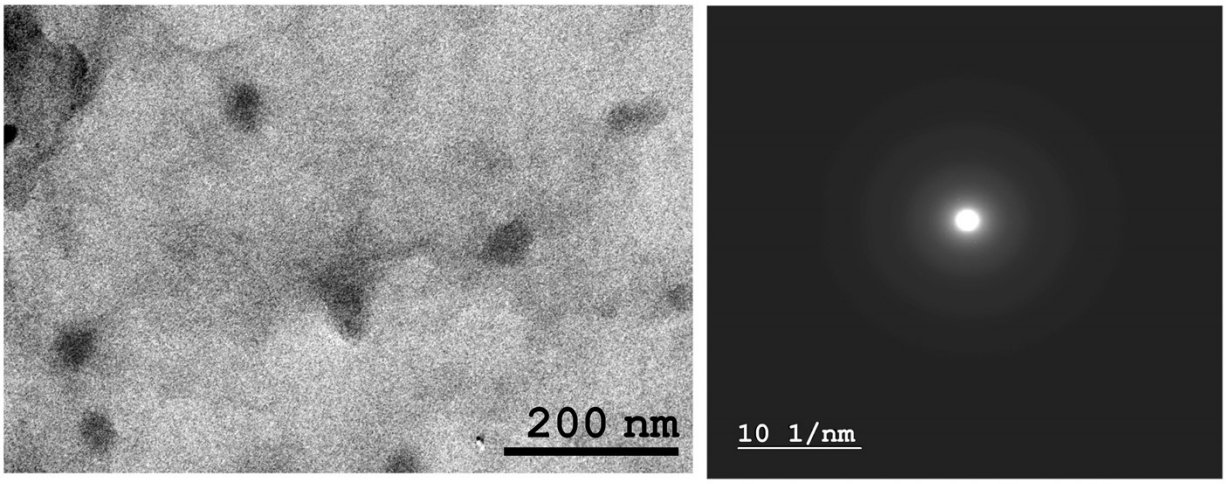

Figure S9. TEM and SAED pattern of $CNP_{ARS\text{-}Tyr}$.

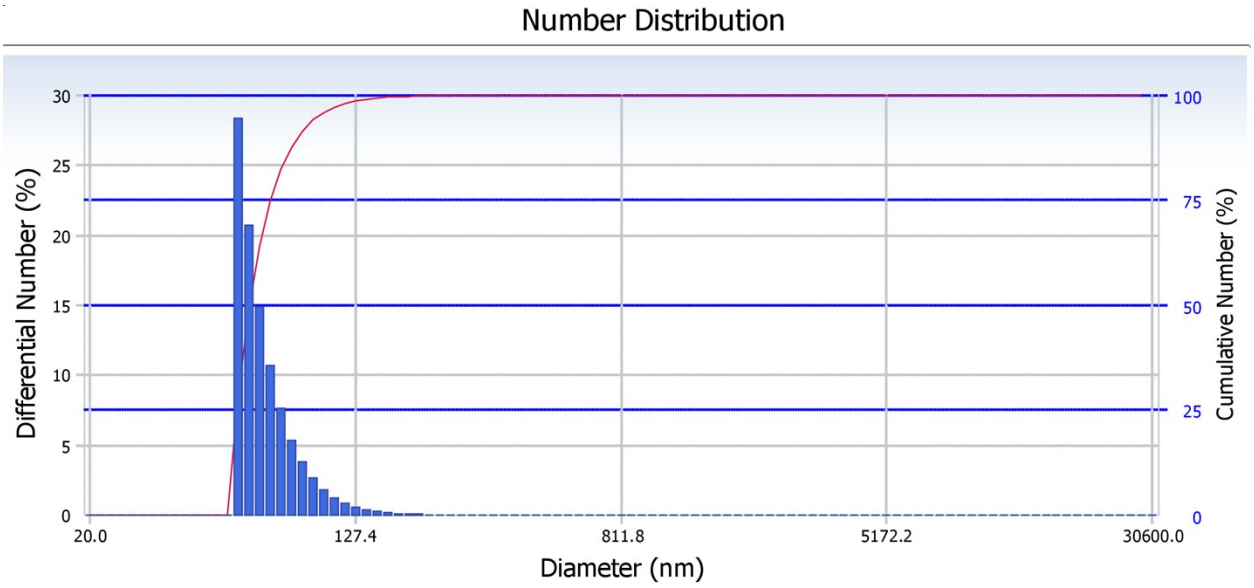

Figure S10. Number distribution diameter of $CNP_{ARS\text{-}Cys}$.

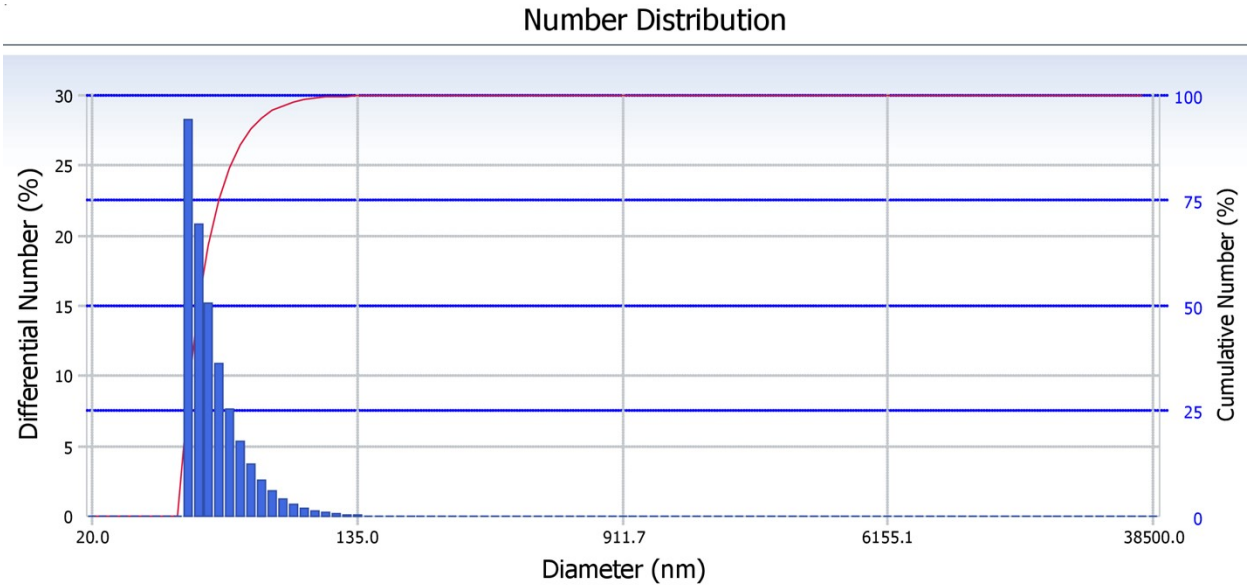

Figure S11. Number distribution diameter of $CNP_{ARS\text{-}DTT}$.

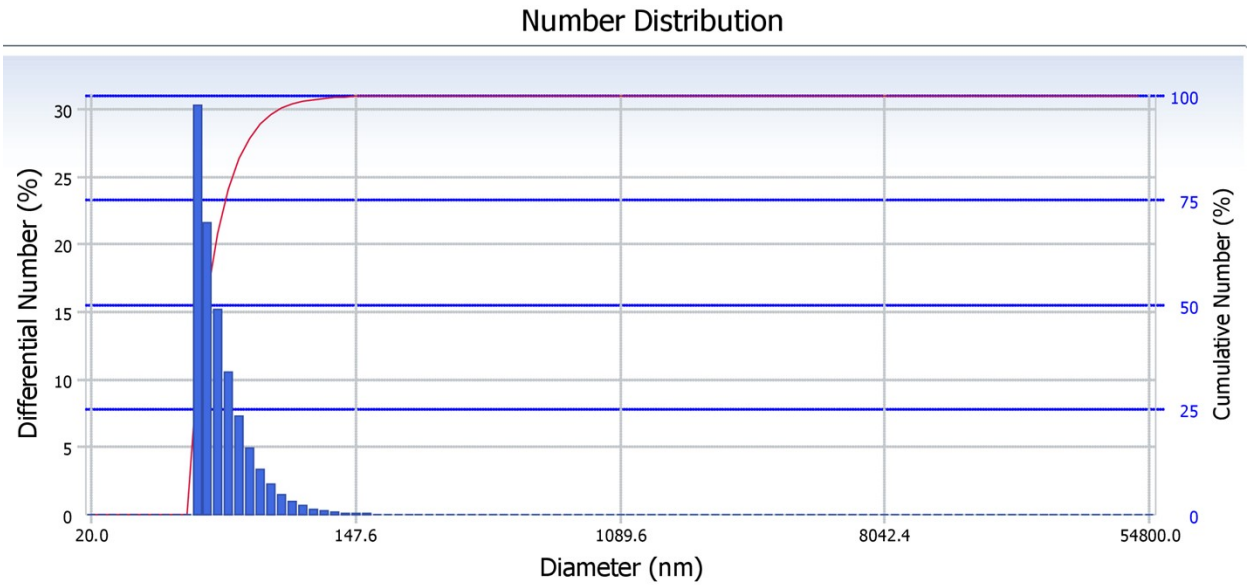

Figure S12. Number distribution diameter of $CNP_{ARS\text{-}Glu}$.

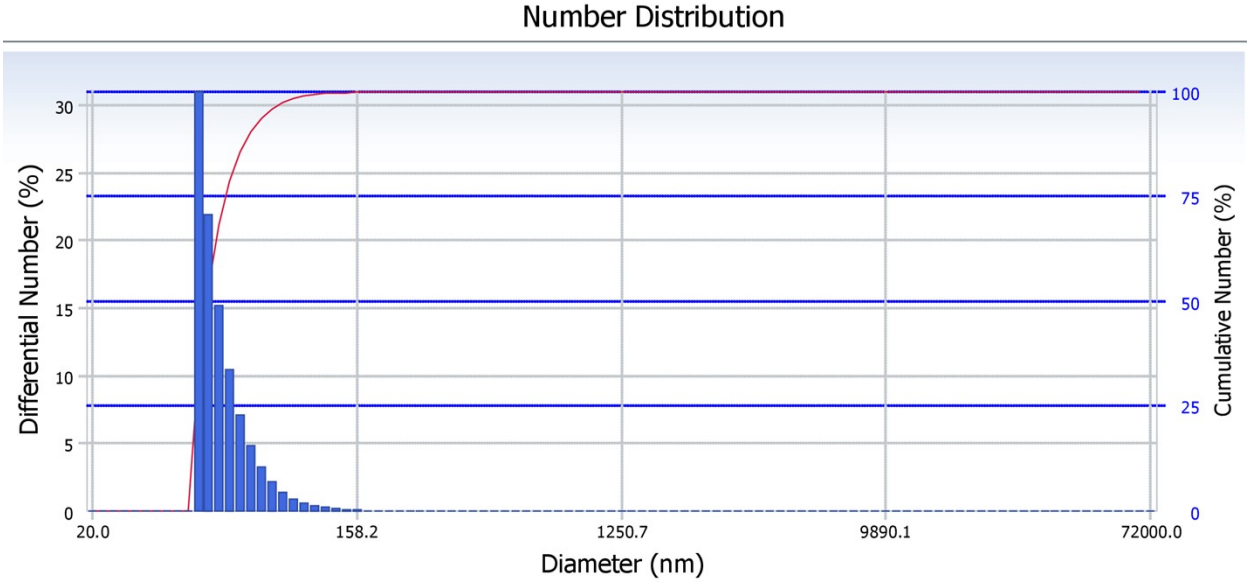

Figure S13. Number distribution diameter of $CNP_{ARS\text{-}His}$.

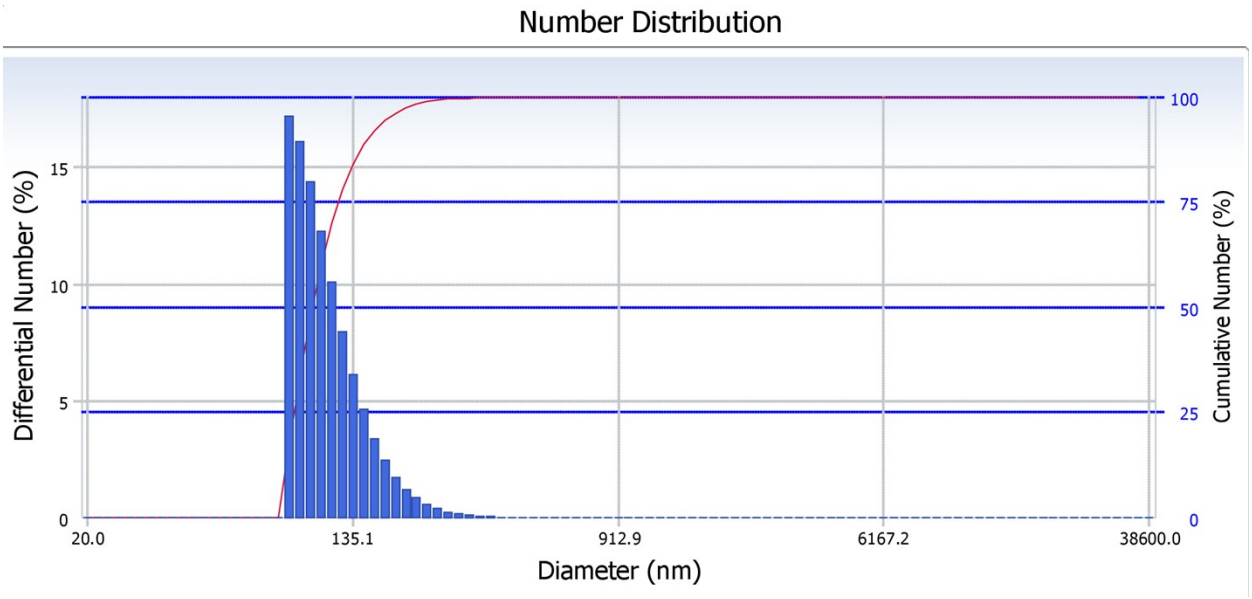

Figure S14. Number distribution diameter of $CNP_{ARS\text{-}Lys}$.

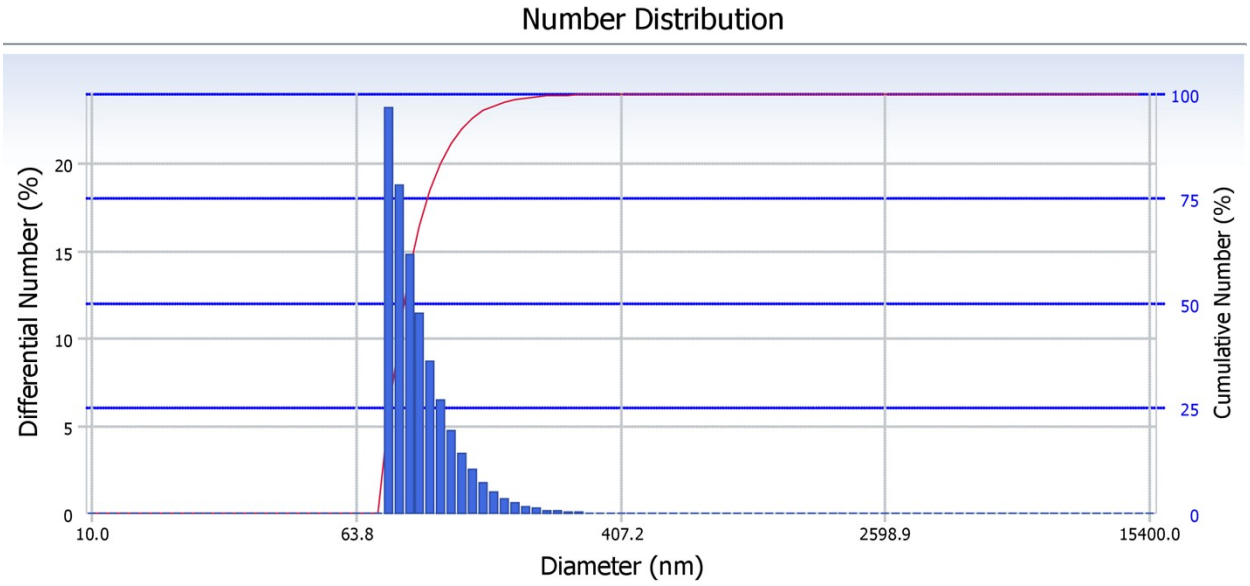

Figure S15. Number distribution diameter of $CNP_{ARS\text{-}pPD}$.

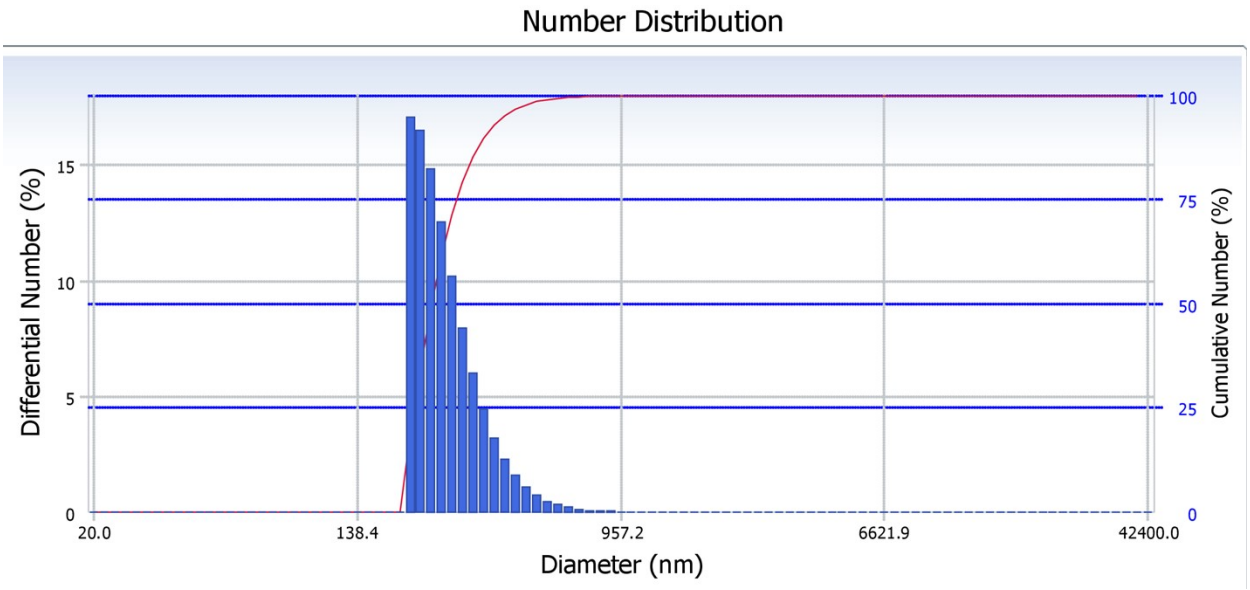

Figure S16. Number distribution diameter of $CNP_{ARS\text{-}PEI}$.

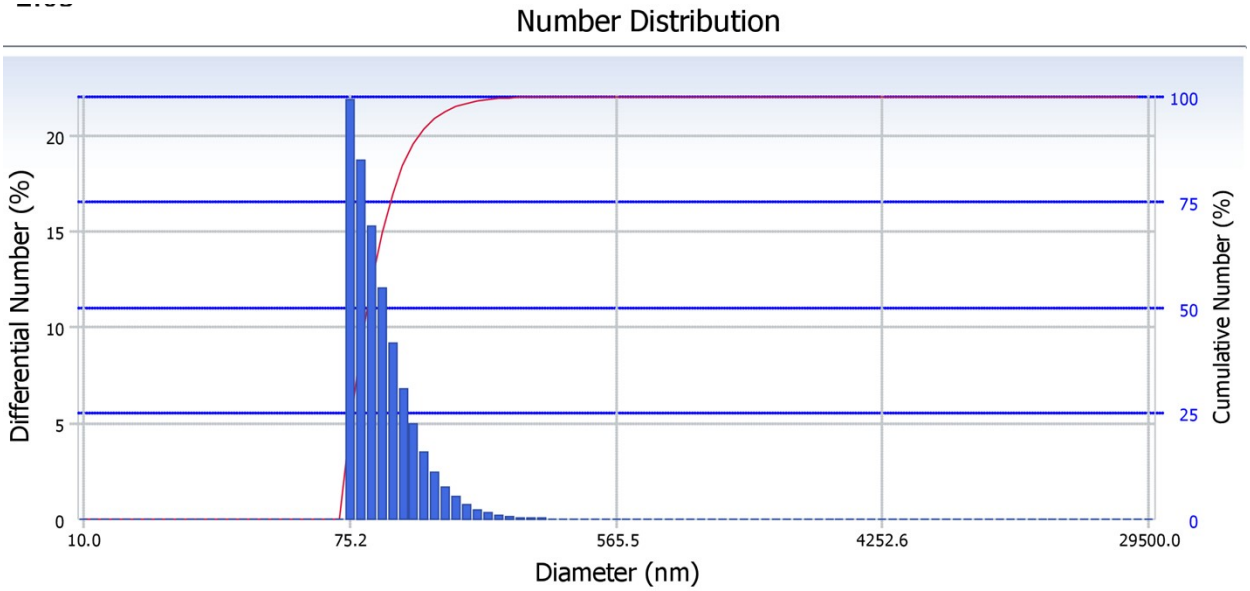

Figure S17. Number distribution diameter of $CNP_{ARS\text{-}Trp}$.

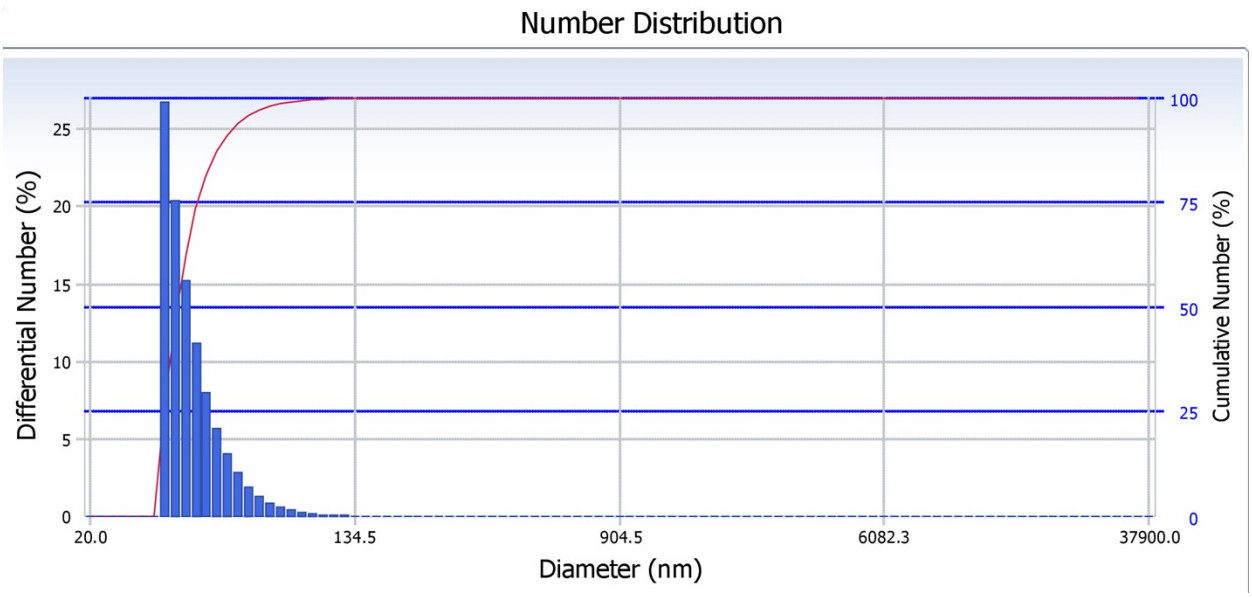

Figure S18. Number distribution diameter of $CNP_{ARS\text{-}Tyr}$.

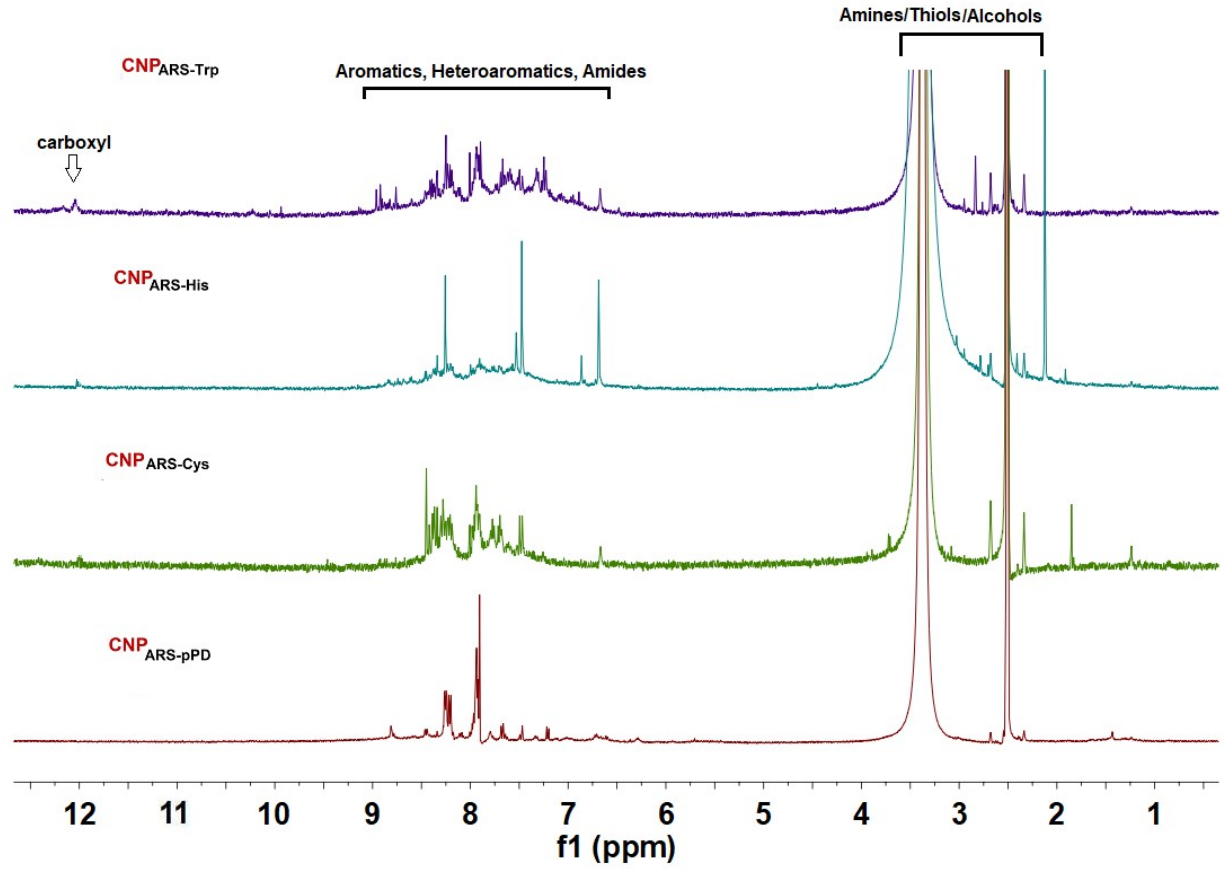

Figure S19. ^{1}H NMR spectra of $CNP_{ARS\text{-}Trp}$, $CNP_{ARS\text{-}His}$, $CNP_{ARS\text{-}Cys}$, and $CNP_{ARS\text{-}pPD}$.

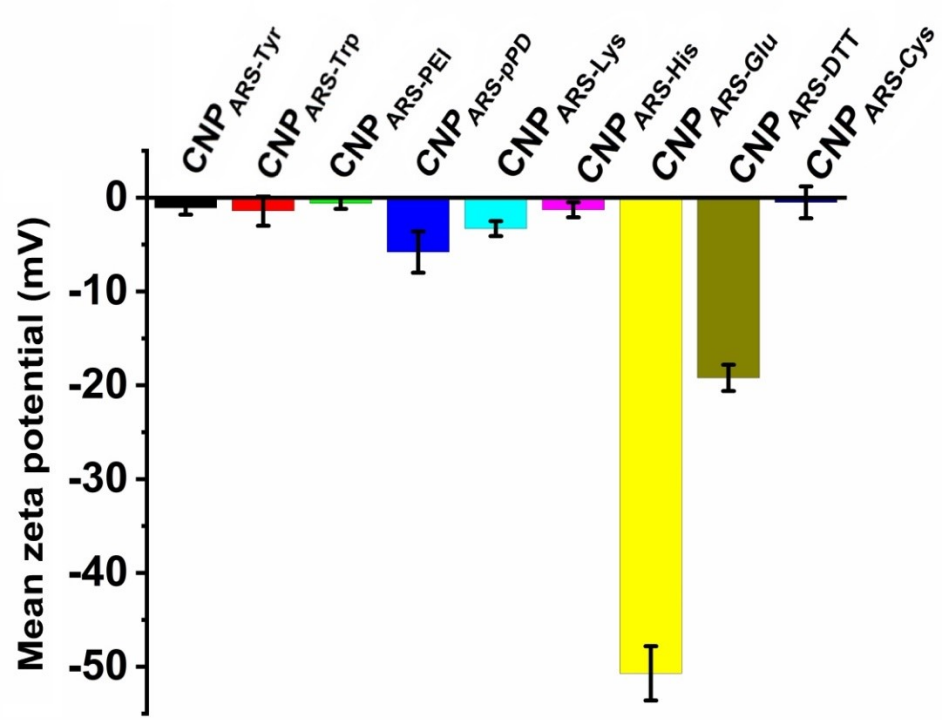

Figure S20. Mean zeta potential distribution of CNPs.

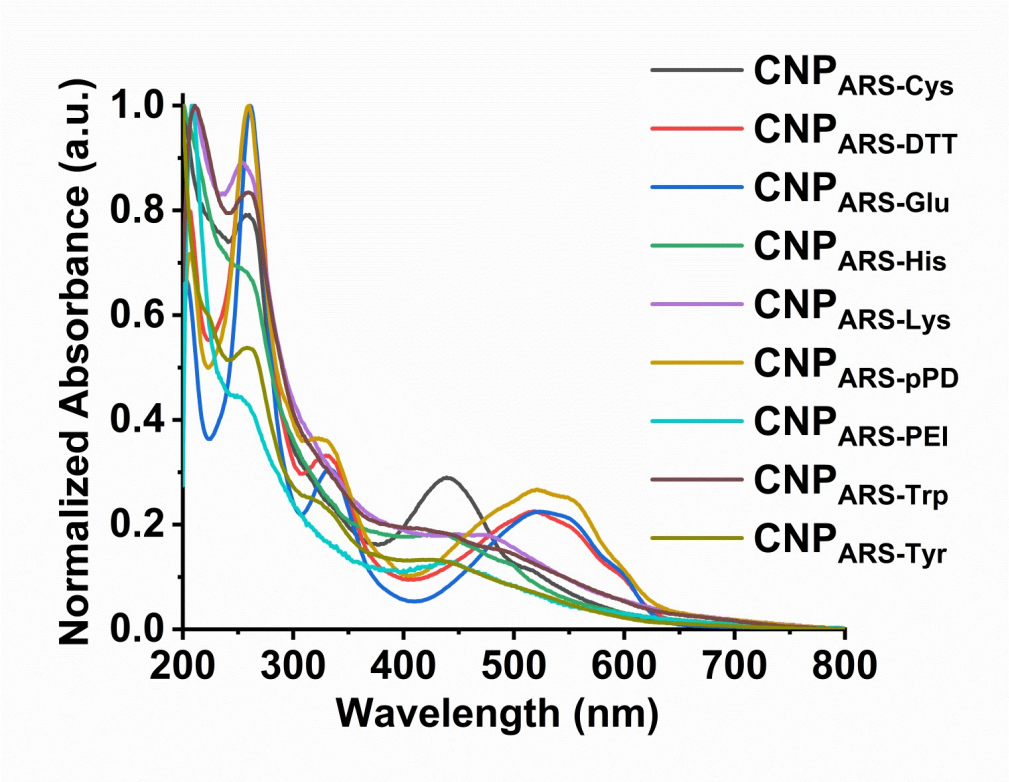

Figure S21. UV-Vis absorption spectroscopy of CNPs.

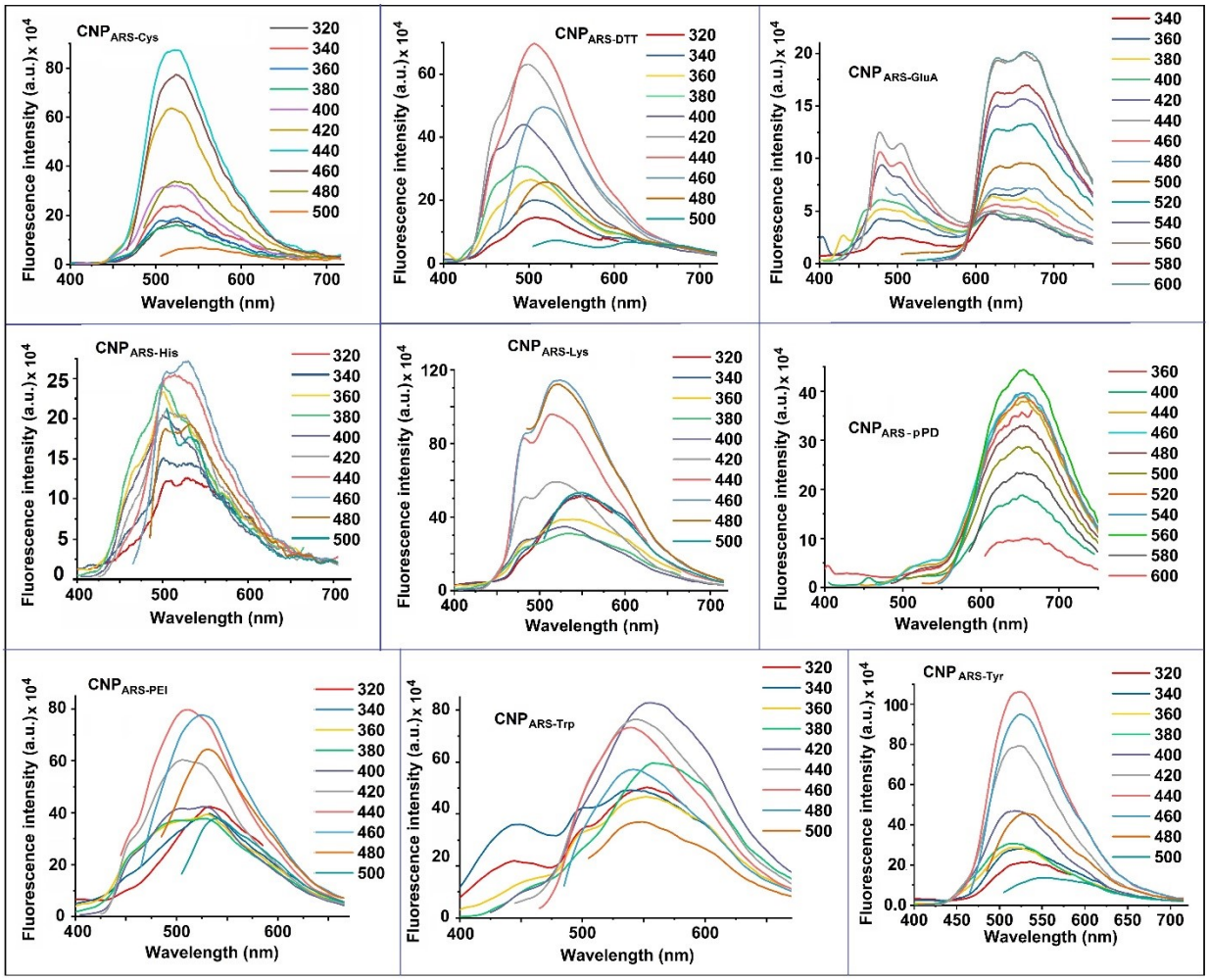

Figure S22. Steady-state fluorescence spectra of CNPs.

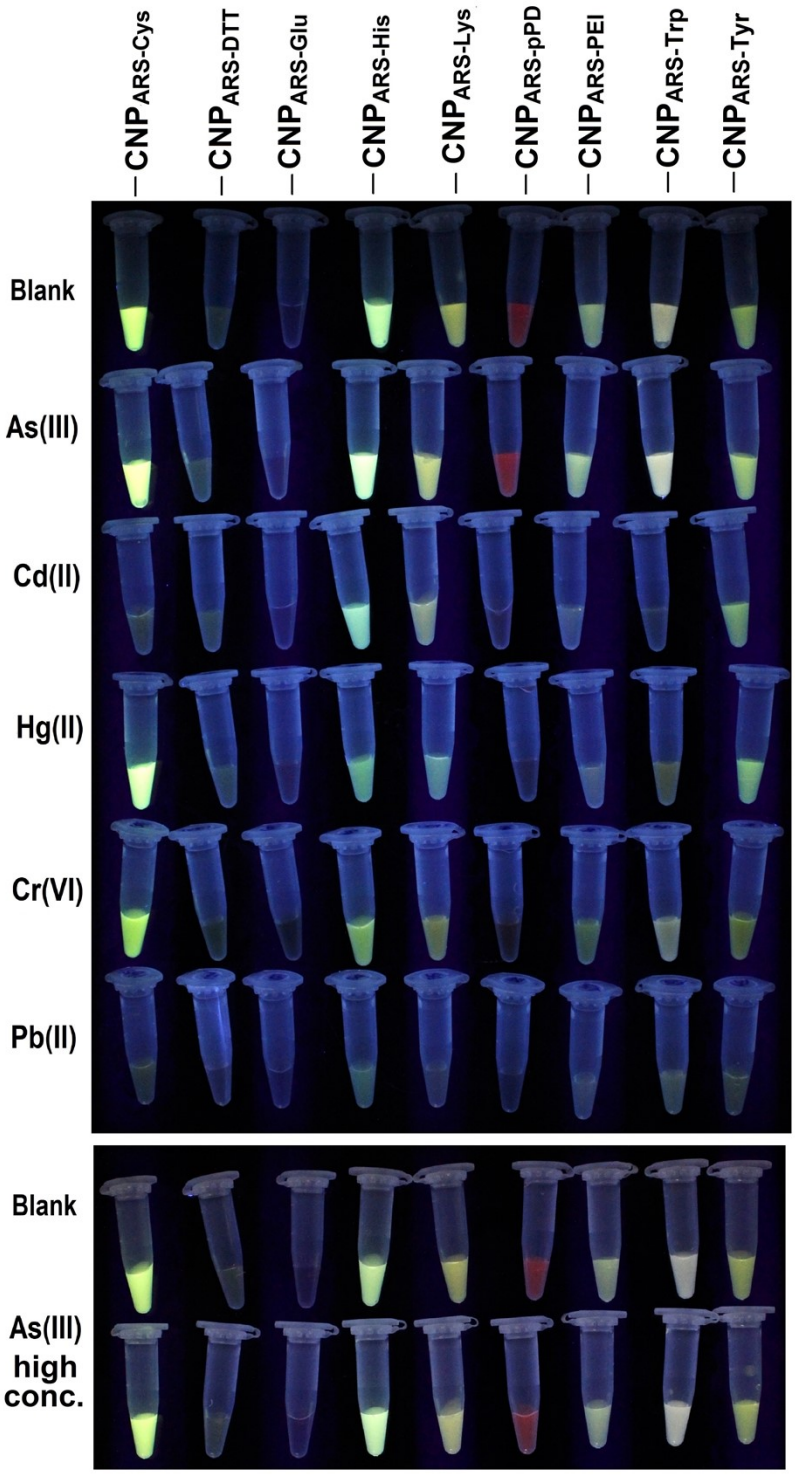

Figure S23. Digital image of CNPs with 100 nmol of the heavy metals in water at pH 7.4±0.1.

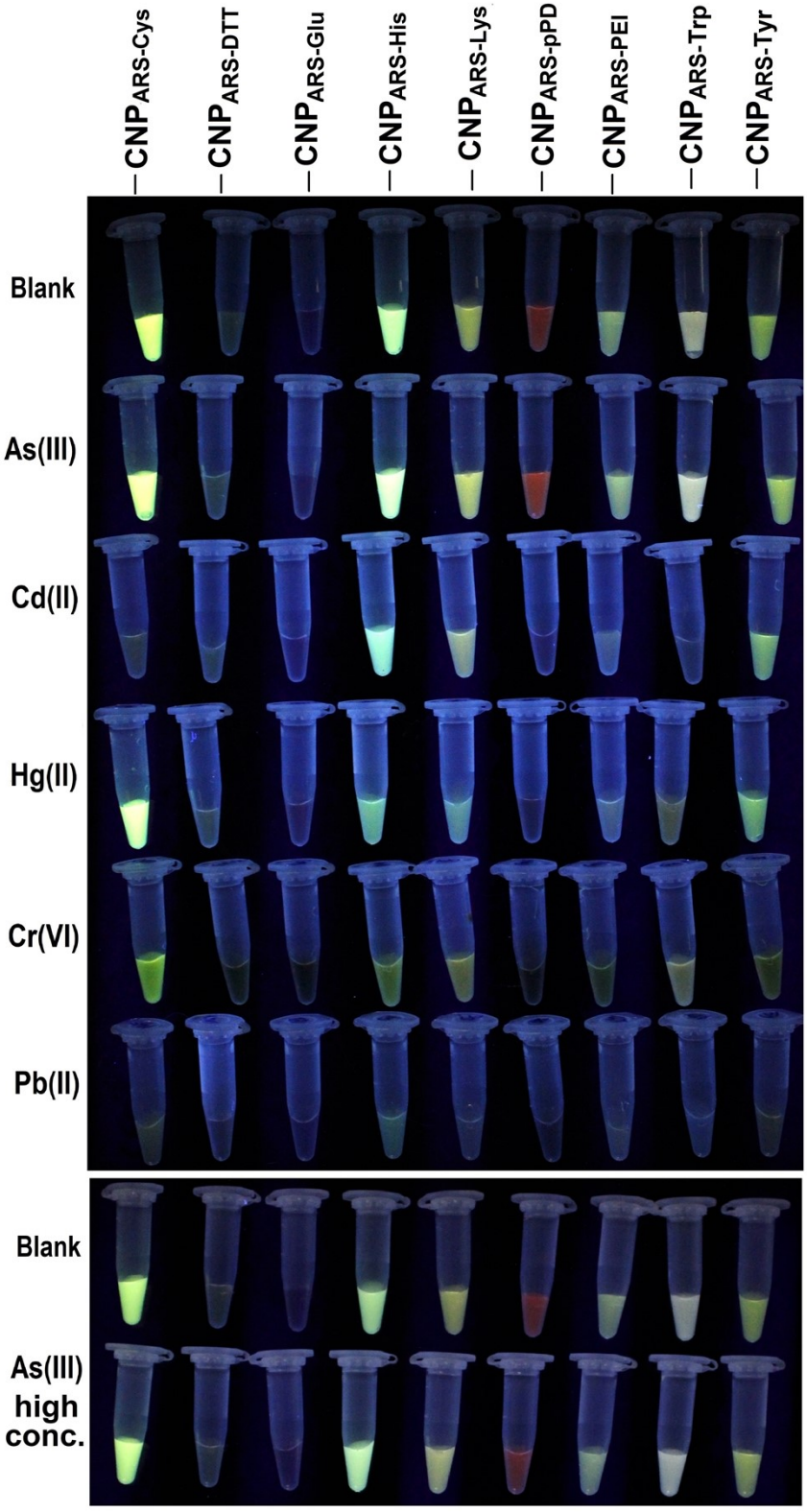

Figure S24. Digital image of CNPs with 200 nmol of the heavy metals in water at pH 7.4±0.1.

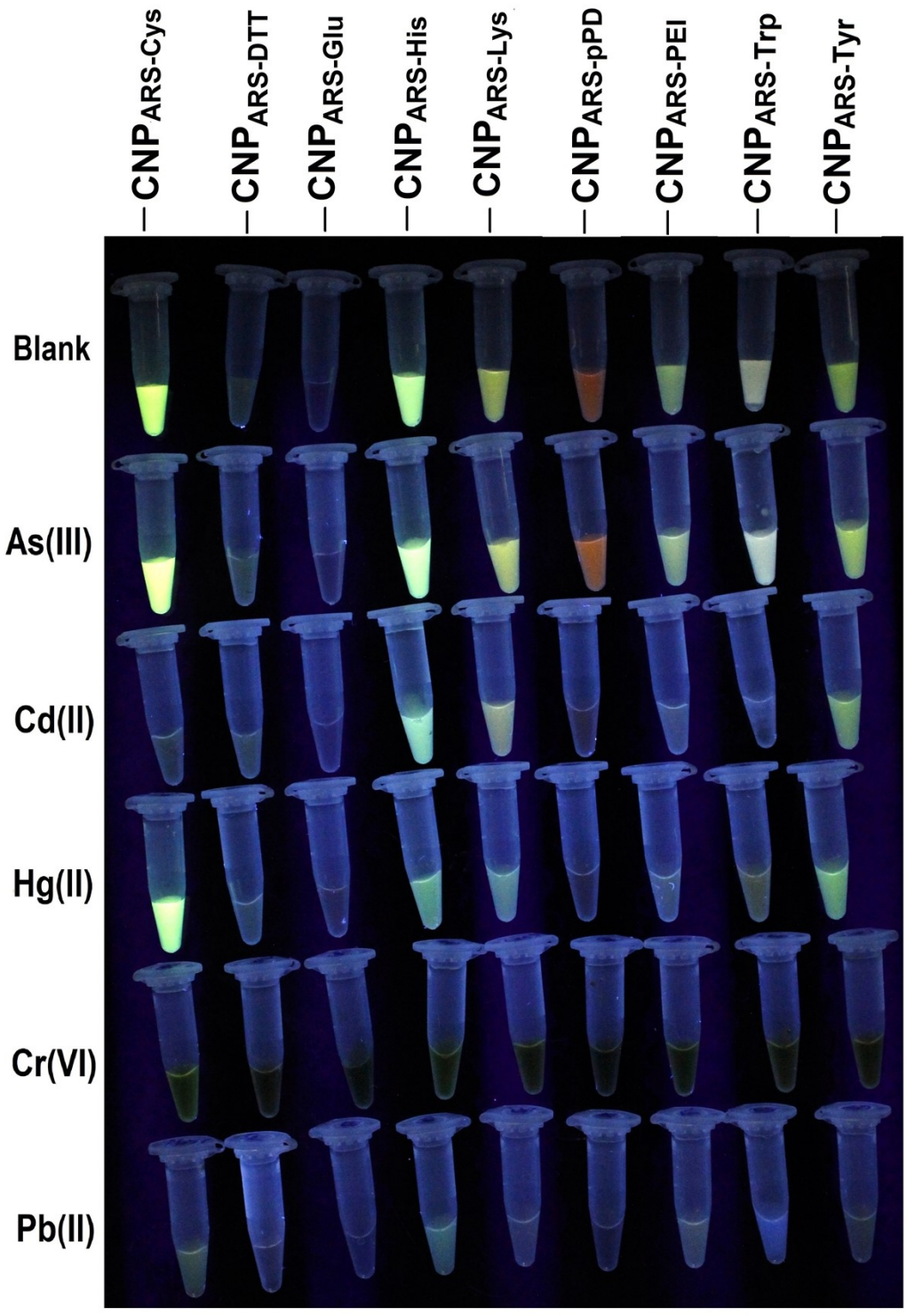

Figure S25. Digital image of CNPs with 800 nmol of the heavy metals in water at pH 7.4±0.1.

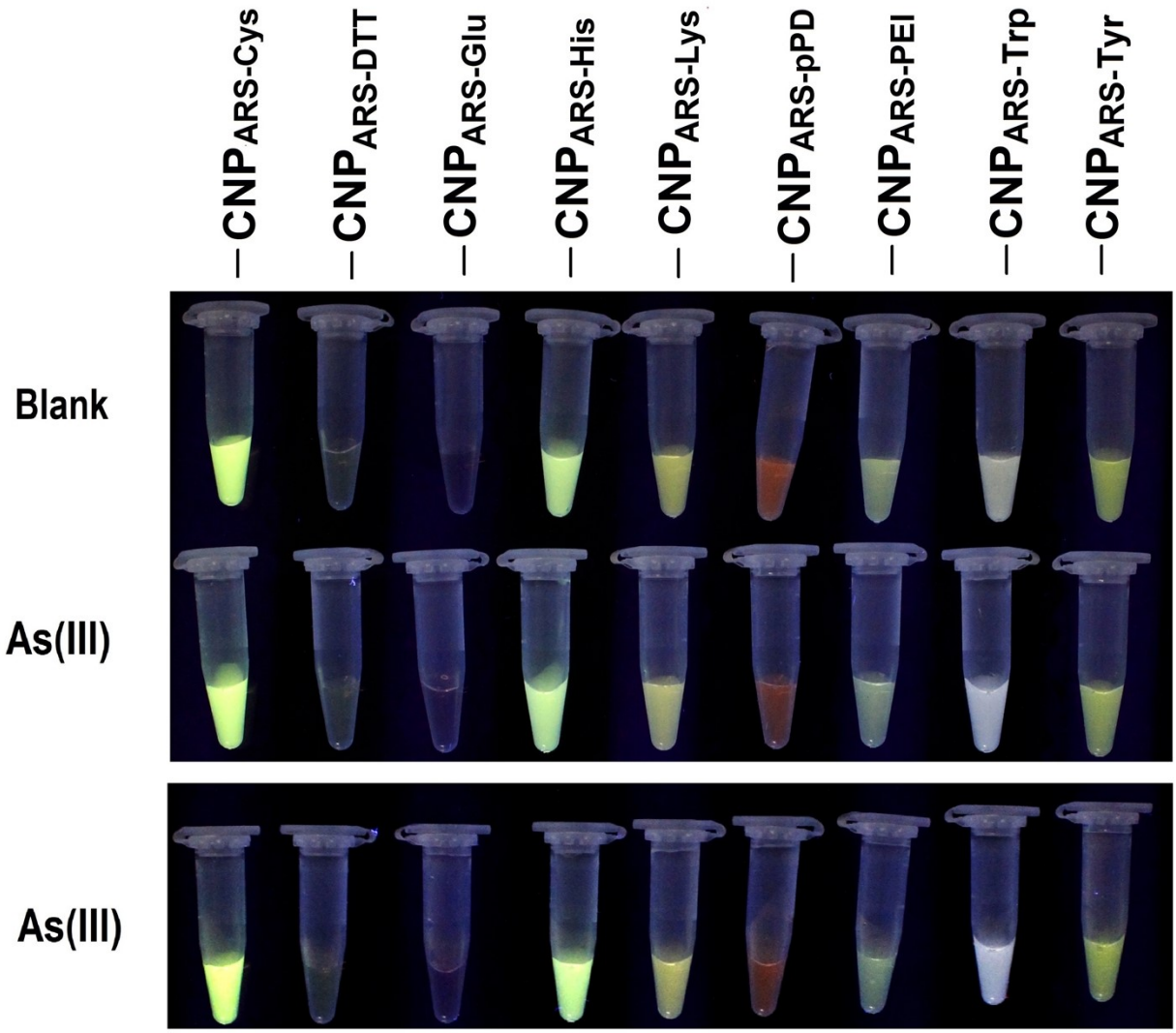

Figure S26. Digital image of CNPs with 1.500 μmol and 2 μmol of As(III) in water at pH 7.4±0.1 respectively.

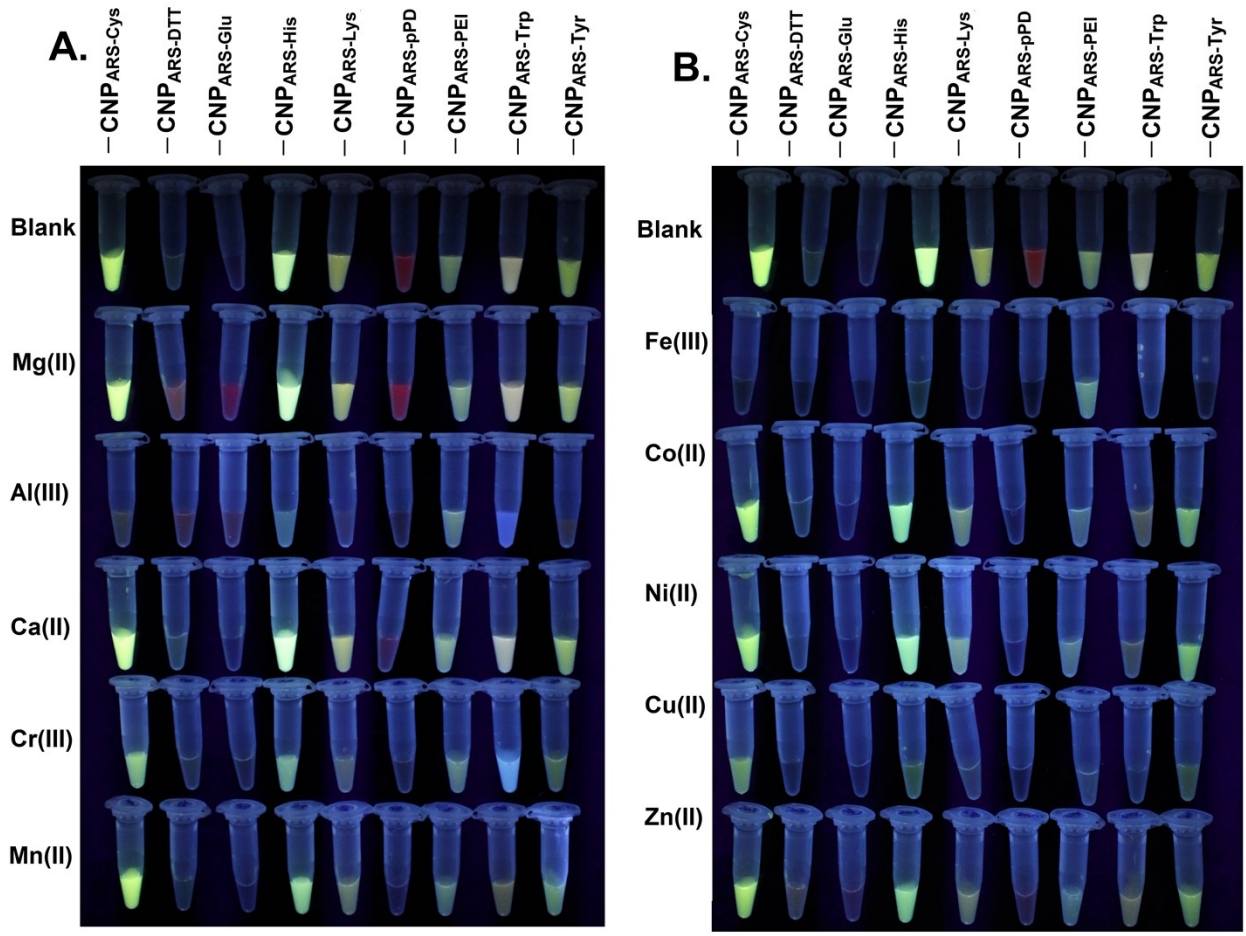

Figure S27. Digital image of CNPs with 400 nmol of other relevant metal ions in water at pH 7.4±0.1.