CIELab Chromaticity Evolution to Measure Binding Free Energy of Non-colored Biomolecules to Gold Nanoparticles.

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Supporting Information

Obtention of CIELab parameters

XYZ colorimetric parameters were obtained from experimental measurements by using the following mathematical expressions:

$$X = K\sum_{\lambda} T_{\lambda}\, S_{\lambda}\, \bar{X}_{10(\lambda)}\, \Delta_{\lambda}$$

$$Y = K\sum_{\lambda} T_{\lambda}\, S_{\lambda}\, \bar{Y}_{10(\lambda)}\, \Delta_{\lambda}$$

$$Z = K\sum_{\lambda} T_{\lambda}\, S_{\lambda}\, \bar{Z}_{10(\lambda)}\, \Delta_{\lambda}$$

$$K = 100/\sum_{\lambda} S_{\lambda}\, \bar{Y}_{10(\lambda)}\, \Delta_{\lambda}$$

where T_λ is the transmittance of the sample; S_λ is a coefficient which depends on both λ and the illuminant (in our case, a D65 illuminant was employed) and $X_{10(\lambda)}$, $Y_{10(\lambda)}$, $Z_{10(\lambda)}$ are functions of both λ and the observer. Conversion from XYZ values to L*a*b* was done directly by using white point values for the D65 illuminant and 10º observer:[2]

$$X_n = 94.825;\ Y_n = 100;\ Z_n = 107.38$$

L*a*b* values were calculated as follows:[3]

$$L^* = 116\,(Y/Y_n)^{1/3} - 16$$

$$a^* = 500[f(X/X_n) - f(Y/Y_n)$$

$$b^* = 200[f(Y/Y_n) - f(Z/Z_n)$$

where:

$$f(X/X_n) = (X/X_n)^{1/3}$$

$$f(Y/Y_n) = (Y/Y_n)^{1/3}$$

$$f(Z/Z_n) = (Z/Z_n)^{1/3}$$

Figures

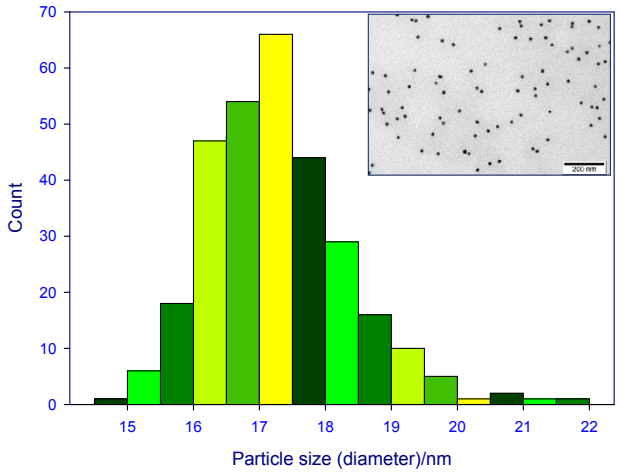

Figure S1. Size distribution of synthesized AuNPs.

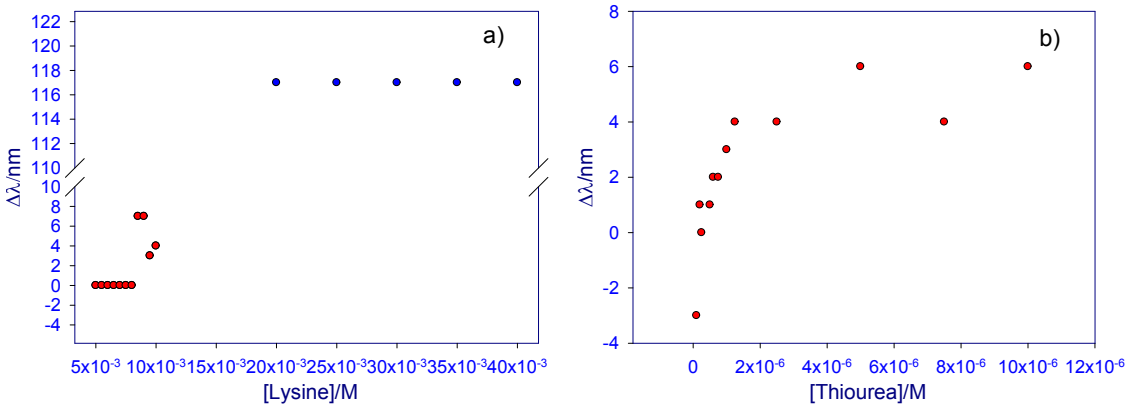

Figure S2. Wavelength shift (Δλ) of the maximum intensity absorbance peak for solutions containing [AuNPs] = 3.2 x 10^{-10} M and varying concentrations of a) lysine, b) thiourea.

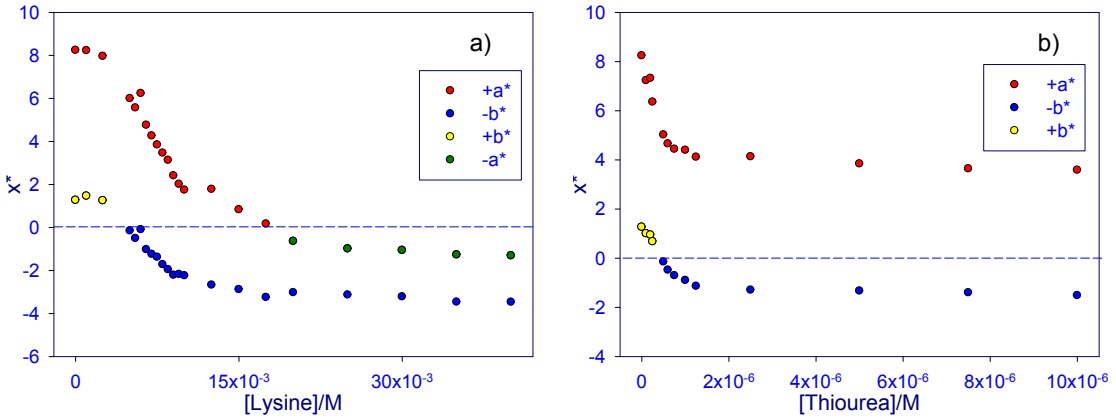

Figure S3. a* and b* parameters for a series of [AuNPs] = 3.2 x 10^{-10} M solutions containing a) lysine and b) thiourea. Green-colored points indicate negative values of a* which account for a green tone in the CIELab color system, and are indicative of fully blue (as opposed to purple) nanoparticle solutions.

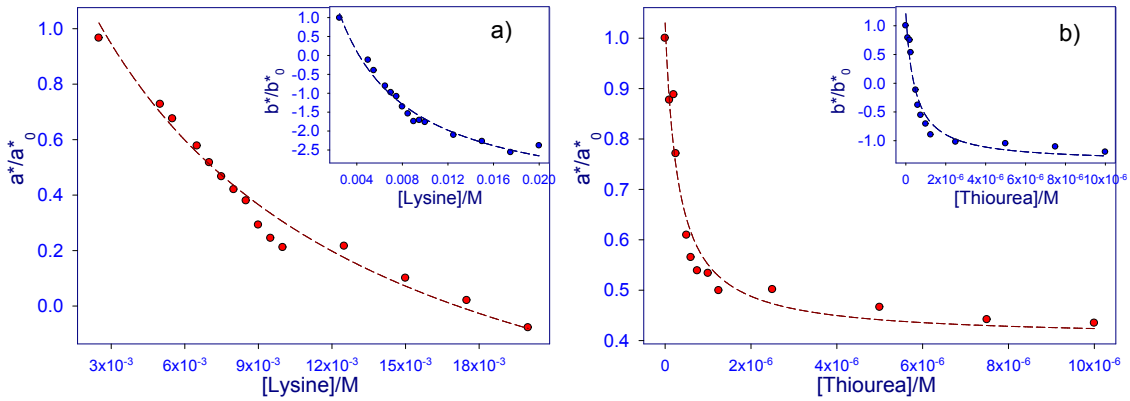

Figure S4. Two-state model fitting for normalized a* and b* (shown in the inset) parameters of AuNPs/biomolecule solutions. a) [AuNPs] = 3.2x10^{-10} M; [Lysine] = 2.5x10^{-3} - 2x10^{-2} M, b) [AuNPs] = 3.2x10^{-10} M; [Thiourea] = 0 - 1x10^{-5} M.

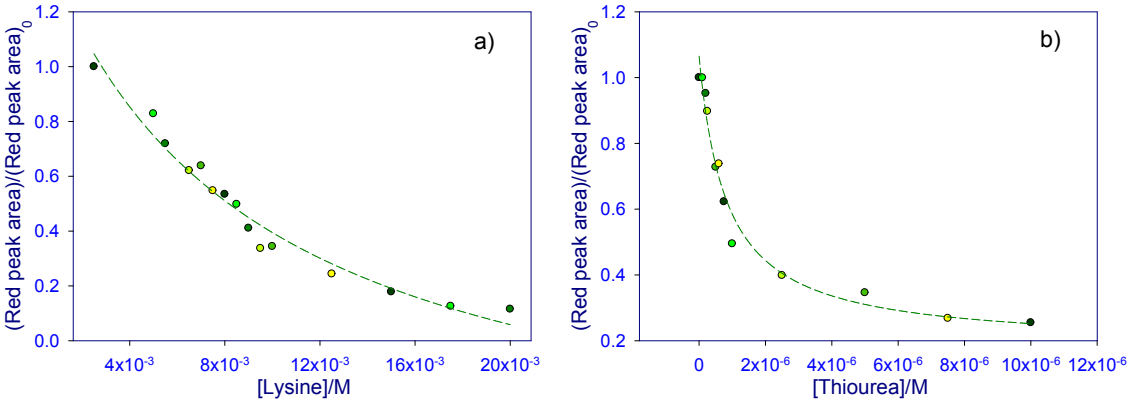

Figure S5. Two-state model fit for the red (non-aggregated) deconvolution peak area for a) a series of AuNPs/lysine solutions ranging from [Lysine] = 2.5x10^{-3} - 2x10^{-2} M and b) a series of AuNPs/thiourea solutions ranging from [Thiourea] = 0 - 1x10^{-5} M.

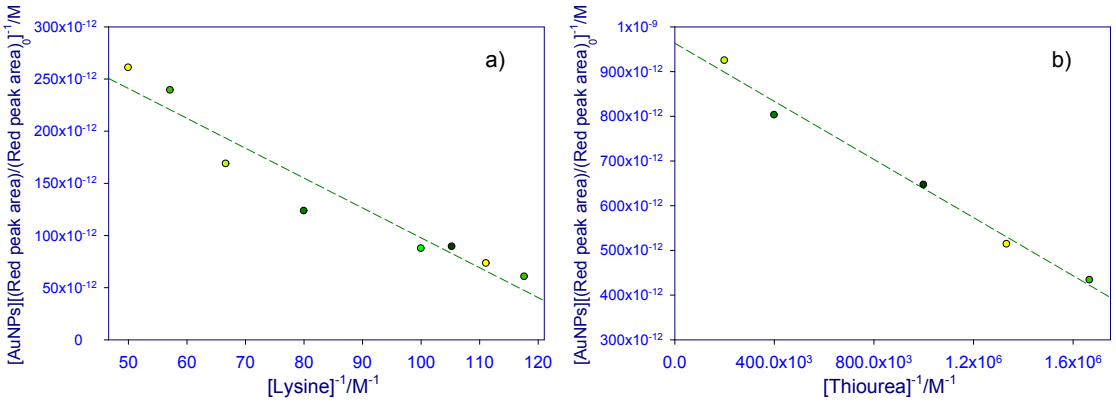

Figure S6. Benesi-Hildebrand fit for the normalized red peak area obtained from deconvolution procedures for a) AuNPs/lysine solutions ranging from [Lysine] = 8.5×10^{-3} to 2×10^{-2} M and b) AuNPs/thiourea solutions ranging from [Thiourea] = 6×10^{-7} to 5×10^{-6} M.

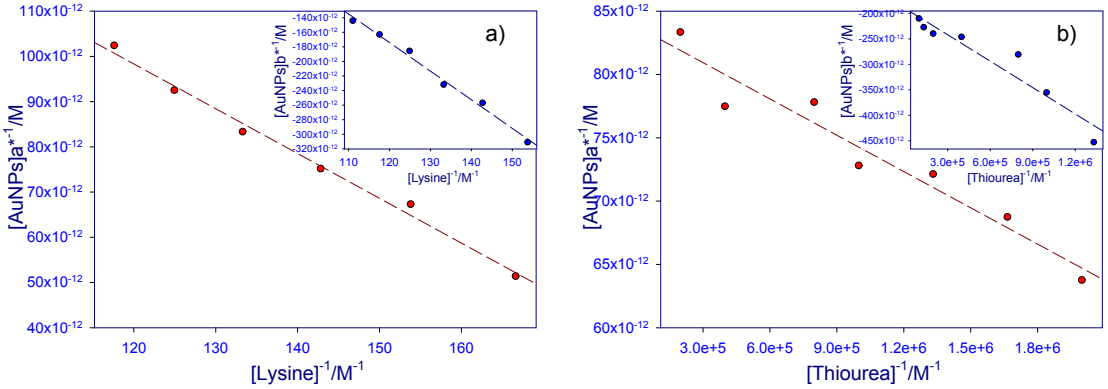

Figure S7. Benesi-Hildebrand fit for a* and b* (shown on inset) for a series of AuNPs solutions ranging from a) [Lysine] = 6×10^{-3} to 9×10^{-3} M and b) [Thiourea] = 5×10^{-7} to 1×10^{-5} M.