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:

\[ X = K \sum_\lambda T_\lambda S_\lambda X_{10(\lambda)} \Delta \lambda \]
\[ Y = K \sum_\lambda T_\lambda S_\lambda Y_{10(\lambda)} \Delta \lambda \]
\[ Z = K \sum_\lambda T_\lambda S_\lambda Z_{10(\lambda)} \Delta \lambda \]
\[ K = \frac{100}{\sum_\lambda S_\lambda Y_{10(\lambda)} \Delta \lambda} \]

where \( T_\lambda \) is the transmittance of the sample; \( S_\lambda \) is a coefficient which depends on both \( \lambda \) 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 \( \lambda \) 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:\(^3\)

\[ L^* = 116 \left( \frac{Y}{Y_n} \right)^{1/3} - 16 \]
\[ a* = 500[f(X/X_n) - f(Y/Y_n)] \]

\[ b* = 200[f(Y/Y_n) - f(Z/Z_n)] \]

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 (\(\Delta \lambda\)) of the maximum intensity absorbance peak for solutions containing [AuNPs] = 3.2 \times 10^{-10} M and varying concentrations of a) lysine, b) thiourea.
**Figure S3.** a* and b* parameters for a series of $[\text{AuNPs}] = 3.2 \times 10^{-10}$ 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) $[\text{AuNPs}] = 3.2 \times 10^{-10}$ M; $[\text{Lysine}] = 2.5 \times 10^{-3} - 2 \times 10^{-2}$ M, b) $[\text{AuNPs}] = 3.2 \times 10^{-10}$ M; $[\text{Thiourea}] = 0 - 1 \times 10^{-5}$ M.

**Figure S5.** Two-state model fit for the red (non-aggregated) deconvolution peak area for a) a series of $\text{AuNPs}/\text{lysine}$ solutions ranging from $[\text{Lysine}] = 2.5 \times 10^{-3} - 2 \times 10^{-2}$ M and b) a series of $\text{AuNPs}/\text{thiourea}$ solutions ranging from $[\text{Thiourea}] = 0 - 1 \times 10^{-5}$ M.
Figure S6. Benesi-Hildebrand fit for the normalized red peak area obtained from deconvolution procedures for a) AuNPs/lysine solutions ranging from [Lysine] = 8.5x10^{-3} to 2x10^{-2} M and b) AuNPs/thiourea solutions ranging from [Thiourea] = 6x10^{-7} to 5x10^{-6} M.

Figure S7. Benesi-Hildebrand fit for a* and b* (shown on inset) for a series of AuNPs solutions ranging from a) [Lysine] = 6x10^{-3} to 9x10^{-3} M and b) [Thiourea] = 5x10^{-7} to 1x10^{-5} M.