

Fig S1. (a) Absorbance spectra of $Au_{16}(RGDC)_{14}$ nanoclusters formed during 30 minutes of irradiation with UVA light, (b) fluorescence EEM contour plot of $Au_{16}(RGDC)_{14}$ nanoclusters after 30 min of UVA irradiation with a single emission peak at 770 nm, and (c) 3D fluorescence EEM plot of the crude product.



Fig S2. (a) absorbance of the Au(RGDC) products at different pHs using 3 mM Au, 9 mM RGDC, and 3 mM Omnirad-2959 after 30 min UVA irradiation along with Fluorescence EEM spectra of the products at pH (b) 9, (c) 11, (d) 12.



Fig S3. Absorbance and emission of Au(RGDC) clusters using 1 mM Au (a and b), 2 mM Au (c and d), and 1 mM of Au with 3 mM of Omnirad-2959 (e and f). EEM plots have been shown at pH 10.



Fig S4. EEM spectra of the nanoclusters using 2-component model calculated with drEEM toolbox for MATLAB.



Fig S5. Structure of RGDC ligand, C-N bond is broken so that just a portion of ligand stays attached to the Au_{16} core.



Fig S6. (a) Femtosecond transient absorption spectra of $Au_{16}(RGDC)_{14}$ clusters excited at 340 nm, (b) three lifetime components, simulated from global analysis, that model the overall transient absorption spectra of $Au_{16}(RGDC)_{14}$, (c) Overlaid transient absorption spectra of $Au_{16}(RGDC)_{14}$ clusters obtained at delay time of t = 1 ps after excitation, and (d) femtosecond transient decay trace of $Au_{16}(RGDC)_{14}$ clusters monitored at 671 nm.

Table S1. Amplitudes and lifetimes obtained from femtosecond transient absorption spectroscopy for $Au_{16}(RGDC)_{14}$ clusters, pumped at 340 nm and probed at 671 nm.

| λ_{probe} | τ ₁ (ps) | A 1 | τ₂ (ps) | A ₂ | τ₃ (ps) | A ₃ |
|-------------------|---------------------|------------------------|----------------|----------------|---------------|----------------|
| 671 nm | 14.3 ± 1.7 | 6.3 x 10 ⁻⁴ | 1541.2 ± 112.5 | 0.00163 | 2212.2± 105.4 | 0.00268 |



Fig S7. (a) Absorbance and (b) emission spectra of the $Au_{16}(RGDC)_{14}$ clusters when brought to acidic, basic, and neutral pHs using minimum amount of either sodium hydroxide or acetic acid.



Fig S8. Viability and uptake of the KB cells incubated with Au₁₆(RGDC)₁₄ clusters following a 20minute irradiation using a 500 nm LED. Viability measurements taken 48 hours after the completion of irradiation.



Fig S9. Absorbance spectra of the (a) $Au_{16}(RGDC)_{14}$ clusters and (b) MB in ABDA aqueous solution. No absorbance decrease was observed for the clusters, indicating they don't generate type II ROS.