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**(a)** 



**Figure SI-1** Figure S1a Molecular structure of Naringin with side chains marked as A and B. Figure S1b UV- Vis scan of absorbance versus wavelength of pure Naringin, [N] = 0.5mM in a buffer of pH 9.







**Figure SI-2** UV-Visible spectra of  $HAuCl_4$  +Naringin mixture in a buffer of pH 9 with [HAuCl\_4] = 0.4mM and [N] = 0.05 (2a), 0.2mM (2b) at 40°C. UV-Visible spectra of HAuCl\_4 +Naringin mixture with [N] = 0.5mM and [Au] = 0.2 (2c), 0.6 (2d), 1.2mM (2e) at 40°C. Blank means no Naringin is added. All the inset shows the SPR peak and colour of AuNPs in each case.

**Figure SI-3** 



**Figure SI-3:** Absorbance versus wavelength scans of  $[AuCl_4] = 0.4mM + [N] = 0.5mM$  at various temperatures. (a) 40°C (b) 50°C (c) 60°C (d) 70°C over a time interval of 120 minutes.





**Figure SI-4:** FTIR spectra of (a) Pure Naringin (b) enlarged view of peaks of Pure Naringin from 400-1800 cm<sup>-1</sup> (c) Naringin stabilized AuNPs.



Figure SI-5: Image of gel-electrophoresis of N-AuNPs.



Figure SI-6: XRD spectrum illustrating the crystalline nature of N-AuNPs.

**(a)** 



**(b)** 



**Figure SI-7:** Minimum energy structure of (a)  $[C_{10}H_7O_2]$  adsorbed on Au<sub>13</sub> cluster and (b)  $[C_6H_5O]^-$  adsorbed on Au<sub>13</sub> cluster (Yellow spheres represent Au, Black C, white H and Red O.

**(a)** 



**Figure SI-8:** NTOs for the excitations which make up the dominant peak in the Vis region (a) Hole part and (b) Particle part of  $[C_6H_5O]^-$ -Au<sub>13</sub>. Phases of the orbitals are indicated in red and blue.

(a)



(b)



**Figure SI-9:** Minimum energy structure of (a)  $[C_{10}H_7O_2]$  adsorbed on Au<sub>32</sub> cluster and (b)  $[C_6H_5O]$ <sup>-</sup> adsorbed on Au<sub>32</sub> cluster.







**Figure SI-10:** (a) UV-Visible absorbance spectra of N-AuNPs with various metal ions. Inset shows a photograph representing the N-AuNPs solution and its response towards  $Al^{3+}$ . (b) The bars represent the calorimetric response of N-AuNPs with various metal ions in terms of change in absorbance  $\Delta A$  with respect to the blank i.e. N-AuNPs. (c) The bars represent the calorimetric response of N-AuNPs of change in wavelength  $\Delta\lambda$  with respect to the blank i.e. N-AuNPs. (c) The bars represent the calorimetric response of N-AuNPs.





**Figure SI-11:** (a) UV-Visible spectrum of N-AuNPs as a function of various concentrations of  $Al^{3+}$  ions (b) plot of absorption ratios  $A_{640}/A_{520}$  of N-AuNPs versus  $Al^{3+}$  concentration.



**Figure SI-12:** (a) Heme Absorption Spectra with different concentrations of N-AuNPs i.e. [N-AuNPs] = 25 and 50  $\mu$ g/ml. (b) Enlarged view of Absorption peaks of heme from 500-600 nm.



T47D Control





N-AuNPs 100 µg/ml



**MDAMB-231** Control



N-AuNPs 100 µg/ml





**Figure SI-13:** Laser Scanning microscope images of cell lines (a, c, and e) represents the morphology in untreated MCF-7, T47D , and MDAMB controls (b, d, and f) represents the changes in morphology in MCF-7, T47D, and MDAMB in the presence of [N-AuNPs] = 100  $\mu$ g/ml.