

*Electronic Supplementary Information*

**Enhanced *in vitro* cytotoxicity and cellular uptake of DNA bases functionalized gold nanoparticles in HeLa cell lines**

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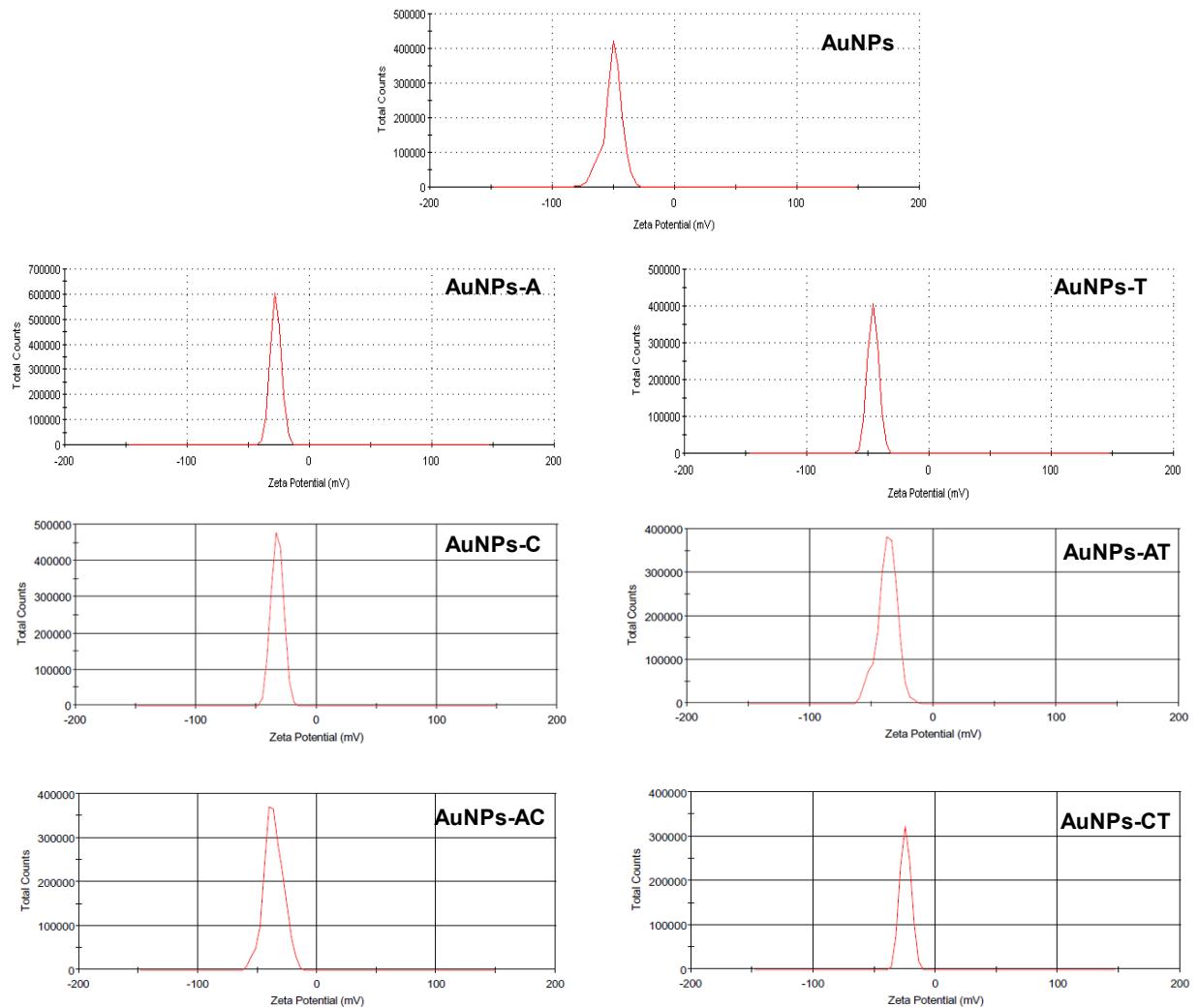
**I. Zeta potential data**

**II. FTIR data**

**III. Structure of adenine, thymine and cytosine and their pair: Binding interaction with gold nanoparticles.**

**IV. Cytotoxicity study of healthy cells line**

## I. Zeta-potential data



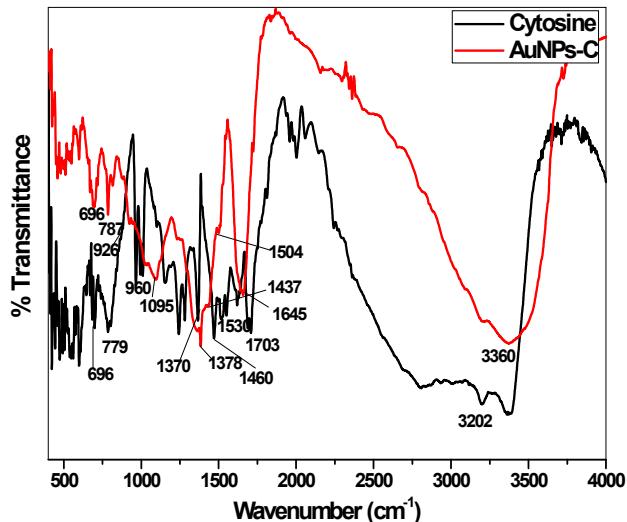
ESI – Figure 1. Zeta potential of functionalized AuNPs.

| Name            | Diameter<br>(TEM)<br>nm | Zeta<br>Potential,<br>mV | pH   |
|-----------------|-------------------------|--------------------------|------|
| <b>AuNPs</b>    | $6.3 \pm 0.04$          | -53.2                    | 8.28 |
| <b>AuNPs-A</b>  | $4.8 \pm 0.11$          | -28.0                    | 7.81 |
| <b>AuNPs-T</b>  | $15.5 \pm 0.2$<br>3     | -41.8                    | 8.32 |
| <b>AuNPs-C</b>  | $7.1 \pm 2.09$          | -31.8                    | 8.31 |
| <b>AuNPs-AC</b> | $6.7 \pm 0.14$          | -34.0                    | 8.18 |
| <b>AuNPs-AT</b> | $6.1 \pm 0.25$          | -37.1                    | 8.10 |
| <b>AuNPs-CT</b> | $9.4 \pm 0.22$          | -24.5                    | 8.30 |

**ESI– Table 1.** Particle diameter (TEM) and zeta potential values and pH of functionalized AuNPs.

### III. FTIR data

The band assignments are reported in this section where the band intensity is indicated as s = strong, m = moderate, w= weak and vw = very weak

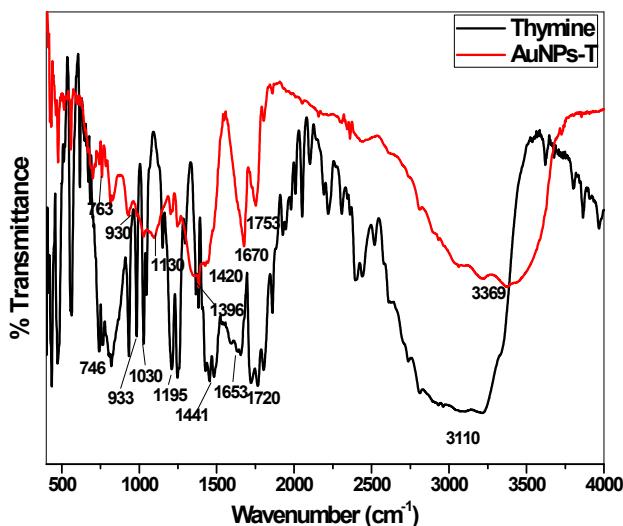


**ESI – Figure 2.** FTIR spectra of cytosine (black line) and AuNPs-Cytosine (red line).

| Modes             | Free (cm <sup>-1</sup> ) | Bound (cm <sup>-1</sup> ) |
|-------------------|--------------------------|---------------------------|
| v NH <sub>2</sub> | 3202                     | 3360 (s)                  |
| v C(2)=O(8)       | 1703                     | 1645 (s)                  |

|                                |      |          |
|--------------------------------|------|----------|
| $\nu$ N(3)=C(4)                | 1536 | 1504 (m) |
| $\nu$ C(5)=C(6)                | 1460 | 1437 (m) |
| $\nu$ C(4)-NH <sub>2</sub>     | 1370 | 1378 (s) |
| $\nu$ C-NH <sub>2</sub>        | 960  | 926 (m)  |
| $\nu$ N-C-N                    | 779  | 787 (w)  |
| Ring breathing<br>of Imidazole | 696  | 696 (w)  |

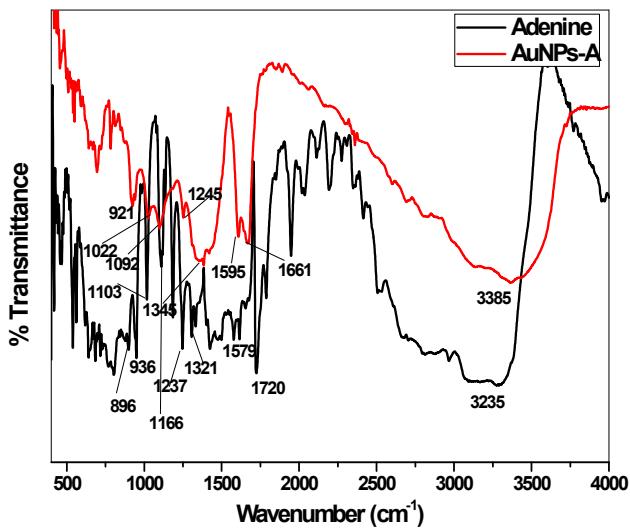
**ESI – Table 2.** Main vibrational modes of free and bound cytosine



**ESI – Figure 3.** FTIR spectra of thymine (black line) and AuNPs-thymine (red line).

| Modes                  | Free (cm <sup>-1</sup> ) | Bound (cm <sup>-1</sup> )      |
|------------------------|--------------------------|--------------------------------|
| $\nu$ N(3)H            | 3110                     | 3369(s)                        |
| $\nu$ N(1) H           |                          |                                |
| $\nu$ C(2)=O(7)        | 1720                     | 1753 (s)                       |
| $\nu$ C(2)=O(7)        | 1653                     | 1670 (s)                       |
| $\delta$ (NH)          | 1441                     | 1420 (s)<br>1396 (s)           |
| $\delta$ (C-O)         | 1195<br>1030<br>933      | 1130 (m)<br>1037(m)<br>950 (m) |
| $\delta$ (C-H(ar) oop) | 746                      | 763 (vw)                       |

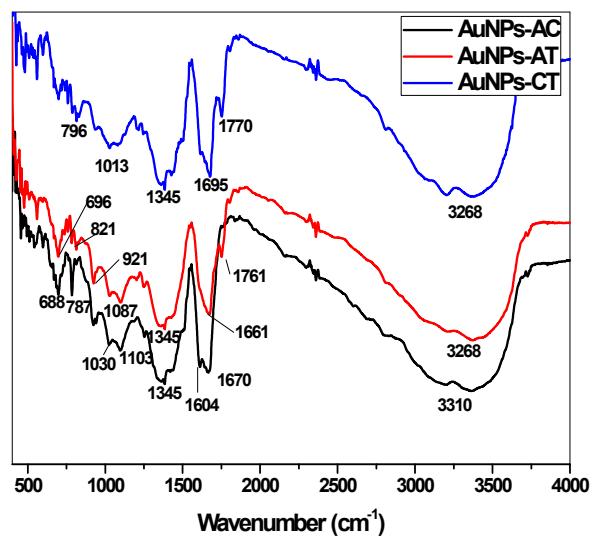
**ESI – Table 3.** Main vibrational modes of free and bound thymine.



**ESI– Figure 4.** FTIR spectra of adenine (black line) and AuNPs-adenine (red line).

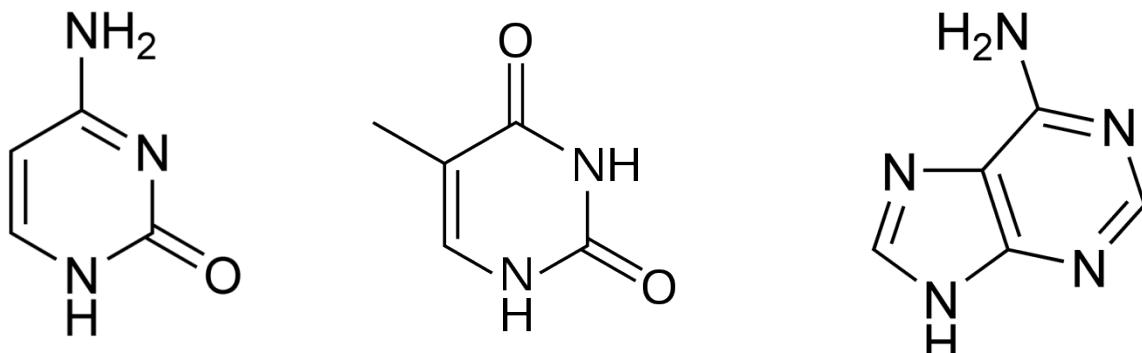
| Modes             | Free (cm <sup>-1</sup> ) | Bound (cm <sup>-1</sup> ) |
|-------------------|--------------------------|---------------------------|
| v NH <sub>2</sub> | 3236                     | 3385 (s)                  |
| v C-N(7)          | 1720                     | 1661 (s)                  |
| v N-H             | 1595                     | 1579 (s)                  |
| v C-C             | 1321                     | 1345 (s)                  |
| v C-H             |                          |                           |
| v C-N             | 1238                     | 1245 (s)                  |
| v C-H             |                          |                           |
| v C-C-N           | 1007                     | 1022 (m)                  |
| v C-H (In plane)  | 1103                     | 1092 (vw)                 |
| v C-H (Out plane) |                          |                           |
| vNH <sub>2</sub>  | 936                      | 921 (vw)                  |
| vN-C-N            | 1166<br>936<br>896       |                           |

**ESI – Table 4.** Main vibrational modes of free and bound adenine.



**ESI – Figure 5.** FTIR spectra of pair of DNA bases functionalized AuNPs.

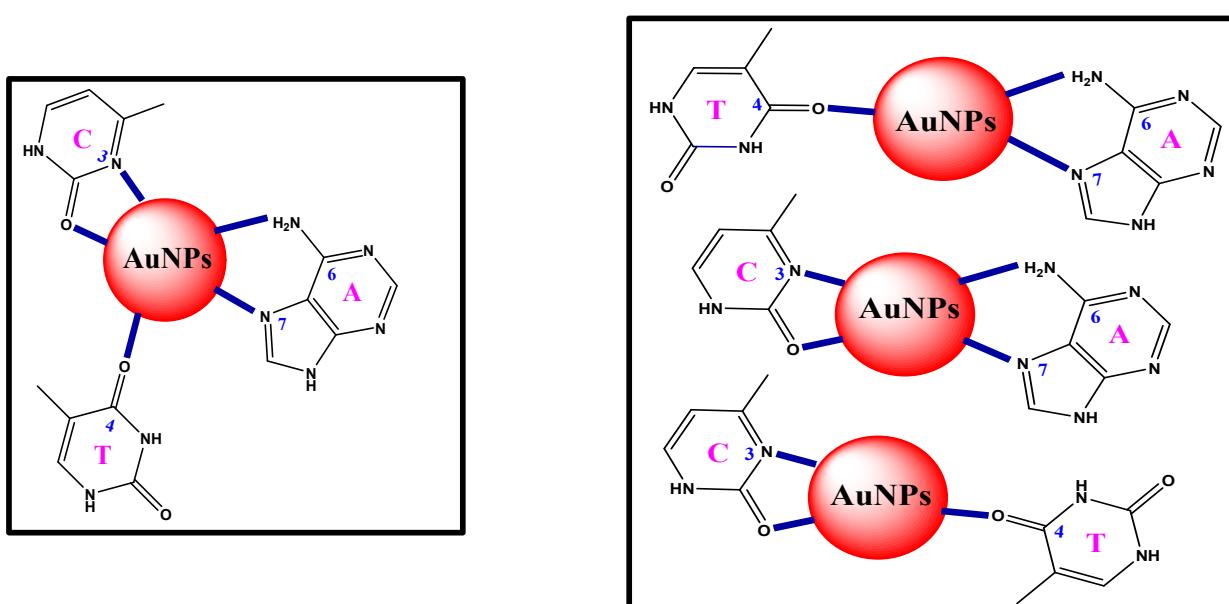
**III. Structure of adenine, thymine and cytosine and their pair: Binding interaction with gold nanoparticles.**



Cytosine

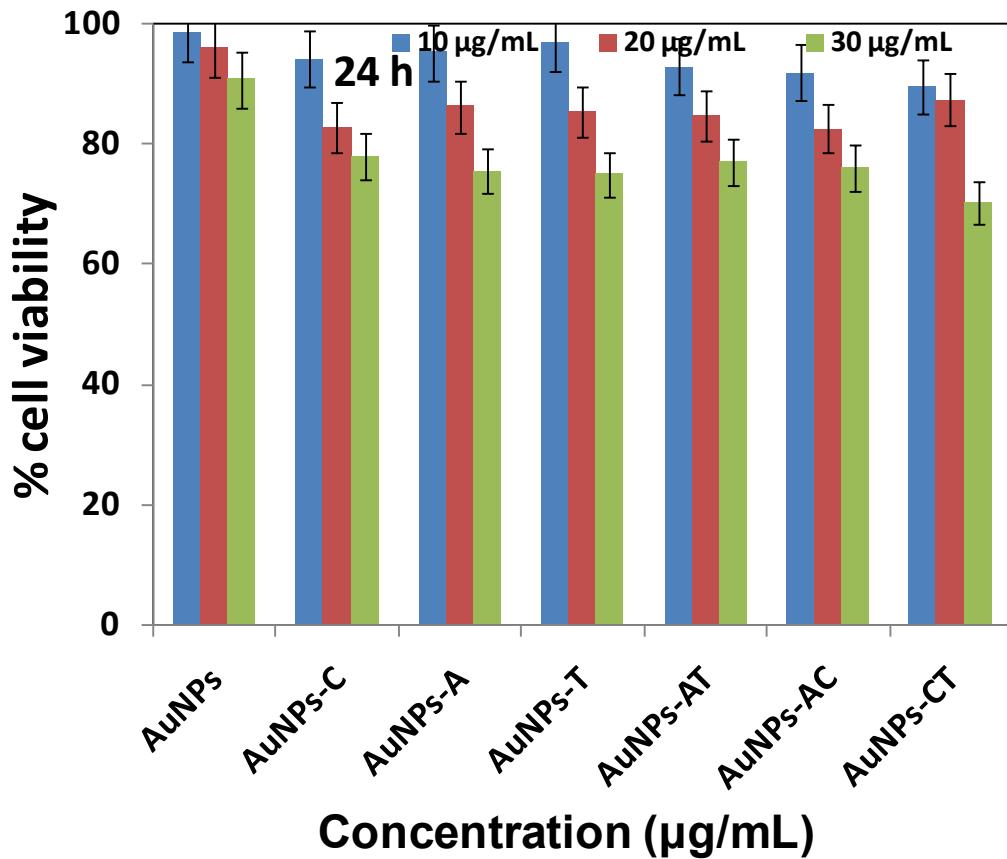
Thymine

Adenine

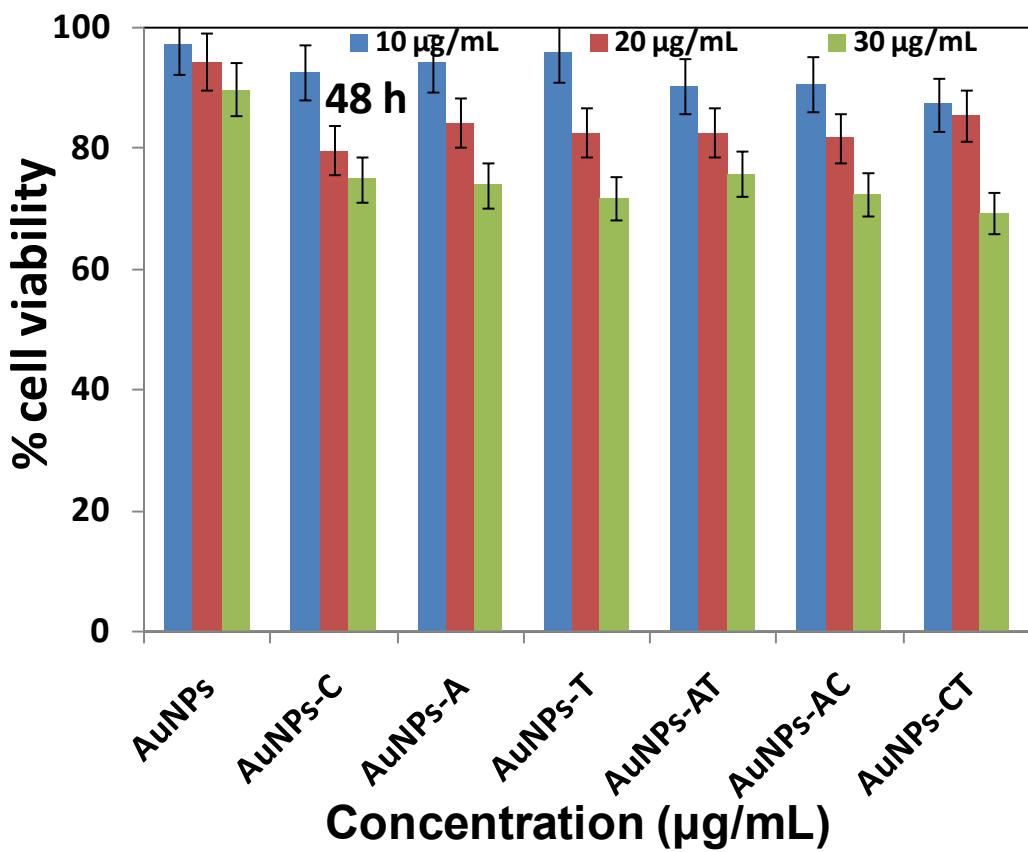


**ESI– Figure 6.** DNA bases (cytosine, thymine and adenine) binding interaction with gold nanoparticles. The numbers in the blue color are the positions of the atoms of the bases. Binding interactions are indicated by the blue lines.

#### IV. Cytotoxicity study of healthy cells line



**ESI–Figure 7.** Cytotoxicity measurements of functionalized AuNPs in healthy cells at various concentrations 2–30  $\mu\text{g/mL}$  for 24 h using MTT cell viability assay.



**ESI–Figure 8.** Cytotoxicity measurements of functionalized AuNPs in healthy cells at various concentrations 2–30  $\mu\text{g/mL}$  for 48 h using MTT cell viability assay.