

Electronic Supplementary Information:

**Experimental and theoretical approach for selective detection of thymine in
real samples using gold nanoparticles as a biochemical sensor**

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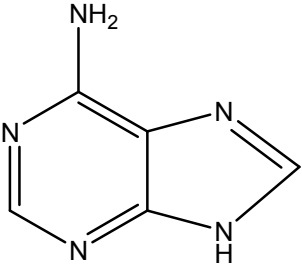
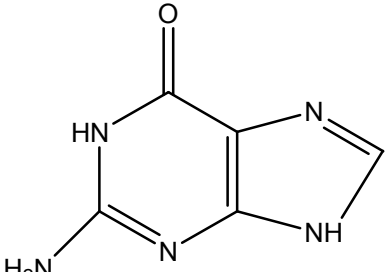
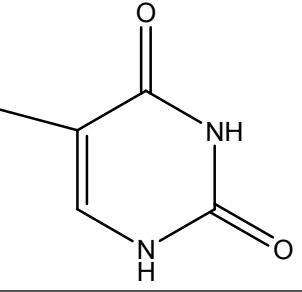
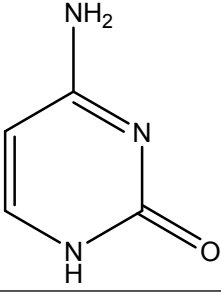
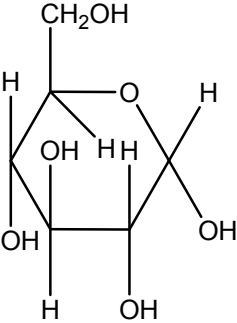
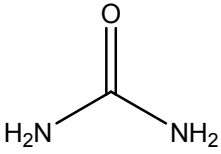
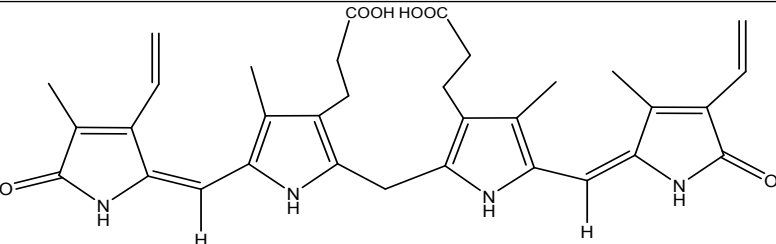
| | |
|---|--|
|  |  |
| Adenine | Guanine |
|  |  |
| Thymine | Cytosine |
|  |  |
| Glucose | Urea |
|  | |
| Bilirubin | |

Fig. S1. Structure of chemical substances

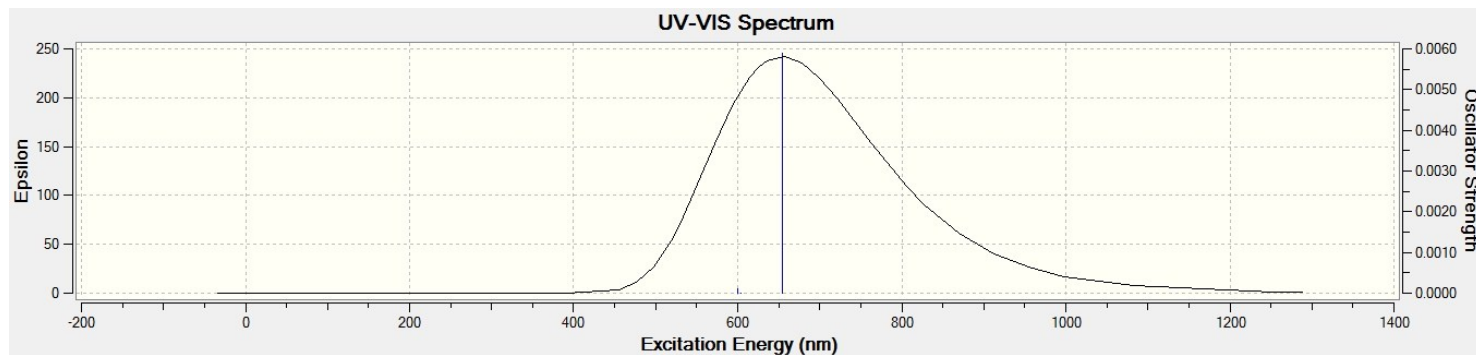


Fig. S2 TD-DFT of AuNPs with thymine calculated using Polarizable Continuum Model (PCM) for the solvent water and integral equation formalism variant (IEFPCM) in self consistent field method (B3LYP method & LANL2DZ basis set).

| Table S1. Absorption band of AuNPs with thymine by TD-DFT calculation | | |
|--|-------|-----------------------|
| Solvent | Model | Absorption band in nm |
| Water | PCM | 654.8 |
| | CPCM | 658.4 |
| | iCEM | 661.04 |
| | iPCM | 661.06 |
| | SMD | 666.0 |

Table S2. The Cartesian coordinates and bond parameters of thiamine gold interaction calculated by density functional theory (DFT) using B3LYP method and LANL2DZ basis set (E= -589.51873015 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|----------|----------|----------|----------|----------|------------|
| 1 | O | | | | -0.2302 | 1.176443 | 0.0005781 |
| 2 | O | 4.654858 | | | -2.55221 | -2.85791 | -0.0001415 |
| 3 | N | 2.319572 | 0.707818 | | -1.41203 | -0.81948 | 0.0002931 |
| 4 | N | 2.328603 | 60.80532 | 0.148403 | -3.74743 | -0.85945 | -0.0000096 |
| 5 | C | 2.408127 | 62.00087 | 179.8409 | -2.63579 | 1.287011 | -0.0000008 |
| 6 | C | 1.26869 | 31.35862 | 179.8443 | -1.35028 | 0.580621 | 0.0003476 |
| 7 | C | 1.367187 | 143.7642 | 0.007657 | -3.77449 | 0.530339 | -0.000118 |
| 8 | C | 1.507528 | 92.28868 | -179.993 | -2.62676 | 2.794512 | -0.0002687 |
| 9 | C | 1.246759 | 30.59026 | -0.00616 | -2.56673 | -1.61123 | 0.000032 |
| 10 | H | 1.084678 | 121.8056 | 179.9927 | -4.7608 | 0.981702 | -0.0003159 |
| 11 | H | 1.022444 | 88.51574 | 179.9821 | -0.51905 | -1.31745 | 0.0001284 |
| 12 | H | 1.013883 | 88.65639 | 179.9986 | -4.60512 | -1.40011 | -0.0001825 |
| 13 | H | 1.096747 | 110.7858 | 59.07446 | -2.09728 | 3.180402 | -0.8798087 |
| 14 | H | 1.096736 | 110.7874 | -59.035 | -2.0971 | 3.180737 | 0.8789981 |
| 15 | H | 1.095781 | 111.1987 | -179.981 | -3.64601 | 3.196859 | -0.0002401 |
| 16 | Au | 2.499972 | 122.5588 | 0.027298 | 1.947153 | -0.05197 | -0.0000508 |

Table S3. The Cartesian coordinates and bond parameters of adenine calculated by density functional theory (DFT) using B3LYP method and 6-31+G(d) basis set (E= -467.25962349 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-----------|-------------|----------|-----------|-----------|-----------|
| 1 | N | | | | 2.034903 | -0.361843 | 0.035194 |
| 2 | C | 1.4946354 | | | 1.489325 | -1.753185 | 0.014049 |
| 3 | N | 1.3109426 | 121.5565605 | | 0.199221 | -1.983825 | -0.017688 |
| 4 | C | 1.4621031 | 118.2172519 | -0.1194 | -0.707943 | -0.837239 | -0.029505 |
| 5 | C | 1.3127704 | 121.2836677 | 4.72112 | -0.252281 | 0.39181 | -0.101456 |
| 6 | C | 1.3016895 | 120.9697972 | -2.5903 | 1.242883 | 0.669243 | -0.027746 |
| 7 | N | 1.4700004 | 121.4487981 | -178.82 | 1.769523 | 2.041656 | -0.033591 |
| 8 | N | 1.4681389 | 128.8772251 | -173.93 | -2.173409 | -0.820744 | 0.057496 |
| 9 | N | 1.4600779 | 109.834637 | 173.719 | -1.365637 | 1.325276 | -0.246049 |
| 10 | C | 1.3113039 | 105.3678617 | 175.054 | -2.503966 | 0.446977 | 0.113473 |
| 11 | H | 1.0700002 | 119.2218531 | 177.534 | 2.167713 | -2.580542 | 0.027105 |
| 12 | H | 0.9999992 | 109.4712018 | -150.14 | 1.103514 | 2.656062 | 0.389417 |
| 13 | H | 0.9999996 | 109.4711683 | -30.142 | 2.625789 | 2.072309 | 0.482033 |
| 14 | H | 1.0000004 | 113.6566051 | 136.316 | -1.283787 | 2.13954 | 0.328647 |
| 15 | H | 1.0699995 | 124.1629312 | -166.22 | -3.473557 | 0.803355 | 0.392376 |

Table S4. The Cartesian coordinates and bond parameters of cytosine calculated by density functional theory (DFT) using B3LYP method and 6-31+G(d) basis set (E= - 394.90515340 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-----------|-------------|--------------|------------|------------|-----------|
| 1 | C | | | | 0.9090589 | 1.273304 | -0.103144 |
| 2 | C | 1.3549062 | | | -0.3644112 | 1.7348837 | -0.071697 |
| 3 | N | 1.4754641 | 121.1234414 | | -1.4852597 | 0.8550808 | 0.3112387 |
| 4 | C | 1.474523 | 111.7667978 | -25.6054526 | -1.1819081 | -0.5634683 | 0.0468257 |
| 5 | N | 1.4703638 | 121.1050844 | 27.6451234 | 0.202521 | -1.0586883 | 0.0559389 |
| 6 | C | 1.2886386 | 120.2332021 | -13.6297026 | 1.1884938 | -0.2292437 | 0.0342916 |
| 7 | N | 1.4700001 | 120.2439992 | 176.4022839 | 2.5712162 | -0.7202698 | 0.1230192 |
| 8 | O | 1.2584001 | 119.4426058 | -152.8093413 | -2.1243565 | -1.3653125 | -0.182102 |
| 9 | H | 1.0700001 | 119.9168927 | -170.2657495 | 1.7217696 | 1.9576758 | -0.22978 |
| 10 | H | 1.0700001 | 119.4445721 | -170.4496428 | -0.5596934 | 2.7570487 | -0.320582 |
| 11 | H | 1.0000001 | 108.9448146 | -146.2882053 | -2.29755 | 1.119091 | -0.208841 |
| 12 | H | 1.0000001 | 109.4712208 | 29.6018724 | 2.6262138 | -1.6354544 | -0.276246 |
| 13 | H | 1.0000001 | 109.4712211 | 149.6018722 | 3.1773692 | -0.1015741 | -0.376775 |

Table S5. The Cartesian coordinates and bond parameters of glucose calculated by density functional theory (DFT) using B3LYP method and 6-31+G(d) basis set (E= -687.16520376 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-----------|-------------|-------------|------------|------------|------------|
| 1 | C | | | | 1.1862307 | -1.4220962 | -0.2097575 |
| 2 | C | 1.5403513 | | | 1.6949879 | -0.0048566 | -0.5342262 |
| 3 | C | 1.5307537 | 108.6551133 | | 0.8172782 | 1.0108274 | 0.2014494 |
| 4 | C | 1.53076 | 108.0443539 | -58.5559624 | -0.6289619 | 0.8079418 | -0.2573024 |
| 5 | C | 1.540368 | 108.6556407 | 58.5630905 | -1.0467426 | -0.6411045 | 0.0564776 |
| 6 | O | 1.4394424 | 109.8976168 | 59.8172041 | -0.181924 | -1.5607941 | -0.6350926 |
| 7 | O | 1.4300001 | 109.8915495 | 179.9219418 | 3.0535965 | 0.1333691 | -0.1099898 |
| 8 | O | 1.4300001 | 110.096523 | -178.821989 | 1.2465463 | 2.3410308 | -0.1005244 |
| 9 | O | 1.4300001 | 109.7573849 | 178.7495729 | -1.4871062 | 1.7215804 | 0.430995 |
| 10 | C | 1.5400001 | 109.2443197 | -179.790067 | -2.4993724 | -0.8617466 | -0.4048077 |
| 11 | O | 1.4300001 | 109.4712206 | -59.8614038 | -3.361472 | 0.0482132 | 0.2834203 |
| 12 | O | 1.4300001 | 109.3451374 | 58.3608711 | 1.2690734 | -1.6465694 | 1.2000826 |
| 13 | H | 0.9600001 | 109.4712208 | 60.2701427 | 3.5994288 | -0.50835 | -0.5702765 |
| 14 | H | 0.9600001 | 109.4712209 | -60.4907417 | 2.1562613 | 2.4559956 | 0.1837324 |
| 15 | H | 0.9600001 | 109.4712204 | -180 | -4.2670075 | -0.08933 | -0.0041342 |
| 16 | H | 0.9600001 | 109.4712207 | -179.703272 | -2.3932853 | 1.587705 | 0.1437374 |
| 17 | H | 0.9600001 | 109.4712207 | 179.7938387 | 2.1814347 | -1.5576677 | 1.4852027 |
| 18 | H | 1.0700001 | 109.5328882 | -119.812996 | 1.7914555 | -2.1402002 | -0.7225244 |
| 19 | H | 1.0700001 | 109.5208602 | 179.9672018 | 1.6340324 | 0.1641313 | -1.5890379 |
| 20 | H | 1.0700001 | 109.6657325 | 60.9340895 | 0.8863536 | 0.8487739 | 1.2568486 |
| 21 | H | 1.0700001 | 109.6528356 | -61.1121667 | -0.6998144 | 0.9803002 | -1.3109497 |
| 22 | H | 1.0700001 | 109.455967 | 60.2796646 | -0.9761196 | -0.8121149 | 1.11036 |
| 23 | H | 1.0700001 | 109.4712209 | 60.1385963 | -2.5687587 | -0.6908303 | -1.4587874 |
| 24 | H | 1.0700001 | 109.4712204 | -179.861403 | -2.7942131 | -1.8668452 | -0.1862991 |

Table S6. The Cartesian coordinates and bond parameters of guanine calculated by density functional theory (DFT) using B3LYP method and 6-31+G(d) basis set (E= -542.49883324 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-----------|-------------|-------------|------------|------------|------------|
| 1 | N | | | | 1.6250048 | 0.9479212 | -0.3121434 |
| 2 | C | 1.4972051 | | | 1.7959029 | -0.5136213 | -0.0358995 |
| 3 | N | 1.3145754 | 123.2243588 | | 0.8039772 | -1.375292 | -0.07732 |
| 4 | C | 1.4622908 | 119.8911515 | -14.9739119 | -0.5777038 | -0.8964899 | -0.0779564 |
| 5 | C | 1.3096361 | 121.6417609 | 3.0186373 | -0.8618443 | 0.3818128 | -0.0967453 |
| 6 | C | 1.4786286 | 112.514342 | 25.2306229 | 0.2478693 | 1.4168759 | -0.047716 |
| | N | 1.4700001 | 118.3841676 | - | 3.1401024 | -1.0104148 | 0.2915515 |
| | | | | 155.0656082 | | | |
| 8 | O | 1.2584001 | 121.3282922 | 157.0958538 | 0.0039601 | 2.6276232 | 0.1934684 |
| 9 | N | 1.460506 | 110.0309657 | 177.2851004 | -2.3086595 | 0.571849 | -0.1574911 |
| 10 | N | 1.4682435 | 128.4611174 | - | -1.8163451 | -1.6817095 | -0.0076949 |
| | | | | 174.4079645 | | | |
| 11 | C | 1.3110863 | 105.3189134 | 171.8116634 | -2.7765925 | -0.8013974 | 0.1403684 |
| 12 | H | 1.0000001 | 108.9027671 | 36.0489683 | 2.2593249 | 1.4653179 | 0.2622595 |
| 13 | H | 1.0000001 | 109.471221 | - | 3.2312931 | -1.9559565 | -0.0209152 |
| | | | | 149.8591561 | | | |
| 14 | H | 1.0000001 | 109.4712201 | -29.8591568 | 3.8255761 | -0.4415835 | -0.1629337 |
| 15 | H | 1.0000001 | 113.6799471 | 134.6550099 | -2.6495515 | 1.2658829 | 0.4766301 |
| 16 | H | 1.0700001 | 124.1777878 | - | -3.7726713 | -1.0442049 | 0.44659 |
| | | | | 165.3547537 | | | |

Table S7. The Cartesian coordinates and bond parameters of urea calculated by density functional theory (DFT) using B3LYP method and 6-31+G(d) basis set (E= -225.25786004 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-------|-------|----------|---|------------|-----------|
| 1 | C | | | | 0 | 0 | 0.1300875 |
| 2 | N | 1.47 | | | 0 | 1.2730575 | -0.604913 |
| 3 | N | 1.47 | 120 | | 0 | -1.2730575 | -0.604913 |
| 4 | O | 1.258 | 120 | 180 | 0 | 0 | 1.3884876 |
| 5 | H | 1 | 120 | 0 | 0 | 2.1390829 | -0.104913 |
| 6 | H | 1 | 120 | 180 | 0 | 1.2730575 | -1.604913 |
| 7 | H | 1 | 120 | 0 | 0 | -2.1390829 | -0.104913 |
| 8 | H | 1 | 120 | -180 | 0 | -1.2730575 | -1.604913 |

Table S8. The Cartesian coordinates and bond parameters of bilirubin calculated by density functional theory (DFT) using B3LYP method and 6-31+G (d) basis set (E= -1949.58777280 a.u.)

| Row | Symbol | Bond | Angle | Dihedral | X | Y | Z |
|-----|--------|-----------|-------------|--------------|------------|------------|------------|
| 1 | O | | | | -6.9809395 | -0.8249639 | 0.6663834 |
| 2 | O | 4.1051209 | | | -3.8796038 | -0.411106 | 3.3239117 |
| 3 | O | 2.2692189 | 133.0000882 | | -7.0851066 | -0.8395122 | -1.6003967 |
| 4 | O | 2.2692892 | 62.9472978 | -91.7186173 | -4.4315261 | -2.5227345 | 2.7025579 |
| 5 | O | 6.0308647 | 126.9347053 | 40.7997018 | 0.7841752 | 3.387607 | 2.8877089 |
| 6 | O | 5.1615942 | 106.6665029 | -98.8447625 | 4.742632 | 0.6617888 | 1.0055321 |
| 7 | N | 5.7112169 | 62.3307218 | -44.3456077 | -0.746813 | 0.517688 | -1.8067173 |
| 8 | N | 3.3141314 | 103.7631056 | -79.7144987 | 0.6022729 | -2.4783832 | -1.3742919 |
| 9 | N | 2.3454981 | 72.2747546 | -29.013468 | 0.0838475 | 2.8638083 | 0.7113502 |
| 10 | N | 2.3450806 | 94.3339122 | 14.3180905 | 3.4080599 | -1.1429952 | 0.3265068 |
| 11 | C | 2.4782027 | 48.0369655 | 128.7321136 | -1.702208 | -1.7649822 | -1.9416679 |
| 12 | C | 1.3469148 | 122.7368114 | 6.8412079 | -1.8506302 | -0.2521726 | -1.86223 |
| 13 | C | 1.370481 | 63.1508407 | 96.0261765 | -0.7102891 | -2.3319097 | -1.0083071 |
| 14 | C | 1.3471437 | 111.0412638 | 69.9904016 | -2.9673451 | 0.5008707 | -1.8363503 |
| 15 | C | 1.377446 | 107.8378884 | -127.9928369 | -0.8416896 | -2.7903461 | 0.2839496 |
| 16 | C | 1.4168083 | 105.8788761 | 0.0134775 | -2.5266683 | 1.8451782 | -1.7589748 |
| 17 | C | 1.416905 | 107.3729316 | 0.0173899 | 0.4370449 | -3.2274269 | 0.7098817 |
| 18 | C | 1.3705779 | 63.9300611 | 102.0913002 | -1.1495639 | 1.8261814 | -1.7425251 |
| 19 | C | 1.3569695 | 106.482811 | 0.0049415 | 1.2819926 | -3.0179079 | -0.3310464 |
| 20 | C | 1.4775244 | 127.6743369 | 179.937367 | -4.3698177 | 0.0380596 | -1.8805637 |
| 21 | C | 1.4774076 | 126.171992 | 179.9372339 | -2.087917 | -2.8177256 | 1.0769824 |
| 22 | C | 1.4778964 | 126.2943215 | -179.9797307 | -3.3865545 | 3.0459751 | -1.7054918 |
| 23 | C | 1.4778174 | 126.2855591 | -179.9772682 | 0.7708343 | -3.7980957 | 2.0315723 |
| 24 | C | 1.542028 | 114.4856824 | 90.0852867 | -4.9961166 | -0.2364652 | -0.4984507 |
| 25 | C | 1.5421043 | 114.4886546 | -89.9155263 | -2.3477996 | -1.542017 | 1.9034896 |
| 26 | C | 1.4041904 | 117.9425584 | 61.7408592 | -0.1572855 | 2.8176724 | -1.6786512 |
| 27 | C | 1.4334998 | 133.3228027 | 179.9217964 | 2.6840652 | -3.2478734 | -0.521388 |
| 28 | C | 1.3545323 | 125.4926707 | -88.3369082 | 0.4081761 | 3.2923906 | -0.5430222 |
| 29 | C | 1.3357854 | 124.6228933 | -88.2880141 | 3.6453875 | -2.3732903 | -0.2127032 |
| 30 | C | 1.4486418 | 129.5418661 | -179.9982383 | 1.4301883 | 4.305265 | -0.3752733 |
| 31 | C | 1.4547455 | 129.3941589 | 179.9962524 | 5.0874219 | -2.4962077 | -0.3600557 |
| 32 | C | 1.222897 | 30.1777756 | 0.9727534 | -6.4443798 | -0.6702623 | -0.5726318 |
| 33 | C | 1.2229654 | 30.1803068 | 109.7997443 | -3.6502624 | -1.5822915 | 2.6735986 |
| 34 | C | 1.3506336 | 109.1317772 | 179.9877577 | 5.6757314 | -1.3638725 | 0.0825727 |
| 35 | C | 1.3470446 | 110.0847371 | -179.9983404 | 1.7045798 | 4.4733707 | 0.9327706 |
| 36 | C | 1.2186439 | 99.6361889 | -25.9685441 | 0.82215 | 3.5258777 | 1.6775304 |
| 37 | C | 1.2184335 | 121.5769446 | 11.7762025 | 4.5857143 | -0.4538536 | 0.5415289 |

| | | | | | | | |
|----|---|-----------|-------------|--------------|------------|------------|------------|
| 38 | C | 1.4924044 | 121.8098535 | 0.0003938 | 2.0372778 | 5.010976 | -1.5417574 |
| 39 | C | 1.4404283 | 126.9348825 | -0.0411658 | 5.8105477 | -3.6250196 | -0.8870341 |
| 40 | C | 1.4852349 | 132.4637917 | 179.9801472 | 7.0965447 | -0.9400139 | 0.1695001 |
| 41 | C | 1.4276948 | 130.2436202 | -179.995564 | 2.6298428 | 5.3500981 | 1.575849 |
| 42 | C | 1.3332523 | 123.4149475 | 140.03132 | 6.8716159 | -3.5092229 | -1.6859628 |
| 43 | C | 1.3403412 | 123.8661581 | 40.0116173 | 2.8476786 | 6.6163797 | 1.1942821 |
| 44 | H | 1.0960952 | 131.7175799 | -153.0904684 | -2.6755127 | -2.2391419 | -1.7705678 |
| 45 | H | 1.0985438 | 85.4109154 | 100.3022706 | -1.4315605 | -2.0184481 | -2.9757392 |
| 46 | H | 1.0118228 | 85.0344201 | -124.3032843 | 0.2138203 | 0.2001832 | -1.8193522 |
| 47 | H | 1.0118218 | 79.0777057 | -124.8784022 | 0.9893439 | -2.2217668 | -2.2732399 |
| 48 | H | 1.0980365 | 109.4755245 | -147.5978492 | -4.9845761 | 0.7822428 | -2.4039636 |
| 49 | H | 1.0978664 | 110.0056418 | -33.1119411 | -4.4470644 | -0.8682034 | -2.495406 |
| 50 | H | 1.0971649 | 109.938529 | 33.2904398 | -2.9464408 | -2.9999533 | 0.4185748 |
| 51 | H | 1.0980518 | 109.6027784 | 147.7291349 | -2.07294 | -3.6796851 | 1.7570702 |
| 52 | H | 1.0946348 | 112.1170931 | 173.1126274 | -2.8091397 | 3.9587758 | -1.527693 |
| 53 | H | 1.094922 | 110.4064905 | -66.7504886 | -3.9263603 | 3.1713569 | -2.6498133 |
| 54 | H | 1.0949008 | 110.6940359 | 53.1593276 | -4.121305 | 2.9600693 | -0.8982932 |
| 55 | H | 1.0946373 | 112.1259649 | -174.8961185 | 1.8451557 | -3.9747431 | 2.1449749 |
| 56 | H | 1.0949556 | 110.4489905 | 65.0003277 | 0.2593611 | -4.7555556 | 2.1750767 |
| 57 | H | 1.0949155 | 110.6499085 | -54.9133298 | 0.4625456 | -3.1199181 | 2.8339894 |
| 58 | H | 1.0958077 | 109.8747733 | 56.9960169 | -4.9374548 | 0.6643789 | 0.1227041 |
| 59 | H | 1.0924317 | 109.0545246 | -62.3286177 | -4.4420524 | -1.0408926 | -0.009251 |
| 60 | H | 1.0955717 | 109.7759238 | 57.2546055 | -2.3687507 | -0.6693127 | 1.2415034 |
| 61 | H | 1.0961727 | 109.5163458 | -61.2595233 | -1.535242 | -1.4017529 | 2.6257574 |
| 62 | H | 1.0874951 | 115.8029672 | 92.2746708 | 0.1611964 | 3.2308057 | -2.6328712 |
| 63 | H | 1.0872973 | 115.7445821 | 91.8232176 | 2.9507504 | -4.2105901 | -0.9506561 |
| 64 | H | 1.0135377 | 100.5227 | -6.5029335 | -0.6095769 | 2.150856 | 0.9065947 |
| 65 | H | 1.0134683 | 100.539925 | 4.7617658 | 2.4854727 | -0.7820811 | 0.5402633 |
| 66 | H | 1.0956818 | 110.6060398 | -47.4041284 | 2.327179 | 4.2940553 | -2.3179666 |
| 67 | H | 1.0947956 | 110.5052905 | 72.5186134 | 1.3232704 | 5.7180998 | -1.9762072 |
| 68 | H | 1.0926354 | 113.0874355 | -165.8173832 | 2.9489413 | 5.5560855 | -1.2856768 |
| 69 | H | 1.0860768 | 117.3326576 | -38.39262 | 5.4448309 | -4.6151257 | -0.6310968 |
| 70 | H | 1.0941492 | 110.4945897 | 96.938032 | 7.3664128 | -0.3251212 | -0.6943521 |
| 71 | H | 1.0955361 | 110.4609552 | -143.6873117 | 7.2637938 | -0.344091 | 1.0734376 |
| 72 | H | 1.0932785 | 112.558351 | -25.2099864 | 7.784033 | -1.787765 | 0.2322366 |
| 73 | H | 1.0862109 | 117.0904949 | -141.2525642 | 3.1662626 | 4.9589125 | 2.4355477 |
| 74 | H | 0.9809217 | 111.8629175 | 0.5691838 | -7.9237845 | -1.0924835 | 0.6253469 |
| 75 | H | 0.9809673 | 70.4585414 | 170.2503309 | -4.7303695 | -0.4250522 | 3.8120716 |
| 76 | H | 1.0856711 | 119.672557 | -179.3918078 | 7.3653718 | -4.4022841 | -2.0565412 |
| 77 | H | 1.0837747 | 123.5589821 | -1.4931815 | 7.2653273 | -2.5581124 | -2.0250024 |
| 78 | H | 1.085427 | 119.8037872 | 179.5169719 | 3.5619869 | 7.2279125 | 1.7364472 |
| 79 | H | 1.0840543 | 123.0185292 | 1.2788611 | 2.3188557 | 7.0848528 | 0.3720576 |

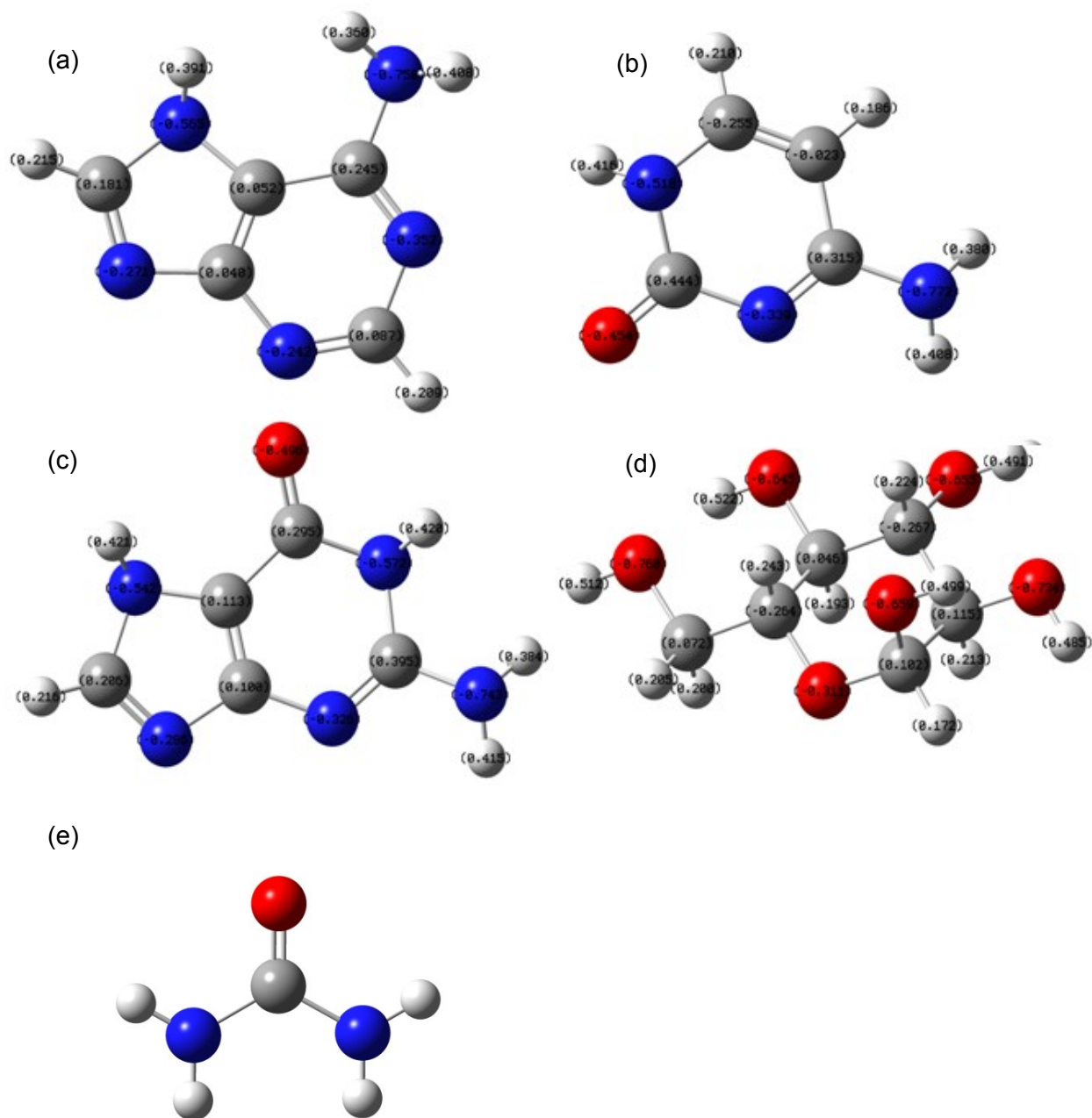


Fig. S3. Optimized structure of (a) adenine, (b) cytosine, (c) guanine, (d) glucose and (e) urea in the present study obtained from density functional theory (DFT) using B3LYP method and 6-31+G (d) basis set

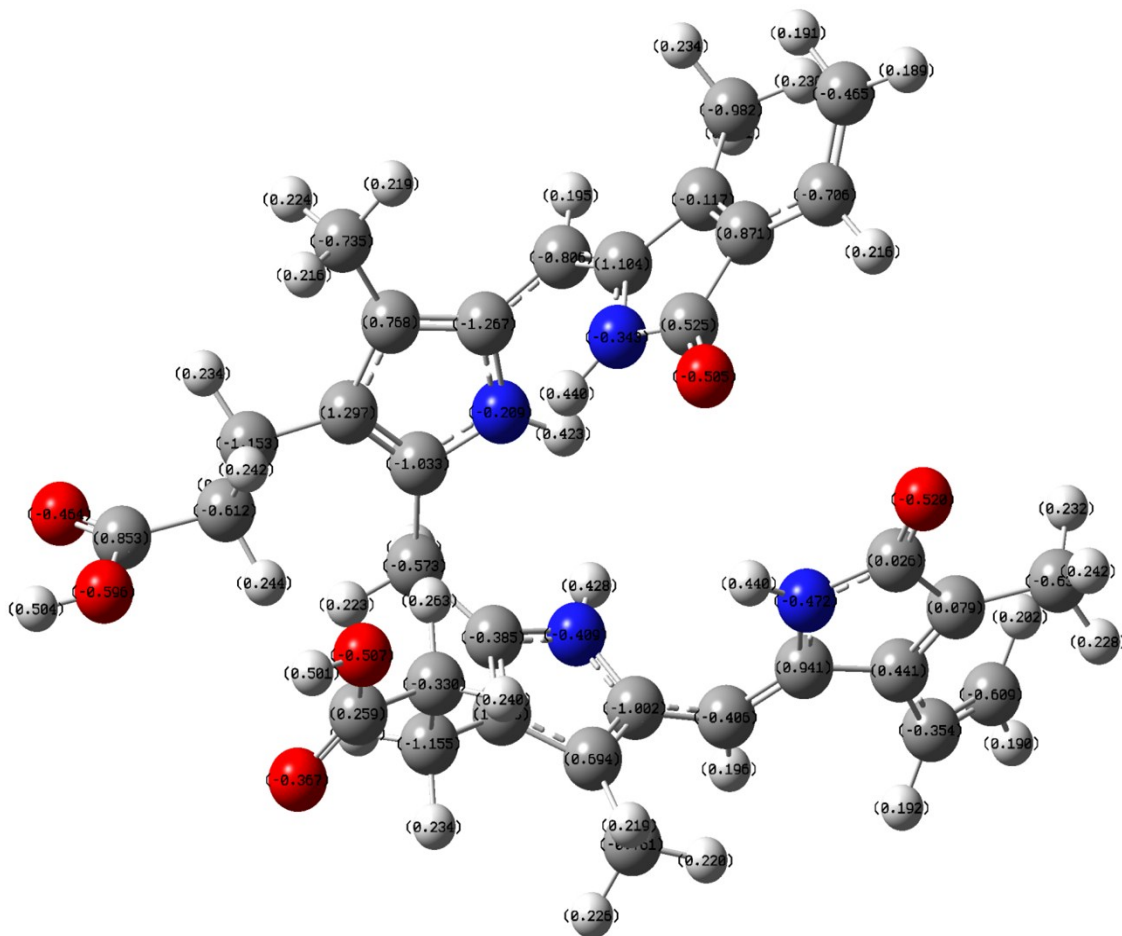


Fig. S4. Optimized structure of bilirubin taken in the present study obtained from density functional theory (DFT) using B3LYP method and 6-31+G (d) basis set.

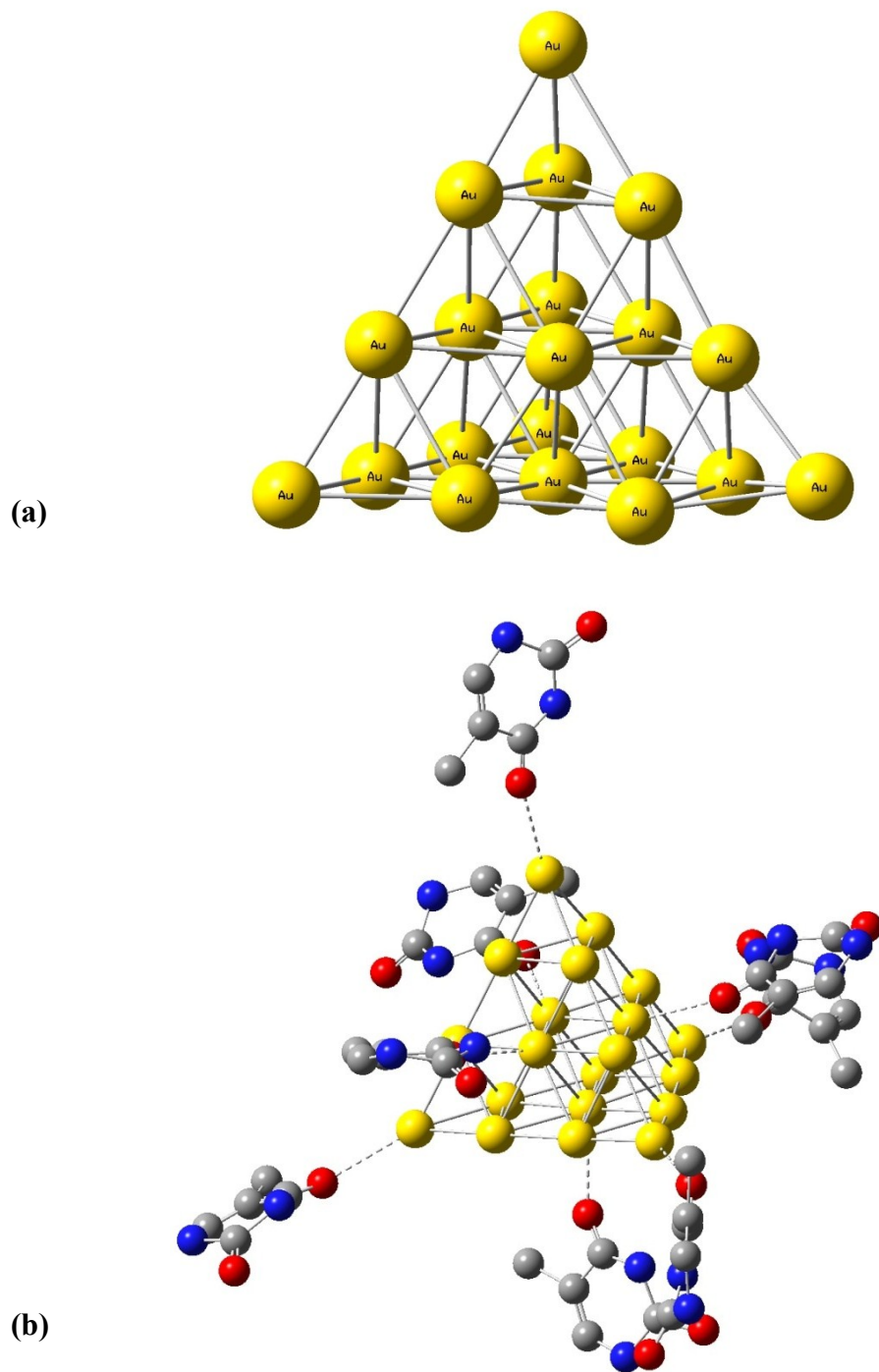


Fig. S5. (a) Optimized omnicauded truncated tetrahedral (v_3 -tetrahedral) Au₂₀ cluster structure model (b) Omnicauded truncated tetrahedral (v_3 -tetrahedral) Au₂₀ cluster interacted with thymine (hydrogen is not shown for clarity)-In both structure optimization is done using B3LYP method and LANL2DZ basis set.

Table S9. The Cartesian coordinates gold nanoparticles (Au₂₀) interacted with thymine calculated by density functional theory (DFT) using B3LYP method and LANL2DZ basis set (E= -2709.74444741 a.u.)

| Row | Symbol | X | Y | Z |
|-----|--------|-----------|-----------|-----------|
| 1 | O | 4.810618 | 3.537719 | -4.924586 |
| 2 | O | 8.316747 | 0.961335 | -6.577398 |
| 3 | N | 6.222534 | 1.95086 | -6.079545 |
| 4 | N | 8.290459 | 3.318847 | -6.855543 |
| 5 | C | 6.655086 | 4.441377 | -5.450655 |
| 6 | C | 5.824802 | 3.233678 | -5.482918 |
| 7 | C | 7.841743 | 4.461535 | -6.023578 |
| 8 | C | 6.006248 | 5.62131 | -4.671069 |
| 9 | C | 7.640775 | 2.021604 | -6.494772 |
| 10 | H | 8.467856 | 5.311499 | -5.885601 |
| 11 | H | 6.081425 | 1.197684 | -5.418016 |
| 12 | H | 9.270955 | 3.229633 | -6.735026 |
| 13 | H | 6.097333 | 5.452023 | -3.612665 |
| 14 | H | 4.961983 | 5.677737 | -4.925785 |
| 15 | H | 6.484977 | 6.534722 | -4.92723 |
| 16 | Au | 2.903248 | 2.018234 | -3.330425 |
| 17 | Au | 1.466701 | 2.451638 | -1.161162 |
| 18 | Au | 2.675081 | 0.101921 | -1.508523 |
| 19 | Au | 0.585919 | 0.699241 | -3.034324 |
| 20 | Au | -0.872774 | 1.191972 | -0.852271 |
| 21 | Au | -1.832283 | -0.574708 | -2.619568 |
| 22 | Au | 1.263995 | 0.565809 | 0.734928 |
| 23 | Au | 0.013862 | 2.909393 | 1.029438 |
| 24 | Au | 0.386701 | -1.228208 | -1.135847 |
| 25 | Au | 2.507086 | -1.772325 | 0.428674 |
| 26 | Au | -3.242538 | -0.128191 | -0.402021 |
| 27 | Au | -1.947485 | -2.468848 | -0.762071 |
| 28 | Au | -4.147012 | -1.927184 | -2.127844 |
| 29 | Au | -2.325328 | 1.71699 | 1.333639 |
| 30 | Au | -1.124403 | -0.730734 | 1.095474 |
| 31 | Au | -1.436877 | 3.444266 | 3.181663 |
| 32 | Au | -0.301936 | 1.047112 | 2.909311 |
| 33 | Au | 0.189286 | -3.055201 | 0.847076 |
| 34 | Au | 1.049138 | -1.281543 | 2.6206 |
| 35 | Au | 2.334243 | -3.58776 | 2.35016 |
| 36 | O | -1.595824 | 5.711704 | 4.988584 |
| 37 | O | -4.943652 | 8.680295 | 5.793803 |
| 38 | N | -3.749424 | 6.663989 | 5.470394 |
| 39 | N | -3.249297 | 8.32037 | 7.420174 |

| | | | | |
|----|---|-----------|-----------|-----------|
| 40 | C | -1.426274 | 6.947332 | 6.613034 |
| 41 | C | -2.332715 | 6.378346 | 5.606813 |
| 42 | C | -1.820812 | 7.927923 | 7.38727 |
| 43 | C | -0.000931 | 6.302987 | 6.632355 |
| 44 | C | -4.022591 | 7.924197 | 6.198385 |
| 45 | H | -1.100586 | 8.430192 | 7.99049 |
| 46 | H | -3.990871 | 6.759696 | 4.494841 |
| 47 | H | -3.279622 | 9.308502 | 7.513672 |
| 48 | H | 0.559156 | 6.627148 | 5.775105 |
| 49 | H | -0.097079 | 5.229364 | 6.599635 |
| 50 | H | 0.513333 | 6.584271 | 7.520837 |
| 51 | O | 3.926821 | -5.662018 | 3.58698 |
| 52 | O | 8.507361 | -5.399546 | 4.00749 |
| 53 | N | 6.200398 | -4.823123 | 4.074329 |
| 54 | N | 7.232478 | -6.757552 | 5.483736 |
| 55 | C | 4.887824 | -6.903604 | 4.883757 |
| 56 | C | 5.007455 | -5.689349 | 4.123873 |
| 57 | C | 5.935528 | -7.476416 | 5.419564 |
| 58 | C | 3.419903 | -7.408345 | 4.930052 |
| 59 | C | 7.366762 | -5.646128 | 4.488502 |
| 60 | H | 5.835539 | -8.459918 | 5.807214 |
| 61 | H | 6.343502 | -4.462499 | 3.14338 |
| 62 | H | 7.949075 | -7.426451 | 5.317771 |
| 63 | H | 3.13705 | -7.785816 | 3.966097 |
| 64 | H | 2.770924 | -6.582203 | 5.18407 |
| 65 | H | 3.320524 | -8.171852 | 5.659053 |
| 66 | O | -9.756123 | -2.748057 | -5.79834 |
| 67 | O | -6.627426 | -3.434006 | -2.699268 |
| 68 | N | -8.168477 | -2.298737 | -4.097458 |
| 69 | N | -8.695947 | -3.46656 | -1.874793 |
| 70 | C | -10.29429 | -3.761114 | -3.668119 |
| 71 | C | -9.415081 | -2.900947 | -4.597366 |
| 72 | C | -9.879877 | -4.079323 | -2.429444 |
| 73 | C | -11.64784 | -4.276763 | -4.159244 |
| 74 | C | -7.762931 | -3.058173 | -2.92253 |
| 75 | H | -10.41972 | -4.787613 | -1.836674 |
| 76 | H | -7.469715 | -2.356799 | -4.812859 |
| 77 | H | -8.248674 | -4.130153 | -1.282746 |
| 78 | H | -11.49666 | -5.054164 | -4.87679 |
| 79 | H | -12.18551 | -3.470684 | -4.610037 |
| 80 | H | -12.20553 | -4.66027 | -3.329751 |
| 81 | O | -3.317725 | -1.768648 | 2.701772 |
| 82 | O | -3.137848 | -5.238612 | 5.617666 |
| 83 | N | -2.678769 | -3.18922 | 4.533318 |

| | | | | |
|-----|---|-----------|-----------|-----------|
| 84 | N | -4.925606 | -3.677696 | 5.755421 |
| 85 | C | -4.958533 | -2.094307 | 3.918312 |
| 86 | C | -3.530687 | -2.356744 | 3.701544 |
| 87 | C | -5.635385 | -2.792896 | 4.799583 |
| 88 | C | -5.553564 | -0.976602 | 3.00189 |
| 89 | C | -3.556802 | -4.092571 | 5.308316 |
| 90 | H | -6.697437 | -2.710834 | 4.815613 |
| 91 | H | -2.048334 | -3.722466 | 3.954663 |
| 92 | H | -5.484266 | -4.490575 | 5.873809 |
| 93 | H | -5.645983 | -1.341452 | 1.996264 |
| 94 | H | -4.89119 | -0.125459 | 3.004235 |
| 95 | H | -6.509907 | -0.679951 | 3.362949 |
| 96 | O | -1.485863 | 3.375218 | -2.600702 |
| 97 | O | -5.334385 | 4.596087 | -4.534321 |
| 98 | N | -3.695103 | 4.108095 | -2.923512 |
| 99 | N | -3.393387 | 5.963003 | -4.722205 |
| 100 | C | -1.397405 | 4.904078 | -3.883128 |
| 101 | C | -2.267689 | 4.055705 | -3.046887 |
| 102 | C | -1.930284 | 5.722458 | -4.744966 |
| 103 | C | 0.152295 | 4.69924 | -3.670631 |
| 104 | C | -4.195173 | 4.865209 | -4.081256 |
| 105 | H | -1.299518 | 6.207612 | -5.45444 |
| 106 | H | -4.072553 | 3.173068 | -2.908513 |
| 107 | H | -3.684638 | 6.060772 | -5.66354 |
| 108 | H | 0.462362 | 3.768256 | -4.111208 |
| 109 | H | 0.370679 | 4.672457 | -2.614884 |
| 110 | H | 0.692064 | 5.500955 | -4.120862 |
| 111 | O | 1.560876 | -3.372945 | -2.685493 |
| 112 | O | 2.908628 | -3.050632 | -7.01468 |
| 113 | N | 2.729263 | -2.627314 | -4.692626 |
| 114 | N | 3.643491 | -4.866633 | -5.670178 |
| 115 | C | 2.633072 | -4.915255 | -3.471016 |
| 116 | C | 2.28102 | -3.51202 | -3.622002 |
| 117 | C | 3.148018 | -5.582817 | -4.469944 |
| 118 | C | 2.292598 | -5.491109 | -2.060617 |
| 119 | C | 3.077673 | -3.489126 | -5.846832 |
| 120 | H | 3.206648 | -6.641464 | -4.400752 |
| 121 | H | 2.004232 | -1.978888 | -4.943261 |
| 122 | H | 3.399977 | -5.417905 | -6.461071 |
| 123 | H | 1.22969 | -5.46618 | -1.912231 |
| 124 | H | 2.763013 | -4.885721 | -1.30114 |
| 125 | H | 2.645813 | -6.49072 | -1.979208 |
| 126 | O | 3.597331 | 0.98722 | 2.413545 |
| 127 | O | 6.707512 | 4.059927 | 1.325842 |

| | | | | |
|-----|---|----------|-----------|----------|
| 128 | N | 4.673291 | 3.017655 | 1.890551 |
| 129 | N | 6.675422 | 3.185661 | 3.535216 |
| 130 | C | 5.150172 | 1.310783 | 3.802157 |
| 131 | C | 4.401907 | 1.803381 | 2.624358 |
| 132 | C | 6.275053 | 1.898424 | 4.155548 |
| 133 | C | 4.531042 | 0.070614 | 4.526528 |
| 134 | C | 6.048268 | 3.44375 | 2.201566 |
| 135 | H | 6.889881 | 1.437058 | 4.894195 |
| 136 | H | 4.571782 | 2.843516 | 0.902234 |
| 137 | H | 7.662308 | 3.166524 | 3.425442 |
| 138 | H | 4.67987 | -0.811148 | 3.931974 |
| 139 | H | 3.473739 | 0.227709 | 4.659336 |
| 140 | H | 4.990848 | -0.061018 | 5.478918 |

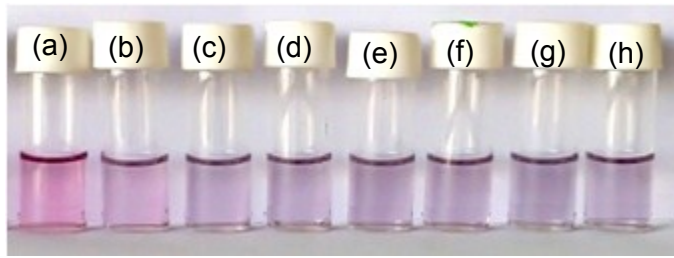


Fig. S6. Glass vial containing different dilution of hydrolyzed product of DNA standard sample and AuNPs that could be differentiated by naked eyes for qualitative determination of thymine

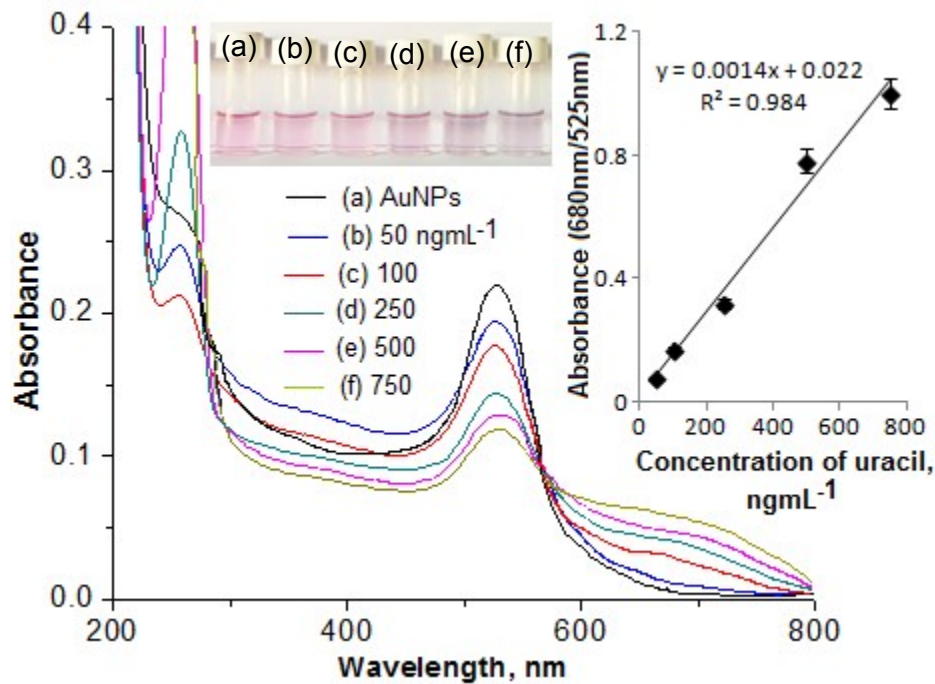


Fig. S7. Glass vial containing AuNPs along with different concentration of uracil (50, 100, 250, 500, 750 ngmL⁻¹) with their respective UV-Vis spectra and inserted graph showing the calibration curve obtained with different concentration of uracil and absorbance ratio (680 nm/525 nm)