Supplementary material for

Evaluation of DNA/BSA interactions and DFT calculations of gold(III), zinc(II), and palladium(II) complexes with dithiocarbamate

By the authors:

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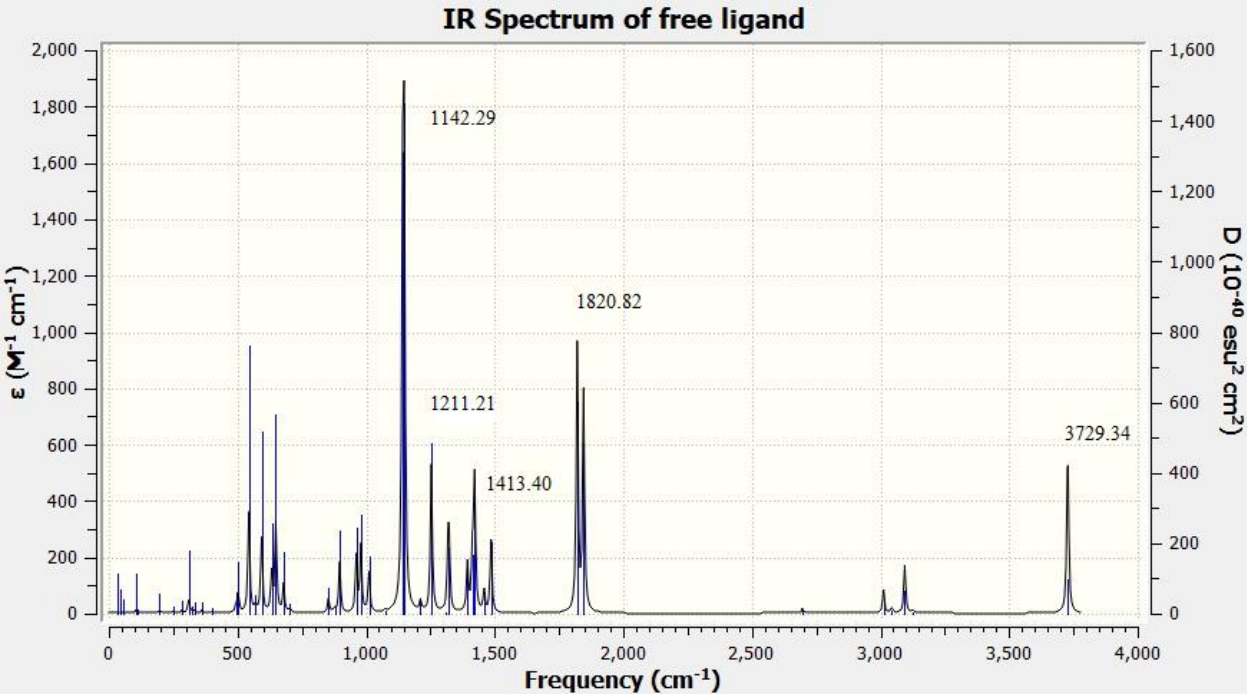
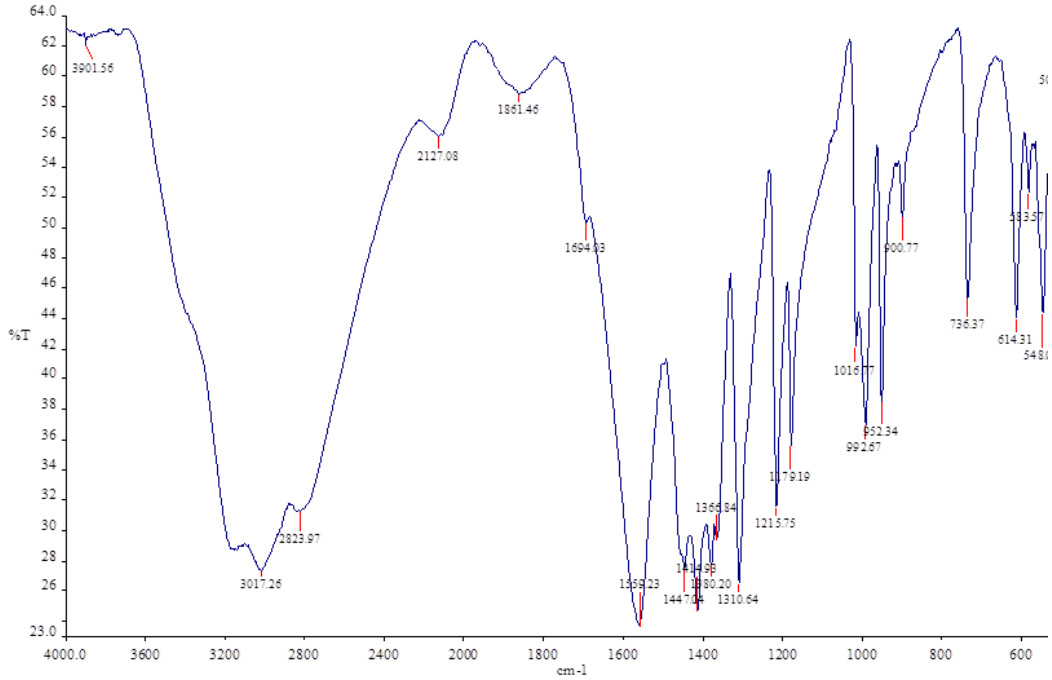
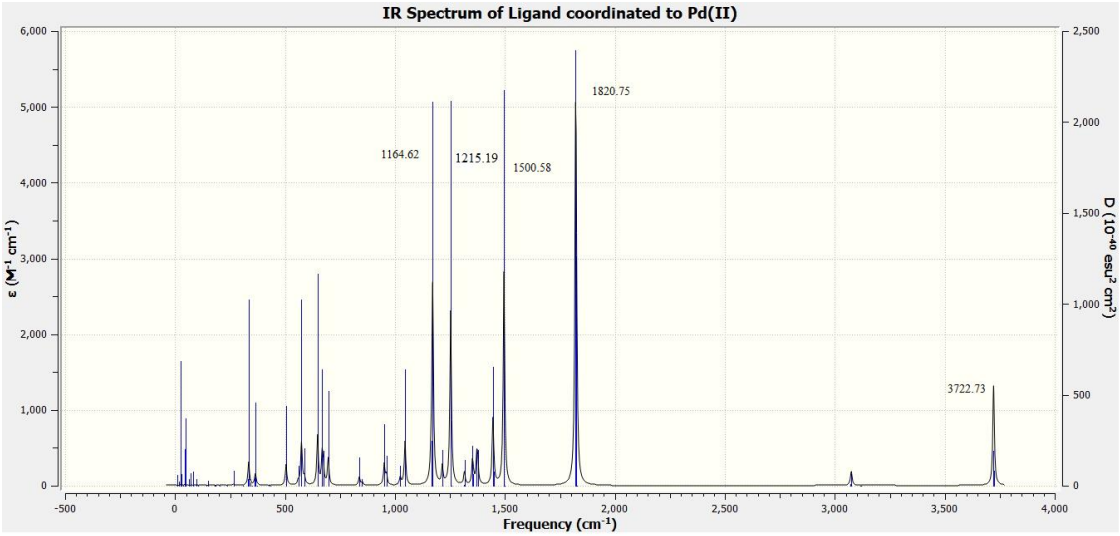


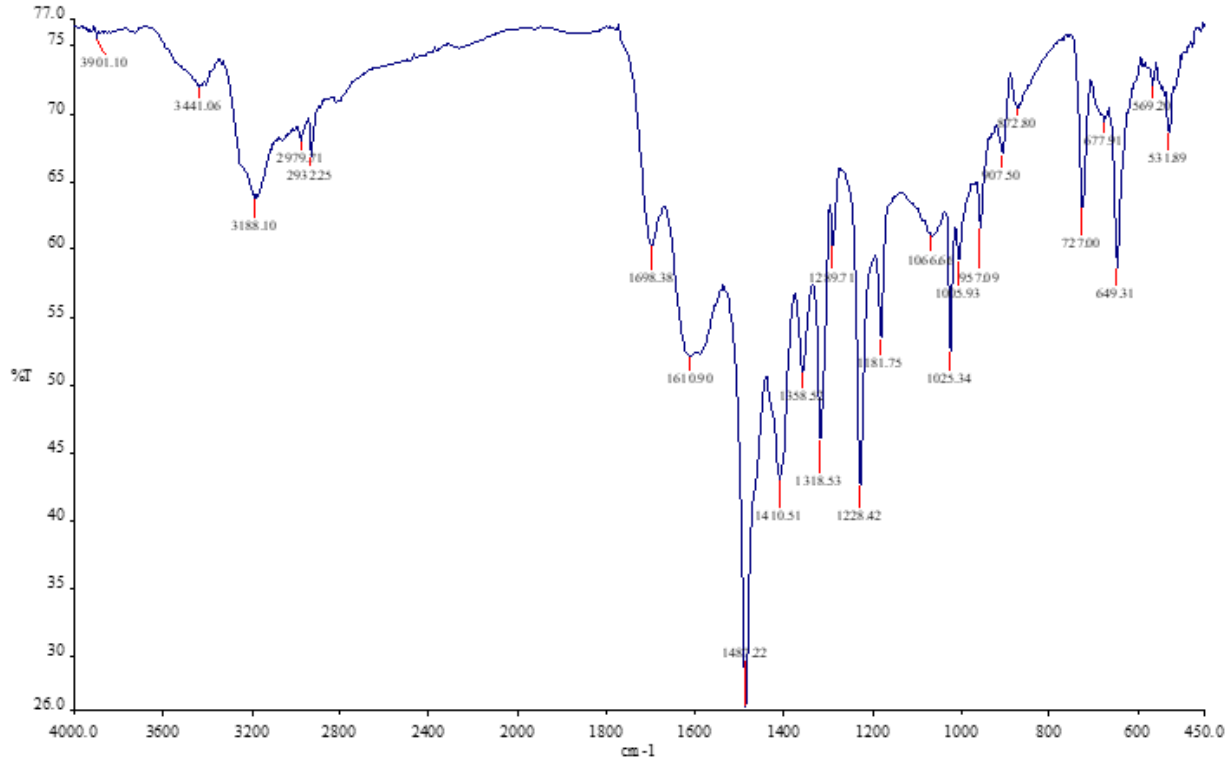
S1. The calculated FTIR spectrum of free ligand (**L**)



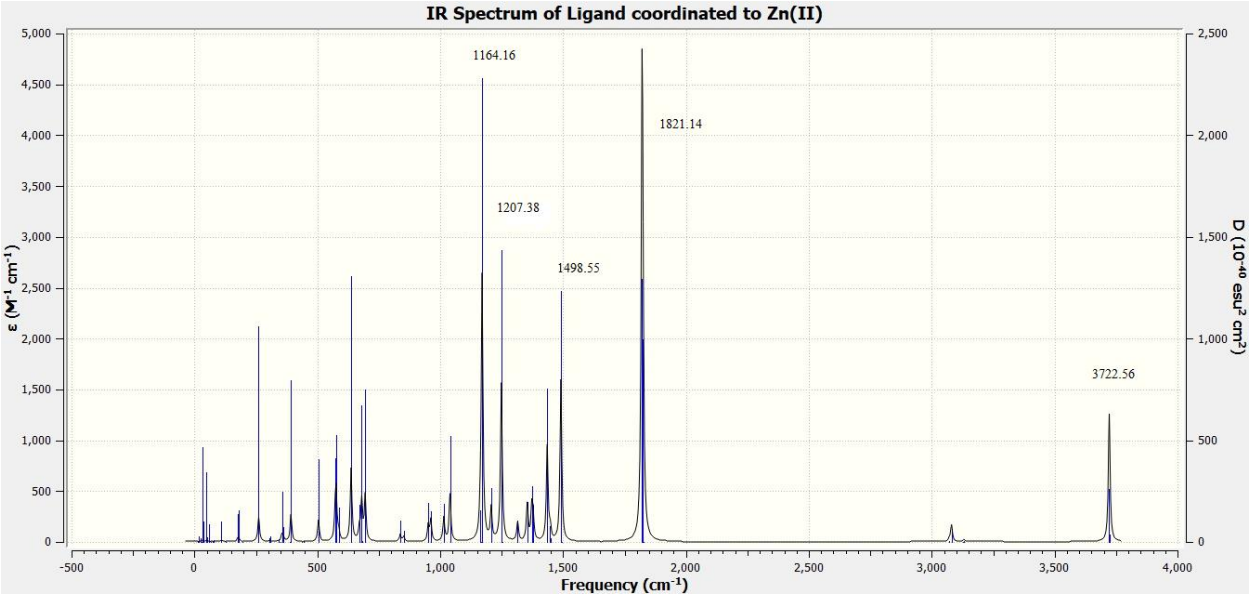
S2. Experimentally obtained FTIR spectrum of free ligand.



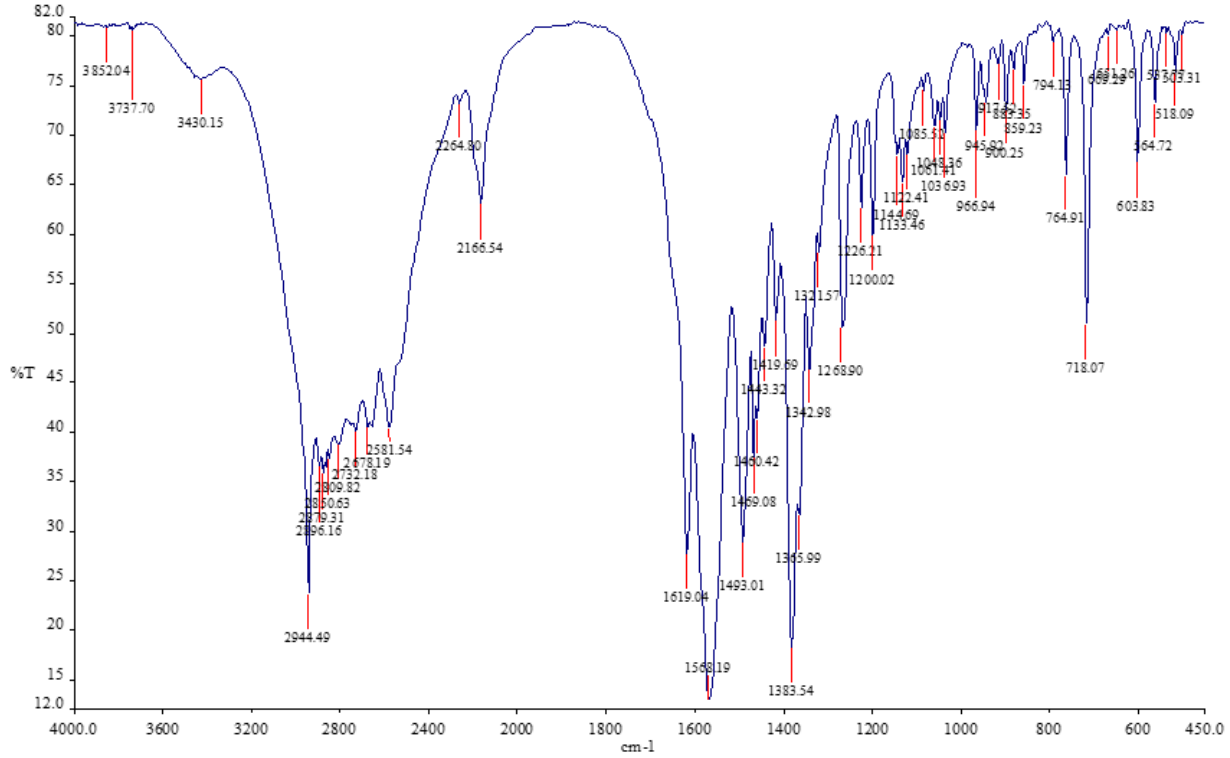
S3. The calculated FTIR spectrum of palladium(II) complex, **C1**



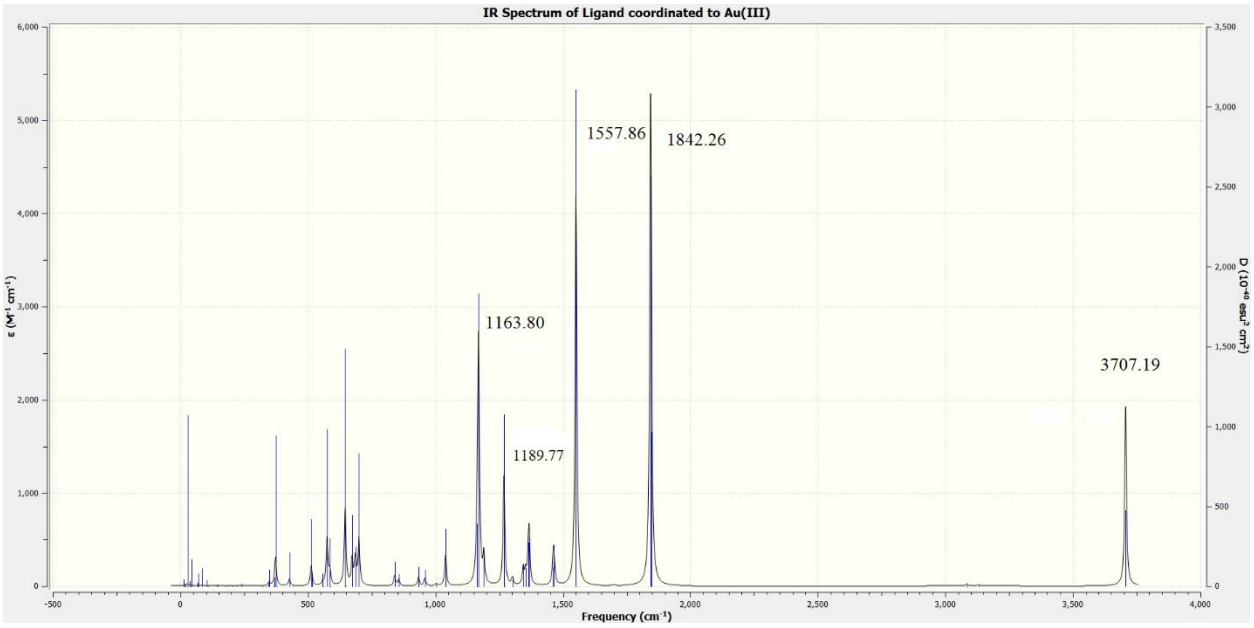
S4. Experimentally obtained FTIR spectrum of palladium(II) complex, **C1**.



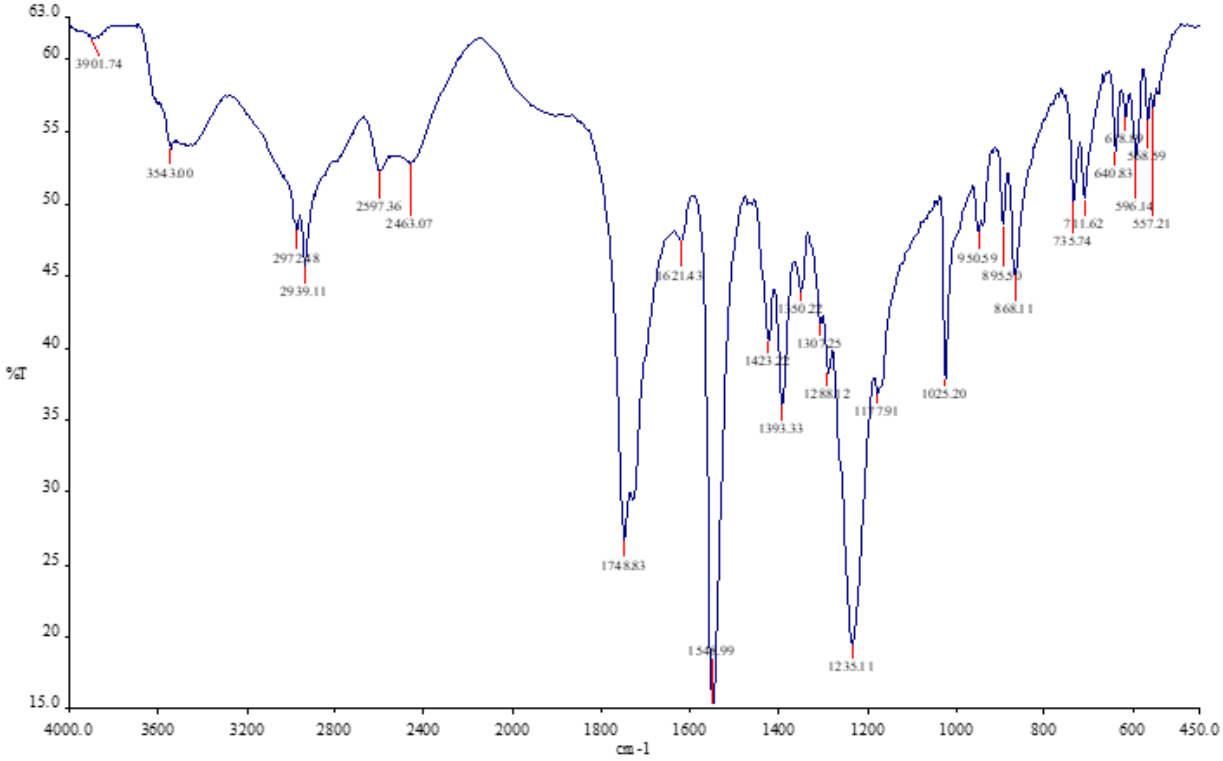
S5. The calculated FTIR spectrum of zinc(II) complex, **C2**



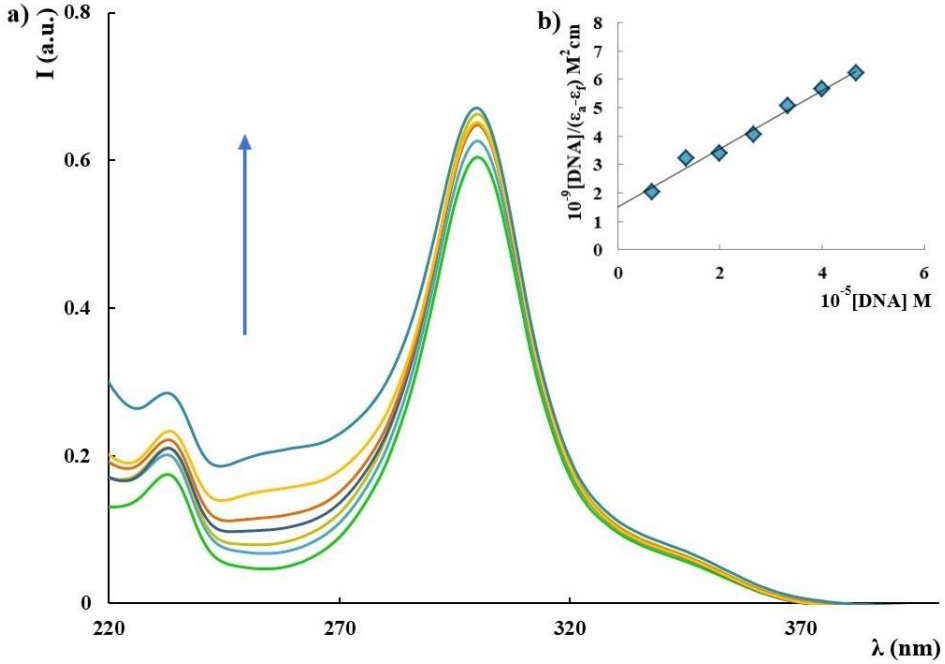
S6. Experimentally obtained FTIR spectrum of zinc(II) complex, **C2**.



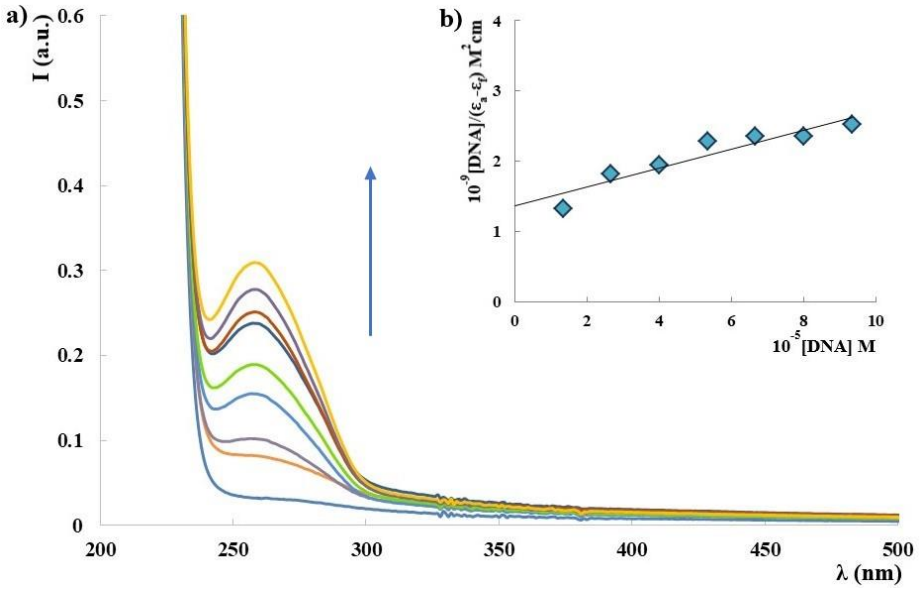
S5. The calculated FTIR spectrum of gold(III) complex, **C3.**



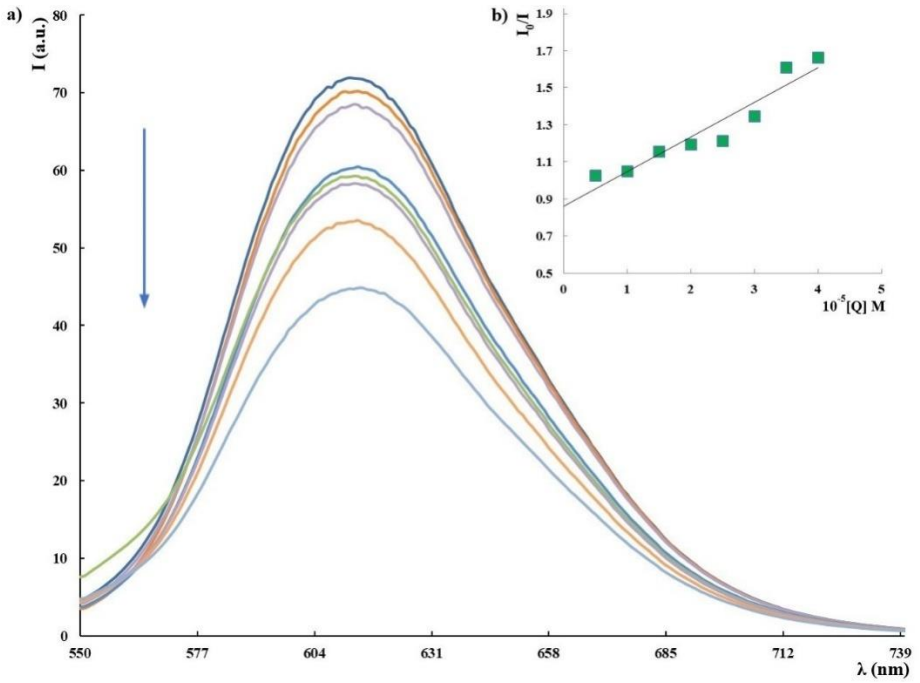
S8. Experimentally obtained FTIR spectrum of gold(III) complex, **C3**.



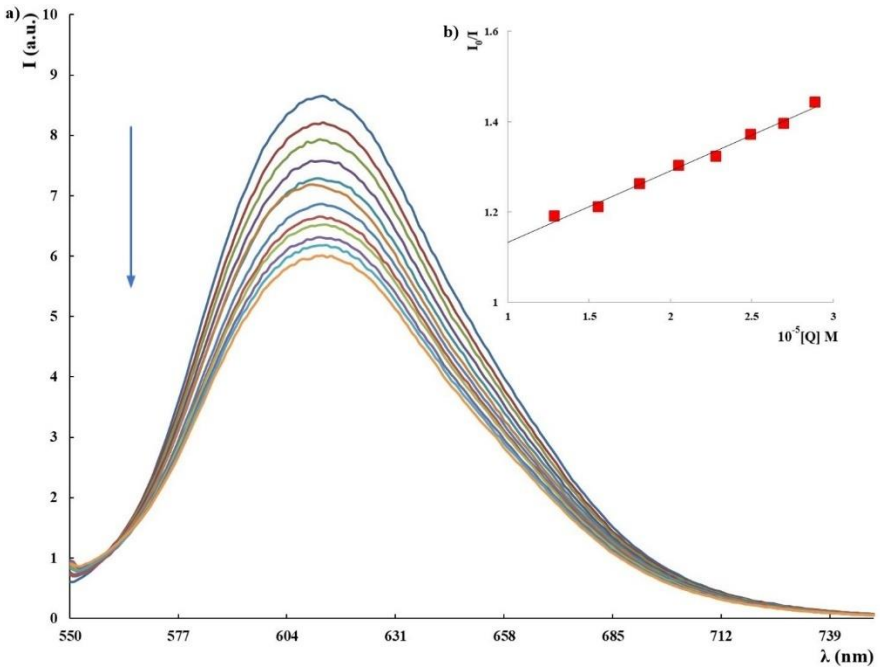
S9. a) Absorption spectra of the interaction of CT-DNA with **C1**in PBS after the addition of DNA. [complex] = 8 μM, [DNA] = 0-40 μM. The arrow shows hyperchromism in the spectral band. b) Insert graph: Plots of [DNA]/($\varepsilon_a - \varepsilon_f$)] vs. [DNA].



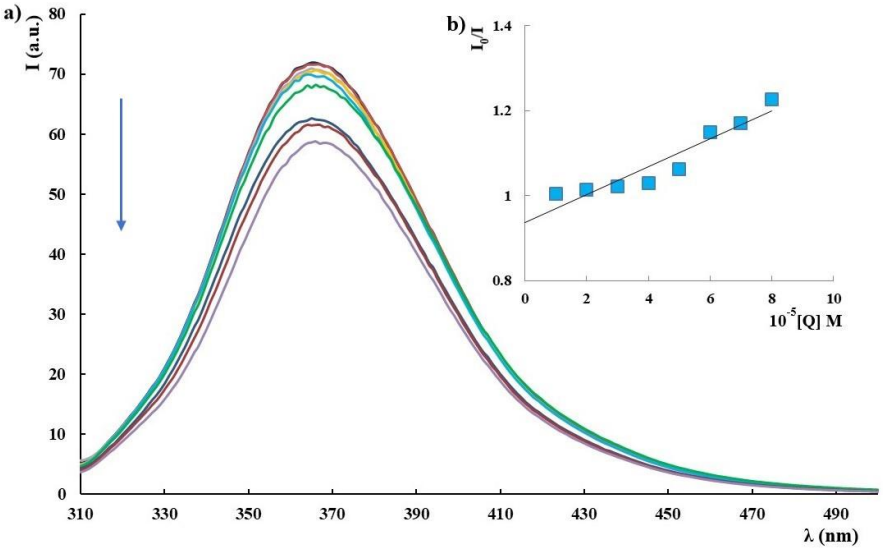
S10. a) Absorption spectra of the interaction of CT-DNA with **C2** in PBS after the addition of DNA. [complex] = 8 μM, [DNA] = 0-40 μM. The arrow shows hyperchromism in the spectral band. b) Insert graph: Plots of [DNA]/($\varepsilon_a - \varepsilon_f$)] vs. [DNA].



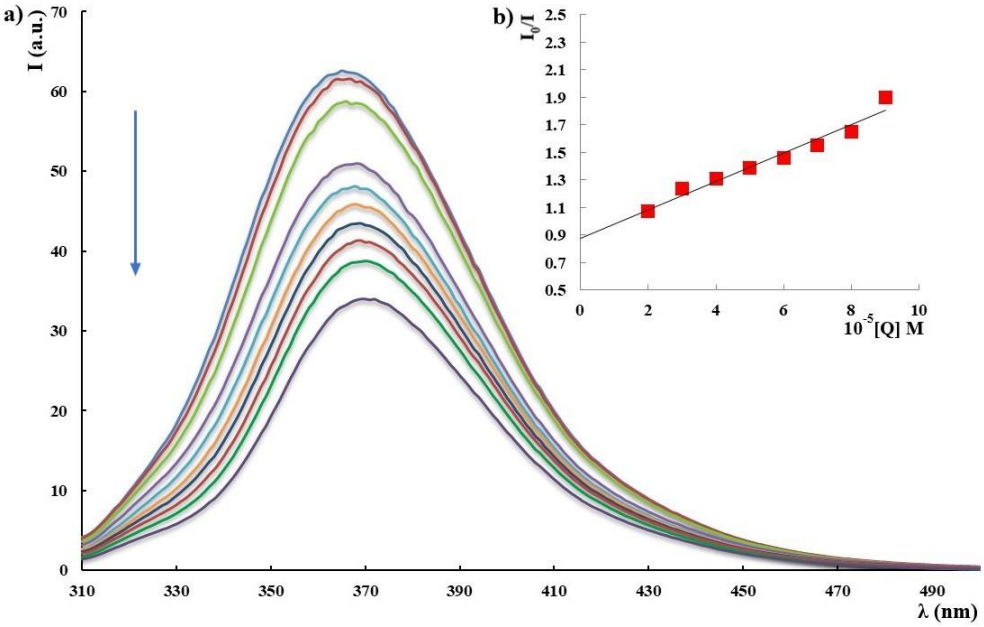
S11.a) EB-DNA emission spectra with increasing concentration of **C1**, [EB] = [DNA] = 10 μM, [complex]/[DNA] = 0-0.9; [Arrow shows changes in fluorescence intensity upon increasing concentration of **C1**]. b) Insert graph: Stern-Volmer plots for EB-DNA fluorescence titration with **C1**. Thedependence of I_0/I on the concentration [Q] (Q = complex) where the full line represents the linear dependence.



S12. a) EB-DNA emission spectra with increasing concentration of **C3**, [EB] = [DNA] = 10 μM, [complex]/[DNA] = 0-0.9; [Arrow shows changes in fluorescence intensity upon increasing concentration of **C3**]. b) Insert graph: Stern-Volmer plots for EB-DNA fluorescence titration with **C3**. Thedependence of I_0/I on the concentration [Q] (Q = complex) where the full line represents the linear dependence.



S13. a) Emission spectra of BSA, and BSA in the presence of different concentration of complex **C2**. The arrow shows that emission intensity changes upon increasing the concentration of the complex. b) Insert graph: The dependence of I_0/I on the concentration [Q] (Q = complex), where the full line represents a linear dependence.



S14. a) Emission spectra of BSA, and BSA in the presence of different concentration of complex **C3**. The arrow shows that emission intensity changes upon increasing the concentration of the complex. b) Insert graph: The dependence of I_0/I on the concentration [Q] (Q = complex), where the full line represents a linear dependence.

S15. The atomic coordinates and calculated vibrational frequencies for free ligand

C 1 6 0.293812 -1.019025 -0.930017
H 2 1 -0.476096 -1.510844 -1.531405
H 3 1 1.154263 -0.878882 -1.580322
C 4 6 0.689778 -1.979134 0.187771
O 5 8 0.372639 -1.898939 1.337626
O 6 8 1.416171 -2.993312 -0.329658
H 7 1 1.625639 -3.598805 0.398932
N 8 7 -0.176812 0.276461 -0.468708
C 9 6 -1.463825 0.501812 -0.084304
C 10 6 0.736061 1.402436 -0.593463
H 11 1 0.892033 1.654087 -1.649674
H 12 1 0.263302 2.269805 -0.134698
C 13 6 2.099100 1.197441 0.029956
O 14 8 2.553386 0.173275 0.463905
O 15 8 2.785393 2.357897 0.002487
H 16 1 3.661444 2.187112 0.383442
S 17 16 -2.081909 1.968714 0.381327
S 18 16 -2.506917 -0.940463 -0.144393
H 19 1 -3.611951 -0.242273 0.149187
[FREQ]

34.678800, 42.373500, 47.113500, 56.005100, 106.145200, 113.090800, 196.804200, 251.112600, 284.984200, 310.246600, 324.034100, 334.374700, 362.655000, 398.753900, 493.397000, 503.246600, 544.069400, 570.815200, 593.839800, 632.933300, 648.905500, 679.061400, 703.842800, 853.883800, 878.177600, 897.409500, 961.901500, 979.584100, 1011.274400, 1073.078500, 1142.287500, 1148.100600, 1211.213400, 1253.751400, 1306.873600, 1318.587700, 1322.890900, 1394.406700, 1413.396000, 1422.156000, 1458.889800, 1485.895800, 1820.822800, 1845.781000, 2697.035100, 3011.978000, 3044.159500, 3094.433200, 3126.445500, 3726.976500, 3729.339800

S16. The atomic coordinates and calculated vibrational frequencies for neutral palladium(II) complex

C 1 6 4.927659 -1.238947 0.058828
H 2 1 5.810717 -1.099626 0.684611
H 3 1 4.325638 -2.011345 0.535525
C 4 6 5.403041 -1.802650 -1.274470
O 5 8 5.969114 -2.856501 -1.364709
O 6 8 5.147870 -0.993853 -2.319941
H 7 1 5.475602 -1.440165 -3.117496
N 8 7 4.177595 0.002256 0.003512
C 9 6 2.834507 0.001660 -0.003807
C 10 6 4.927051 1.244316 -0.042059
H 11 1 5.816040 1.107174 -0.659787
H 12 1 4.328668 2.016991 -0.522990
C 13 6 5.388506 1.805977 1.296756
O 14 8 5.955131 2.859007 1.393849
O 15 8 5.120825 0.996869 2.338668
H 16 1 5.440136 1.442284 3.140045
S 17 16 1.886011 1.428084 -0.001193
S 18 16 1.886831 -1.425162 -0.016453
C 19 6 -4.928172 1.237989 0.058339
H 20 1 -5.810662 1.098588 0.684859
H 21 1 -4.326345 2.011194 0.534030
C 22 6 -5.404951 1.800250 -1.275086
O 23 8 -5.973781 2.852658 -1.365300
O 24 8 -5.147736 0.992149 -2.320467
H 25 1 -5.476555 1.437571 -3.118065
N 26 7 -4.177234 -0.002693 0.003555
C 27 6 -2.834142 -0.001113 -0.004579
C 28 6 -4.926033 -1.245089 -0.041041
H 29 1 -5.814725 -1.109332 -0.659495

H 30 1 -4.326915 -2.017987 -0.520725
C 31 6 -5.387867 -1.805390 1.298231
O 32 8 -5.956356 -2.857336 1.396136
O 33 8 -5.119294 -0.995702 2.339411
H 34 1 -5.439330 -1.439914 3.141251
S 35 16 -1.884449 -1.427425 -0.001216
S 36 16 -1.888454 1.427455 -0.017921
Pd 37 46 0.000705 0.000001 -0.017186
[FREQ]
9.576300, 15.913100, 18.717500, 24.832900, 26.925000, 27.819900, 36.850600, 44.249400, 45.870700, 46.824400, 47.382000, 62.908900, 69.327200, 80.216300, 97.014700, 105.214600, 143.030400, 148.490100, 180.417300, 185.083100, 201.495700, 235.724700, 266.055200, 308.689100, 333.001100, 334.763900, 342.317500, 342.413700, 351.864900, 361.153700, 361.199600, 365.764200, 372.876100, 424.014300, 431.583300, 504.612300, 504.888800, 504.975200, 505.309100, 560.299000, 560.849100, 574.372000, 574.776900, 588.180100, 588.959900, 647.892300, 648.488200, 668.582000, 668.900900, 673.948100, 674.152900, 696.343600, 696.512800, 837.536500, 837.897100, 850.498300, 850.534700, 951.053200, 951.882900, 961.022600, 961.460600, 1021.897200, 1024.166800, 1045.627800, 1046.814900, 1164.620300, 1166.528900, 1170.713100, 1171.436300, 1214.693600, 1215.188900, 1253.095400, 1258.259000, 1315.212900, 1315.600500, 1352.173900, 1352.250700, 1356.734800, 1356.880000, 1371.881700, 1371.961900, 1376.504100, 1377.113100, 1444.907500, 1446.135300, 1448.643400, 1448.969500, 1495.571600, 1500.577400, 1820.752100, 1821.111800, 1824.212700, 1825.788500, 3070.005800, 3070.086400, 3075.447100, 3075.602800, 3117.290100, 3117.420100, 3117.622500, 3117.776200, 3721.718200, 3721.758100, 3721.956600, 3722.725400

S17. The atomic coordinates and calculated vibrational frequencies for neutral zinc(II) complex
C 1 6 4.862962 -0.839799 0.909582
H 2 1 5.777631 -0.317080 1.193479
H 3 1 4.297831 -1.009098 1.823345
C 4 6 5.273774 -2.207303 0.378855
O 5 8 5.805683 -3.034258 1.066226
O 6 8 5.012278 -2.373914 -0.931310
H 7 1 5.302061 -3.268750 -1.171877
N 8 7 4.100483 -0.000027 0.000046
C 9 6 2.754042 -0.000065 0.000011
C 10 6 4.862972 0.839697 -0.909520
H 11 1 5.777642 0.316957 -1.193383
H 12 1 4.297853 1.008961 -1.823296
C 13 6 5.273780 2.207225 -0.378830

O 14 8 5.805518 3.034250 -1.066245
O 15 8 5.012508 2.373768 0.931398
H 16 1 5.302289 3.268609 1.171951
S 17 16 1.874611 1.065387 -1.032120
S 18 16 1.874543 -1.065453 1.032100
C 19 6 -4.863093 -0.839766 -0.909506
H 20 1 -5.777747 -0.316998 -1.193366
H 21 1 -4.298009 -1.009128 -1.823285
C 22 6 -5.273947 -2.207235 -0.378723
O 23 8 -5.805861 -3.034213 -1.066068
O 24 8 -5.012488 -2.373803 0.931451
H 25 1 -5.302297 -3.268622 1.172051
N 26 7 -4.100522 -0.000002 -0.000041
C 27 6 -2.754081 -0.000077 -0.000114
C 28 6 -4.862891 0.839770 0.909579
H 29 1 -5.777602 0.317106 1.193457
H 30 1 -4.297723 1.008963 1.823335
C 31 6 -5.273591 2.207343 0.378931
O 32 8 -5.805099 3.034460 1.066420
O 33 8 -5.012563 2.373800 -0.931350
H 34 1 -5.302274 3.268670 -1.171878
S 35 16 -1.874573 1.065430 1.031914
S 36 16 -1.874678 -1.065559 -1.032143
Zn 37 30 0.000093 0.000142 -0.000078
[FREQ]
14.580100, 17.317700, 18.012500, 25.371600, 27.796900, 31.898800, 35.780900, 47.797700,
49.562200, 49.908100, 52.100600, 60.947800, 66.560200, 75.729100, 78.802800, 107.681700,
109.898300, 126.846400, 176.673700, 179.243600, 180.209900, 193.742500, 261.246600,
306.059000, 307.529900, 340.694100, 340.964400, 348.377800, 355.877500, 362.823200,
363.200600, 386.049800, 392.631500, 438.544600, 443.076600, 504.335800, 504.476000,
504.808300, 504.952100, 572.773400, 573.182300, 576.213400, 576.422000, 586.544300,
587.265700, 637.367400, 637.675500, 670.807600, 671.216300, 680.560600, 680.779500,
694.752000, 694.982100, 837.350400, 837.640900, 851.793300, 851.802200, 951.188300,
951.482500, 961.542000, 961.998700, 1014.657000, 1015.079300, 1039.765600, 1040.357700,
1164.102200, 1165.157600, 1170.057800, 1170.510800, 1207.381000, 1207.423900,
1248.821400, 1251.798700, 1315.009000, 1315.320000, 1353.968600, 1354.053700,
1356.657900, 1356.740000, 1372.411700, 1372.521200, 1378.199100, 1378.679400,
1435.384400, 1435.885400, 1447.590000, 1448.004500, 1491.037900, 1493.551600,
1821.136500, 1821.298600, 1824.636300, 1825.805000, 3071.994400, 3072.005200,

3080.582100, 3080.678700, 3129.081700, 3129.138300, 3130.274800, 3130.282400, 3722.249400, 3722.272100, 3722.418800, 3722.557900

S18. The atomic coordinates and calculated vibrational frequencies for singly charged gold(III) complex

C 1 6 4.950867 -1.251575 0.019551
H 2 1 5.855405 -1.098548 0.608514
H 3 1 4.378991 -2.027467 0.525724
C 4 6 5.366929 -1.794519 -1.346647
O 5 8 5.820486 -2.891549 -1.479337
O 6 8 5.193007 -0.902008 -2.337416
H 7 1 5.498428 -1.307756 -3.166577
N 8 7 4.193910 0.000660 0.000249
C 9 6 2.875506 -0.000096 0.000117
C 10 6 4.949426 1.253765 -0.019004
H 11 1 5.854312 1.101689 -0.607700
H 12 1 4.376817 2.028952 -0.525414
C 13 6 5.364531 1.797328 1.347244
O 14 8 5.815994 2.895200 1.480108
O 15 8 5.192420 0.904290 2.337856
H 16 1 5.497173 1.310426 3.167073
S 17 16 1.906619 1.429535 0.013802
S 18 16 1.908286 -1.430827 -0.013681
C 19 6 -4.949393 1.253801 0.019378
H 20 1 -5.854339 1.101590 0.607930
H 21 1 -4.376797 2.028828 0.526047
C 22 6 -5.364283 1.797670 -1.346808
O 23 8 -5.815456 2.895676 -1.479530
O 24 8 -5.192389 0.904710 -2.337531
H 25 1 -5.497013 1.311037 -3.166700
N 26 7 -4.193917 0.000654 -0.000101
C 27 6 -2.875523 -0.000132 -0.000106
C 28 6 -4.950900 -1.251581 -0.019637
H 29 1 -5.855679 -1.098241 -0.608166
H 30 1 -4.379243 -2.027263 -0.526355
C 31 6 -5.366465 -1.795030 1.346519
O 32 8 -5.818824 -2.892544 1.479227
O 33 8 -5.193633 -0.902262 2.337264
H 34 1 -5.498734 -1.308251 3.166423
S 35 16 -1.908332 -1.430980 0.013427

S 36 16 -1.906668 1.429647 -0.013672
Au 37 79 -0.000187 -0.001672 -0.000109
[FREQ]
13.351300, 18.504400, 20.909400, 26.671500, 27.703100, 27.887500, 35.127300, 39.217100,
40.653500, 42.836800, 43.938500, 66.744600, 70.440100, 84.222200, 103.578900, 107.730600,
144.427100, 146.777600, 176.849500, 188.871000, 204.267100, 218.383300, 241.385900,
320.880500, 338.566200, 345.044300, 347.497700, 348.872300, 349.556400, 367.509900,
368.792000, 373.098800, 378.269900, 427.364300, 440.333100, 512.424700, 512.810800,
515.088200, 515.114100, 558.177600, 558.755400, 574.541200, 575.045600, 585.909400,
586.977400, 646.017100, 646.761500, 672.509000, 673.043200, 685.818000, 685.856700,
699.914500, 700.134200, 839.971200, 840.434600, 856.567200, 856.577700, 933.730000,
934.144000, 958.935100, 959.237900, 1002.514400, 1002.729900, 1039.560200, 1040.339400,
1163.800100, 1165.970300, 1168.653900, 1169.214600, 1189.771300, 1189.958500,
1268.599300, 1271.799200, 1301.781500, 1301.838400, 1344.546200, 1344.580700,
1354.003500, 1354.183900, 1365.347800, 1366.192600, 1367.695400, 1367.843300,
1460.609200, 1461.118500, 1464.591400, 1465.164300, 1551.256000, 1557.863900,
1842.963100, 1843.417100, 1845.832900, 1847.307700, 3084.820300, 3084.874300,
3087.916100, 3088.020000, 3129.681500, 3129.789000, 3130.798900, 3130.981500,
3706.678700, 3706.746700, 3706.909700, 3707.191900