Photochemical synthesis and catalytic applications of gold nanoplates fabricated using Quercetin Diphosphate macromolecules

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Supporting Information Content:

-Computed images of nine of the other conformers that could be taking place
-Determination of the $\Delta G$ and $\Delta H$ for each conformer
-The computed energy for each conformer
-TEM images of P, Q, R, S, T, U with calculated edge length

| Conformer 2 | $\Delta G=1.3\text{kcal/mol}$ |
|-------------|-----------------------------|
|             | $\Delta H=2\text{kcal/mol}$ |

| Conformer 3 | $\Delta G=0.17\text{kcal/mol}$ |
|-------------|--------------------------------|
|             | $\Delta H=0.012\text{Kcal/mol}$ |

| Conformer 4 | $\Delta G=0.223\text{kcal/mol}$ |
|-------------|---------------------------------|
|             | $\Delta H=0.03\text{Kcal}$     |
Conformer 5 $\Delta G=0.47$ kcal/mol  
$\Delta H=0.43$ kcal/mol

Conformer 6 $\Delta G=0.225$ kcal/mol  
$\Delta H=0.24$ kcal/mol

Conformer 7 $\Delta G=0.280$ kcal/mol  
$\Delta H=0.024$ kcal/mol

Conformer 8 $\Delta G=0.65$ kcal/mol  
$\Delta H=0.076$ kcal/mol

Conformer 9 $\Delta G=0.23$ kcal/mol  
$\Delta H=0.031$ kcal/mol
### COMPUTED STRUCTURES AND ENERGIES

**Conformer 1 (A)**

Energy = -2239.411349

| Element | x        | y        | z        |
|---------|----------|----------|----------|
| C       | 4.52049200 | 1.94587300 | 0.40627600 |
| C       | 4.08030000 | 0.64072600 | 0.47012000 |
| C       | 2.70984800 | 0.30512200 | 0.27683900 |
| C       | 1.82560300 | 1.39127600 | 0.06548400 |
| C       | 2.24981400 | 2.71552800 | -0.00736800 |
| C       | 3.60396300 | 2.98864400 | 0.15243900 |
| H       | 5.57015900 | 2.16092000 | 0.57696500 |
| C       | 2.14801400 | -1.02400100 | 0.27995300 |
| H       | 1.53519300 | 3.51171900 | -0.17712200 |
| C       | -0.09569900 | -0.03882000 | -0.00835600 |
| C       | 0.70343600 | -1.13181700 | 0.17858500 |
| C       | -1.55048100 | 0.02778400 | -0.18341000 |
| C       | -2.16317000 | 1.26056000 | -0.48897900 |
| C       | -2.35620200 | -1.11532900 | -0.04427800 |
| C       | -3.53863000 | 1.32564500 | -0.66725500 |
| H       | -1.56763400 | 2.15778100 | -0.59552200 |
| C       | -3.74227500 | -1.05828200 | -0.21745500 |
| H       | -1.92542300 | -2.07524200 | 0.20323300 |
| C       | -4.32224900 | 0.18220400 | -0.54235100 |
| H       | -4.02283400 | 2.26215800 | -0.92375800 |
| O       | 0.22424300 | -2.39635100 | 0.22573500 |
| H       | 1.03262300 | -2.95403600 | 0.30518700 |
| O       | 2.78182300 | -2.11681400 | 0.35377200 |
| O       | 4.98713900 | -0.32632100 | 0.85990700 |
| O       | 3.99278600 | 4.28000800 | 0.07662100 |
| H       | 4.95252000 | 4.35190400 | 0.21361900 |
| O       | -4.43980600 | -2.21649600 | -0.09886600 |
| H       | -5.36894800 | -2.03139600 | 0.17674000 |
| O       | -5.68292900 | 0.29320600 | -0.86933200 |
| P       | 5.97461600 | -1.18433700 | -0.12580000 |
| P       | -6.87341400 | 0.04765500 | 0.18670400 |
| O       | 6.53458500 | -0.15145900 | -1.22450300 |
| H       | 7.41993900 | 0.17592000 | -0.98732900 |
| O       | 4.98646600 | -2.05154900 | -1.00630600 |
| H       | 4.12382400 | -2.20669100 | -0.49211000 |
| O       | 7.00107100 | -1.86184800 | 0.69730600 |
| O       | -6.84842900 | -1.29757900 | 0.82915700 |
| O       | -8.16484000 | 0.38733600 | -0.68842800 |
| H       | -8.52120000 | -0.39164500 | -1.15250800 |
| O       | -6.74180300 | 1.31017200 | 1.15622900 |
| H       | -7.16003800 | 1.16667700 | 2.02464400 |
Conformer 2(B)
Energy= -2239.40921

C                   4.43534000  1.91148500  0.51997500
C                   4.03685300  0.59143300  0.51799800
C                   2.67856200  0.22254000  0.30211700
C                   1.76135100  1.28928200  0.13793500
C                   2.14345500  2.62820300  0.13001100
C                   3.48763100  2.93582100  0.31012300
H                   5.47650000  2.15035100  0.70839800
C                   2.15927100 -1.12243300  0.23828500
H                   1.40467900  3.40863200 -0.00621200
C                 -0.11338400 -0.19090300 -0.01223600
C                   0.71931200 -1.27102400  0.12624500
C                 -1.56894200 -0.16967700 -0.18929200
C                 -2.35010100 -1.33491500 -0.05327000
C                 -2.20214100  1.04904800 -0.50072400
C                 -3.73101600 -1.27721700 -0.22779900
H                 -1.88559600 -2.28054400  0.18559000
C                 -3.58129600  1.10806100 -0.67184400
H                 -1.63155000  1.96205600 -0.61451200
C                 -4.33944300 -0.06407200 -0.52629600
H                 -4.34015500 -2.16809700 -0.12717400
O                   0.27983600 -2.55082200  0.10868800
H                   1.10520600 -3.08609100  0.16306200
O                   2.82764300 -2.19687900  0.26083100
O                   0.43474900  1.06061000 -0.01758800
O                   4.97354800 -0.36455200  0.86236100
O                   3.83603900  4.24084700  0.29711800
H                   4.79320900  4.33568100  0.43815100
O                 -4.16347300  2.29710100 -0.97793700
H                 -5.11972800  2.14757800 -1.08642000
O                 -5.70903900  0.06968400 -0.77526300
P                   5.99232500 -1.13449100 -0.16387700
P                 -6.83914700 -0.41680800  0.28959300
O                   6.50105200 -0.03074800 -1.21781900
H                   7.36544900  0.33582600  0.96130200
O                   5.03745000 -2.00399100 -0.10793500
H                   4.17705800 -2.20453900 -0.58243500
O                   7.05162700 -1.80313600  0.62409400
O                 -6.80052100 -1.84166600  0.68740500
O                 -8.16397900  0.08241700 -0.46037200
H                 -8.58172000 -0.62779100 -0.97926500
O                 -6.63926300  0.67621100  1.44493700
H                 -6.99907500  0.38200900  2.30084300

Conformer 3(C)
Energy= -2239.411082
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 4.3883400 | 1.99818700 | -0.26903900 |
| C    | 4.05432400 | 0.66480700 | -0.37507300 |
| C    | 2.69859600 | 0.23096400 | -0.33570400 |
| C    | 1.71971300 | 1.24975800 | -0.23800500 |
| C    | 2.03596000 | 2.60092200 | -0.12243400 |
| C    | 3.37644100 | 2.97098800 | -0.12498100 |
| H    | 5.43235000 | 2.28926700 | -0.32266600 |
| C    | 2.23893100 | -1.13556700 | -0.38666800 |
| H    | 1.25108200 | 3.34308400 | -0.04135900 |
| C    | -0.08861900 | -0.31115100 | -0.39013800 |
| C    | 0.80453600 | -1.34875900 | -0.46323700 |
| C    | -1.55430600 | -0.35678000 | -0.41963500 |
| C    | -2.25817000 | -1.56297000 | -0.61400500 |
| C    | -2.81841000 | 0.83421000 | -0.24893500 |
| C    | -3.64779300 | -1.55015000 | -0.64973900 |
| H    | -1.72908400 | -2.49521000 | -0.74490000 |
| C    | -3.67617000 | 0.85598900 | -0.27891400 |
| H    | -1.77414100 | 1.77674800 | -0.08753700 |
| C    | -4.35297200 | -0.36132000 | -0.49287500 |
| H    | -4.20547500 | -2.46527400 | -0.81902300 |
| O    | 0.42886100 | -2.64521100 | -0.55876600 |
| H    | 1.27975400 | -3.14125900 | -0.53150600 |
| O    | 2.95511500 | -2.17876800 | -0.36624900 |
| O    | 0.39630600 | 0.95949300 | -0.25811000 |
| O    | 5.06546800 | -0.23390000 | -0.65739100 |
| O    | 3.66053600 | 4.28646800 | -0.00901400 |
| H    | 4.62231100 | 4.42648200 | -0.02810000 |
| O    | -4.29578400 | 2.05614300 | -0.14071600 |
| H    | -5.19849900 | 1.93564800 | 0.23911200 |
| O    | -5.74391500 | -0.40563200 | -0.67608600 |
| P    | 5.99697900 | -1.01796400 | 0.43815500 |
| P    | -6.80601200 | -0.05268100 | 0.48115800 |
| O    | 4.97550600 | -1.92306600 | 1.23946400 |
| H    | 4.18929000 | -2.15397600 | 0.64499500 |
| O    | 6.38884300 | 0.06236900 | 1.56380200 |
| H    | 7.26985200 | 0.44311200 | 1.40165700 |
| O    | 7.13419800 | -1.64928600 | -0.26761600 |
| O    | -6.63320800 | 1.30522400 | 1.07204900 |
| O    | -6.65652300 | -1.29626200 | 1.47227800 |
| H    | -7.01633300 | -1.11907000 | 2.36279600 |
| O    | -8.19682600 | -0.32804400 | -0.25337300 |
| H    | -8.55604200 | 0.46602300 | -0.68882700 |

**Conformer 4 (D)**

**Energy= -2239.410993**

| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | 4.33714700 | 2.01311200 | 0.43738600 |
| C    | 4.01489800 | 0.67333200 | 0.48490800 |
| C    | 2.67769700 | 0.22097000 | 0.29791300 |
Conformer 5 (E)  
Energy= -2239.410606

C  -4.59758600  1.88762600 -0.29292200  
C  -4.12772000  0.59452800 -0.38433500  
C  -2.73464500  0.30219600 -0.34465800  
C  -1.86572500  1.41722900 -0.25670800  
C  -2.31925000  2.72994500 -0.15644600  
C  -3.69055100  2.96093300  0.16221200  

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|   |         |         |         |
|---|---------|---------|---------|
| H | -5.66590600 | 2.06818200 | -0.34634200 |
| C | -2.13688600 | -1.01062900 | -0.38798400 |
| H | -1.61468800 | 3.54950900 | -0.08310800 |
| C | 0.09269100 | 0.04884100 | -0.38798400 |
| C | -0.68821600 | -1.07511000 | -0.46306100 |
| C | 1.55542000 | 0.15377700 | -0.38324700 |
| C | 2.16356100 | 1.39204500 | -0.09250400 |
| C | 2.37148800 | -0.95694000 | -0.65642400 |
| C | 3.54786200 | 1.49906700 | -0.08674600 |
| H | 1.55890200 | 2.26266000 | 0.12552300 |
| C | 3.76631000 | -0.85956800 | -0.65084200 |
| H | 1.94170100 | -1.92281200 | -0.88183300 |
| C | 4.34454400 | 0.39189300 | -0.36580300 |
| H | 4.03114700 | 2.44835900 | 0.12044700 |
| O | -0.17804400 | -2.32589200 | -0.54475800 |
| H | -0.97135300 | -2.90903500 | -0.50948400 |
| O | -2.74170500 | -2.12171200 | -0.35754300 |
| O | -0.51940300 | 1.26482600 | -0.27116700 |
| O | -5.04323800 | -0.40664700 | -0.64835000 |
| O | -4.10746800 | 4.24179100 | -0.06073200 |
| H | -5.07860700 | 4.28583000 | -0.07493900 |
| O | 4.47624800 | -1.97265300 | -0.96369200 |
| H | 5.36615200 | -1.94200900 | -0.53701200 |
| O | 5.72908100 | 0.60517000 | -0.46298300 |
| P | -5.80053100 | -1.26496000 | 0.46801700 |
| P | 6.81339500 | -0.09362000 | 0.51338200 |
| O | -6.35856600 | -0.21482300 | 1.58898200 |
| H | -7.27493000 | 0.07636400 | 1.43761200 |
| O | -4.76602200 | -2.05960800 | 1.26217800 |
| H | -3.96610600 | -2.21497500 | 0.66149400 |
| O | -6.96150700 | -2.01067100 | -0.21414100 |
| O | 8.17221100 | 0.57426700 | 0.00828900 |
| H | 8.48245700 | 0.23361300 | -0.85016100 |
| O | 6.72838900 | -1.57895500 | 0.51958300 |
| O | 6.62584700 | 0.51753300 | 1.97334100 |
| H | 6.66391100 | 1.49026600 | 2.01634100 |

Conformer 6 (F)

Energy= -2239.41099

|   |         |         |         |
|---|---------|---------|---------|
| C | 4.51536200 | 1.94599600 | 0.41565400 |
| C | 4.07674700 | 0.64002600 | 0.47336800 |
| C | 2.70666100 | 0.30368000 | 0.27872600 |
| C | 1.82123000 | 1.38973100 | 0.07172600 |
| C | 2.24387500 | 2.71495500 | 0.00498700 |
| C | 3.59760400 | 2.98883700 | 0.16666600 |
| H | 5.56470700 | 2.16075300 | 0.58757500 |
| C | 2.14633200 | -1.02613700 | 0.27677000 |
| H | 1.52833200 | 3.51087800 | -0.16134900 |
| C    | -0.09822100 | -0.03726700 | -0.00836400 |
| C    | 0.70179800  | -1.13504600 | 0.17505300  |
| C    | -1.55276900 | 0.02283700  | -0.18601300 |
| C    | -2.16402600 | 1.25157400  | -0.51017000 |
| C    | -2.35884000 | -1.11795100 | -0.03166500 |
| C    | -3.53923600 | 1.31488000  | -0.69125200 |
| H    | -1.56762800 | 2.14667400  | -0.62890000 |
| C    | -3.74473400 | -1.06272900 | -0.20740300 |
| H    | -1.92847900 | -2.07437200 | 0.22982700  |
| C    | -4.32290700 | 0.17363700  | -0.55055700 |
| H    | -4.02268900 | 2.24782600  | -0.96175200 |
| O    | 0.22354300  | -2.40010600 | 0.21650200  |
| H    | 1.03226500  | -2.95762800 | 0.29323600  |
| O    | 2.78127800  | -2.11851800 | 0.34595600  |
| O    | 0.48767700  | 1.19563000  | -0.06877800 |
| O    | 4.98482200  | -0.32780300 | 0.85827000  |
| O    | 3.98480400  | 4.28105200  | 0.09737100  |
| H    | 4.94435200  | 4.35350100  | 0.23535200  |
| O    | -4.44183700 | -2.21912600 | -0.07200200 |
| H    | -5.37856800 | -2.03498600 | 0.17611300  |
| O    | -5.68432500 | 0.27612600  | -0.87829200 |
| P    | 5.97351000  | -1.17935100 | -0.13194700 |
| P    | -6.87051200 | 0.03740300  | 0.18394500  |
| O    | 6.52745500  | -0.14107700 | -1.22861900 |
| H    | 7.41222400  | 0.18860300  | -0.99244700 |
| O    | 4.98657600  | -2.04767500 | -1.01265400 |
| H    | 4.12394800  | -2.20426300 | -0.50590300 |
| O    | 7.00419400  | -1.85562700 | 0.68687800  |
| O    | -6.68309500 | 1.27955900  | 1.18105400  |
| H    | -7.08250800 | 1.12530000  | 2.05688800  |
| O    | -6.88638000 | -1.31282500 | 0.80821900  |
| O    | -8.17069700 | 0.29754700  | -0.70103800 |
| H    | -8.25631900 | 1.20848100  | -1.03633700 |

**Conformer 7 (G)**

**Energy=-2239.410903**

| C    | 4.33716700  | 2.01316100  | 0.43722900  |
| C    | 4.01484400  | 0.67340000  | 0.48495800  |
| C    | 2.67765600  | 0.22104000  | 0.29777900  |
| C    | 1.69851600  | 1.22752900  | 0.11254400  |
| C    | 2.00341700  | 2.58495500  | 0.05406200  |
| C    | 3.33012200  | 2.97394400  | 0.20360500  |
| H    | 5.36485200  | 2.31762700  | 0.60407600  |
| C    | 2.23649500  | -1.15251800 | 0.28068700  |
| H    | 1.21993100  | 3.31711300  | -0.09923900 |
C  -0.08977900  -0.36182700   0.03210200
C   0.80599700  -1.38740700   0.19217000
C  -1.54650200  -0.42981300  -0.12414200
C  -2.24944300  -1.65323100  -0.06807100
C  -2.27168300   0.75738600  -0.32871700
C  -3.62484900  -1.66621800  -0.23647800
H  -1.71841500  -2.58158300   0.09747000
C  -3.65826200   0.75463200  -0.49200500
H  -1.76907600   1.71554000   0.36588400
C  -4.32585500  -0.48488000  -0.45480800
H  -4.17620900  -2.60054400  -0.21631100
O   0.44323100   2.69065900   0.22515400
H   1.30074000   3.17337900   0.28674700
O   2.96632100  -2.18533400   0.32745600
O   0.38577400   0.91815700  -0.01777700
O   5.00756700   0.21588200   0.85057000
O   6.03985000   4.29508000   0.13811200
H   4.55701700   4.47863000   0.25387100
O  -4.27389300   1.94281000  -0.71879600
H  -5.20608800   1.91079400  -0.39692800
O  -5.69374200  -0.58781200  -0.75182700
P   6.05643000  -0.96199800   0.63673600
P  -6.85136800   0.02482500   0.18543500
O   6.51309000   0.13992000  -1.24215900
H   7.35819200   0.55401300  -0.99396600
O   5.13928500  -1.89079900  -1.05701900
H   7.14543000  -1.56624800   1.45794700
O  -8.17334700  -0.43289000  -0.58400000
H  -8.46167300   0.21273200  -1.25423500
O  -6.71170900   1.48610300   0.44642600
O  -6.81514300  -0.93962700   0.18543500
H  -7.19767600  -0.53007100   2.25497300

Conformer 8 (H)

Energy= -2239.410319

C  -4.59562500   1.88639500  -0.29076000
C  -4.12510500   0.59370500  -0.38392000
C  -2.73193800   0.30191700  -0.34342300
C  -1.86355800   1.41717900  -0.25314100
C  -2.31774800   2.72953000  -0.15098000
C  -3.68913900   2.95990100  -0.15737800
H  -5.66395700   2.06677700  -0.34491100
C  -2.13360800  -1.01054900  -0.38779500
H  -1.61361600   3.54929600  -0.07577400
C   0.09556100   0.04987500  -0.38547500
C  -0.68487200  -1.07434700  -0.46183100
C   1.55825900   0.15579400  -0.38191300

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C                  2.16567500    1.39552200   -0.09540000
C                  2.37473300   -0.95522000   -0.65282100
C                  3.54985500    1.50445200   -0.09263600
H                  1.56033100    2.26585900    0.12180300
C                  3.76931500   -0.85566900   -0.64981600
H                  1.94550800   -1.92224400   -0.87426600
C                  4.34628700    0.39753200   -0.37151100
H                  4.03315700    2.45402300    0.11241300
O                 -0.17426000   -2.32489200   -0.54478900
H                 -0.96750900   -2.90823800   -0.51120700
O                 -2.73792200   -2.12200100   -0.35927000
O                 -5.03967400   -0.40764200   -0.65061600
O                 -4.10675100    4.24035400   -0.05403400
H                 -5.07789200    4.28068100   -0.06870200
O                 -6.35628400   -0.21933800    1.58615200
H                 -7.27218600    0.07336800    1.43507200
O                 -4.76550500   -2.06527900    1.25602400
O                 -3.96419000   -2.21775100    0.65625600
O                 -6.96019700   -2.01045400   -0.22117400
O                 -8.17051200    0.59230000   -0.66794600
O                 -6.76689000   -1.56943500    0.50241600
H                 -6.50808700    0.64503100    1.89953000
C                 -5.37517200   -1.93351900   -0.54460700
O                 -5.73048800    0.60834100   -0.47574000
P                 -5.87875600   -1.26746300    0.46324600
P                 -6.80512900   -0.07897000    0.50703100
O                 -6.35628400   -0.21933800    1.58615200
H                 -7.27218600    0.07336800    1.43507200
O                 -4.76550500   -2.06527900    1.25602400
H                 -3.96419000   -2.21775100    0.65625600
O                 -6.96019700   -2.01045400   -0.22117400
O                 -8.17051200    0.59230000   -0.66794600
O                 -6.76689000   -1.56943500    0.50241600
O                 -6.50808700    0.64503100    1.89953000
H                 -6.83388700    0.14003000    2.66644400

Conformer 9 (I)

Energy= -2239.410983

C                  4.33717200    2.01312500    0.43736400
C                  4.01490000    0.67335200    0.48491200
C                  2.67769300    0.22100900    0.29790600
C                  1.69849200    1.22749400    0.11294300
C                  2.00334000    2.58493100    0.05461200
C                  3.33006400    2.97393100    0.20401700
H                  5.36486700    2.31763000    0.60407200
C                  2.23603000   -1.15252200    0.28074100
H                  1.21981900    3.31710400   -0.09844000
C                  0.08972700   -0.36194500    0.03270900
C                  0.80615100   -1.38750900    0.19242200
C                 -1.54646100   -0.43004600   -0.12342000
C                 -2.24489400   -1.65342100   -0.06628300
C                 -2.27162800    0.75697800   -0.32896300
Figure S1: Computed optimized QDP structures (B-I) and energies for conformers 1 to 9(A-I).
Conformer A $\Delta G=2.1\text{kcal/mol}$

Conformer B $\Delta G=3.01\text{kcal/mol}$

Conformer C $\Delta G=3.21\text{kcal/mol}$

Conformer D $\Delta G=6\text{kcal/mol}$
COMPUTED STRUCTURES AND ENERGIES

Conformer 1(A)

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| C | 7.23505900| 1.62493800| -0.16708000|
| C | 6.65066300| 0.42228500| 0.17467800 |
| C | 5.23632700| 0.24535500| 0.15866400|
| C | 4.47372900| 1.38402600| -0.20517600|
| C | 5.04289200| 2.60312100| -0.56849300|
| C | 6.42800200| 2.71671700| -0.55286900|
| H | 8.31452100| 1.72330000| -0.11662600|
| C | 4.51563500| -0.95847700| 0.50160800 |
| H | 4.41374300| 3.44145700| -0.84194200|
| C | 2.39693900| 0.25852700| 0.15936800 |
| C | 3.06877900| -0.88214600| 0.51920700 |
| C | 0.94921500| 0.48462300| 0.08317300 |
| C | 0.45590300| 1.60812200| -0.61360000|

Conformer E $\Delta G=3.1$ Kcal/mol

Conformer F $\Delta G=0.5$ Kcal/mol

Conformer G $\Delta G=4.3$ Kcal/mol

$\Delta G=2.9$ Kcal/mol
| At  | X     | Y     | Z     |
|-----|-------|-------|-------|
| C   | 0.03944300 | -0.38357500 | 0.71156700 |
| C   | -0.91414000 | 1.83119600 | -0.68700400 |
| H   | 1.13618000 | 2.29389800 | -1.10204000 |
| C   | -1.33933200 | -0.15787400 | 0.65243100 |
| H   | 0.38175400 | -1.24558300 | 1.26744500 |
| C   | -1.80575100 | 0.95746300 | -0.06754600 |
| H   | -1.31139000 | 2.67709300 | -1.23794000 |
| O   | 2.42674800 | -2.02392300 | 0.86685600 |
| H   | 3.13610900 | -2.68154900 | 1.02122100 |
| O   | 5.01118500 | -2.09061000 | 0.78911800 |
| O   | 3.11827400 | 1.35447800 | -0.20906400 |
| O   | 7.47999700 | -0.57518900 | 0.64721100 |
| O   | 6.96043100 | 3.91173100 | -0.90162900 |
| H   | 7.92718300 | 3.89465600 | -0.84336800 |
| O   | -2.15589800 | -1.05529900 | 1.26759500 |
| H   | -2.99691900 | -0.62761600 | 1.55059900 |
| O   | -3.17463300 | 1.17389300 | -0.27804100 |
| P   | 8.21648600 | -1.77210800 | -0.20023500 |
| P   | -4.21950500 | 1.54743200 | 0.89656400 |
| O   | 8.12025500 | -1.32678000 | -1.74642500 |
| H   | 8.90787600 | -0.85540300 | -2.06136700 |
| O   | 7.01233300 | -2.97187800 | -0.09473100 |
| H   | 6.29764200 | -2.65818400 | 0.27752200 |
| O   | 9.59209900 | -2.01094900 | 0.30592400 |
| O   | -4.25980000 | 0.53143000 | 1.99431900 |
| O   | -5.56281300 | 1.79144300 | 0.08381400 |
| H   | -6.07723600 | 0.97400500 | -0.12002700 |
| O   | -3.78422200 | 3.02437800 | 1.32465700 |
| H   | -3.90842600 | 3.21431500 | 2.26851900 |
| Au  | -7.45011100 | -0.95157800 | -0.55059900 |

Conformer 1(B)

| At  | X     | Y     | Z     |
|-----|-------|-------|-------|
| C   | 3.19376300 | -1.84719300 | -1.89541700 |
| C   | 2.75880500 | -0.54228400 | -1.78159700 |
| C   | 1.43269000 | -0.23134300 | -1.36655800 |
| C   | 0.58158800 | -1.33570300 | -1.11737200 |
| C   | 1.00285200 | -2.66088700 | -1.22084000 |
| C   | 2.31678600 | -2.90918000 | -1.59727400 |
| H   | 4.21471700 | -2.03321200 | -2.21289700 |
| C   | 0.88359300 | 1.09380600 | -1.18123800 |
| H   | 0.32095700 | -3.47421600 | -1.00555500 |
| C   | -1.29507200 | 0.06625100 | -0.62065600 |
| C   | -0.52377100 | 1.18124200 | -0.83095600 |
| C   | -2.71039200 | -0.01934400 | -0.24264400 |
Conformer 1(C)

C   -2.69795500  -0.99603500  1.16340500
C   -2.11141000  0.23791400  0.97980800
C   -0.73475900  0.36706900  0.63998800
C    0.00602500  -0.83853200  0.56688300
C   -0.57007900  -2.09732700  0.73554900
C   -1.93191900  -2.16939200  1.00755900
H   -3.75459300  -1.04778000  1.40914300
C   -0.03854400  1.60123000  0.35733300
H    0.02895400  -2.99493800  0.64337100
C    2.05760600  0.31298300  0.11612500
|   | x      | y      | z       |
|---|--------|--------|---------|
| C | 1.3943500 | 1.51436600 | 0.13747500 |
| C | 3.48219000 | 0.05134700 | -0.11895700 |
| C | 3.93793100 | -1.28109800 | -0.22663100 |
| C | 4.41190500 | 1.09971100 | -0.22840300 |
| C | 5.28365200 | -1.53599300 | -0.45646400 |
| H | 3.24418600 | -2.10692900 | -0.14079000 |
| C | 5.77185000 | 0.85173500 | -0.45136900 |
| H | 4.10662100 | 2.13310700 | -0.14517100 |
| C | 6.19076600 | -0.48536800 | -0.57667600 |
| H | 5.64973500 | -2.55153900 | -0.56470700 |
| O | 2.01337500 | 2.69668200 | -0.08448900 |
| H | 1.29603200 | 3.36406400 | -0.06219900 |
| O | -0.54173600 | 2.75860600 | 0.26931000 |
| O | 1.33914100 | -0.83327400 | 0.31489500 |
| O | -2.86942100 | 1.36299600 | 1.22433500 |
| O | -2.48439000 | -3.39897200 | 1.13875200 |
| H | -3.44822200 | -3.33212300 | 1.20626500 |
| O | 6.59019000 | 1.92431600 | -0.57712700 |
| H | 7.50756900 | 1.71387100 | -0.29776000 |
| O | 7.50840500 | -0.81695600 | -0.93781100 |
| P | -3.84816100 | 2.07702900 | 0.10985300 |
| P | 8.79646700 | -0.52885400 | -0.02110700 |
| O | -4.98317300 | 2.74321600 | 1.02366600 |
| H | -4.69589900 | 3.55822100 | 1.46099800 |
| O | -4.40518000 | 1.12337800 | -0.88506200 |
| O | -2.96088100 | 3.28035300 | -0.40172000 |
| O | 8.96771200 | 0.89457000 | 0.37164200 |
| O | 9.97053500 | -1.17224600 | -0.89623800 |
| H | 10.31235400 | -0.57388900 | -1.57718500 |
| O | 8.66015600 | -1.56882800 | 1.18936600 |
| H | 8.98522300 | -1.20736600 | 2.02743500 |
| Au | -5.85595100 | -0.95063200 | -0.51872900 |
| H | -1.98442900 | 3.13713700 | -0.16131300 |

Conformer 1(D)

|   | x      | y      | z       |
|---|--------|--------|---------|
| C | 5.22772000 | 2.25672100 | -0.55078400 |
| C | 4.70276400 | 1.24704100 | 0.23162700 |
| C | 3.30133800 | 0.99241500 | 0.27160700 |
| C | 2.48274700 | 1.85765100 | -0.49585600 |
| C | 2.99463000 | 2.87875200 | -1.29399900 |
| C | 4.37256200 | 3.06306700 | -1.32716800 |
| H | 6.30201800 | 2.41062100 | -0.55441300 |
| C | 2.65064600 | -0.05819100 | 1.02293900 |
| H | 2.33366400 | 3.50937200 | -1.87565200 |
| C | 0.46453600 | 0.79844600 | 0.23681200 |

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| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 1.195169   | -0.081796  | 0.990871   |
| C       | -0.989522  | 0.888835   | 0.084105   |
| C       | -1.550235  | 1.889271   | -0.731478  |
| C       | -1.860535  | -0.005754  | 0.753277   |
| C       | -2.931504  | 2.011262   | -0.85198   |
| H       | -0.907106  | 2.579842   | -1.260759  |
| C       | -3.246313  | 0.133961   | 0.631014   |
| H       | -1.458991  | -0.73776   | 1.443069   |
| C       | -3.786539  | 1.146408   | -0.173179  |
| H       | -3.369947  | 2.784853   | -1.473185  |
| O       | 0.628223   | -1.059454  | 1.736523   |
| H       | 1.389625   | -1.547267  | 2.119227   |
| O       | 3.19628    | -0.967103  | 1.706314   |
| O       | 1.129709   | 1.738895   | -0.499238  |
| O       | 5.552166   | 0.545799   | 1.048806   |
| O       | 4.848666   | 4.055401   | -2.119844  |
| H       | 5.815317   | 4.073352   | -2.101398  |
| O       | -4.121933  | -0.692986  | 1.291915   |
| H       | -3.635686  | -1.387042  | 1.758125   |
| O       | -5.148394  | 1.259681   | -0.363264  |
| P       | 6.359861   | -0.824482  | 0.579119   |
| P       | -6.200478  | 1.643114   | 0.846392   |
| O       | 6.481027   | -0.943583  | -0.886248  |
| O       | 5.603586   | -1.936775  | 1.426980   |
| O       | 7.769833   | -0.673383  | 1.333645   |
| O       | -6.841350  | 0.217751   | 1.238788   |
| O       | -7.407831  | 2.314798   | 0.040041   |
| H       | -7.91887   | 1.688757   | -0.494088  |
| O       | -5.608372  | 2.478259   | 1.906201   |
| Au      | -1.696176  | -2.373387  | -1.011954  |
| H       | 4.654743   | -1.652425  | 1.589210   |
| H       | -6.135632  | -0.414920  | 1.465006   |
| H       | 7.720429   | -0.896254  | 2.274810   |

Conformer 1 (E)

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| C       | 5.780006   | 2.386282   | 0.383999   |
| C       | 5.712985   | 1.011060   | 0.476833   |
| C       | 4.491087   | 0.306890   | 0.267012   |
| C       | 3.352360   | 1.106899   | -0.003430  |
| C       | 3.400219   | 2.494969   | -0.115574  |
| C       | 4.622444   | 3.130302   | 0.070107   |
| H       | 6.724148   | 2.885087   | 0.575017   |
| C       | 4.300770   | -1.122528  | 0.324226   |
| H       | 2.501007   | 3.058936   | -0.331777  |
| C       | 1.887567   | -0.783880  | -0.057495  |
| C       | 2.946902   | -1.620064  | 0.194723   |
| C       | 0.476809   | -1.126726  | -0.268758  |
| C       | -0.402759  | -0.136079  | -0.747875  |
Conformer 1(F)

O1 6.93178500 1.48436400 -0.49796600
C 6.69928200 0.25830000 -0.44582900
C 4.87982600 0.15385200 -0.36191000
C 4.16458700 1.37774200 -0.37964300
C 4.78324600 2.62577900 -0.41807100
C 6.17159800 2.67318400 -0.46609700
H 8.01253900 1.51946000 -0.58474700
C 4.10996200 -1.06429000 -0.28296600
H 4.10980500 3.53196700 -0.42092200
C 2.04147100 0.27618300 -0.36344000
C 2.66826700 -0.94501200 -0.33220900
C 0.60467700 0.57242100 -0.36478200
C -0.35252300 -0.44112900 -0.56738100
C 0.16959100 1.90058600 -0.16938800
C -1.71190000 -0.13505000 -0.56649500
H -0.05821000 -1.46870000 -0.72802800
C -1.18892800 2.20697000 -0.17039500
H 0.88918300 2.69448000 -0.01743700
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -2.12148500  | 1.18997100   | -0.35965800  |
| O       | 1.98438400   | -2.11445700  | -0.28834700  |
| H       | 2.66915900   | -2.81062900  | -0.21022000  |
| O       | 4.56567900   | -2.24396500  | -0.16280000  |
| O       | 2.80925500   | 1.40220300   | -0.36818800  |
| O       | 7.08298900   | -0.86827900  | -0.60693400  |
| H       | 6.75361200   | 3.89511800   | -0.53950400  |
| O       | 7.71892100   | 3.82247400   | -0.53950400  |
| O       | -3.49756000  | 1.40768100   | -0.42364600  |
| P       | 7.82149800   | -1.75980400  | 0.55576500   |
| O       | -4.33817900  | 2.29654700   | 0.64917800   |
| H       | 6.65642300   | -2.61392200  | 1.18460100   |
| O       | 5.78998900   | -2.52416400  | 0.63733400   |
| O       | 8.18322300   | -0.73753300  | 1.74659000   |
| O       | 8.98159700   | -2.47579400  | -0.03441300  |
| O       | -4.06247700  | 1.47617900   | 2.00596000   |
| O       | -5.82953500  | 1.99184400   | 0.17849700   |
| H       | -6.06808400  | 1.03597200   | 0.12602600   |
| O       | -4.04018600  | 3.74838400   | 0.70166300   |
| Au      | -6.52978900  | -1.32387900  | -0.08676300  |
| H       | 9.08693600   | -0.38915500  | 1.68546700   |
| H       | -1.52719200  | 3.22594300   | -0.02513400  |
| O       | -2.61155700  | -1.13691800  | -0.77059700  |
| H       | -3.51402900  | -0.77664200  | -0.74231200  |
| H       | -4.08895600  | 2.03039800   | 2.80268600   |

Conformer 1(G)

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -5.88355000  | 2.33139600   | -0.34074500  |
| C       | -5.76676900  | 0.96171500   | -0.46283200  |
| C       | -4.52199500  | 0.29693900   | -0.25844500  |
| C       | -3.41454400  | 1.13111300   | 0.03781700   |
| C       | -3.51288900  | 2.51361600   | 0.18054600   |
| C       | -4.75565900  | 3.10900900   | -0.00094700  |
| H       | -6.84303000  | 2.80050200   | -0.52938500  |
| C       | -4.28020200  | -1.12329000  | -0.34432400  |
| H       | -2.63596200  | 3.10435100   | 0.41601900   |
| C       | -1.88297100  | -0.70623100  | 0.05855100   |
| C       | -2.90751500  | -1.57460200  | -0.21752600  |
| C       | -0.46066600  | -1.00192200  | 0.26632700   |
| C       | 0.38024300   | 0.00949200   | 0.76932300   |
| C       | 0.08726100   | -2.26717100  | -0.03151400  |
| C       | 1.73672100   | -0.23009000  | 0.97631200   |
| H       | -0.00833400  | 0.99144800   | 1.00851300   |
| C       | 1.44393900   | -2.50804700  | 0.17759900   |
| H       | -0.53568000  | -3.05884100  | -0.42111800  |
| C       | 2.26109800   | -1.49606600  | 0.67116100   |
| O       | -2.72300200  | -2.91136800  | -0.33620000  |
| H       | -3.61795600  | -3.28536300  | -0.47398800  |
| O       | -5.14995700  | -2.03324500  | -0.51276600  |
| O       | -2.16896800  | 0.61930300   | 0.19396000   |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| O    | -6.87320000 | 0.26743500 | -0.91414800 |
| O    | -4.83029700 | 4.45337100 | 0.13974800 |
| H    | -5.73247500 | 4.77197100 | -0.01174900 |
| O    | 3.61139600  | -1.70273500 | 0.98033800  |
| P    | -8.07033100 | -0.41667800 | -0.02438000 |
| P    | 4.77251000  | -2.02079600 | -0.10551200 |
| O    | -8.18075200 | 0.45507900  | 1.32548100  |
| H    | -8.85442500 | 1.15165100  | 1.27357900  |
| O    | -7.44254900 | -1.76708800 | 0.48935600  |
| O    | -9.31404000 | -0.48592100 | -0.83374000 |
| O    | 4.99579900  | -1.00330500 | -1.16740300 |
| P    | 4.34429800  | -3.48209200 | -0.61595200 |
| O    | 6.04521900  | -2.18440500 | 0.84429900  |
| Au   | 5.80424100  | 1.48036800  | -0.23256500 |
| H    | -6.51783700 | -1.93383400 | 0.07208800  |
| H    | 1.87054200  | -3.47956600 | -0.04179000 |
| O    | 2.50483600  | 0.77318100  | 1.47964100  |
| H    | 3.43381400  | 0.49381100  | 1.52315100  |
| H    | 5.97926100  | -2.88367400 | 1.51541100  |

### Conformer 1(H)

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.59732600 | 3.89371200 | -0.77833800 |
| C    | 3.37504200 | 2.56396700 | -0.48268200 |
| C    | 2.06532300 | 2.06449900 | -0.22181400 |
| C    | 1.01207300 | 3.00849700 | -0.31431300 |
| C    | 1.21503600 | 4.35816300 | -0.59567300 |
| C    | 2.51409000 | 4.79775900 | -0.82076000 |
| H    | 4.60692200 | 4.22698000 | -0.99575400 |
| C    | 1.71080300 | 0.70098300  | 0.09494500  |
| H    | 0.37465000 | 5.03971400  | -0.64667800 |
| C    | -0.66815600 | 1.36004000 | 0.11521300  |
| C    | 0.30017600 | 0.39177300  | 0.22002400  |
| C    | -2.12454400 | 1.23127500 | 0.24623600  |
| C    | -2.73416300 | -0.00154000 | 0.54151600 |
| C    | -2.94095000 | 2.36992800 | 0.06946500  |
| C    | -4.12188100 | -0.11588000 | 0.67381000 |
| H    | -2.14671900 | -0.89816600 | 0.67796600 |
| C    | -4.32022800 | 2.26300100 | 0.20014000 |
| H    | -2.50176500 | 3.33081100 | -0.16363000 |
| C    | -4.90862400 | 1.03808600 | 0.50736400 |
| O    | 0.00443900 | -0.90445600 | 0.47774500 |
| H    | 0.86321300 | -1.37727900 | 0.50950800 |
| O    | 2.50879100 | -0.26862600 | 0.27586500 |
| O    | -0.28008000 | 2.64306000 | -0.13344300 |
| O    | 4.45500200 | 1.70698800 | -0.56509700 |
| H    | 2.68877100 | 6.11169500 | -1.09706700 |
| H    | 3.62361200 | 6.31728800 | -1.24517500 |
|        | X         | Y         | Z         |
|--------|-----------|-----------|-----------|
| O      | -6.28918000 | 1.03216800 | 0.75416100 |
| P      | 5.49353400  | 1.26286900 | 0.62574800 |
| P      | -7.37201300 | 0.21054100 | -0.11393700 |
| O      | 4.79982200  | 0.00821500 | 1.27767300 |
| H      | 3.86685100  | -0.15285100 | 0.87797400 |
| O      | 5.35978900  | 2.39418200 | 1.76564200 |
| O      | 6.86104500  | 1.07688600 | 0.07694800 |
| O      | -7.42969000 | 1.00004300 | -1.49957400 |
| O      | -8.74163000 | 0.63558800 | 0.58244700 |
| H      | -8.94362000 | 0.15521900 | 1.40206300 |
| O      | -7.08052900 | -1.25355800 | -0.19779600 |
| Au     | 1.75762000  | -4.13018500 | -0.33847300 |
| H      | 6.01953200  | 3.10117400 | 1.68432400 |
| H      | -4.95830900 | 3.13284700 | 0.08335200 |
| O      | -4.62519700 | -1.33671800 | 1.00099400 |
| H      | -5.54608500 | -1.43960500 | 0.66864200 |
| H      | -7.61182100 | 0.43663700 | -2.26916700 |

**Figure S2:** Computed optimized QDP – gold structures and energies for conformers A to G.
Figure S3: TEM images for the samples P, Q, R, S, T and U and the corresponding histogram showing edge length distribution of gold nanoplates formed after 55 minutes.