**Supplementary information for article:**

# On the Role of Mercury in the Non-Covalent Stabilisation of Consecutive U-Hg$^{II}$-U Metal-Mediated Nucleic Acid Base Pairs

**by**

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## The geometries of monomers (in XMol format in Å)

```
23
U-Hg-U
N     0.0000000    4.0149899   -1.1594949
C     0.0000000    2.6314408   -1.2240810
N     0.0000000    2.0056721    0.0027977
C     0.0000000    2.6333501    1.2531508
C     0.0000000    4.0846721    1.2101248
C     0.0000000    4.7133066    0.0172693
H     0.0000000    4.4880439   -2.0512324
O     0.0000000    2.0295141   -2.2857013
O     0.0000000    1.9542371    2.2719346
H     0.0000000    4.6322030    2.1403771
H     0.0000000    5.7919324   -0.0774140
Hg    0.0000000    0.0000000    0.0131449
N     0.0000000   -4.0149899   -1.1594949
C     0.0000000   -2.6314408   -1.2240810
N     0.0000000   -2.0056721    0.0027977
C     0.0000000   -2.6333501    1.2531508
C     0.0000000   -4.0846721    1.2101248
C     0.0000000   -4.7133066    0.0172693
H     0.0000000   -4.4880439   -2.0512324
O     0.0000000   -2.0295141   -2.2857013
O     0.0000000   -1.9542371    2.2719346
H     0.0000000   -4.6322030    2.1403771
H     0.0000000   -5.7919324   -0.0774140

24
U-U
N     0.0000000    3.9649649   -1.1853773
C     0.0000000    2.5815396   -1.2286862
N     0.0000000    2.0056721    0.0240166
C     0.0000000    2.6395171    1.2751106
C     0.0000000    4.0895601    1.1881529
C     0.0000000    4.6861888   -0.0205631
H     0.0000000    4.4218930   -2.0851571
O     0.0000000    1.9517319   -2.2679148
O     0.0000000    1.9820283    2.3011905
H     0.0000000    4.6627129    2.1023685
H     0.0000000    5.7622966   -0.1394127
H     0.0000000    0.9917996    0.0362721
N     0.0000000   -3.9649649   -1.1853773
C     0.0000000   -2.5815396   -1.2286862
N     0.0000000   -2.0056721    0.0240166
C     0.0000000   -2.6395171    1.2751106
C     0.0000000   -4.0895601    1.1881529
C     0.0000000   -4.6861888   -0.0205631
H     0.0000000   -4.4218930   -2.0851571
O     0.0000000   -1.9517319   -2.2679148
O     0.0000000   -1.9820283    2.3011905
H     0.0000000   -4.6627129    2.1023685
H     0.0000000   -5.7622966   -0.1394127
H     0.0000000   -0.9917996    0.0362721

3
H-Hg-H
H     0.0000000    0.0000000    1.6172810
Hg    0.0000000    0.0000000    0.0000000
H     0.0000000    0.0000000   -1.6172810
```

**The geometry of the T-p-T dinucleoside monophosphate dimer linked with two $Hg^{II}$ (a complex containing two T-$Hg^{II}$-T base pairs) obtained at the RI-MP2/def2-TZVP(T-$Hg^{II}$-T), MWB60 effective core potential ($Hg^{II}$), def2-SVP (all other atoms) level of theory (in XMol format in Å)**

```
124
2TpT.2Hg
H      6.658537  -0.734095   5.032087
O      6.592741  -0.706871   4.063138
C      7.249606  -1.846306   3.529363
H      6.857585  -2.781332   3.979470
H      8.342925  -1.796408   3.718645
C      7.028102  -1.914496   2.032104
H      7.695924  -2.691590   1.616083
O      5.675075  -2.275384   1.753549
C      5.028885  -1.257602   0.989524
H      4.930580  -1.556691  -0.068102
N      3.666911  -1.116731   1.502681
C      3.496929  -0.896538   2.853250
H      4.427641  -0.729620   3.406151
C      2.584673  -1.377448   0.661415
O      2.691393  -1.622973  -0.530947
N      1.347811  -1.328331   1.294722
C      1.115153  -1.249826   2.667863
O     -0.018516  -1.446635   3.110227
C      2.283759  -0.920884   3.471179
C      2.084582  -0.650413   4.930532
H      1.411959   0.217423   5.050032
H      3.050584  -0.434300   5.420922
H      1.610149  -1.514175   5.430679
C      5.900408  -0.018506   1.147310
H      5.628010   0.535621   2.060617
H      5.836543   0.656094   0.289743
C      7.300678  -0.597835   1.286722
H      7.964178   0.083427   1.850347
O      7.881074  -0.952940   0.050322
P      8.442674   0.240659  -1.011958
O      8.168644   1.586491  -0.401004
O      9.747215  -0.245930  -1.555483
O      7.268889   0.050003  -2.210245
C      7.138536  -1.240075  -2.756780
H      7.055348  -1.992910  -1.950770
H      8.017567  -1.502903  -3.381048
C      5.870222  -1.295729  -3.582651
H      5.721379  -2.328197  -3.954990
O      4.762642  -0.935184  -2.760689
C      4.124954   0.229608  -3.254515
H      3.189068  -0.053437  -3.762338
N      3.727124   1.100222  -2.163747
C      4.674959   1.804950  -1.448153
H      5.716936   1.630268  -1.737928
C      2.381440   1.076656  -1.774311
O      1.512247   0.461033  -2.368468
N      2.108256   1.839697  -0.649121
C      2.985263   2.670331   0.047285
O      2.567982   3.346315   0.990097
C      4.371947   2.615297  -0.395533
C      5.411229   3.379043   0.370077
H      5.309207   4.466297   0.191909
H      6.424594   3.042813   0.085801
H      5.268265   3.216054   1.453040
C      5.123074   0.868585  -4.223732
H      5.851482   1.498926  -3.694562
H      4.616280   1.475450  -4.997426
C      5.829071  -0.352198  -4.786635
```

| | | | |
|---|---|---|---|
| H | 6.845876 | -0.127105 | -5.166583 |
| O | 5.041300 | -0.995454 | -5.784987 |
| H | 4.778952 | -0.320819 | -6.434324 |
| Hg | 0.329878 | 1.633078 | 0.236407 |
| H | -6.658537 | 0.734095 | 5.032087 |
| O | -6.592741 | 0.706871 | 4.063138 |
| C | -7.249606 | 1.846306 | 3.529363 |
| H | -6.857585 | 2.781332 | 3.979470 |
| H | -8.342925 | 1.796408 | 3.718645 |
| C | -7.028102 | 1.914496 | 2.032104 |
| H | -7.695924 | 2.691590 | 1.616083 |
| O | -5.675075 | 2.275384 | 1.753549 |
| C | -5.028885 | 1.257602 | 0.989524 |
| H | -4.930580 | 1.556691 | -0.068102 |
| N | -3.666911 | 1.116731 | 1.502681 |
| C | -3.496929 | 0.896538 | 2.853250 |
| H | -4.427641 | 0.729620 | 3.406151 |
| C | -2.584673 | 1.377448 | 0.661415 |
| O | -2.691393 | 1.622973 | -0.530947 |
| N | -1.347811 | 1.328331 | 1.294722 |
| C | -1.115153 | 1.249826 | 2.667863 |
| O | 0.018516 | 1.446635 | 3.110227 |
| C | -2.283759 | 0.920884 | 3.471179 |
| C | -2.084582 | 0.650413 | 4.930532 |
| H | -1.411959 | -0.217423 | 5.050032 |
| H | -3.050584 | 0.434300 | 5.420922 |
| H | -1.610149 | 1.514175 | 5.430679 |
| C | -5.900408 | 0.018506 | 1.147310 |
| H | -5.628010 | -0.535621 | 2.060617 |
| H | -5.836543 | -0.656094 | 0.289743 |
| C | -7.300678 | 0.597835 | 1.286722 |
| H | -7.964178 | -0.083427 | 1.850347 |
| O | -7.881074 | 0.952940 | 0.050322 |
| P | -8.442674 | -0.240659 | -1.011958 |
| O | -8.168644 | -1.586491 | -0.401004 |
| O | -9.747215 | 0.245930 | -1.555483 |
| O | -7.268889 | -0.050003 | -2.210245 |
| C | -7.138536 | 1.240075 | -2.756780 |
| H | -7.055348 | 1.992910 | -1.950770 |
| H | -8.017567 | 1.502903 | -3.381048 |
| C | -5.870222 | 1.295729 | -3.582651 |
| H | -5.721379 | 2.328197 | -3.954990 |
| O | -4.762642 | 0.935184 | -2.760689 |
| C | -4.124954 | -0.229608 | -3.254515 |
| H | -3.189068 | 0.053437 | -3.762338 |
| N | -3.727124 | -1.100222 | -2.163747 |
| C | -4.674959 | -1.804950 | -1.448153 |
| H | -5.716936 | -1.630268 | -1.737928 |
| C | -2.381440 | -1.076656 | -1.774311 |
| O | -1.512247 | -0.461033 | -2.368468 |
| N | -2.108256 | -1.839697 | -0.649121 |
| C | -2.985263 | -2.670331 | 0.047285 |
| O | -2.567982 | -3.346315 | 0.990097 |
| C | -4.371947 | -2.615297 | -0.395533 |
| C | -5.411229 | -3.379043 | 0.370077 |
| H | -5.309207 | -4.466297 | 0.191909 |
| H | -6.424594 | -3.042813 | 0.085801 |
| H | -5.268265 | -3.216054 | 1.453040 |
| C | -5.123074 | -0.868585 | -4.223732 |
| H | -5.851482 | -1.498926 | -3.694562 |
| H | -4.616280 | -1.475450 | -4.997426 |
| C | -5.829071 | 0.352198 | -4.786635 |
| H | -6.845876 | 0.127105 | -5.166583 |
| O | -5.041300 | 0.995454 | -5.784987 |
| H | -4.778952 | 0.320819 | -6.434324 |
| Hg | -0.329878 | -1.633078 | 0.236407 |

**Summary of the interaction energy profiles for U-Hg$^{II}$-U•U-Hg$^{II}$-U dimer**

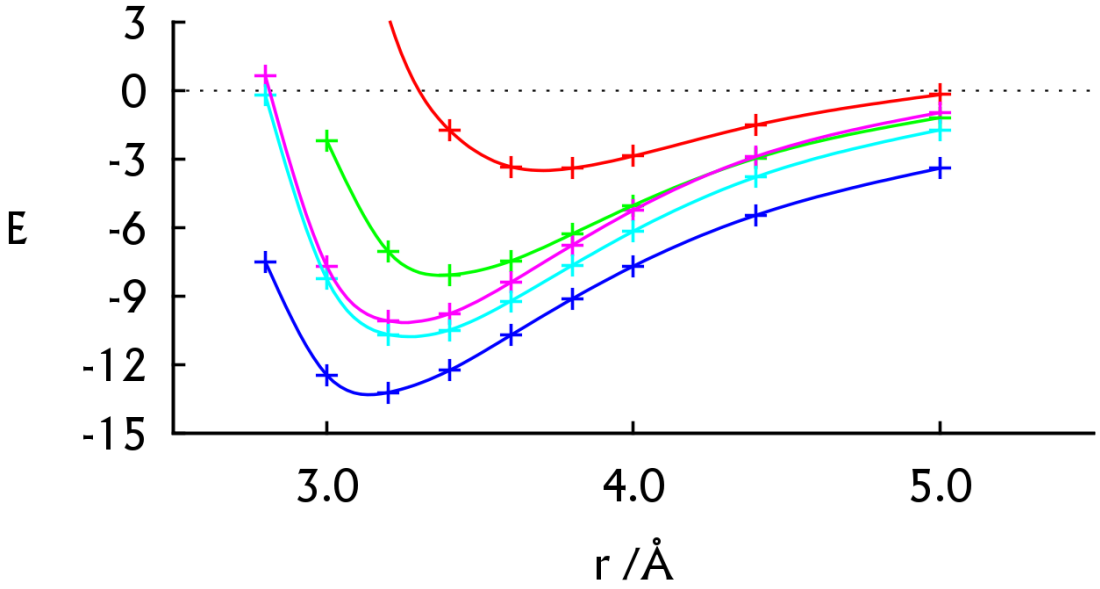


**Figure S1:** Interaction energy profiles (in kcal/mol) in U-Hg$^{II}$-U•U-Hg$^{II}$-U dimer for various mutual orientations of the U-Hg$^{II}$-U monomers: φ = 0°, *d* = 0 Å (red), φ = 30°, *d* = 0 Å (green), φ = 90°, *d* = 0 Å (blue), φ = 0°, *d* = 2.0 Å (magenta), φ = 30°, *d* = 2.0 Å (cyan).