

## SUPPORTING INFORMATION

### Interaction of Au(III) with amino acids. A vademecum for medicinal chemistry and nanotechnology

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**Table S1.** Cartesian coordinates for the complexes of Au(III) and peptide/protein backbone (Figure 1 in main text).

*N-terminal*•AuCl<sub>3</sub>

MP2=-1816.4457213

N	1.006000	0.367000	0.542000
H	1.310000	-0.305000	1.254000
C	1.970000	0.293000	-0.562000
H	1.712000	-0.549000	-1.206000
C	3.347000	0.028000	0.037000
O	3.437000	-0.481000	1.148000
N	4.388000	0.344000	-0.728000
H	4.226000	0.771000	-1.625000
H	1.927000	1.208000	-1.148000
C	5.748000	0.069000	-0.321000
H	6.421000	0.425000	-1.098000
H	5.983000	0.580000	0.614000
H	5.902000	-1.002000	-0.179000
Au	-0.962000	0.004000	0.063000
Cl	-1.320000	2.283000	0.121000
Cl	-3.160000	-0.397000	-0.457000
Cl	-0.471000	-2.250000	0.022000
H	1.026000	1.291000	0.971000

*N-terminal*

*N-backbone*•AuCl<sub>3</sub>

MP2=-1968.2078233

C	-1.247000	1.711000	0.878000
O	-2.380000	2.212000	0.835000
N	-0.812000	0.898000	-0.093000
C	-1.625000	0.660000	-1.267000
H	-2.153000	1.587000	-1.515000
C	-2.648000	-0.460000	-1.108000
O	-2.629000	-1.462000	-1.815000
H	-0.980000	0.397000	-2.104000
C	-0.313000	1.994000	2.020000
H	-0.144000	1.083000	2.599000
H	0.656000	2.344000	1.660000
H	-0.757000	2.749000	2.665000
N	-3.565000	-0.240000	-0.159000
H	-3.491000	0.631000	0.355000
C	-4.594000	-1.197000	0.158000
H	-5.187000	-0.814000	0.985000
H	-5.253000	-1.370000	-0.697000
H	-4.161000	-2.158000	0.450000
Au	0.935000	-0.095000	-0.000000
Cl	2.962000	-1.262000	0.059000
Cl	-0.058000	-1.673000	1.374000

Cl 1.855000 1.534000 -1.366000

*C-backbone*•AuCl<sub>3</sub>

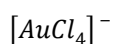
MP2=-1969.4980381

H 2.110000 3.730000 0.094000  
C 1.342000 3.215000 0.665000  
H 0.956000 3.879000 1.442000  
H 1.771000 2.339000 1.157000  
C 0.238000 2.787000 -0.259000  
O 0.233000 3.007000 -1.457000  
N -0.762000 2.089000 0.349000  
H -0.754000 2.011000 1.354000  
C -1.908000 1.630000 -0.373000  
H -2.755000 2.318000 -0.293000  
H -1.631000 1.570000 -1.431000  
C -2.343000 0.255000 0.056000  
O -1.550000 -0.683000 0.348000  
N -3.628000 0.015000 0.115000  
H -4.261000 0.781000 -0.050000  
C -4.175000 -1.289000 0.435000  
H -3.714000 -2.048000 -0.196000  
H -3.983000 -1.535000 1.481000  
H -5.246000 -1.265000 0.258000  
Au 0.487000 -0.647000 0.031000  
Cl 0.789000 -0.325000 2.301000  
Cl 2.728000 -0.734000 -0.297000  
Cl 0.092000 -0.916000 -2.225000

*C-terminal*•AuCl<sub>3</sub>

MP2=-2004.9812642

H -6.788000 -0.881000 1.093000  
C -6.148000 -0.001000 1.168000  
H -5.652000 -0.001000 2.138000  
H -6.788000 0.880000 1.094000  
C -5.191000 0.000000 0.007000  
O -5.582000 0.001000 -1.156000  
N -3.885000 -0.000000 0.319000  
H -3.573000 -0.000000 1.278000  
C -2.855000 0.001000 -0.677000  
H -2.923000 -0.877000 -1.328000  
C -1.495000 0.000000 -0.005000  
O -1.373000 -0.000000 1.206000  
H -2.923000 0.879000 -1.327000  
Au 1.342000 0.000000 -0.108000  
Cl 1.301000 -2.308000 -0.118000  
Cl 3.506000 -0.000000 0.648000  
Cl 1.302000 2.308000 -0.117000  
O -0.537000 0.000000 -0.875000



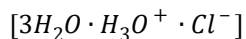
MP2=-1973,679602

Au	0.000000	0.000000	0.000066
Cl	0.000000	2.314079	-0.000005
Cl	0.000000	0.000000	-2.314350
Cl	0.000000	-2.314079	-0.000005
Cl	0.000000	0.000000	2.314054



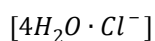
MP2=-305.3095165

O	0.006347	1.842653	0.183424
H	0.082369	2.516619	-0.497388
H	0.778290	1.257917	0.063118
O	-2.076969	0.068580	-0.000208
H	-2.490366	0.146753	-0.864004
H	-1.403158	0.781588	0.030569
O	-0.177107	-2.031285	0.085800
H	0.622946	-1.491598	0.026099
H	-0.900372	-1.379807	0.049972
O	2.013339	-0.084186	-0.083793
H	2.673081	-0.106318	0.616849
H	2.512324	-0.091249	-0.906999



MP2=-765,6281806

O	1.642179	1.454089	0.749396
H	1.617104	1.504935	1.709540
H	0.708090	1.528343	0.457202
O	2.264150	-0.876937	-0.316704
H	2.645526	-1.503887	0.305895
H	2.158875	-0.009332	0.163804
O	-0.073654	-1.297489	-0.993501
H	-0.596874	-1.634971	-0.193838
H	0.948418	-1.197573	-0.708646
O	-1.526464	-1.535536	1.099210
H	-1.772080	-0.600330	0.989299
H	-2.350954	-2.032128	1.087801
Cl	-1.257036	1.314384	-0.415768
H	-0.438184	-0.352596	-1.050217



MP2=-765,190263

O	-0.011295	2.256746	-0.298063
H	-0.276785	2.994786	0.257402
H	-0.734371	1.592265	-0.209154
O	2.380951	1.157699	0.359960

H	2.439448	1.160567	1.318818
H	1.514411	1.577088	0.152389
O	2.178852	-1.507611	-0.537633
H	1.303550	-1.791876	-0.222617
H	2.267952	-0.588667	-0.227718
O	-0.385046	-2.292951	0.390319
H	-0.983600	-1.523612	0.261787
H	-0.760856	-2.990896	-0.152962
Cl	-2.239849	0.156428	-0.029095

**Table S2.** Cartesian coordinates for the complexes of Au(III) and sulfur/selenium containing amino acids (Figure 5 in main text).

*Sec*•AuCl<sub>3</sub>

MP2=-4408,434291

H	4.394854	-3.865532	-0.100985
C	4.460332	-3.017546	-0.785187
H	4.537139	-3.415362	-1.798105
H	5.356500	-2.442066	-0.554800
C	3.190213	-2.219218	-0.677447
O	2.098265	-2.703426	-0.952732
N	3.329814	-0.947361	-0.259572
H	4.239499	-0.563889	-0.051944
C	2.216793	-0.048818	-0.097310
H	1.463227	-0.304552	-0.845421
C	1.614943	-0.222989	1.302290
H	1.361746	-1.272000	1.449406
H	2.341916	0.076548	2.062751
Se	0.034559	0.845939	1.690667
C	2.742734	1.366005	-0.321929
O	3.892159	1.657342	-0.003031
N	1.887161	2.229183	-0.868812
H	0.920702	1.953898	-0.983930
C	2.212762	3.626465	-1.022270
H	3.158831	3.737064	-1.553077
H	1.424084	4.106872	-1.598302
H	2.301221	4.126725	-0.053719
Au	-1.470061	-0.102364	-0.005689
Cl	-2.984516	-1.023615	-1.658452
Cl	-1.529565	1.971318	-1.062004
Cl	-1.348106	-2.138793	1.081076

*Sec*

MP2=-2895,019169

C	4.46274	-3.02161	-0.71441
C	3.18951	-2.22445	-0.65146
N	3.32082	-0.92729	-0.31614
C	2.19295	-0.03977	-0.20165

C	2.7223	1.38239	-0.35113
N	1.89101	2.25546	-0.92366
C	2.20467	3.66083	-1.03048
O	2.09763	-2.72773	-0.89192
C	1.5109	-0.23699	1.15656
Se	-0.2018	0.67502	1.38033
O	3.83959	1.6781	0.05878
H	4.40964	-3.81918	0.02896
H	4.53166	-3.48986	-1.69731
H	5.35737	-2.42591	-0.53551
H	4.22204	-0.53185	-0.09434
H	1.47992	-0.2755	-0.99456
H	1.26978	-1.29448	1.26464
H	2.17728	0.05366	1.96816
H	0.96979	1.94162	-1.18126
H	3.21767	3.7865	-1.4129
H	1.50293	4.1268	-1.71914
H	2.13715	4.16058	-0.06033
H	0.36199	2.01565	1.57991

*Cys*•AuCl<sub>3</sub>

MP2= -2406,025408

H	2.771	1.103	-0.420
C	2.635	2.022	0.162
H	2.362	1.724	1.180
H	1.812	2.599	-0.272
C	3.940	2.771	0.206
O	4.969	2.265	0.651
N	3.908	4.040	-0.271
H	3.060	4.460	-0.638
C	5.081	4.878	-0.261
H	5.639	4.680	0.665
C	5.971	4.546	-1.471
H	6.029	3.457	-1.587
H	5.520	4.957	-2.388
S	7.655	5.227	-1.403
C	4.610	6.327	-0.317
O	3.561	6.612	-0.892
N	5.428	7.219	0.269
H	6.290	6.880	0.692
C	5.187	8.646	0.236
H	4.226	8.817	-0.253
H	5.150	9.056	1.251
H	5.972	9.165	-0.326
Au	8.471	3.886	0.411
Cl	9.308	2.513	2.273
Cl	8.649	2.056	-1.098
Cl	8.223	5.766	1.865

Cys(H)•AuCl<sub>3</sub>

MP2= -2406,437529

H	1.677	1.771	0.266
C	1.868	2.837	0.428
H	1.446	3.099	1.406
H	1.353	3.418	-0.343
C	3.353	3.065	0.469
O	4.106	2.408	1.176
N	3.815	4.081	-0.323
H	3.194	4.542	-0.979
C	5.225	4.388	-0.387
H	5.656	4.104	0.583
C	5.872	3.533	-1.477
H	5.890	2.482	-1.172
H	5.324	3.631	-2.422
S	7.597	3.970	-1.924
H	7.281	5.181	-2.451
C	5.394	5.878	-0.671
O	5.315	6.296	-1.825
N	5.635	6.639	0.411
H	5.666	6.193	1.321
C	5.817	8.075	0.349
H	5.856	8.367	-0.703
H	4.989	8.597	0.840
H	6.759	8.353	0.834
Au	8.537	4.881	0.121
Cl	9.381	5.792	2.144
Cl	9.015	6.896	-1.035
Cl	8.059	2.809	1.183

Cys

MP2=-892.620411

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.090847
H	1.028173	0.000000	1.451725
H	-0.494593	-0.915226	1.421631
C	-0.802977	1.177142	1.570691
O	-1.955057	1.370972	1.198090
N	-0.182310	2.002457	2.433757
H	0.761171	1.824469	2.743727
C	-0.820008	3.166630	2.987363
H	-1.428378	3.639737	2.212979
C	-1.737590	2.760262	4.150658
H	-2.417112	1.992410	3.778224
H	-1.149992	2.328558	4.961927
S	-2.812811	4.066053	4.787841
H	-1.885121	4.746764	5.478799

C	0.284746	4.105903	3.458193
O	1.359571	3.662474	3.848335
N	-0.010290	5.407298	3.438422
H	-0.930754	5.687661	3.142769
C	0.898250	6.407850	3.947298
H	1.892812	6.257986	3.526178
H	0.533955	7.391758	3.659846
H	0.974381	6.360299	5.036705

Met•AuI<sub>3</sub>

MP2= -2484,879375

H	1.693	2.152	1.793
C	2.035	2.234	0.755
H	1.311	2.826	0.187
H	2.064	1.219	0.343
C	3.427	2.807	0.745
O	4.347	2.308	1.387
N	3.600	3.914	-0.020
H	2.850	4.302	-0.582
C	4.881	4.569	-0.138
H	5.374	4.546	0.846
C	5.764	3.840	-1.166
H	5.764	2.774	-0.906
H	5.290	3.946	-2.154
C	7.184	4.373	-1.182
H	7.240	5.445	-1.407
H	7.700	4.180	-0.229
S	8.189	3.487	-2.419
C	9.756	4.385	-2.256
H	10.164	4.162	-1.265
H	10.430	4.009	-3.032
H	9.590	5.460	-2.378
C	4.614	5.996	-0.605
O	3.709	6.219	-1.405
N	5.458	6.934	-0.130
H	6.117	6.675	0.594
C	5.401	8.322	-0.538
H	4.695	8.400	-1.369
H	5.059	8.963	0.282
H	6.387	8.663	-0.871
Au	7.517	4.290	-4.618
Cl	8.415	2.235	-5.410
Cl	6.722	6.361	-3.781
Cl	6.951	4.963	-6.834

Met

MP2=-971.052792

H	0.000000	0.000000	0.000000
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C	0.000000	0.000000	1.091146
H	1.028850	0.000000	1.450247
H	-0.494614	-0.915030	1.421613
C	-0.803315	1.177688	1.570959
O	-1.972184	1.340798	1.236930
N	-0.160128	2.037414	2.381183
H	0.791905	1.865206	2.664817
C	-0.794841	3.200267	2.947429
H	-1.513122	3.581641	2.217526
C	-1.533993	2.842484	4.243929
H	-2.218024	2.024004	4.004402
H	-0.803376	2.460891	4.963334
C	-2.305763	4.004238	4.840679
H	-1.633170	4.812506	5.139155
H	-3.018725	4.406596	4.114332
S	-3.215419	3.449620	6.299545
C	-3.964355	5.008084	6.791742
H	-4.619559	5.390022	6.007194
H	-4.557349	4.814089	7.685840
H	-3.199257	5.749717	7.026970
C	0.298692	4.224584	3.220124
O	1.382418	3.873287	3.673788
N	-0.011887	5.500001	2.974451
H	-0.904104	5.715459	2.563887
C	0.903615	6.578694	3.263856
H	1.205491	6.553396	4.312519
H	1.801543	6.507255	2.646134
H	0.406204	7.524214	3.059438

**Table S3.** Cartesian coordinates for the complexes of Au(III) and histidine (Figure 6 in main text).

*His(N $\delta$ )•AuCl<sub>3</sub>*

MP2=-2233,356548

H	2.082	1.209	-0.182
C	2.092	2.160	0.363
H	1.761	1.950	1.386
H	1.380	2.847	-0.106
C	3.502	2.683	0.405
O	4.427	2.040	0.894
N	3.688	3.920	-0.125
H	2.938	4.419	-0.592
C	4.991	4.532	-0.179
H	5.520	4.318	0.760
C	5.821	3.961	-1.356
H	6.023	2.904	-1.147
H	5.208	4.012	-2.266
C	7.077	4.732	-1.539
N	7.196	5.736	-2.480

H 6.533 5.932 -3.224  
C 8.326 6.420 -2.263  
H 8.679 7.254 -2.855  
N 8.939 5.893 -1.213  
C 8.185 4.838 -0.749  
H 8.472 4.268 0.126  
C 4.806 6.029 -0.389  
O 3.938 6.441 -1.155  
N 5.695 6.825 0.234  
H 6.371 6.421 0.873  
C 5.764 8.249 -0.026  
H 5.548 8.434 -1.084  
H 5.044 8.812 0.581  
H 6.775 8.599 0.202  
Au 10.541 6.735 -0.251  
Cl 11.800 6.597 -2.256  
Cl 9.199 6.898 1.711  
Cl 12.361 7.713 0.870

*His(Nε)•AuCl<sub>3</sub>*

MP2=-2233,363102

H 2.627 2.655 2.752  
C 2.622 2.514 1.665  
H 1.716 2.969 1.254  
H 2.598 1.434 1.479  
C 3.893 3.081 1.094  
O 5.003 2.646 1.399  
N 3.747 4.111 0.226  
H 2.838 4.448 -0.076  
C 4.897 4.733 -0.377  
H 5.630 4.954 0.413  
C 5.569 3.803 -1.428  
H 5.212 2.785 -1.239  
H 5.243 4.063 -2.444  
C 7.051 3.781 -1.332  
N 7.931 4.548 -2.081  
C 9.170 4.286 -1.679  
H 10.073 4.729 -2.075  
N 9.121 3.382 -0.697  
H 9.929 3.004 -0.215  
C 7.808 3.055 -0.458  
H 7.501 2.357 0.309  
C 4.424 6.014 -1.050  
O 3.269 6.129 -1.448  
N 5.368 6.959 -1.240  
H 6.261 6.880 -0.764  
C 5.040 8.214 -1.889  
H 4.545 8.018 -2.846

H 4.372 8.824 -1.268  
H 5.967 8.763 -2.076  
Au 7.523 5.929 -3.555  
Cl 8.626 7.577 -2.239  
Cl 6.495 4.247 -4.878  
Cl 7.088 7.523 -5.227

*His - N $\delta$  tautomer*

MP2=-719.520934

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091372
H	1.039944	0.000000	1.421686
H	-0.490684	-0.904687	1.449031
C	-0.655271	1.265968	1.569922
O	-0.214894	2.372696	1.276646
N	-1.748722	1.111072	2.337647
H	-2.099433	0.194396	2.571574
C	-2.484992	2.222756	2.869925
H	-1.778716	3.001737	3.166953
C	-3.438998	2.816415	1.807695
H	-2.820392	3.078853	0.947592
H	-4.131082	2.034110	1.485447
C	-4.184337	4.011161	2.278787
N	-5.493748	3.972955	2.679270
H	-6.095912	3.165911	2.655197
C	-5.837654	5.206259	3.109452
H	-6.828455	5.436917	3.470976
N	-4.831878	6.043230	3.016606
C	-3.796452	5.307048	2.500179
H	-2.826113	5.741484	2.309640
C	-3.266107	1.727055	4.080279
O	-3.615506	0.554770	4.169111
N	-3.559881	2.656375	4.993965
H	-3.290158	3.609020	4.808638
C	-4.420418	2.385400	6.120733
H	-4.119750	1.455242	6.602789
H	-4.332363	3.201415	6.835121
H	-5.465741	2.293781	5.812400

*His - N $\epsilon$  tautomer*

MP2=-719.523555

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091526
H	1.040026	0.000000	1.421587
H	-0.490881	-0.905267	1.447892
C	-0.657227	1.265094	1.572193
O	-0.209276	2.372557	1.288649
N	-1.764961	1.108242	2.314635

H	-2.057112	0.196002	2.636689
C	-2.463975	2.214670	2.908878
H	-1.733153	2.893680	3.362251
C	-3.276378	3.013747	1.863512
H	-2.783527	2.883841	0.900141
H	-4.277284	2.578355	1.774378
C	-3.361271	4.474945	2.142061
N	-3.810444	4.978957	3.339412
C	-3.742440	6.286244	3.237623
H	-4.016243	6.999137	3.999957
N	-3.272772	6.650492	2.030974
H	-3.129511	7.594435	1.711994
C	-3.018677	5.510897	1.318525
H	-2.626095	5.532487	0.315662
C	-3.335630	1.630566	4.029244
O	-3.345721	0.420455	4.252983
N	-4.059491	2.510384	4.713835
H	-4.038404	3.494681	4.423853
C	-4.949502	2.094168	5.768924
H	-4.403256	1.586957	6.567587
H	-5.436414	2.976082	6.181800
H	-5.715724	1.409507	5.396090

**Table S4.** Cartesian coordinates for the complexes of Au(III) and aromatic amino acids (Figure 7 in main text).

*Trp*•AuCl<sub>3</sub>

MP2=-2370,619766

H	2.031	2.694	2.429
C	2.366	2.558	1.395
H	1.544	2.803	0.715
H	2.622	1.499	1.273
C	3.599	3.387	1.169
O	4.572	3.339	1.919
N	3.578	4.198	0.079
H	2.816	4.180	-0.592
C	4.713	5.009	-0.260
H	5.087	5.495	0.652
C	5.843	4.132	-0.875
H	5.924	3.234	-0.250
H	5.534	3.827	-1.883
C	7.147	4.833	-0.883
C	7.776	5.510	-2.013
H	7.180	6.072	-2.737
N	8.908	6.155	-1.503
H	9.563	6.682	-2.068
C	9.078	5.833	-0.200
C	10.094	6.185	0.695

H	10.938	6.795	0.386
C	9.965	5.723	1.988
H	10.737	5.980	2.711
C	8.868	4.927	2.427
H	8.834	4.610	3.466
C	7.874	4.567	1.560
H	7.014	3.973	1.872
C	7.973	5.019	0.216
C	4.280	6.022	-1.310
O	3.430	5.729	-2.144
N	4.956	7.188	-1.311
H	5.535	7.430	-0.516
C	4.710	8.192	-2.329
H	4.801	7.743	-3.324
H	3.704	8.620	-2.233
H	5.450	8.988	-2.227
Au	8.299	3.792	-3.277
Cl	8.858	1.982	-4.813
Cl	6.332	4.325	-4.521
Cl	10.186	3.260	-1.933

*Trp*

MP2=-856.787575

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091431
H	1.040023	0.000000	1.421524
H	-0.490704	-0.905028	1.448523
C	-0.656264	1.265575	1.570641
O	-0.211725	2.372847	1.279924
N	-1.753996	1.112250	2.329339
H	-2.087547	0.197766	2.595422
C	-2.475623	2.229399	2.871445
H	-1.754726	2.984262	3.196456
C	-3.407004	2.870735	1.815241
H	-2.822644	2.919941	0.892164
H	-4.251528	2.201444	1.630997
C	-3.877783	4.231919	2.184952
C	-5.147303	4.623117	2.512749
H	-6.053446	4.037759	2.556390
N	-5.164869	5.958163	2.814469
H	-5.982140	6.478994	3.079682
C	-3.901565	6.467172	2.692368
C	-3.420476	7.758813	2.889596
H	-4.078784	8.564426	3.194561
C	-2.070777	7.973608	2.680411
H	-1.663141	8.967663	2.825907
C	-1.216925	6.931836	2.282502
H	-0.164652	7.141950	2.126762

C	-1.695477	5.650523	2.087138
H	-1.034708	4.846121	1.778110
C	-3.057581	5.403612	2.294705
C	-3.271197	1.727535	4.069109
O	-3.517169	0.534108	4.216494
N	-3.691431	2.672481	4.914958
H	-3.528142	3.635440	4.668780
C	-4.566476	2.378070	6.024431
H	-4.176674	1.533260	6.592592
H	-4.616125	3.249757	6.674062
H	-5.576140	2.129229	5.685849

*Tyr•AuCl<sub>3</sub>*

MP2=-2313,974421

H	2.703	1.000	0.962
C	2.555	2.050	1.235
H	2.380	2.085	2.316
H	1.667	2.433	0.723
C	3.810	2.819	0.919
O	4.919	2.451	1.302
N	3.641	3.955	0.198
H	2.734	4.250	-0.149
C	4.759	4.786	-0.164
H	5.423	4.885	0.709
C	5.559	4.173	-1.344
H	5.579	3.086	-1.186
H	5.017	4.366	-2.280
C	6.957	4.695	-1.401
C	7.367	5.621	-2.307
H	6.683	5.989	-3.073
C	8.714	6.144	-2.284
H	9.171	6.330	-3.261
C	9.705	5.561	-1.316
O	10.886	5.894	-1.348
C	9.188	4.575	-0.370
H	9.887	4.182	0.365
C	7.898	4.182	-0.420
H	7.518	3.444	0.290
C	4.210	6.140	-0.593
O	3.087	6.225	-1.086
N	5.053	7.178	-0.442
H	5.973	7.026	-0.033
C	4.761	8.500	-0.953
H	3.679	8.598	-1.074
H	5.119	9.257	-0.248
H	5.244	8.670	-1.927
Au	8.477	8.246	-1.729
Cl	8.271	10.686	-1.185

Cl 8.496 8.718 -4.085  
Cl 8.272 7.687 0.609

*Tyr*

MP2=-800.589660

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091113
H	1.028741	0.000000	1.450604
H	-0.494238	-0.915336	1.421459
C	-0.802965	1.177606	1.571821
O	-1.970992	1.343720	1.233911
N	-0.164306	2.032467	2.388895
H	0.796018	1.880465	2.657852
C	-0.796506	3.197993	2.942858
H	-1.454175	3.630251	2.184396
C	-1.645537	2.838309	4.182412
H	-2.320206	2.038254	3.868148
H	-0.979654	2.428167	4.946137
C	-2.424265	3.997414	4.727548
C	-2.018214	4.667067	5.877004
H	-1.139823	4.323010	6.413550
C	-2.706451	5.773440	6.351516
H	-2.372486	6.279138	7.251941
C	-3.826187	6.235766	5.669030
O	-4.541400	7.312816	6.078448
H	-4.152609	7.676488	6.880875
C	-4.249836	5.578769	4.518066
H	-5.127266	5.940670	3.994845
C	-3.552990	4.473173	4.060953
H	-3.896062	3.967616	3.163453
C	0.302216	4.184452	3.316697
O	1.420247	3.790457	3.632508
N	-0.050290	5.473529	3.302082
H	-1.013640	5.699274	3.115128
C	0.815979	6.518183	3.792705
H	1.837402	6.328816	3.465115
H	0.483398	7.473806	3.391343
H	0.804828	6.568490	4.885577

*Phe•AuCl<sub>3</sub>*

MP2=-2239,26168

H	2.409	1.264	1.285
C	2.329	2.342	1.468
H	2.111	2.474	2.534
H	1.495	2.741	0.882
C	3.651	2.989	1.158
O	4.688	2.682	1.738
N	3.625	3.949	0.195

H	2.787	4.141	-0.344
C	4.821	4.624	-0.230
H	5.445	4.830	0.652
C	5.624	3.727	-1.218
H	5.817	2.779	-0.700
H	4.980	3.536	-2.087
C	6.898	4.377	-1.624
C	6.930	5.221	-2.751
H	6.038	5.320	-3.369
C	8.075	5.911	-3.069
H	8.121	6.544	-3.952
C	9.234	5.819	-2.223
H	10.210	6.052	-2.658
C	9.199	4.908	-1.119
H	10.092	4.788	-0.509
C	8.050	4.215	-0.829
H	8.013	3.543	0.027
C	4.408	5.901	-0.953
O	3.444	5.884	-1.715
N	5.197	6.968	-0.737
H	5.984	6.884	-0.098
C	5.064	8.206	-1.475
H	4.074	8.232	-1.936
H	5.173	9.059	-0.798
H	5.826	8.282	-2.265
Au	8.988	7.882	-1.299
Cl	8.191	7.141	0.830
Cl	8.824	10.130	-0.480
Cl	9.831	8.719	-3.360

*Phe*

MP2=-725.460395

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091430
H	1.039945	0.000000	1.421670
H	-0.490731	-0.904966	1.448725
C	-0.655628	1.266270	1.569608
O	-0.209735	2.372644	1.282066
N	-1.753757	1.111688	2.329561
H	-2.113136	0.195084	2.549235
C	-2.500501	2.223824	2.849271
H	-1.797445	3.006369	3.145235
C	-3.458763	2.799481	1.783348
H	-2.844638	3.020305	0.907096
H	-4.170530	2.018584	1.504103
C	-4.178118	4.033116	2.240323
C	-5.517861	3.986314	2.616150
H	-6.058426	3.047983	2.543418



C	-6.164156	5.120072	3.088729
H	-7.208180	5.064558	3.376110
C	-5.475327	6.320455	3.196181
H	-5.977760	7.206509	3.567068
C	-4.139120	6.380400	2.821703
H	-3.594952	7.315178	2.897106
C	-3.498002	5.245648	2.345874
H	-2.454482	5.299703	2.050781
C	-3.285259	1.729504	4.057639
O	-3.664747	0.565171	4.126679
N	-3.545352	2.648707	4.992068
H	-3.262864	3.598926	4.816015
C	-4.418887	2.388692	6.111009
H	-4.208363	1.400420	6.518148
H	-4.241626	3.137413	6.880885
H	-5.471362	2.425699	5.814674

**Table S5.** Cartesian coordinates for the complexes of Au(III) and charged amino acids (Figure 8 in main text).

*Asp•AuCl<sub>3</sub>*

MP2=-2196,592226

H	1.847	1.395	-0.522
C	2.036	2.196	0.201
H	1.900	1.768	1.202
H	1.299	2.992	0.054
C	3.463	2.658	0.059
O	4.412	1.881	0.129
N	3.631	3.987	-0.145
H	2.849	4.634	-0.178
C	4.937	4.588	-0.249
H	5.596	4.158	0.518
C	5.550	4.315	-1.631
H	5.507	3.230	-1.796
H	4.958	4.801	-2.417
C	6.998	4.730	-1.802
O	7.713	4.486	-0.727
O	7.433	5.205	-2.837
C	4.760	6.089	-0.023
O	3.653	6.613	-0.135
N	5.891	6.761	0.263
H	6.768	6.251	0.333
C	5.929	8.198	0.425
H	4.901	8.568	0.447
H	6.428	8.462	1.365
H	6.466	8.677	-0.403
Au	9.702	4.956	-0.983
Cl	9.263	7.077	-0.007

Cl 10.049 2.822 -1.960  
Cl 12.001 5.470 -1.182

*Asp*

MP2=-682.761821

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091356
H	1.029110	0.000000	1.450088
H	-0.493301	-0.916069	1.421085
C	-0.802571	1.179269	1.572739
O	-1.978786	1.328947	1.249926
N	-0.159323	2.041339	2.372620
H	0.829565	1.947058	2.555500
C	-0.760929	3.249705	2.875769
H	-1.343930	3.717567	2.077395
C	-1.708156	2.970916	4.048769
H	-2.256514	2.054476	3.820512
H	-1.135195	2.768811	4.959504
C	-2.759370	4.046681	4.369375
O	-3.603592	3.733959	5.227931
O	-2.700371	5.144241	3.750630
C	0.385877	4.188183	3.258259
O	1.555345	3.800270	3.270520
N	0.003649	5.419613	3.578123
H	-1.015119	5.571057	3.611111
C	0.936518	6.414387	4.040656
H	1.726605	6.581234	3.304962
H	0.402133	7.349880	4.198012
H	1.409761	6.117536	4.981286

*Glu•AuCl<sub>3</sub>*

MP2=-2235,803638

H	1.954	1.608	0.262
C	2.372	2.126	-0.608
H	1.637	2.847	-0.982
H	2.550	1.370	-1.381
C	3.689	2.746	-0.220
O	4.596	2.090	0.283
N	3.803	4.076	-0.461
H	3.065	4.597	-0.922
C	5.021	4.809	-0.189
H	5.472	4.391	0.722
C	6.006	4.670	-1.354
H	6.176	3.595	-1.515
H	5.529	5.066	-2.264
C	7.344	5.371	-1.121
H	7.215	6.460	-1.093
H	7.795	5.044	-0.174

C 8.284 4.982 -2.242  
O 8.049 5.671 -3.331  
O 9.104 4.082 -2.142  
C 4.632 6.269 -0.002  
O 3.790 6.780 -0.738  
N 5.292 6.930 0.970  
H 5.938 6.414 1.555  
C 5.087 8.336 1.248  
H 4.401 8.730 0.494  
H 4.647 8.481 2.241  
H 6.033 8.885 1.195  
Au 9.063 4.909 -4.944  
Cl 10.806 6.477 -4.565  
Cl 10.162 4.074 -6.870  
Cl 7.276 3.366 -5.218

*Glu*

MP2=-721.969974

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091292
H	1.029228	0.000000	1.449658
H	-0.493864	-0.915544	1.421389
C	-0.804153	1.178175	1.571467
O	-1.977637	1.329926	1.244426
N	-0.157436	2.045111	2.367558
H	0.804194	1.887180	2.625964
C	-0.781938	3.217882	2.929539
H	-1.520501	3.581900	2.210277
C	-1.488319	2.898302	4.252520
H	-2.175402	2.071892	4.062837
H	-0.740375	2.530955	4.962469
C	-2.254680	4.063624	4.844088
H	-1.583721	4.874843	5.137896
H	-2.926149	4.490446	4.087247
C	-3.134504	3.720989	6.060808
O	-3.535038	4.702998	6.728727
O	-3.397693	2.516945	6.274267
C	0.314484	4.252775	3.137368
O	1.433888	3.916018	3.511650
N	-0.026663	5.525951	2.917555
H	-0.969504	5.732061	2.635000
C	0.876488	6.619628	3.185572
H	1.825145	6.463532	2.669933
H	0.425637	7.542874	2.827796
H	1.078711	6.714044	4.255655

*Lys•Au/Cl<sub>3</sub>*

MP2=-2181,652789

H 2.157 1.253 -0.436  
 C 2.096 2.174 0.156  
 H 1.734 1.895 1.151  
 H 1.371 2.848 -0.311  
 C 3.477 2.763 0.285  
 O 4.407 2.141 0.792  
 N 3.620 4.026 -0.186  
 H 2.854 4.511 -0.641  
 C 4.888 4.723 -0.166  
 H 5.419 4.437 0.754  
 C 5.740 4.344 -1.382  
 H 5.839 3.248 -1.379  
 H 5.178 4.614 -2.291  
 C 7.118 4.986 -1.405  
 H 7.029 6.081 -1.485  
 H 7.638 4.787 -0.453  
 C 7.960 4.464 -2.561  
 H 8.081 3.373 -2.472  
 H 7.440 4.651 -3.514  
 C 9.323 5.129 -2.585  
 H 9.239 6.216 -2.708  
 H 9.882 4.933 -1.661  
 N 10.150 4.625 -3.712  
 H 9.694 4.811 -4.612  
 H 10.287 3.612 -3.641  
 C 4.575 6.213 -0.187  
 O 3.676 6.643 -0.907  
 N 5.361 6.988 0.588  
 H 6.056 6.540 1.173  
 C 5.245 8.430 0.638  
 H 4.478 8.729 -0.080  
 H 4.950 8.766 1.638  
 H 6.194 8.906 0.369  
 Au 12.053 5.501 -3.796  
 Cl 12.852 3.725 -2.442  
 Cl 14.185 6.503 -3.864  
 Cl 11.110 7.222 -5.129

Lys

MP2=-668.270834

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091390
H	1.039901	0.000000	1.421812
H	-0.490367	-0.905066	1.448897
C	-0.655748	1.266108	1.570503
O	-0.210249	2.372096	1.282004
N	-1.751531	1.107589	2.333650
H	-2.109932	0.186959	2.534507

C	-2.507375	2.217839	2.857243
H	-1.807707	3.031998	3.062483
C	-3.555521	2.699243	1.848143
H	-3.023805	2.915441	0.917025
H	-4.242617	1.871631	1.644156
C	-4.328956	3.927298	2.296027
H	-4.897607	3.704265	3.204579
H	-3.627942	4.729242	2.554927
C	-5.280587	4.420757	1.216767
H	-4.714610	4.669919	0.313082
H	-5.981445	3.622656	0.949848
C	-6.046720	5.634104	1.690459
H	-6.662036	5.407270	2.560715
H	-5.380701	6.459654	1.940702
N	-6.970820	6.138464	0.631158
H	-7.647431	5.426103	0.355244
H	-7.495638	6.952908	0.950527
H	-6.459587	6.413959	-0.208180
C	-3.176393	1.743926	4.140408
O	-3.676727	0.626079	4.207245
N	-3.212553	2.621820	5.146277
H	-2.748560	3.507149	5.037000
C	-3.882937	2.332011	6.392001
H	-4.919338	2.042160	6.209790
H	-3.387252	1.517530	6.925021
H	-3.867267	3.224095	7.014375

*Arg•AuCl<sub>3</sub>*

MP2=-2290,995221

H	2.040	1.417	-0.299
C	2.020	2.358	0.263
H	1.654	2.126	1.270
H	1.318	3.045	-0.221
C	3.423	2.896	0.366
O	4.324	2.268	0.916
N	3.622	4.119	-0.185
H	2.880	4.605	-0.678
C	4.920	4.758	-0.201
H	5.433	4.510	0.739
C	5.757	4.259	-1.384
H	5.813	3.164	-1.302
H	5.208	4.488	-2.311
C	7.158	4.848	-1.444
H	7.109	5.935	-1.611
H	7.677	4.693	-0.484
C	7.966	4.209	-2.556
H	8.069	3.129	-2.370
H	7.444	4.339	-3.518

N 9.289 4.818 -2.628  
H 9.470 5.615 -2.029  
C 10.274 4.409 -3.436  
N 10.024 3.464 -4.350  
H 9.127 3.000 -4.383  
H 10.810 2.982 -4.778  
N 11.508 4.914 -3.306  
H 11.568 5.711 -2.676  
C 4.676 6.256 -0.325  
O 3.813 6.676 -1.092  
N 5.482 7.044 0.416  
H 6.135 6.606 1.054  
C 5.421 8.490 0.381  
H 4.699 8.777 -0.387  
H 5.096 8.894 1.347  
H 6.400 8.913 0.132  
Au 12.801 5.165 -4.877  
Cl 12.345 7.487 -4.762  
Cl 13.215 2.812 -4.952  
Cl 14.325 5.505 -6.664

#### Arg

MP2=-777.621172

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091282
H	1.040034	0.000000	1.421645
H	-0.490115	-0.904938	1.449459
C	-0.654852	1.266557	1.569781
O	-0.222835	2.372535	1.261717
N	-1.734591	1.111047	2.356654
H	-2.088971	0.192301	2.572944
C	-2.484712	2.225893	2.876993
H	-1.781841	3.035755	3.088910
C	-3.520904	2.714203	1.858004
H	-2.983487	2.894255	0.922910
H	-4.232152	1.902833	1.673948
C	-4.252009	3.975820	2.281058
H	-4.818622	3.798199	3.200482
H	-3.528587	4.770305	2.493953
C	-5.200166	4.446378	1.196522
H	-4.638387	4.639044	0.276837
H	-5.940728	3.666235	0.988284
N	-5.869686	5.665750	1.614328
H	-5.726684	5.978074	2.561078
C	-6.681855	6.378320	0.847042
N	-6.947177	5.982604	-0.391593
H	-6.601950	5.108459	-0.744779
H	-7.566706	6.509523	-0.981667

N	-7.233113	7.493117	1.317932
H	-6.975820	7.856314	2.218484
H	-7.824666	8.062903	0.739757
C	-3.169163	1.754655	4.153416
O	-3.663754	0.634447	4.217462
N	-3.228870	2.640258	5.151691
H	-2.747831	3.518029	5.053484
C	-3.910288	2.353039	6.392219
H	-4.904725	1.953315	6.189912
H	-3.359714	1.621059	6.988247
H	-4.005589	3.274577	6.962602

**Table S6.** Cartesian coordinates for the complexes of Au(III) and polar amino acids (Figure 9 in main text).

*Asn•AuCl<sub>3</sub>*

MP2= -2176,728037

H	1.624	2.504	-1.440
C	1.976	2.591	-0.405
H	1.828	1.618	0.074
H	1.372	3.345	0.110
C	3.446	2.906	-0.421
O	4.287	2.067	-0.753
N	3.772	4.181	-0.105
H	3.051	4.871	0.094
C	5.115	4.708	-0.031
H	5.649	4.272	0.829
C	5.971	4.391	-1.272
H	6.900	4.970	-1.249
H	6.221	3.328	-1.264
C	5.251	4.729	-2.544
O	5.271	5.948	-2.889
N	4.647	3.755	-3.190
H	4.152	3.903	-4.065
H	4.617	2.828	-2.765
C	4.966	6.219	0.206
O	3.861	6.751	0.214
N	6.110	6.897	0.401
H	6.987	6.399	0.487
C	6.096	8.331	0.613
H	5.603	8.589	1.559
H	7.125	8.695	0.634
H	5.558	8.825	-0.204
Au	4.311	6.764	-4.562
Cl	5.670	5.449	-5.998
Cl	3.300	7.783	-6.400
Cl	2.959	8.036	-3.089

*Asn*

MP2=-663.3543395

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091553
H	1.039685	0.000000	1.422103
H	-0.492991	-0.903569	1.448840
C	-0.655276	1.263180	1.570652
O	-0.196930	2.373326	1.303415
N	-1.778573	1.118588	2.292533
H	-2.101069	0.212731	2.600877
C	-2.446916	2.253347	2.861379
H	-1.705446	2.844922	3.413415
C	-3.083332	3.160357	1.782919
H	-2.600512	2.951561	0.830514
H	-4.150500	2.963060	1.683671
C	-2.881172	4.605501	2.165313
O	-3.681039	5.201752	2.883675
N	-1.744137	5.148799	1.714935
H	-1.469957	6.060852	2.042125
H	-1.049329	4.553507	1.287690
C	-3.463536	1.748484	3.886612
O	-3.507680	0.564697	4.204087
N	-4.260696	2.685213	4.401463
H	-4.206056	3.632827	4.039689
C	-5.269468	2.363426	5.382386
H	-4.824916	1.852757	6.238490
H	-5.732029	3.287618	5.722907
H	-6.041873	1.714957	4.961090

*Gln•AuCl<sub>3</sub>*

MP2= -2215,942717

H	1.611	1.955	0.495
C	2.018	2.423	-0.408
H	1.344	3.223	-0.731
H	2.049	1.651	-1.186
C	3.421	2.889	-0.126
O	4.282	2.140	0.328
N	3.673	4.193	-0.406
H	2.974	4.789	-0.836
C	4.985	4.774	-0.229
H	5.432	4.343	0.678
C	5.876	4.450	-1.434
H	5.905	3.357	-1.540
H	5.403	4.863	-2.337
C	7.302	4.988	-1.290
H	7.326	6.085	-1.301
H	7.741	4.648	-0.342
C	8.150	4.440	-2.396



O 8.487 3.224 -2.282  
N 8.451 5.209 -3.423  
H 9.049 4.885 -4.178  
H 8.155 6.177 -3.447  
C 4.797 6.281 -0.104  
O 3.999 6.861 -0.835  
N 5.583 6.894 0.804  
H 6.159 6.324 1.412  
C 5.562 8.325 1.024  
H 4.960 8.779 0.234  
H 5.117 8.569 1.996  
H 6.577 8.734 0.985  
Au 9.330 2.042 -3.785  
Cl 11.292 3.381 -3.803  
Cl 10.248 0.614 -5.384  
Cl 7.318 0.786 -3.773

*Gln*

MP2=-702.569336

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091145
H	1.028898	0.000000	1.450191
H	-0.494308	-0.915261	1.421491
C	-0.803992	1.177534	1.570865
O	-1.971955	1.340841	1.233162
N	-0.162654	2.035466	2.383842
H	0.790094	1.864306	2.665433
C	-0.796385	3.200457	2.948591
H	-1.518971	3.576679	2.219814
C	-1.526517	2.851542	4.249473
H	-2.207220	2.026577	4.033633
H	-0.790536	2.485094	4.971431
C	-2.311338	4.008316	4.838726
H	-1.654850	4.835664	5.117858
H	-3.012723	4.404021	4.093730
C	-3.148536	3.583526	6.027213
O	-3.637643	2.465788	6.116432
N	-3.340144	4.528912	6.963403
H	-3.934308	4.330503	7.750963
H	-2.938776	5.446081	6.882971
C	0.298337	4.227732	3.205934
O	1.384853	3.880743	3.656780
N	-0.013458	5.501717	2.953161
H	-0.905183	5.713953	2.539792
C	0.905511	6.581913	3.225522
H	1.234544	6.549246	4.265594
H	1.787650	6.519469	2.584227
H	0.399338	7.527092	3.041839

*Ser•Au/Cl<sub>3</sub>*

MP2=-2083,401118

H 6.677 -1.081 -0.205  
C 6.090 -0.315 0.310  
H 6.659 0.622 0.267  
H 5.966 -0.595 1.361  
C 4.784 -0.125 -0.413  
O 4.697 -0.109 -1.636  
N 3.696 0.053 0.385  
H 3.763 0.062 1.398  
C 2.399 0.355 -0.162  
H 2.514 1.001 -1.045  
C 1.751 -0.954 -0.605  
H 2.414 -1.441 -1.328  
H 1.568 -1.621 0.247  
O 0.507 -0.674 -1.294  
H 0.322 -1.378 -1.942  
C 1.589 1.048 0.931  
O 1.830 0.851 2.114  
N 0.565 1.822 0.495  
H 0.553 2.107 -0.479  
C -0.256 2.566 1.437  
H -0.600 1.892 2.229  
H 0.302 3.392 1.894  
H -1.125 2.963 0.905  
Au -1.357 -0.270 -0.232  
Cl -3.376 0.210 0.805  
Cl -0.760 -1.672 1.575  
Cl -1.919 1.158 -2.038

*Ser*

MP2=-570.0331055

H 0.000000 0.000000 0.000000  
C 0.000000 0.000000 1.091227  
H 1.040153 0.000000 1.421400  
H -0.490930 -0.904722 1.448638  
C -0.654499 1.265944 1.571459  
O -0.229171 2.372423 1.258614  
N -1.739065 1.109184 2.353846  
H -1.982735 0.200462 2.720941  
C -2.406816 2.217433 2.974086  
H -1.662937 2.947965 3.314366  
C -3.320555 2.937230 1.982896  
H -2.767689 3.061939 1.047345  
H -4.211975 2.329776 1.787976  
O -3.662548 4.195256 2.539116  
H -4.374823 4.579763 2.021006  
C -3.157968 1.683148 4.195590

O	-3.065806	0.507518	4.535831
N	-3.898062	2.582475	4.845684
H	-3.996702	3.494684	4.421134
C	-4.696962	2.226944	5.993250
H	-4.082700	1.727027	6.743631
H	-5.112708	3.135093	6.425211
H	-5.516268	1.556270	5.720416

*Thr•AuCl<sub>3</sub>*

MP2=-2122,620542

H	1.676	1.312	0.723
C	1.794	2.396	0.645
H	1.404	2.844	1.568
H	1.199	2.773	-0.194
C	3.255	2.729	0.519
O	4.137	2.073	1.056
N	3.532	3.835	-0.242
H	2.781	4.491	-0.455
C	4.840	4.441	-0.217
H	5.377	4.098	0.682
C	5.688	4.030	-1.425
H	6.648	4.559	-1.397
C	5.885	2.546	-1.588
H	4.928	2.038	-1.767
H	6.561	2.332	-2.425
H	6.320	2.128	-0.675
O	5.018	4.600	-2.600
C	4.658	5.964	-0.201
O	3.568	6.464	-0.457
N	5.775	6.666	0.067
H	6.613	6.169	0.343
C	5.811	8.114	0.077
H	4.838	8.478	-0.261
H	6.004	8.495	1.087
H	6.589	8.484	-0.599
H	4.191	4.098	-2.767
Au	6.074	4.708	-4.455
Cl	7.651	6.154	-3.440
Cl	7.177	4.868	-6.486
Cl	4.458	3.229	-5.357

*Thr*

MP2=-609.255219

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.091474
H	1.039860	0.000000	1.421591
H	-0.491465	-0.904956	1.447671
C	-0.655021	1.267109	1.569426

O	-0.198237	2.369621	1.289592
N	-1.772994	1.104960	2.303380
H	-2.044911	0.181087	2.598817
C	-2.475356	2.194090	2.918534
H	-1.827808	3.072999	2.871985
C	-3.784132	2.539041	2.195436
H	-4.225884	3.400292	2.715718
C	-3.560709	2.901048	0.743512
H	-3.102529	2.067629	0.207856
H	-4.514974	3.138557	0.266815
H	-2.910759	3.773822	0.657653
O	-4.630410	1.410390	2.333973
H	-5.439210	1.576632	1.841205
C	-2.754489	1.831413	4.378363
O	-2.675650	0.678336	4.781367
N	-3.112042	2.853905	5.163563
H	-3.105446	3.787061	4.788879
C	-3.462051	2.664984	6.551392
H	-4.270392	1.937777	6.647603
H	-2.607164	2.305378	7.129002
H	-3.791284	3.617063	6.962357