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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•$AuICl_3$

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•$AuICl_3$

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-backbonel•AulCl₃

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•AulCl₃

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

$[AuCl_4]^-$

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

$4H_2O$

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

$[3H_2O \cdot H_3O^+ \cdot Cl^-]$

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

$[4H_2O \cdot Cl^-]$

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•$AuCl_3$

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•AuICl$_3$

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)•AuICl₃

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•$AuICl_3$

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

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(Nδ)•AuIICl$_3$

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)•AuICl$_3$
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 - Nδ 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 – Nε 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•$AuICl_3$

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•AulCl$_3$

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•AulCl$_3$
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•$AuICl_3$

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•$AuICl_3$
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•AulCl$_3$
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•AulCl$_3$

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•AuICl₃

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•$AuICl_3$

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•AuICl$_3$

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•AulCl$_3$

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