Supporting information:

The calculations are based on Density functional theory within the local density approximation. Core electrons are described by Trouillier-Martins pseudopotentials and valence electrons are expanded in localized numerical basis sets as implemented in the SIESTA program. We use a Double ζ+Polarization basis set for the molecule, and a single ζ for the gold *s*, *p* and *d* channels. The relaxed molecular coordinates of the molecule and the coordinates of the first gold layers are given below.

Au	1.443009	-0.833121	8.247346
Au	2.885970	-3.332431	8.247348
Au	4.328956	-5.831724	8.247343
Au	2.885977	1.666217	8.247344
Au	4.328956	-0.833107	8.247350
Au	5.771942	-3.332431	8.247348
Au	4.328956	4.165530	8.247343
Au	5.771936	1.666217	8.247344
Au	7.214901	-0.833123	8.247342
S	2.883010	-0.028921	10.047609
C	2.515770	-0.364941	14.579670
C	1.386960	-0.060178	13.784806
C	1.493840	0.022841	12.402747
C	2.738610	-0.190367	11.789884
C	3.872760	-0.496504	12.558133
C	3.756960	-0.584849	13.938200
H	0.412306	0.117718	14.279955
H	0.623489	0.254596	11.751366
H	4.838910	-0.670372	12.039426
H	4.636000	-0.831444	14.564670
N	0.116939	-0.766809	18.570578
H	0.215527	-0.699637	17.550885
H	-0.808278	-0.821543	18.995571
C	1.237820	-0.801263	20.716481
C	1.247940	-0.725323	19.311175
C	2.502260	-0.620700	18.635030
C	3.682710	-0.608381	19.402060
C	3.648320	-0.699253	20.787321
H	4.650130	-0.530244	18.863803
C	2.503620	-0.535959	17.225330
C	2.441510	-0.454087	15.991412
C	2.417620	-0.805556	21.460042
C	2.379430	-0.928045	22.955634
H	3.111390	-1.705174	23.293659
H	1.373390	-1.289010	23.285373
H	4.594420	-0.712100	21.364095
H	0.517566	0.269465	25.368547
C	2.698660	0.380351	23.682319
H	3.697220	0.757920	23.346036
H	1.951280	1.155597	23.375868
H	4.894200	0.113394	25.435391
H	0.263930	-0.889413	21.242063
N	5.134910	-0.182005	27.938882
O	6.146040	0.004577	27.258223
O	5.135820	-0.463509	29.133945
C	2.456950	-0.211247	30.655927
C	2.629060	-0.195104	29.432450
C	2.661660	-0.105501	28.023168
C	1.462160	0.009581	27.280595
C	1.487880	0.164129	25.899314
C	2.693220	0.216972	25.171767
C	3.881570	0.083701	25.891704
C	3.861300	-0.072875	27.275368
H	0.489465	-0.012195	27.815184
C	1.367030	-0.069753	32.874311
C	2.515680	-0.233356	32.068689

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C   3.777100  -0.405249  32.686324
C   3.892810  -0.392451  34.070245
C   1.475350  -0.052003  34.258891
C   2.740130  -0.198432  34.849174
H   0.597567   0.081259  34.928321
H   0.384603   0.055921  32.379880
H   4.654980  -0.537615  32.019507
H   4.866720  -0.520292  34.588365
S   2.885000  -0.048884  36.591014
Au   1.443020  -0.833130  38.388500
Au   2.885970  -3.332431  38.388500
Au   4.328954  -5.831725  38.388500
Au   2.885977   1.666218  38.388500
Au   4.328958  -0.833107  38.388500
Au   5.771942  -3.332430  38.388500
Au   4.328956   4.165530  38.388500
Au   5.771936   1.666217  38.388500
Au   7.214909  -0.833117  38.388500
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