

Supramolecular gold(I) vesicles. In-depth study of the aggregation process

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Supporting information

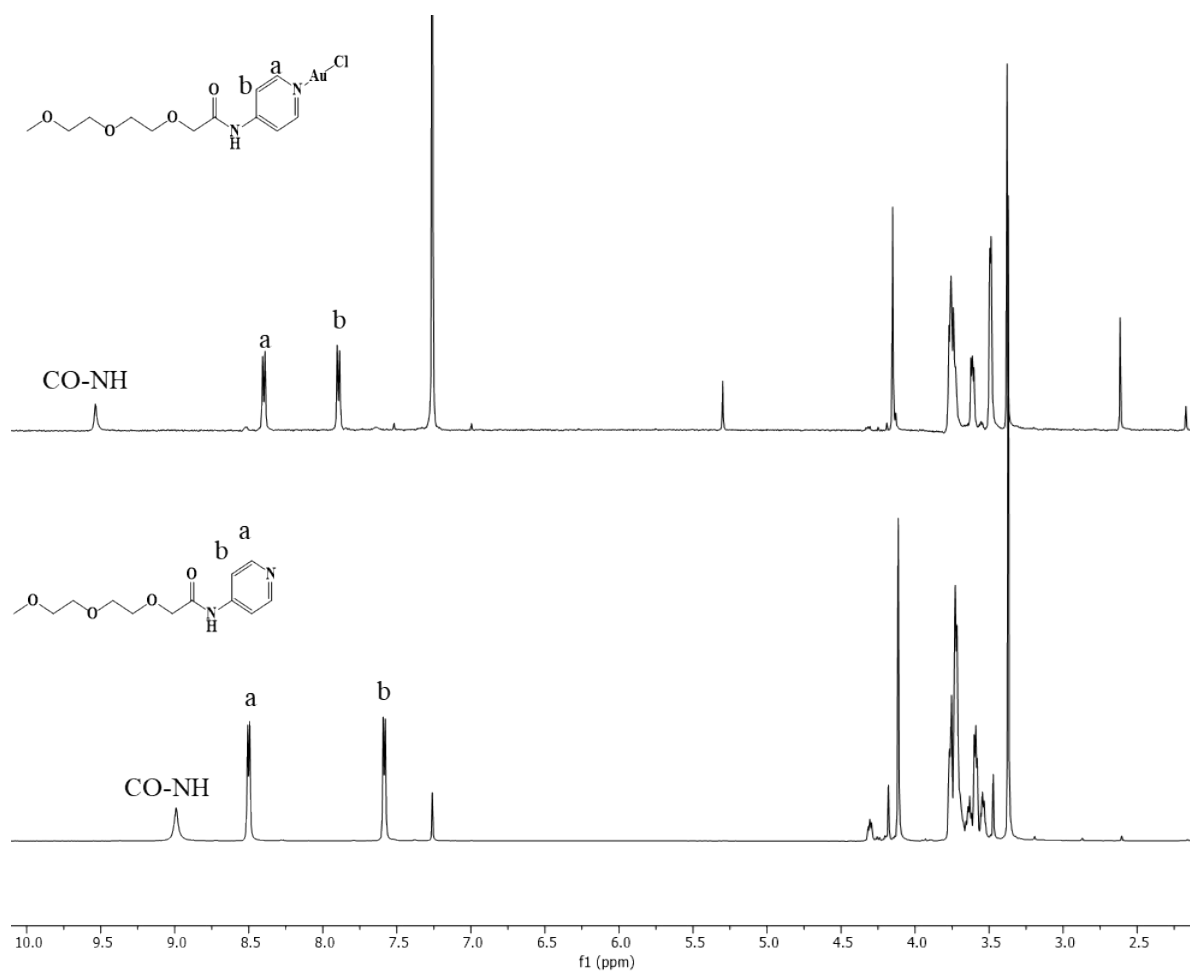


Figure S1. ¹H NMR of **2** (above) and **1** (below) in CDCl₃.

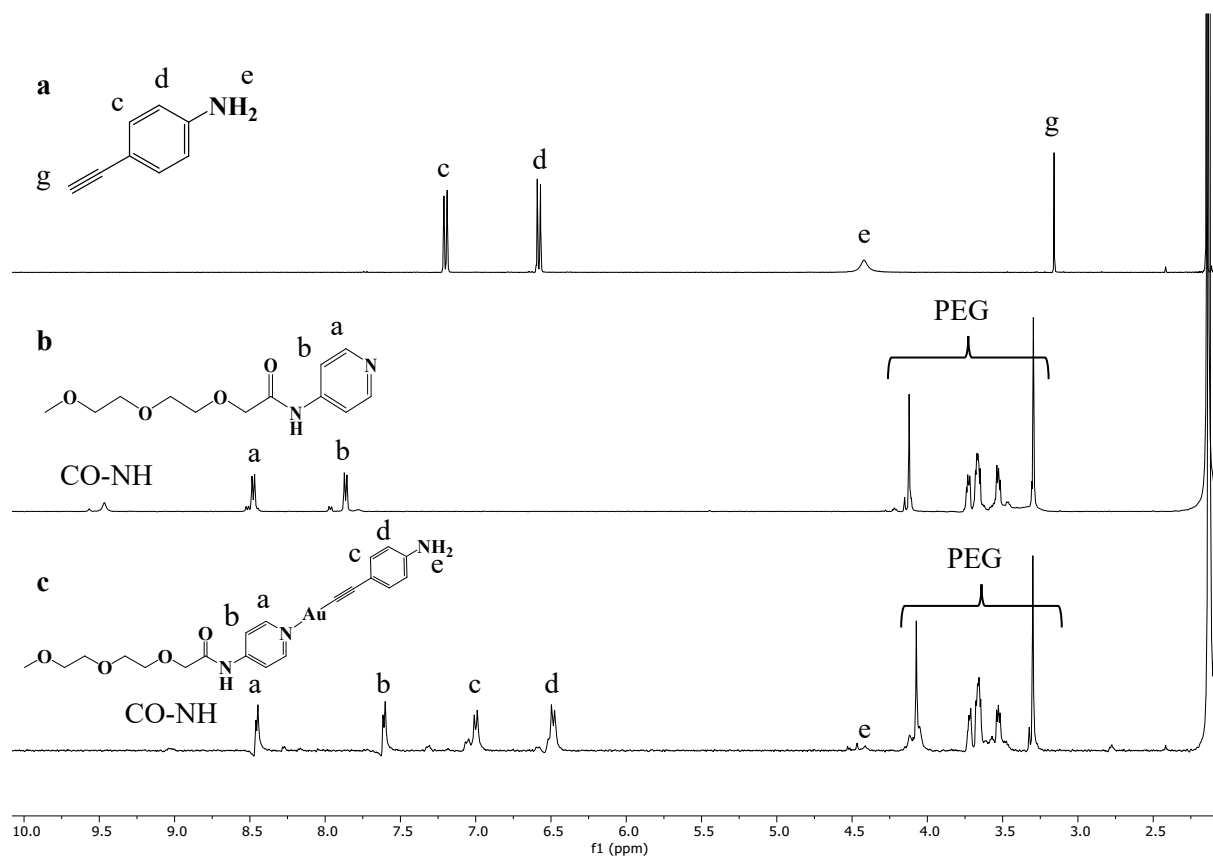


Figure S2. $^1\text{H-NMR}$ spectra of 4-ethynylaniline (a), **1** (b) and **3** (c) in $\text{ACN-}d_3$.

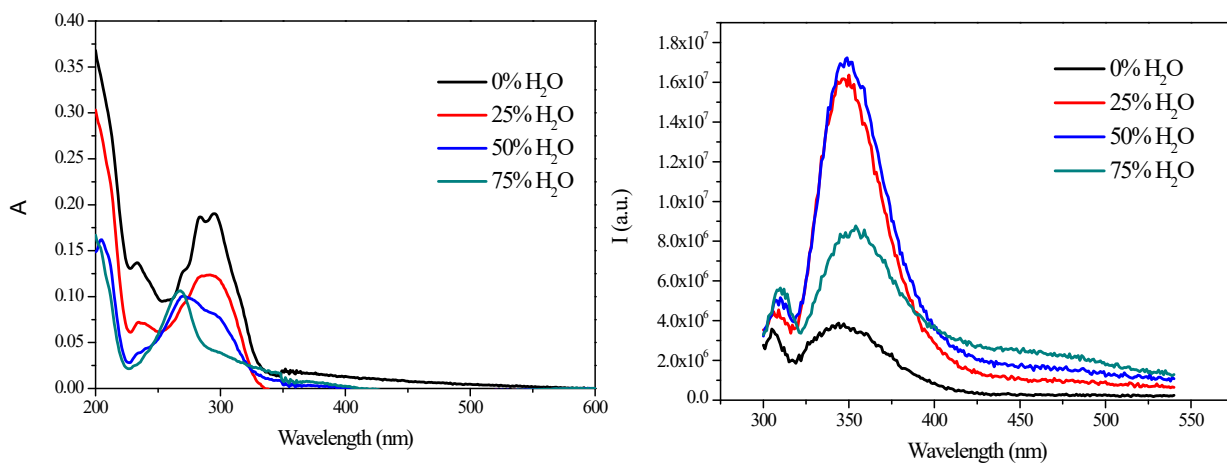


Figure S3. Absorption (left) and emission (right) spectra of **3** in acetonitrile/water mixtures.

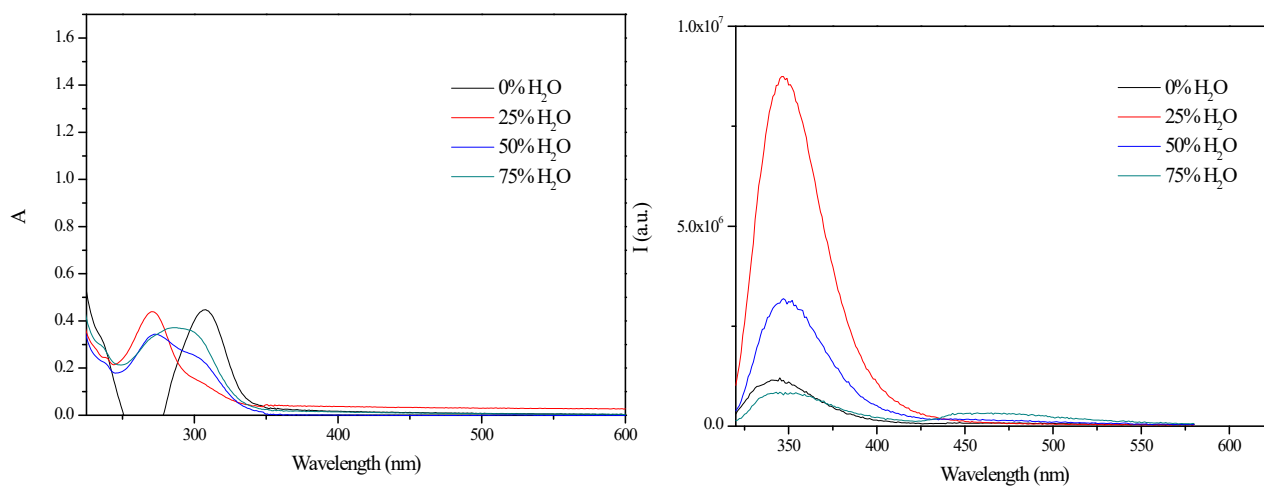


Figure S4. Absorption (left) and emission (right) spectra of **6** in acetonitrile/water mixtures.

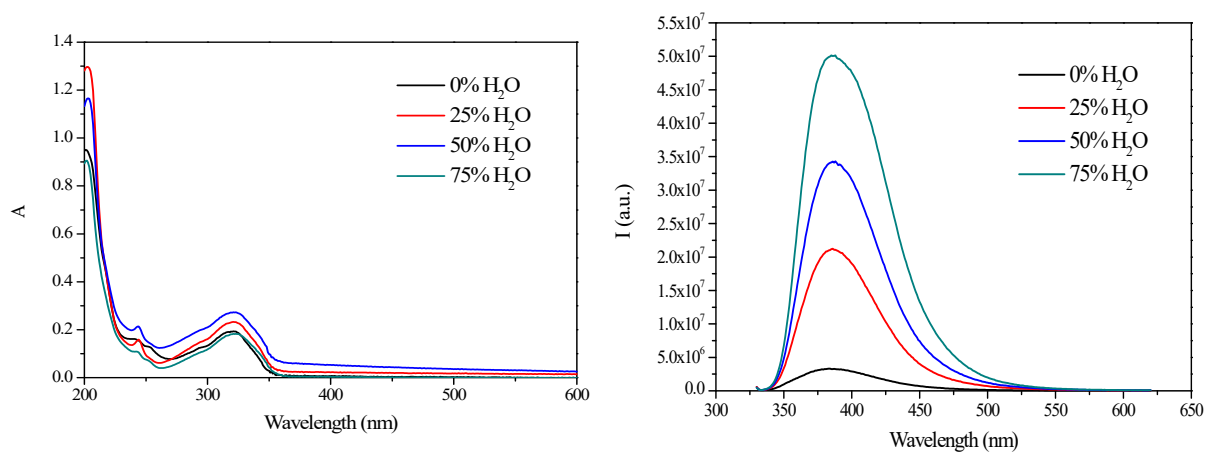


Figure S5. Absorption (left) and emission (right) spectra of **7** in acetonitrile/water mixtures.

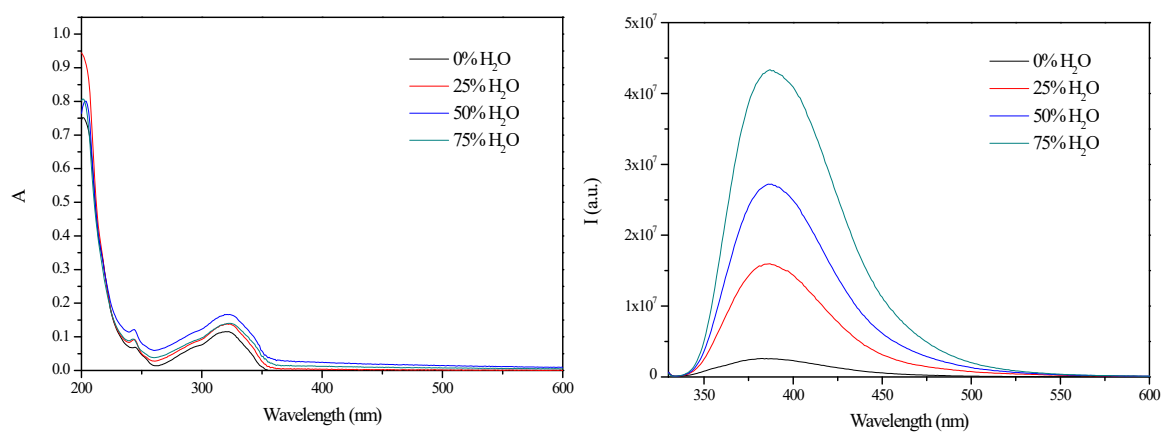


Figure S6. Absorption (left) and emission (right) spectra of **8** in acetonitrile/water mixtures.

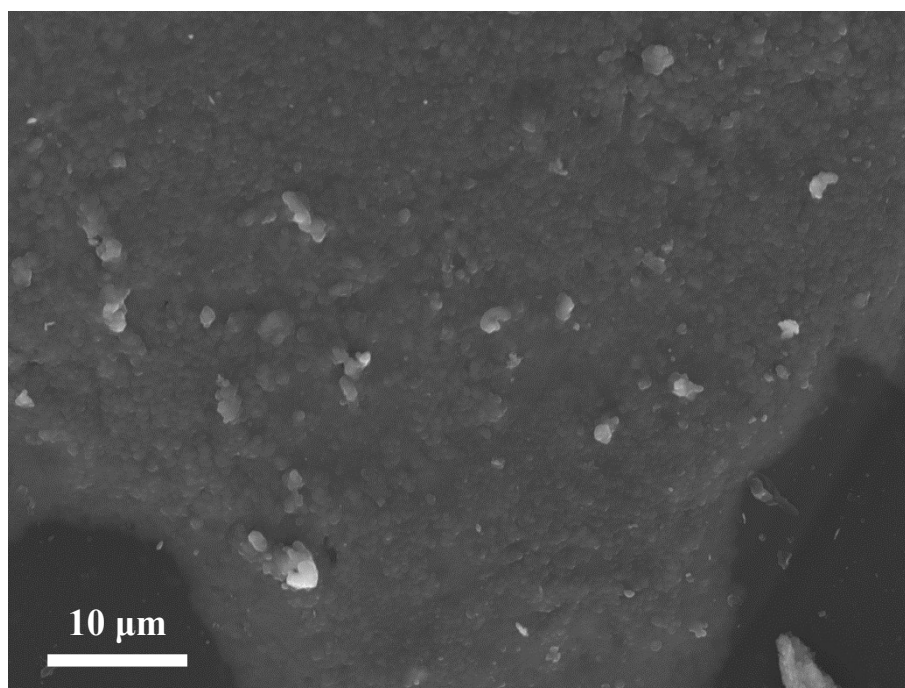


Figure S7. SEM micrograph of **4** in acetonitrile/water mixtures (25/75).

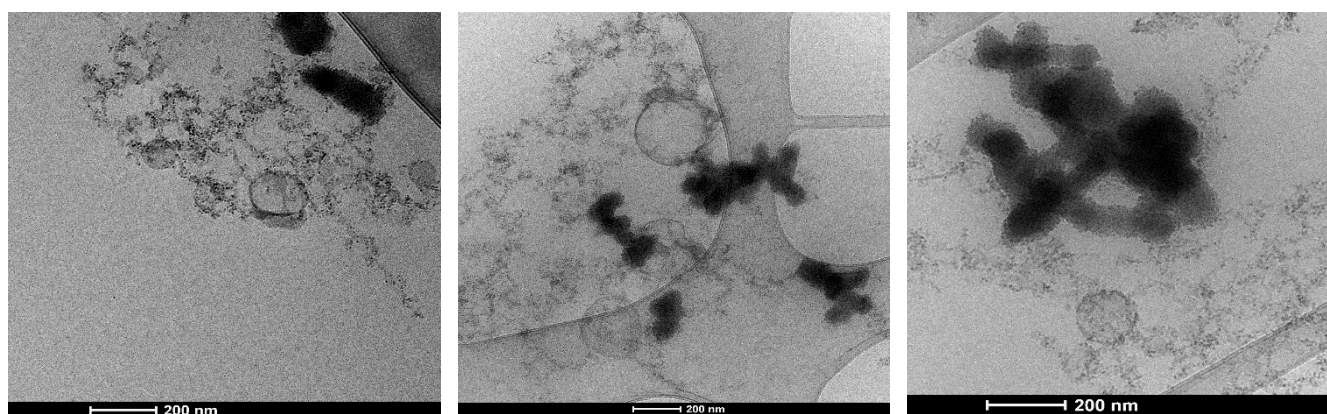


Figure S8. Cryo-TEM micrograph of **4** DMSO/water mixtures (25/75).

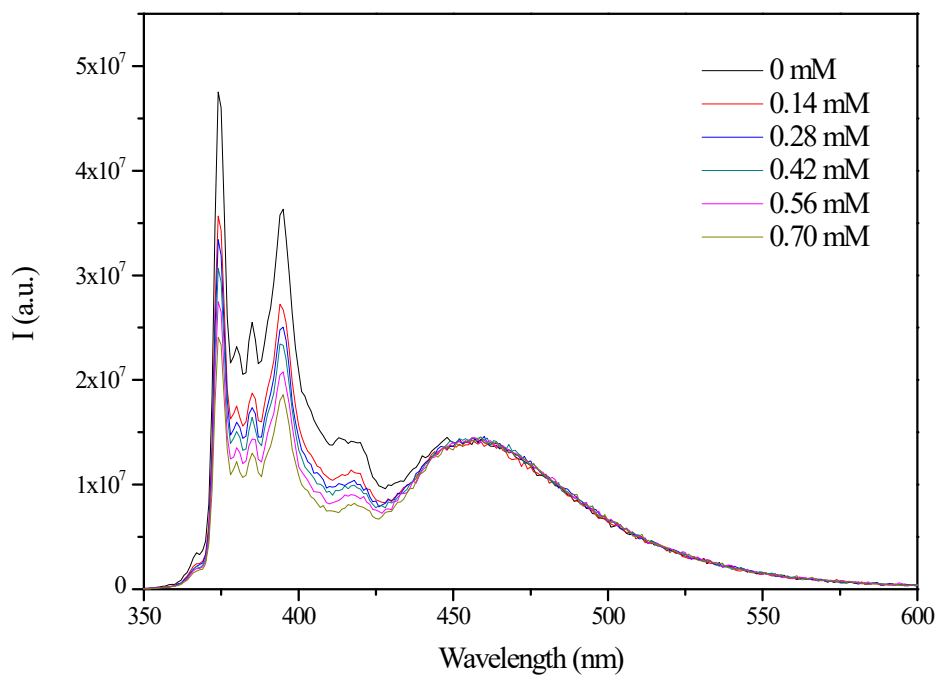


Figure S9. Emission spectra of gold(I) aggregates in the presence of pyrene and at different amounts of quencher.

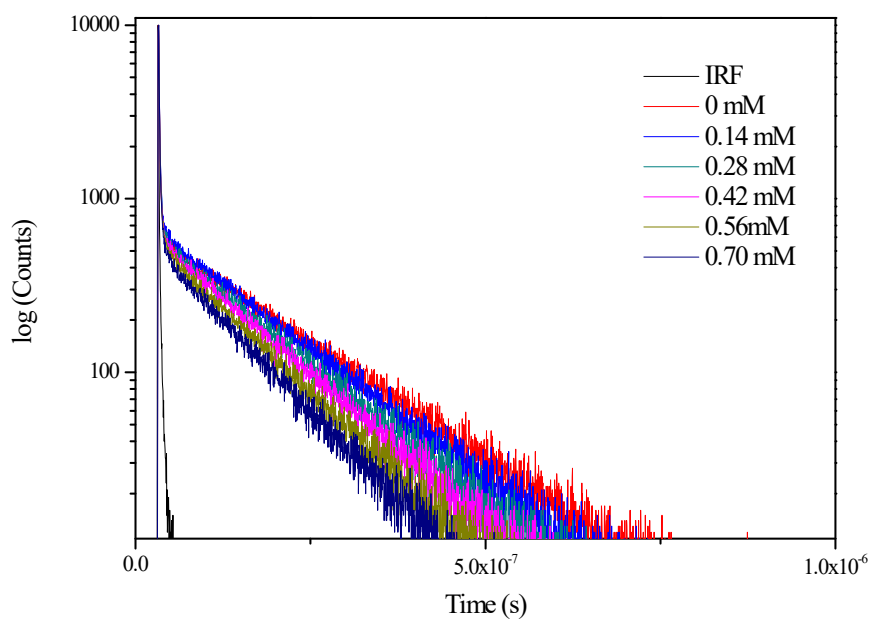


Figure S10. Decay profiles for pyrene fluorescence quenching by CPC in gold(I) aggregates.

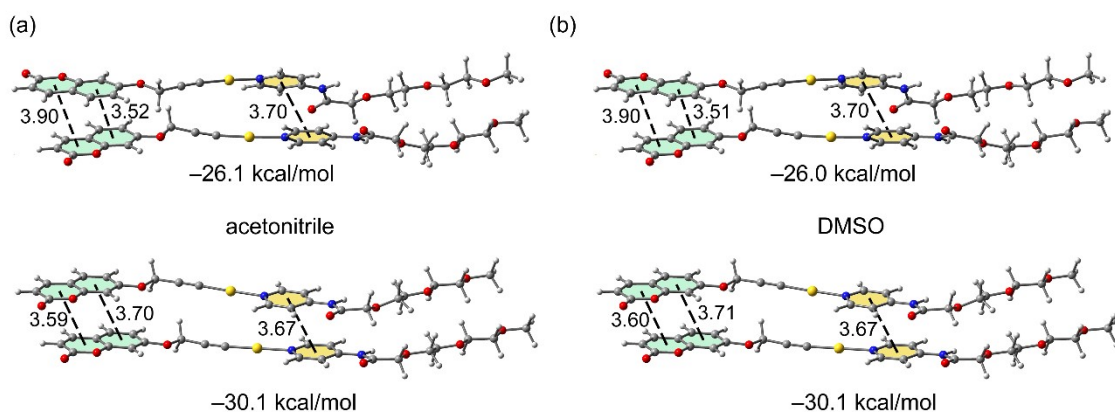


Figure S11. Representative π -stacked dimers of the vesicle optimized using acetonitrile (a) or DMSO as solvents. Level of theory: RI-BP86-COSMO/def2-TZVP. Distances in Å

For the XYZ coordinates of the vesicle, please contact toni.frontera@uib.es. The file occupies 3451 lines!. The Cartesian coordinates of the π -stacking dimers in Figure 13 (main text) follow:

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π-π (Fig 13b)
C      3.62574848    7.25645946    4.70225935
H      3.93060308    8.05810198    4.01810861
H      2.95768804    7.67357361    5.47792403
H      4.52167083    6.83745580    5.19566403
O      2.95509409    6.26624355    3.91959317
C      2.51656491    5.16747258    4.71622002
H      3.37530309    4.67835111    5.21587158
H      1.81471718    5.50827260    5.50171462
C      1.82271891    4.17865025    3.79296822
H      0.95628428    4.66054846    3.30146871
H      2.52114353    3.84061998    3.00426080
O      1.39767757    3.07611448    4.59545551
C      0.72174946    2.07708849    3.83453639
H      -0.18536361    2.49272279    3.35676236
H      1.37816003    1.67798294    3.03808922
C      0.34162699    0.96700518    4.80039813
H      1.24643944    0.54607554    5.27485845
H      -0.31851349    1.36054093    5.59424827
O      -0.33743767    -0.04208454    4.04368489
C      -0.74006682    -1.14789460    4.83925870
H      0.10891351    -1.56017302    5.41669845
H      -1.53166662    -0.86730057    5.55742519
C      -1.28183737    -2.27917263    3.97688431
O      -1.76498910    -3.28450260    4.49508287
N      -1.16036145    -2.06183346    2.62370669
H      -0.73189210    -1.16393567    2.38624994
C      -1.53815104    -2.87880323    1.56801291
C      -2.12531531    -4.14832051    1.72222326
C      -1.32118419    -2.41356932    0.25689877
C      -2.45887068    -4.87475924    0.59090861
H      -2.31777183    -4.56427965    2.70534002
C      -1.68350656    -3.20107275    -0.81930660
H      -0.87034772    -1.43801236    0.07579634
H      -2.91292319    -5.85958617    0.68664415
H      -1.52292966    -2.85718650    -1.83942106
N      -2.24950496    -4.42611385    -0.67098085
Au      -2.77665745    -5.58792691    -2.31373054
C      -3.27968236    -6.69449322    -3.83248081
C      -3.60771538    -7.41086387    -4.77370015
C      -3.99823434    -8.24825580    -5.89297154
H      -4.70812281    -7.71912984    -6.55192663
H      -3.12105710    -8.54399952    -6.49359661
O      -4.64139888    -9.45011145    -5.36388459

```


C	-5.11851534	-10.36223353	-6.25173197
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C	-6.25815884	-12.46323692	-6.50867052
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C	-5.55292359	-11.23318036	-8.46595996
H	-4.54616050	-9.37485731	-8.11442129
C	-6.18256325	-12.36876670	-7.91912689
H	-5.48413825	-11.14141608	-9.55097692
C	-6.75077341	-13.42795430	-8.69128976
C	-7.34692485	-14.49362142	-8.08394256
H	-6.70183083	-13.37146713	-9.78081462
H	-7.78871697	-15.31289434	-8.64810655
O	-6.85910110	-13.54184313	-5.90651358
C	-7.42502763	-14.59056140	-6.64582416
O	-7.93522075	-15.49463536	-5.99492333
C	0.67563928	8.81316505	3.13024446
H	0.98049388	9.61480757	2.44609372
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H	1.57156163	8.39416139	3.62364914
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H	-1.99382492	6.21725405	1.72945382
H	-0.42896567	5.39732557	1.43224591
O	-1.55243163	4.63282007	3.02344062
C	-2.22835974	3.63379408	2.26252150
H	-3.13547281	4.04942838	1.78474747
H	-1.57194917	3.23468853	1.46607433
C	-2.60848221	2.52371077	3.22838324
H	-1.70366976	2.10278113	3.70284356
H	-3.26862269	2.91724652	4.02223338
O	-3.28754687	1.51462105	2.47167000
C	-3.69017602	0.40881099	3.26724381
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H	-4.48177582	0.68940502	3.98541030
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O	-4.71509830	-1.72779701	2.92306798
N	-4.11047065	-0.50512787	1.05169180
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O	-9.80921030	-11.98513754	-7.47852847
C	-10.37513683	-13.03385581	-8.21783905
O	-10.88532995	-13.93792977	-7.56693822
π-π (Fig 13d)			
C	3.62574848	7.25645946	4.70225935

H	3.93060308	8.05810198	4.01810861
H	2.95768804	7.67357361	5.47792403
H	4.52167083	6.83745580	5.19566403
O	2.95509409	6.26624355	3.91959317
C	2.51656491	5.16747258	4.71622002
H	3.37530309	4.67835111	5.21587158
H	1.81471718	5.50827260	5.50171462
C	1.82271891	4.17865025	3.79296822
H	0.95628428	4.66054846	3.30146871
H	2.52114353	3.84061998	3.00426080
O	1.39767757	3.07611448	4.59545551
C	0.72174946	2.07708849	3.83453639
H	-0.18536361	2.49272279	3.35676236
H	1.37816003	1.67798294	3.03808922
C	0.34162699	0.96700518	4.80039813
H	1.24643944	0.54607554	5.27485845
H	-0.31851349	1.36054093	5.59424827
O	-0.33743767	-0.04208454	4.04368489
C	-0.74006682	-1.14789460	4.83925870
H	0.10891351	-1.56017302	5.41669845
H	-1.53166662	-0.86730057	5.55742519
C	-1.28183737	-2.27917263	3.97688431
O	-1.76498910	-3.28450260	4.49508287
N	-1.16036145	-2.06183346	2.62370669
H	-0.73189210	-1.16393567	2.38624994
C	-1.53815104	-2.87880323	1.56801291
C	-2.12531531	-4.14832051	1.72222326
C	-1.32118419	-2.41356932	0.25689877
C	-2.45887068	-4.87475924	0.59090861
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H	-2.91292319	-5.85958617	0.68664415
H	-1.52292966	-2.85718650	-1.83942106
N	-2.24950496	-4.42611385	-0.67098085
Au	-2.77665745	-5.58792691	-2.31373054
C	-3.27968236	-6.69449322	-3.83248081
C	-3.60771538	-7.41086387	-4.77370015
C	-3.99823434	-8.24825580	-5.89297154
H	-4.70812281	-7.71912984	-6.55192663
H	-3.12105710	-8.54399952	-6.49359661
O	-4.64139888	-9.45011145	-5.36388459
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C	-5.73726088	-11.48275500	-5.67646577
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C	-6.25815884	-12.46323692	-6.50867052
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C	-5.55292359	-11.23318036	-8.46595996
H	-4.54616050	-9.37485731	-8.11442129
C	-6.18256325	-12.36876670	-7.91912689
H	-5.48413825	-11.14141608	-9.55097692
C	-6.75077341	-13.42795430	-8.69128976
C	-7.34692485	-14.49362142	-8.08394256
H	-6.70183083	-13.37146713	-9.78081462
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C	-7.42502763	-14.59056140	-6.64582416
O	-7.93522075	-15.49463536	-5.99492333
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H	-13.19975813	-18.98539412	-17.67550338
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H	-12.57413897	-17.87036885	-15.56068035
H	-14.50152909	-20.77071389	-13.28018540
N	-13.50463759	-19.26138704	-14.32077996
Au	-12.92862145	-18.25971598	-12.59127530
C	-12.37743097	-17.30293249	-10.98975108
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H	-12.47788892	-15.66462742	-8.19841222
H	-10.92163807	-16.54814498	-8.19004829
O	-10.91320562	-14.73283314	-9.24517814
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C	-9.82801987	-12.72546642	-8.77283181
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C	-9.34604888	-11.79268713	-7.86570943
H	-9.71529036	-12.56848866	-9.84488944
C	-10.12377500	-13.13423492	-6.01185683
H	-11.10883473	-14.97074655	-6.50924829
C	-9.47860517	-11.96741043	-6.46716480
H	-10.23595117	-13.28790784	-4.93751283
C	-8.95242908	-10.94973295	-5.61367321
C	-8.34353720	-9.84630501	-6.13483636
H	-9.04615745	-11.06783668	-4.53204615
H	-7.93556745	-9.05580986	-5.50766214
O	-8.72927692	-10.67845210	-8.38067406
C	-8.20842124	-9.66696063	-7.56076105
O	-7.68517774	-8.72134402	-8.13812065
π-π (Fig 13c)			
C	3.8890024	6.4818602	5.3316406
H	4.1852257	7.4696288	4.9576886
H	3.3005095	6.6036046	6.2589191
H	4.7933341	5.8915459	5.5654405
O	3.1117035	5.8566075	4.3089861
C	2.6049718	4.5927566	4.7325317
H	3.4277075	3.9290874	5.0590374
H	1.9152373	4.7208696	5.5894940
C	1.8577192	3.9764164	3.5599491
H	1.1771508	4.7309866	3.1238349
H	2.5645384	3.6484361	2.7771037
O	1.1141654	2.8687802	4.0727520
C	0.5701464	2.0218887	3.0576520
H	0.0599135	2.6098463	2.2730321
H	1.3631282	1.4179524	2.5803763
C	-0.4368053	1.1401146	3.7745102
H	0.0624753	0.5683286	4.5774807
H	-1.2133478	1.7739534	4.2403525
O	-1.0387755	0.2419624	2.8324538
C	-2.0660439	-0.5237956	3.4507386
H	-1.7369115	-0.9168555	4.4314688
H	-2.9746677	0.0804428	3.6238070
C	-2.4669574	-1.7262994	2.6147125
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N	-1.6067930	-2.0171525	1.5811033
H	-0.8390336	-1.3510160	1.4724903
C	-1.7523133	-2.9999557	0.6083808
C	-2.6430645	-4.0815388	0.7268309
C	-0.9802913	-2.9126092	-0.5636694
C	-2.7614785	-4.9704377	-0.3274937
H	-3.2505766	-4.2173616	1.6143478
C	-1.1576191	-3.8459886	-1.5703417
H	-0.2612535	-2.1062506	-0.7050564
H	-3.4607995	-5.8018396	-0.2675002
H	-0.5883838	-3.7802520	-2.4955185
N	-2.0515532	-4.8596316	-1.4765269

Au	-2.5602518	-6.0693211	-3.0957779
C	-3.1300361	-7.1792579	-4.5885728
C	-3.5885796	-7.8505273	-5.5082373
C	-4.1502696	-8.5847720	-6.6259466
H	-5.0325040	-8.0604367	-7.0339373
H	-3.4104142	-8.7049367	-7.4354264
O	-4.5676645	-9.9052257	-6.1608047
C	-5.0881668	-10.7625944	-7.0777910
C	-5.5030646	-11.9998821	-6.5658834
C	-5.2363163	-10.4714732	-8.4534853
C	-6.0712498	-12.9258385	-7.4278013
H	-5.4107985	-12.2137069	-5.5025865
C	-5.7923758	-11.4213748	-9.2967757
H	-4.9365504	-9.5088869	-8.8596522
C	-6.2243857	-12.6709830	-8.8107120
H	-5.9160939	-11.1974645	-10.3572607
C	-6.8361561	-13.6813652	-9.6122197
C	-7.2676930	-14.8496112	-9.0570424
H	-6.9657720	-13.5006104	-10.6811666
H	-7.7453487	-15.6311501	-9.6448046
O	-6.5124028	-14.1045800	-6.8765497
C	-7.1251303	-15.1056754	-7.6445360
O	-7.4849684	-16.1067159	-7.0358653
C	0.8832702	7.7825414	7.7584961
H	1.1161344	7.4773792	8.7859175
H	1.8192990	8.0652442	7.2430538
H	0.2160318	8.6632781	7.7790969
O	0.2514064	6.6713315	7.1205486
C	-0.0379768	6.9391754	5.7492120
H	-0.5789354	7.8987242	5.6432186
H	0.8954570	7.0042604	5.1572012
C	-0.8936884	5.7963421	5.2277617
H	-0.3912534	4.8292288	5.4196559
H	-1.8753341	5.7796199	5.7361679
O	-1.0469196	5.9988151	3.8221446
C	-1.6857256	4.9012673	3.1723141
H	-1.2631453	3.9484672	3.5349072
H	-2.7719971	4.8928467	3.3743843
C	-1.3890534	5.0482752	1.6880319
H	-1.9601677	5.8790742	1.2381649
H	-0.3127813	5.2665599	1.5644480
O	-1.7117901	3.8122008	1.0347140
C	-1.2015622	3.7802672	-0.2911730
H	-1.6139607	4.6038963	-0.9034813
H	-0.1001630	3.8777030	-0.2992786
C	-1.5476222	2.4865590	-1.0075756
O	-1.1318502	2.2854751	-2.1463726
N	-2.3495991	1.6236601	-0.2922443
H	-2.6025012	1.9576523	0.6400970
C	-2.9472938	0.4479067	-0.7291544
C	-2.6768637	-0.1538592	-1.9716166
C	-3.8868808	-0.1824958	0.1085483
C	-3.3585490	-1.3076845	-2.3216089
H	-1.9515967	0.2694573	-2.6576756
C	-4.5164629	-1.3393995	-0.3123781
H	-4.1375733	0.2338020	1.0841556
H	-3.1666820	-1.7857187	-3.2806530
H	-5.2393176	-1.8421877	0.3266682
N	-4.2736573	-1.9043014	-1.5221904
Au	-5.2077543	-3.6540171	-2.1569184
C	-5.9897144	-5.3141356	-2.7939165
C	-6.3539015	-6.3983253	-3.2387714
C	-6.7061906	-7.7245131	-3.7061496
H	-5.8501720	-8.4143656	-3.5995459
H	-7.5623679	-8.1215806	-3.1356038
O	-7.0597795	-7.6567943	-5.1244584
C	-7.6054176	-8.7621924	-5.6949638
C	-7.8648862	-8.6554563	-7.0696061
C	-7.9101662	-9.9560662	-5.0012943
C	-8.4424016	-9.7303830	-7.7311426
H	-7.6125099	-7.7436276	-7.6086818
C	-8.5048448	-11.0064562	-5.6816143
H	-7.6793516	-10.0683376	-3.9450928
C	-8.7953991	-10.9229359	-7.0574293
H	-8.7432872	-11.9285208	-5.1497454
C	-9.4008966	-11.9664566	-7.8182019
C	-9.6117134	-11.8230382	-9.1573842

H	-9.6824434	-12.8924122	-7.3122787
H	-10.0568038	-12.6086970	-9.7641149
O	-8.6528393	-9.5972368	-9.0794242
C	-9.2127800	-10.6249692	-9.8527997
O	-9.3078874	-10.4040160	-11.0545694