

Electronic Supplementary Information

Selective and reversible self-assembly of C₆₀ fullerene on 9,10-bis(S-acetylthiomethyl)anthracene modified gold surface

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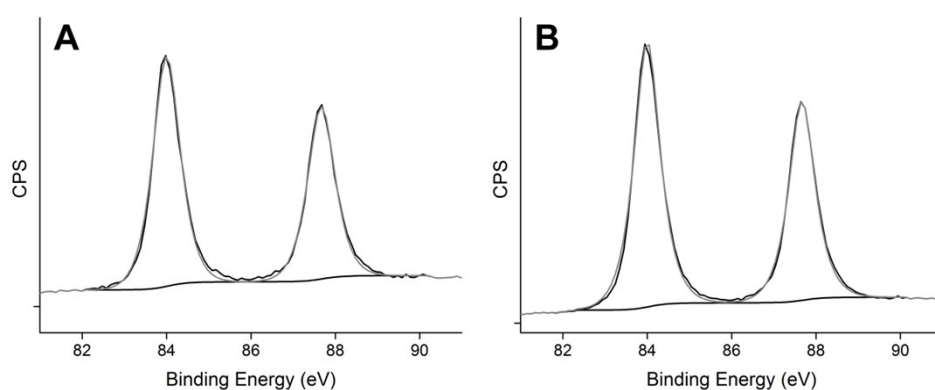


Figure S1. Au 4f XPS core level spectra of the ADMTA (A) and its Diels-Alder adduct with C₆₀ (B) self-assembled on the surface of gold electrode.

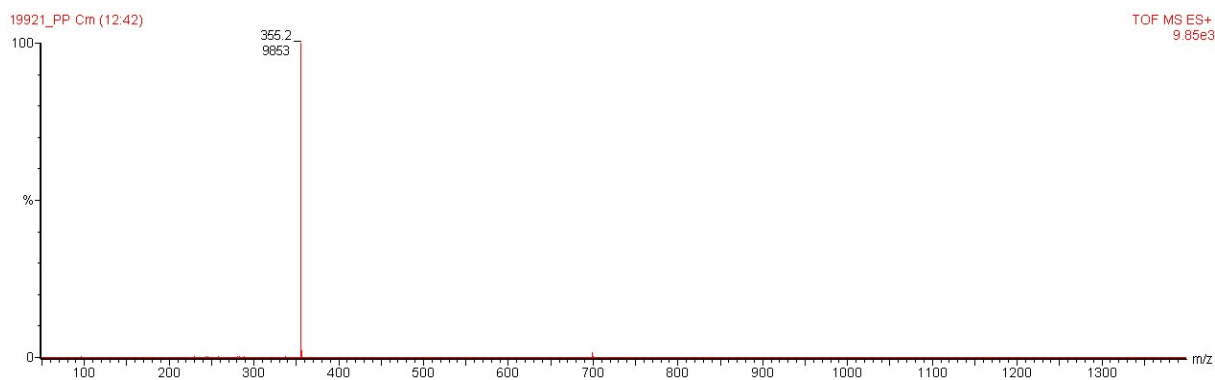


Figure S2. ESI-MS spectrum of 9,10-anthracenedimethanethiol diacetate as a [M + H]⁺ cation.

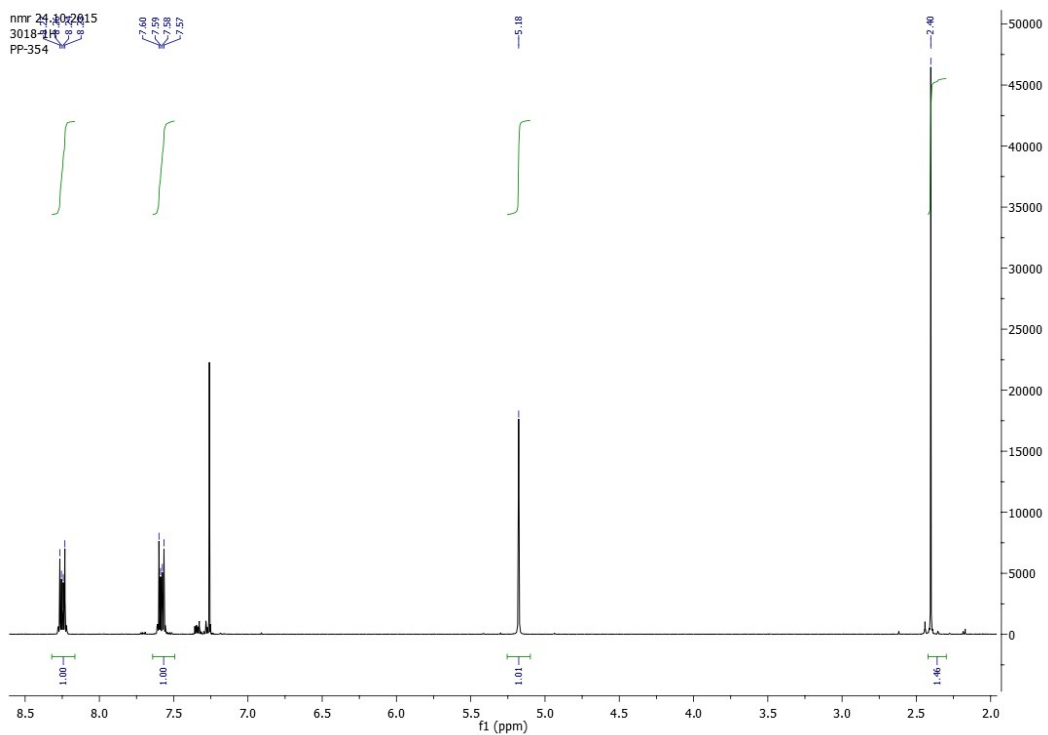


Figure S3. ^1H NMR spectrum of 9,10-anthracenedimethanethiol diacetate in CDCl_3 .

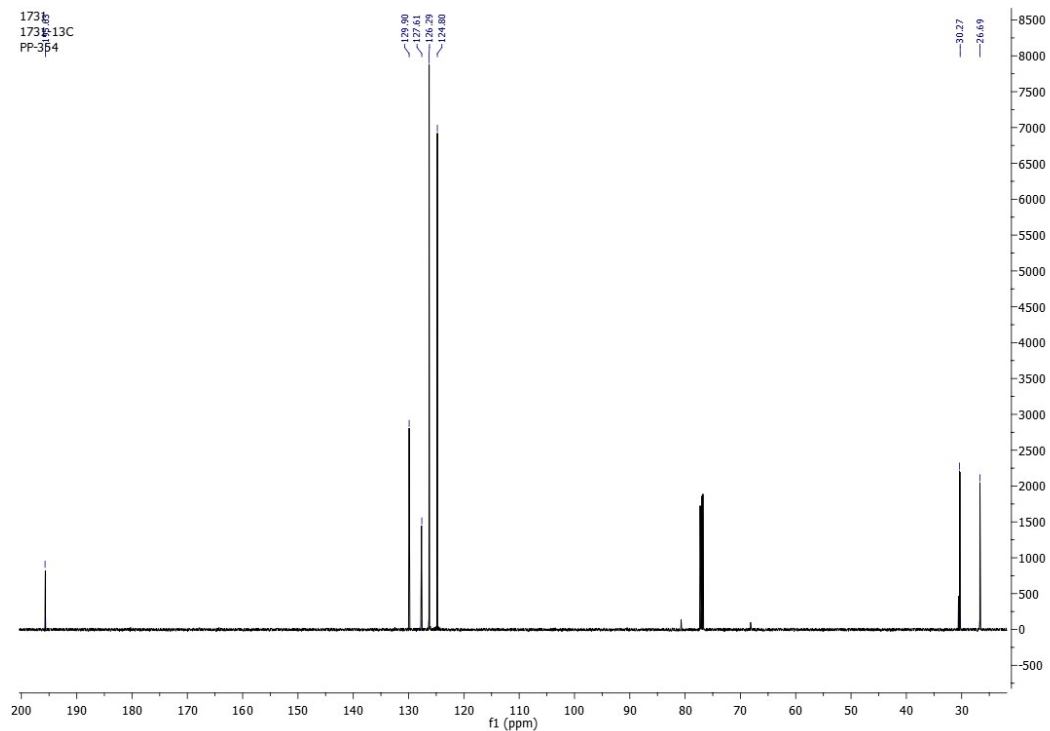


Figure S4. ^{13}C NMR spectrum of 9,10-anthracenedimethanethiol diacetate in CDCl_3 .

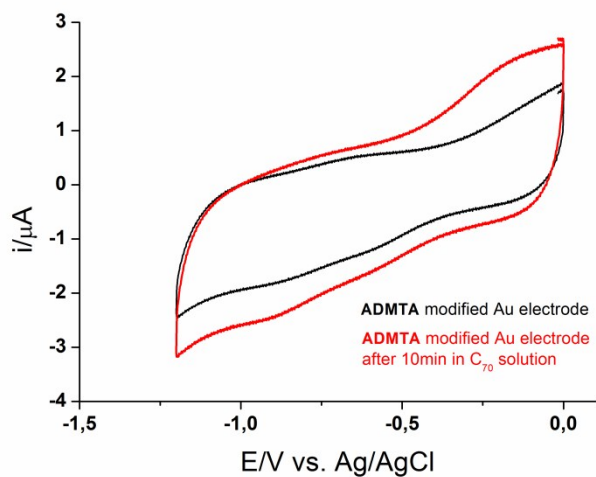


Figure S5. Voltammograms of ADMTA covered gold electrode before and after immersion in: $1 \cdot 10^{-3} \text{M}$ C_{70} solution. CV curves recorded in 0.1M TBAHFP solution in acetonitrile, $\nu = 1 \text{V/s}$.

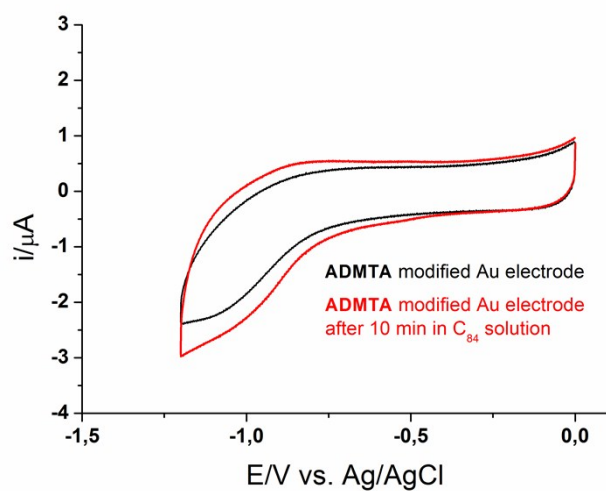


Figure S6. Voltammograms of ADMTA covered gold electrode before and after immersion in: $1 \cdot 10^{-4} \text{M}$ C_{84} solution. CV curves recorded in 0.1M TBAHFP solution in acetonitrile, $\nu = 1 \text{V/s}$.

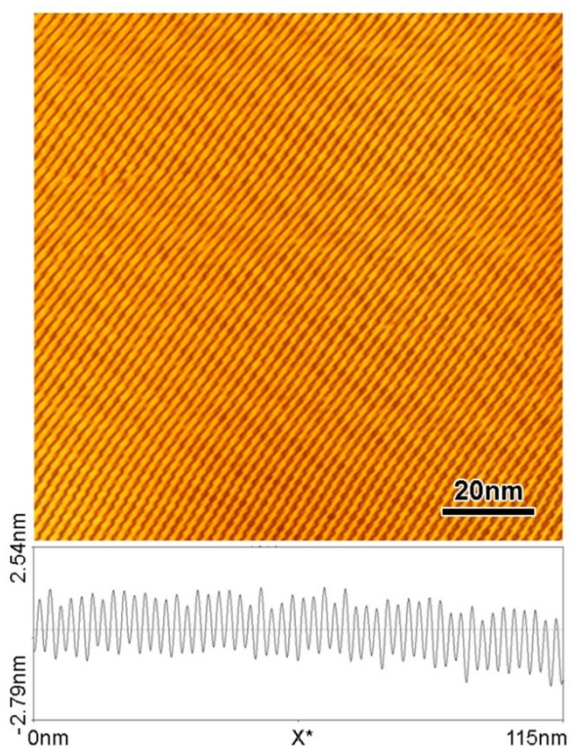


Figure S7. Diels-Alder adduct of ADMTA and C_{60} self-assembled on the gold surface AFM image and its cross-section.

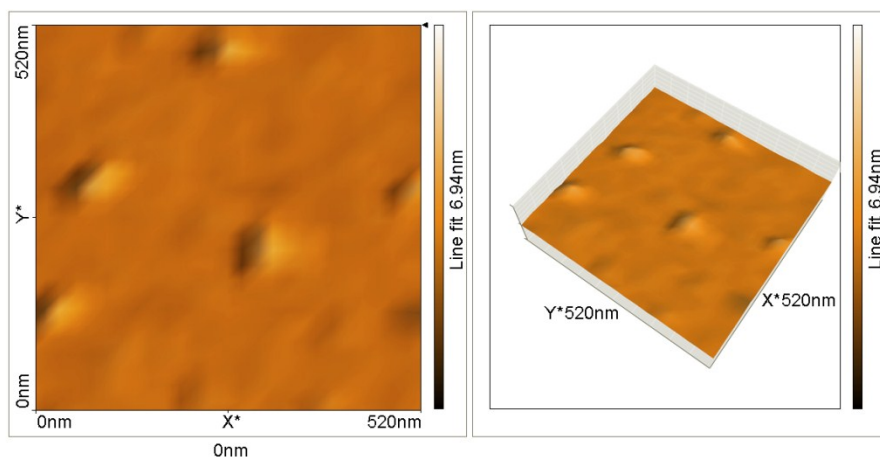


Figure S8. AFM image of ADMTA functionalized gold plate immersed in the $1 \cdot 10^{-3} M$ solution of C_{70} fullerene.

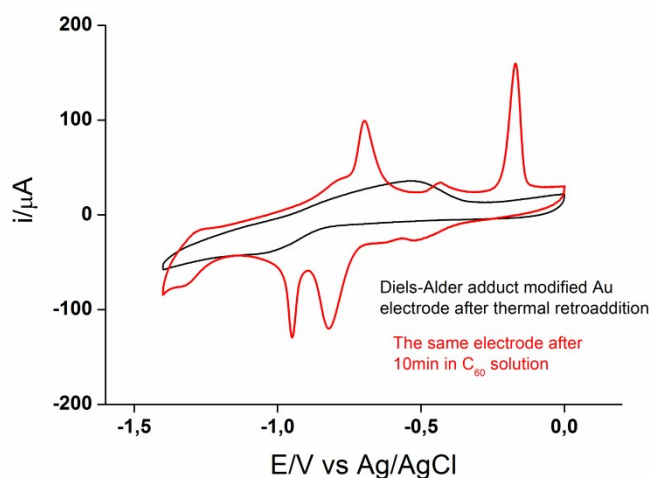


Figure S9. Cyclic voltammograms obtained for gold electrode after thermal retroaddition followed by immersion in C_{60} fullerene solution, recorded 0.1 M TBAHFP solution in acetonitrile, $v = 1V/s$.

Table S1 Cartesian coordinates for ADMTA in Molpro format

C	0.172243000000	-0.606300000000	-0.087050000000
C	0.094983000000	-0.480633000000	1.274734000000
C	1.264011000000	-0.274637000000	2.079016000000
C	1.428908000000	-0.533887000000	-0.742045000000
C	2.572180000000	-0.335708000000	-0.014754000000
C	2.547070000000	-0.197875000000	1.411988000000
C	1.195559000000	-0.152187000000	3.486240000000
C	2.385000000000	-0.041727000000	4.243666000000
C	3.668065000000	0.035026000000	3.576633000000
C	3.728632000000	-0.000959000000	2.164202000000
C	2.369640000000	-0.010620000000	5.676859000000
C	3.521925000000	0.088729000000	6.410108000000
C	4.778116000000	0.166384000000	5.754786000000
C	4.846264000000	0.140547000000	4.386981000000
C	-0.139433000000	-0.136052000000	4.187852000000
S	-0.690380000000	-1.803763000000	4.788719000000
C	-2.293512000000	-1.938686000000	3.978436000000
C	-3.003578000000	-3.246146000000	4.270275000000
O	-2.759322000000	-1.083539000000	3.254394000000
C	5.046393000000	0.171750000000	1.451181000000
S	5.895361000000	-1.428890000000	1.047344000000
C	7.487633000000	-1.175256000000	1.850568000000
C	8.424783000000	-2.358679000000	1.708881000000

O	7.783821000000	-0.170123000000	2.462506000000
H	-0.731846000000	-0.769277000000	-0.667172000000
H	-0.876286000000	-0.562167000000	1.747950000000
H	1.484538000000	-0.643178000000	-1.821688000000
H	3.520939000000	-0.306466000000	-0.538097000000
H	1.425518000000	-0.090662000000	6.203275000000
H	3.475171000000	0.100805000000	7.495620000000
H	5.690408000000	0.239408000000	6.340336000000
H	5.821410000000	0.179518000000	3.916322000000
H	-0.120552000000	0.519027000000	5.059057000000
H	-0.953151000000	0.207350000000	3.547953000000
H	-4.042608000000	-3.029924000000	4.537174000000
H	-3.011202000000	-3.849319000000	3.355207000000
H	-2.526322000000	-3.818438000000	5.069432000000
H	4.919203000000	0.704138000000	0.508381000000
H	5.777921000000	0.729922000000	2.036706000000
H	8.067124000000	-3.098666000000	0.988847000000
H	9.410665000000	-1.992154000000	1.406775000000
H	8.531056000000	-2.837209000000	2.689152000000

Cartesian coordinates for ADMTA Diels-Alder adduct with C₆₀ fullerene in Molpro format

C	4.604028000000	-1.567847000000	-3.212698000000
C	4.139376000000	-1.960257000000	-1.955995000000
C	3.726921000000	-0.999570000000	-1.029713000000
C	4.628624000000	-0.219261000000	-3.558951000000
C	4.176868000000	0.741122000000	-2.652199000000
C	3.737644000000	0.358864000000	-1.381797000000
C	3.127793000000	-1.289474000000	0.339600000000
C	3.737692000000	-0.358823000000	1.381623000000
C	3.726934000000	0.999614000000	1.029541000000
C	3.127769000000	1.289511000000	-0.339756000000
C	4.176959000000	-0.741075000000	2.652012000000
C	4.628721000000	0.219315000000	3.558754000000
C	4.604076000000	1.567902000000	3.212511000000
C	4.139378000000	1.960305000000	1.955823000000
C	3.180325000000	-2.772980000000	0.746181000000
S	4.875083000000	-3.455325000000	1.010471000000
C	4.788509000000	-4.956546000000	0.015824000000
C	6.017224000000	-5.832780000000	0.156865000000
O	3.845488000000	-5.245681000000	-0.689999000000
C	3.180283000000	2.773012000000	-0.746350000000

S	4.875001000000	3.455398000000	-1.010707000000
C	4.788558000000	4.956438000000	-0.015872000000
C	6.017781000000	5.832157000000	-0.155802000000
O	3.845417000000	5.245767000000	0.689722000000
H	4.932760000000	-2.322110000000	-3.922277000000
H	4.084937000000	-3.016805000000	-1.725317000000
H	4.980295000000	0.090311000000	-4.539195000000
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H	4.166388000000	-1.781576000000	2.957285000000
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H	6.853283000000	5.314766000000	-0.633925000000
C	-1.549974000000	0.909926000000	3.326021000000
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