Supporting Information

Structure and Dynamics of DL- Homocysteine Functionalized Fullerene-C_{60} - Gold Nanocomposite: a Femtomolar L-Histidine Sensor

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Table S1. HOMO-LUMO energy gap of the investigated compounds

Compound	Energy (eV)	HOMO-LUMO gap (eV)
Hcys	-1.89 x 10^4	6.33
C_{60}	-6.22 x 10^4	2.76
$(Hcys)_2$-C_{60}	-1.00 x 10^5	2.45
Au_3(Hcys)-C_{60}-(Hcys)Au_3	-1.01 x 10^5	1.65

IR spectral characteristics

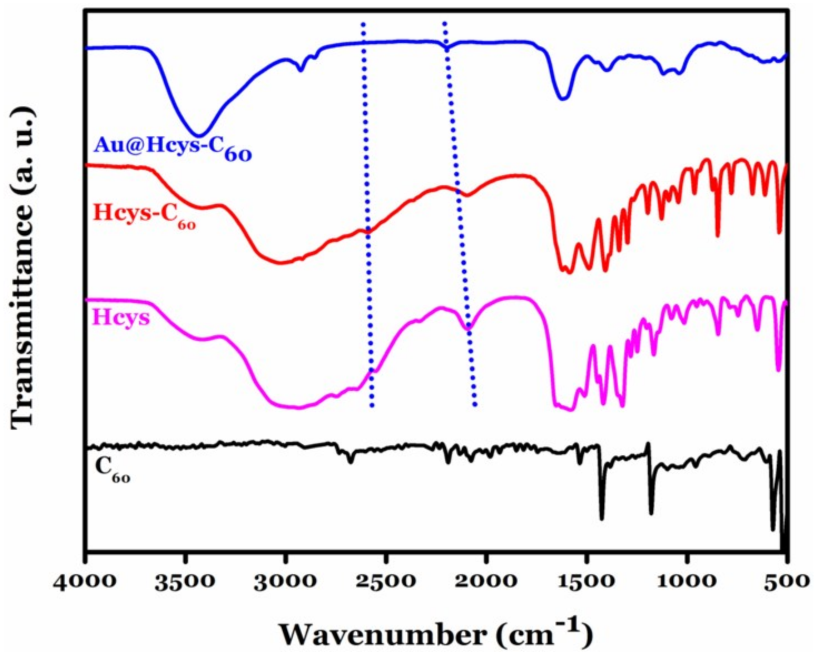

Fig. S1 FTIR spectra of Hcys, C_{60}, Hcys-C_{60}, Au@Hcys-C_{60} nanocomposite.

Table S2. Characteristic IR frequencies of the compounds used in the present investigation.

Compound	N-H (cm^{-1})	S-H (cm^{-1})	C=O (cm^{-1})	C-N (cm^{-1})	C-S (cm^{-1})	Characteristic frequency (cm^{-1})
Hcys	2144	2595	1650	1473	1222	-
C_{60}	-	-	-	-	-	1425, 1178, 569, 524
Hcys-C_{60}	2148	2646	1669	1479	1238	1444, 1184, 594, -
Au@Hcys-C_{60}	2190	Disappeared	1694	1478	1174	1447, 1110, 584, -

Optical spectra and FESEM micrograph of the nanocomposite:

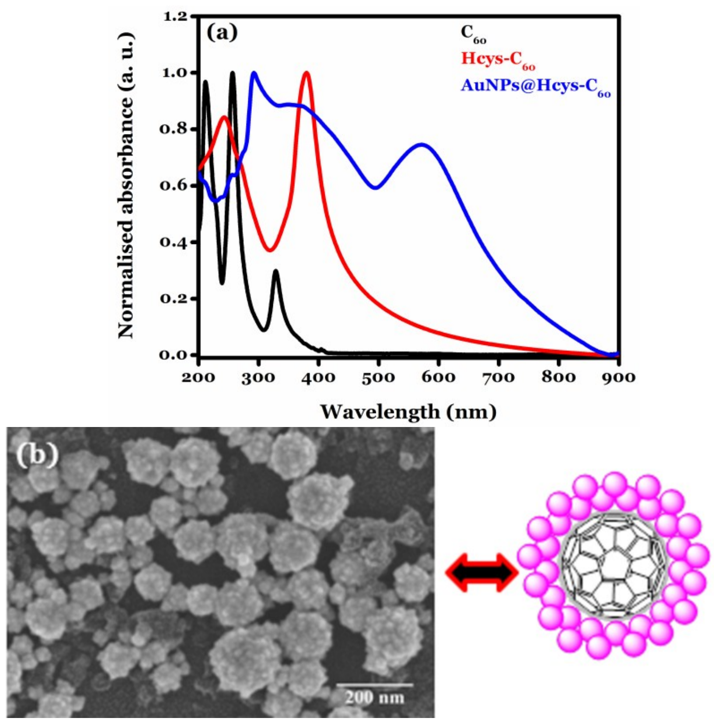

Fig. S2 (a) UV-visible of C_{60}, Hcys-C_{60}, Au@Hcys-C_{60} nanocomposite. (b) FE-SEM image of the AuNPs@C_{60} nanocomposite.

EDX analysis and elemental mapping of the nanocomposite

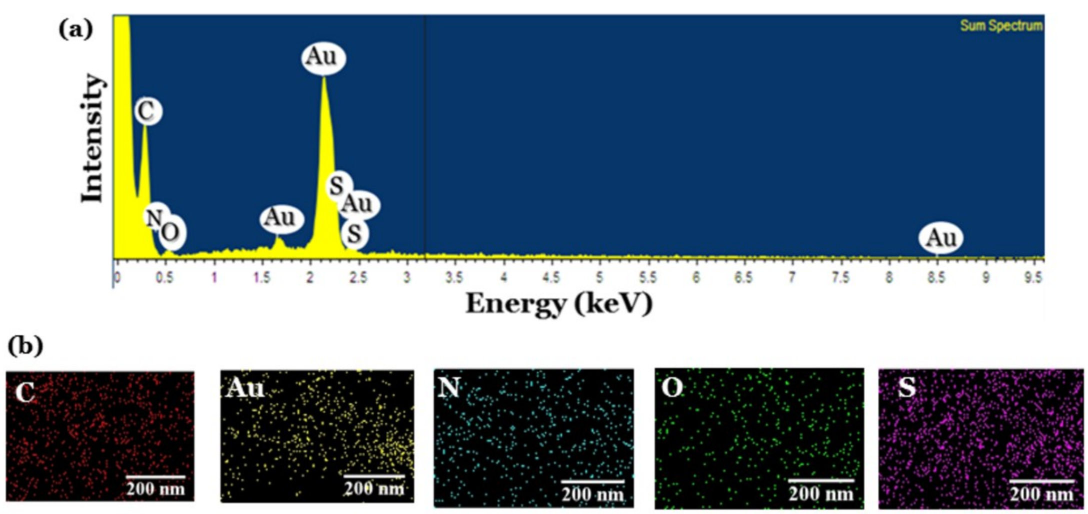

Fig. S3 (a) EDX analysis and (b) FESEM-EDX elemental mapping of the Au@Hcys-C_{60} nanocomposite on conductive carbon tape for different elements: C, N, S, Au.

Cyclic voltammetry and the corresponding potential plots as a function of scan rate of the modified and bare GCE

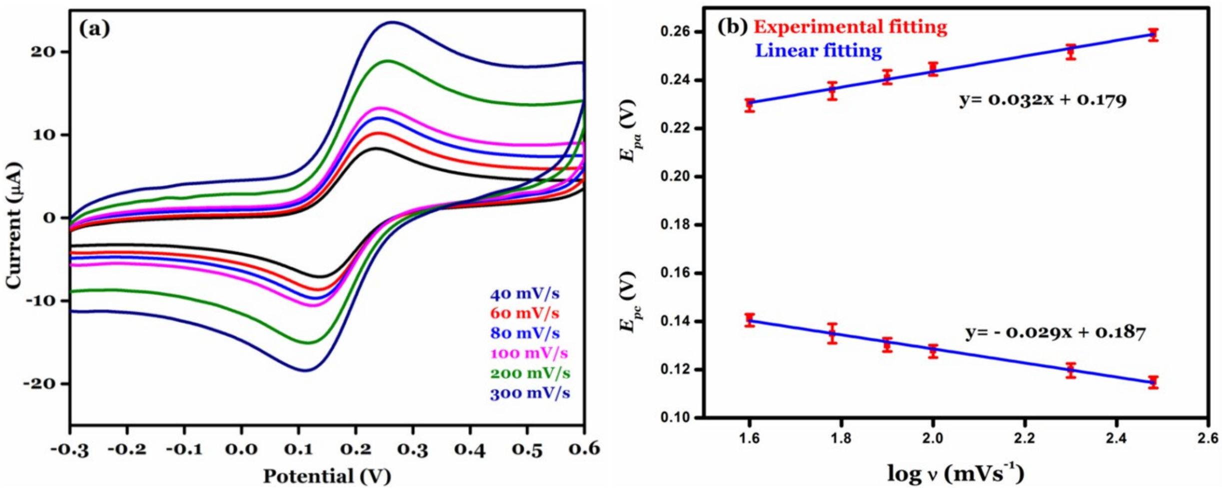

Fig. S4 (a) CVs of nanocomposite modified GCE with different scan rates in 0.1 M KCl containing 5 mM $K_3[Fe(CN)_6/K_4[Fe(CN)_6]$ (1:1) redox couple (*vs.* Ag/AgCl); (b) Peak potential *vs.* log scan rate (ν)

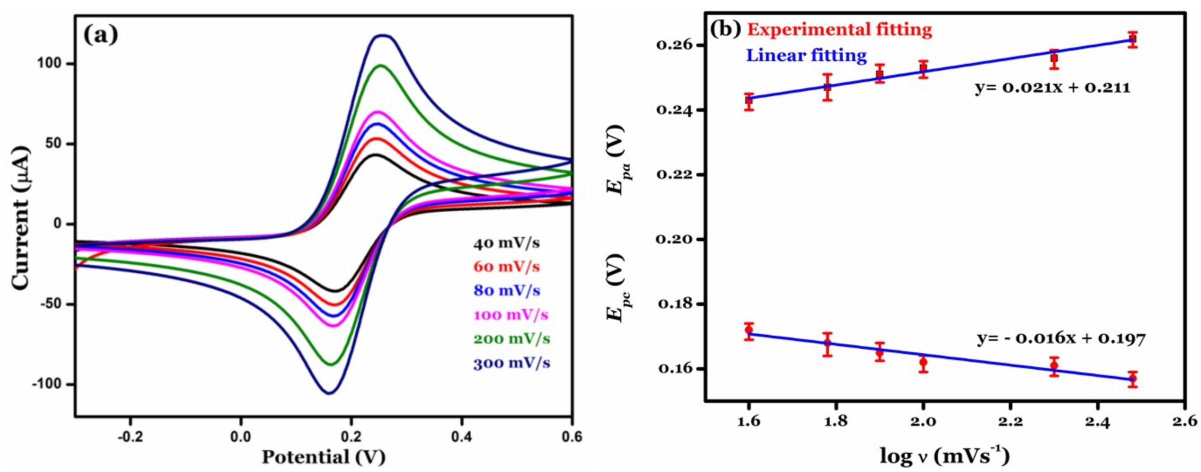

Fig. S5 (a) CVs of bare GCE with different scan rates in 0.1 M KCl containing 5 mM $K_3[Fe(CN)_6/K_4[Fe(CN)_6]$ (1:1) redox couple (*vs.* Ag/AgCl); (b) Peak potential *vs.* log scan rate (ν)

Calculation of effective working area of AuNPs@C_{60}/GCE electrode

Effective working area of this working electrode for the reversible process was calculated using Randles-Sevcik equation.[1]

$$I_{pa} = (2.69 \times 10^{5}) n^{\frac{2}{3}} A D^{\frac{1}{2}} \nu^{\frac{1}{2}} C$$

Here,

I_{pa} = Peak current in A

n = Number of electrons transferred

A = Effective working area of the modified electrode in cm^2

D = Diffusion coefficient of redox probe $K_3[Fe(CN)_6]$ = 7.6 x 10^{-6} cm^2s^{-1}

C = Concentration of redox probe = 5 mM = 5 x 10^{-6} $molcm^{-3}$

ν = Scan rate in Vs^{-1}

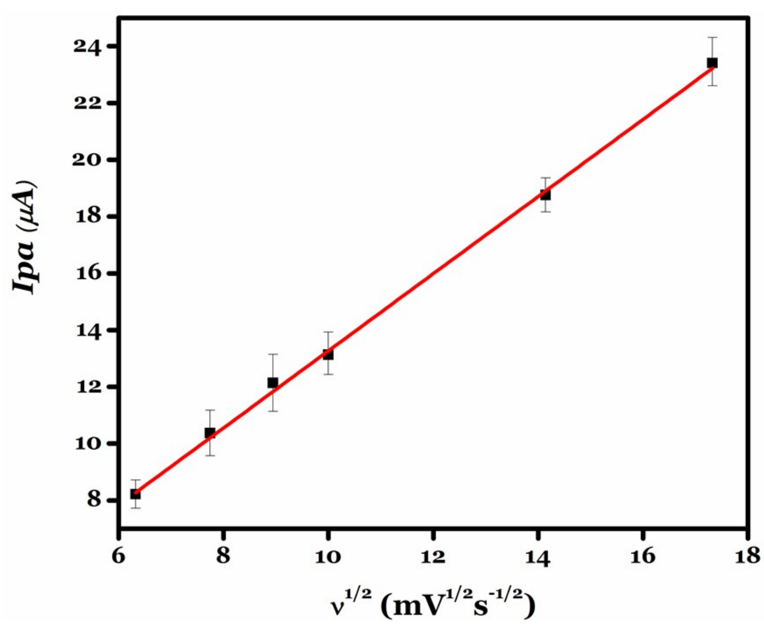

Fig. S6 A plot of anodic peak current as a function of scans rate for estimation of electrochemical area of the electrode.

The slope of the straight line for I_{pa} vs $\nu^{1/2}$ plot amounted to 4.3 x 10^{-4} $AV^{-1/2}s^{1/2}$. Accordingly, the estimated area was found to be 0.037 cm^2.

Reproducibility of the AuNPs@C_{60}/GCE sensor

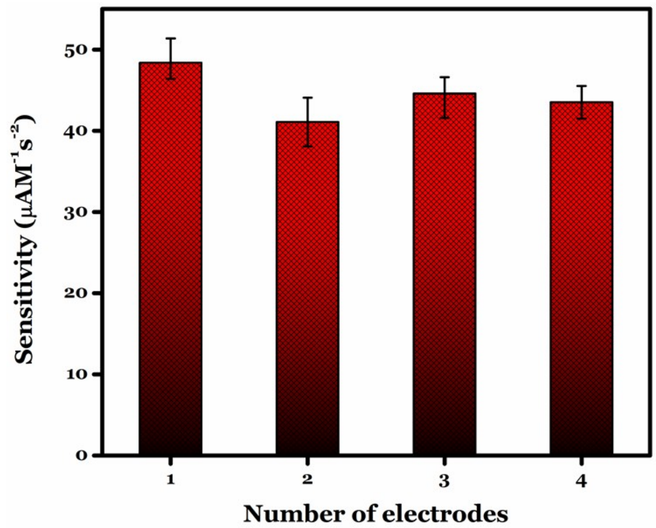

Fig. S7 A plot of sensitivity response of four same electrodes of Au@Hcys-C_{60}/GCE in a 0.1 M PBS (pH 7.5) containing 0.1 M KCl (*vs.* Ag/AgCl) with L-histidine concentration varying as 0.01 pM - 0.1 mM.

Specificity of Au@Hcys-C_{60}/GCE sensor

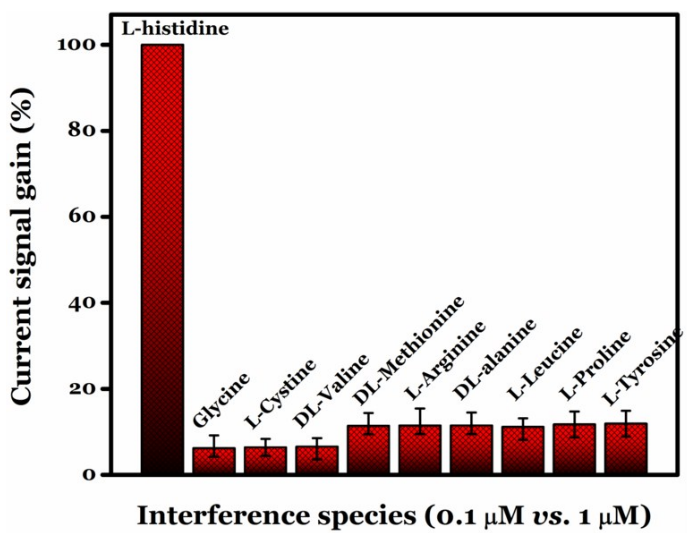

Fig. S8 Relative response of the fabricated Au@Hcys-C_{60}/GCE sensor by SWV to different amino acids in 0.1 M PBS buffer (pH 7.5) containing 0.1 M KCl (*vs.* Ag/AgCl).

Stability of Au@Hcys-C_{60}/GCE sensor

Here, I_0 is the initial current response and I is the current response of the investigation day.

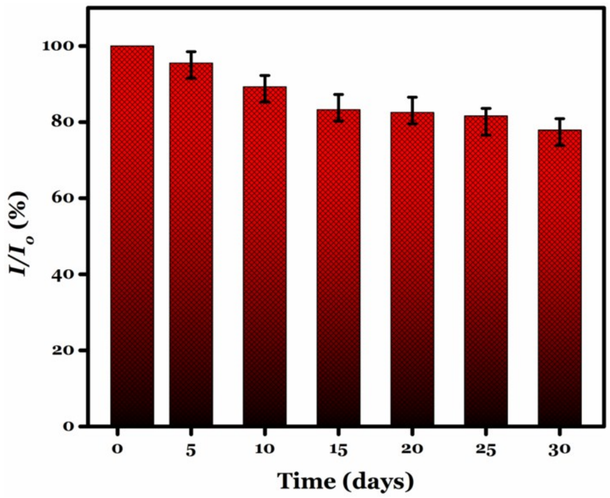

Fig. S9 Stability performance of the Au@Hcys-C_{60}/GCE sensor over a period of 30 days with a interval of 5 days to 1 mM L-histidine in a 0.1 M PBS (pH 7.5) containing 0.1 M KCl (*vs.* Ag/AgCl).

MD simulated geometries for higher simulation time scales

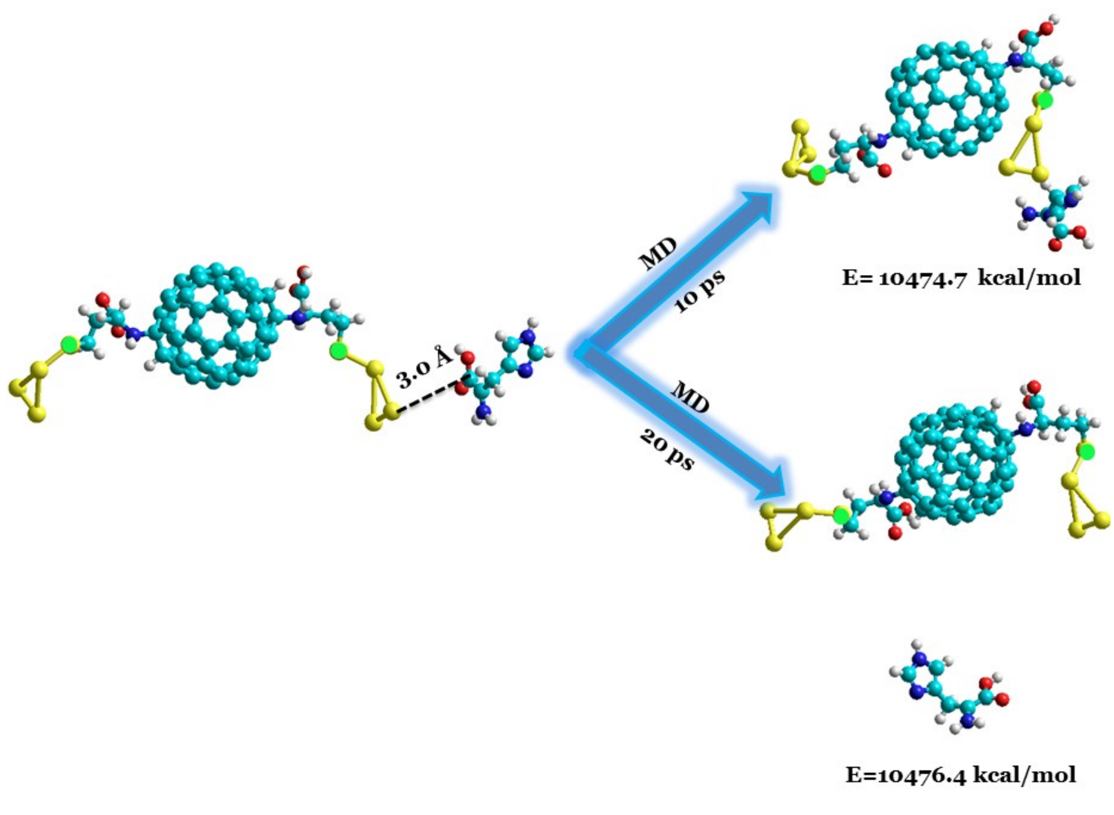

Fig. S10 Snapshots of the MD simulated geometries for higher simulation time scales depicting the 2 components diverging from each other.

Reference:

1. J.-S. Ye, Y. Wen, W. De Zhang, H. F. Cui, G. Q. Xu and F.-S. Sheu, *Electroanalysis*, 2005, **17**, 89-96.