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Novel Salen-Based Dual Channel Sensor for Easy and Selective Nanomolar Detection of L-Cysteine

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Table S1 Details of final refinement for EDH

CCDC number	2297263
Empirical formula	$C_{24}H_{30}N_2O_4\,H_2O$
Formula weight	428.52
Color	Yellow
Crystal system	Orthorhombic
Space group	*P* $2_1/c$
Cell parameters	
a (Å)	9.824(18)
b (Å)	11.69(19)
c (Å)	21.88(4)
α (°)	90
β (°)	111.1(8)
γ (°)	90
Volume V ($Å^3$)	2345.2(7)
Z	4

Calculated density (ρ) (Mg m^{-3})	1.214
Absorption coefficient, μ (mm^{-1})	0.085
F(000)	920.0
Crystal size mm^3	0.40 x 0.35 x 0.35
θ (°) range for data collection	2.39 to 25.50
Limiting indices	-12≤h≤12, -15≤k≤15, -28≤l≤28
Reflections collected	5672
Unique Reflections (R_{int})	2701
Absorption correction	Semi-empirical from equivalents
Maximum and minimum transmission	0.980 and 0.977
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.028
Final R indices [I > 2σ (I)]	R_1 = 0.079, wR_2 = 0.1606
R indices (all data)	R_1 = 0.1280, wR_2 = 0.1950
Largest difference peak and hole (e $Å^{-3}$)	0.495 and -0.485

$R_1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o| wR_2 = [\Sigma w(F_o^2-F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths and bond angles of probe, EDH

Bond lengths (Å)			**Bond angles (°)**		
	Experimental	B3LYP/def2-TZVP		Experimental	B3LYP/def2-TZVP
O(1)–C(4)	1.365(4)	1.354	N(1)–C(8)–C(9)	110.6(3)	111.1
O(1)–C(24)	1.433(3)	1.416	O(1)–C(4)–C(5)	115.3(4)	115.1
O(2)–C(5)	1.351(3)	1.329	C(13)–C(8)–C(10)	110.6(3)	111.9
N(1)–C(7)	1.272(3)	1.285	N(2)–C(9)–C(10)	110.6(3)	111.1
N(2)–C(9)	1.460(3)	1.447	C(10)–C(11)–C(12)	111.0(4)	112.4
C(8)–C(9)	1.531(3)	1.539	O(4)–C(21)–C(22)	107.1(3)	108.0

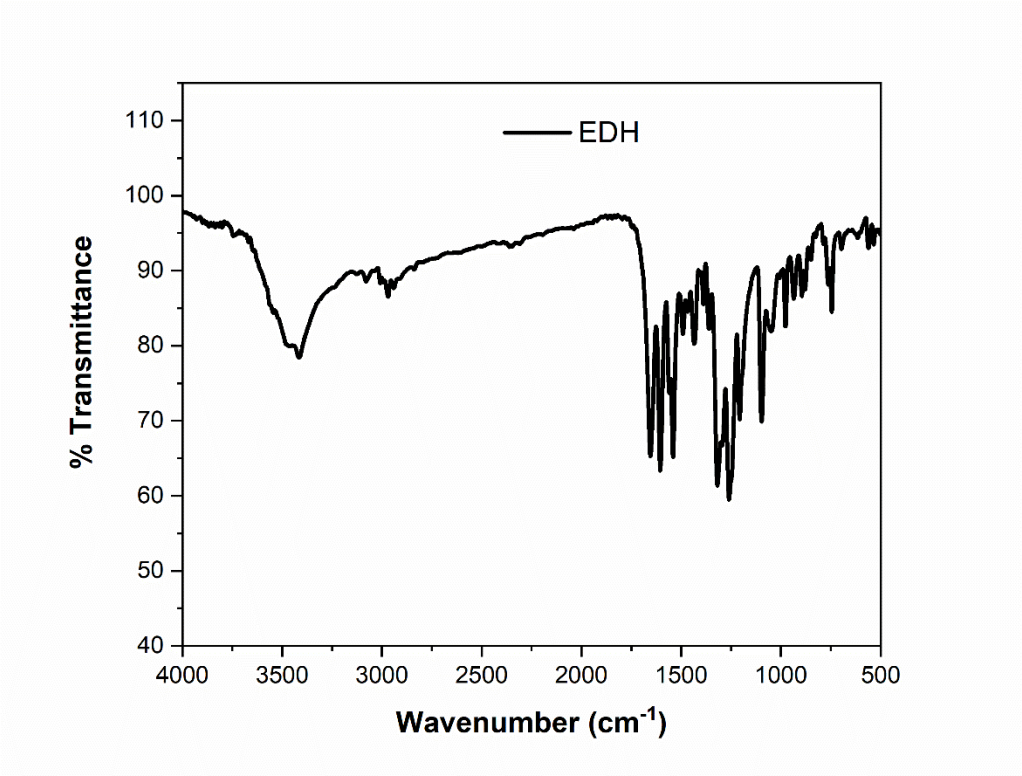

Fig S1 IR spectrum of the probe.

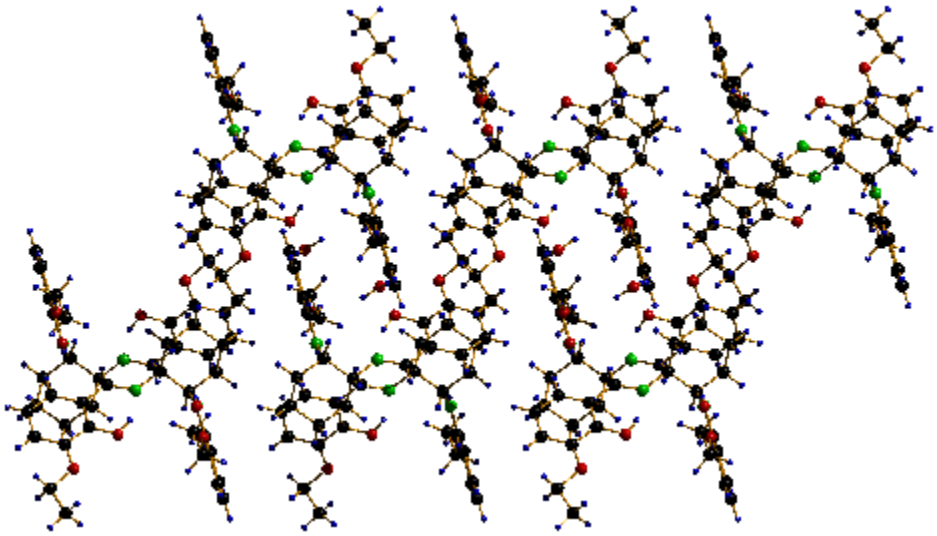

Fig S2 Packing diagram of EDH viewed along ‘a’ axis

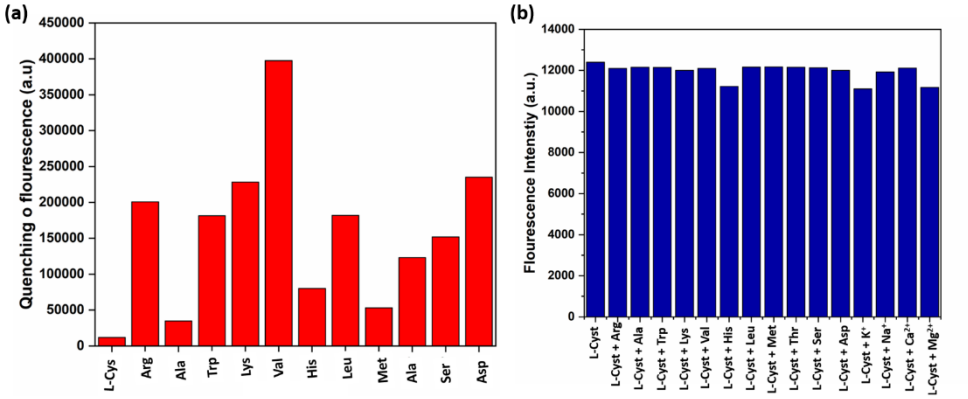

Fig S3 (a) Selectivity of EDH towards L-cysteine in presence of other amino acids ((L- Arginine (Arg), Alanine (Ala), L-Cysteine (Cys), Tryptophan (Trp), Lysine (Lys), Valine (Val), Histidine (His), Leucine (Leu), Methionine (Met), Alanine (Ala), Serine(Ser), L- Aspartic acid (Asp)). **(b)** Interference study from other common amino acids and metal ions.

Quantum Yield calculation

Quantum yield of the probe EDH was calculated using Rhodamine 6G as reference in ethanol ith the following equation[1, 2]

$$\Phi_S = \Phi_R \times \frac{I_S}{I_R} \times \frac{A_g}{A_s} \times \frac{\eta_S^2}{\eta_R^2}$$

Where,

Φ_S and Φ_R are the quantum yields of sample and reference, I_S and I_R are area under PL curve for sample and reference. A_S and A_R are the absorbance of sample and reference and η_S and η_R are the refractive index values for the sample and reference solutions. The quantum yield (Q.Y.) of the EDH is calculated to be 72 % amd in the resence of analyte (L-Cysteine) it was found to reduce to 58%. Q.Y. of Rhodamine = 0.94 and refractive index of ethanol = 1.36.

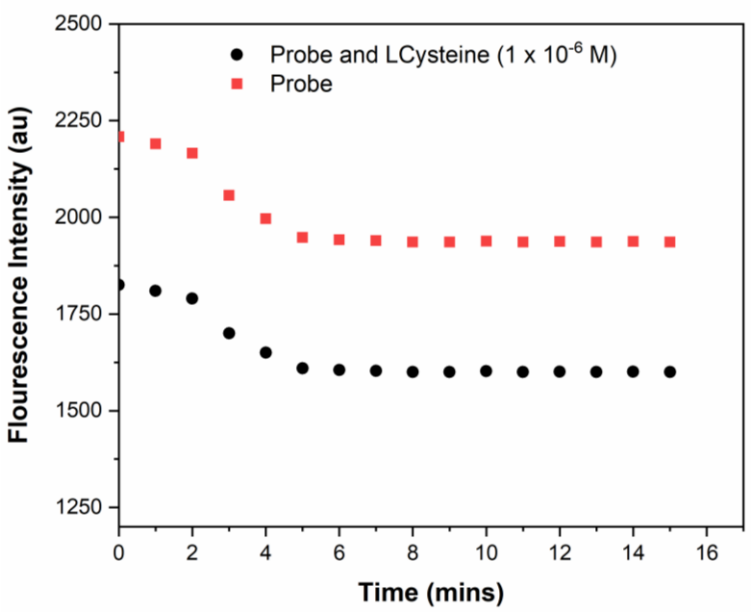

Fig S4 Time dependent fluorescent intensity of

EDH in the absence and presence of L-Cysteine (1 x 10^{-6} M)

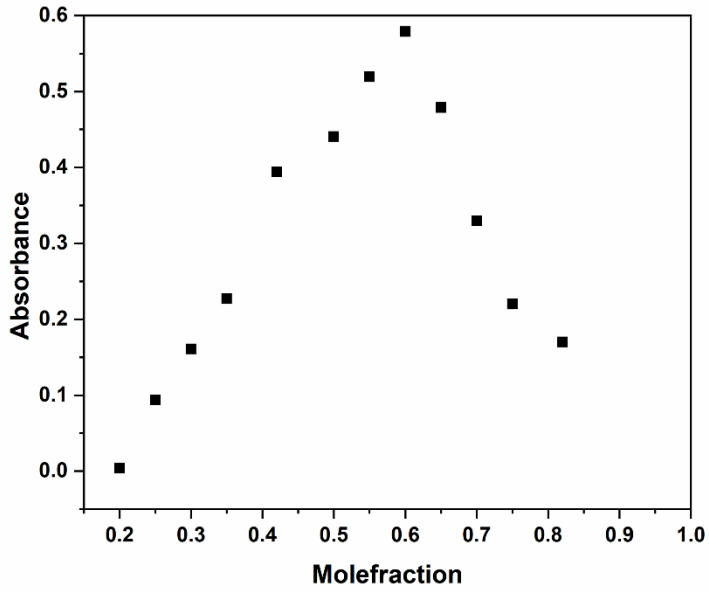

Fig S5 Jobs plot of the probe with analyte showing a 1:2 association

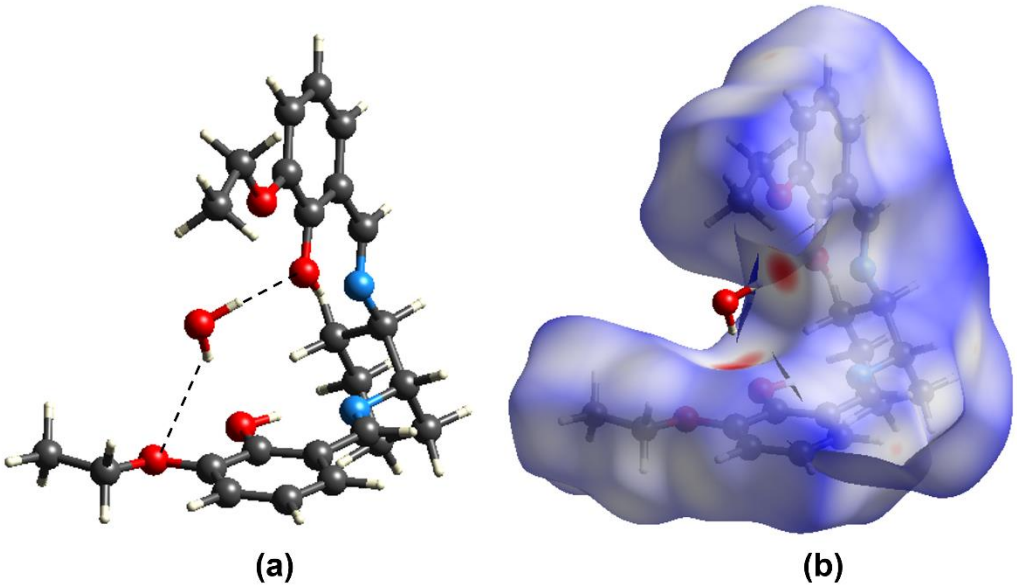

Fig S6 Hirshfeld surface of EDH mapped with (b) d_{norm} function.

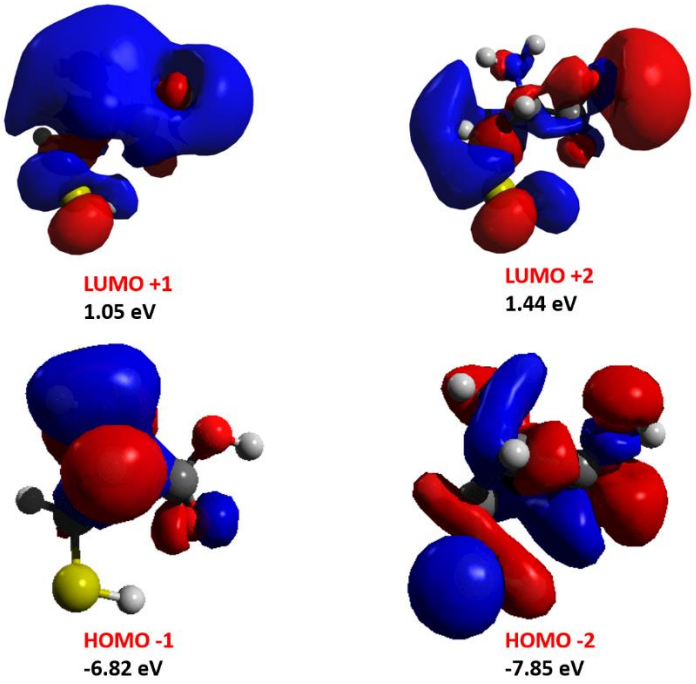

Fig S7 Contour plots of frontier orbitals of L-Cysteine along with their energy values.

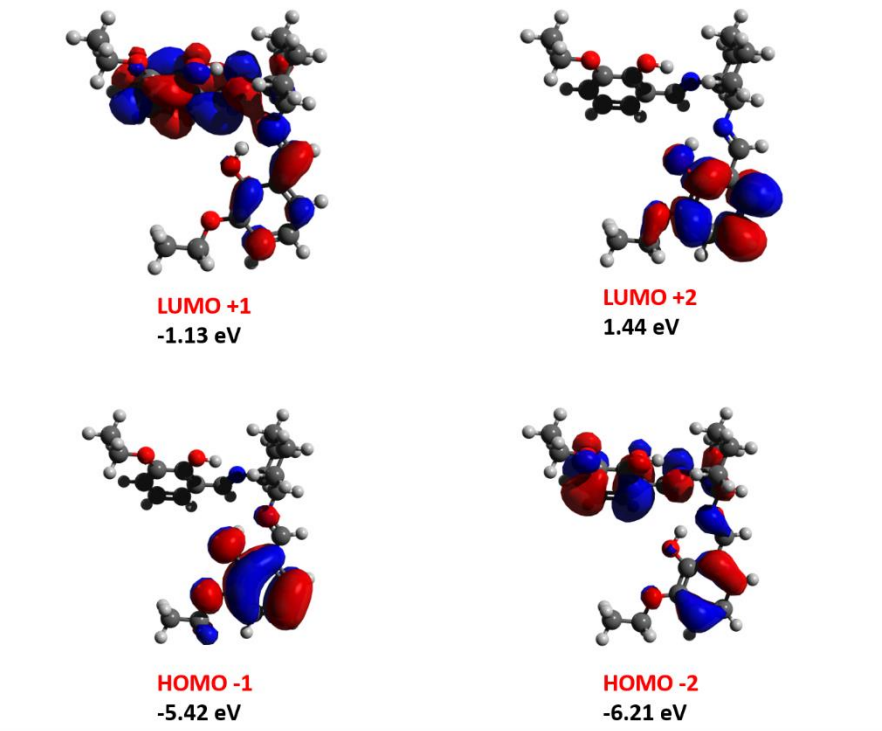

Fig S8 Contour plots of frontier orbitals of EDH along with their energy values.

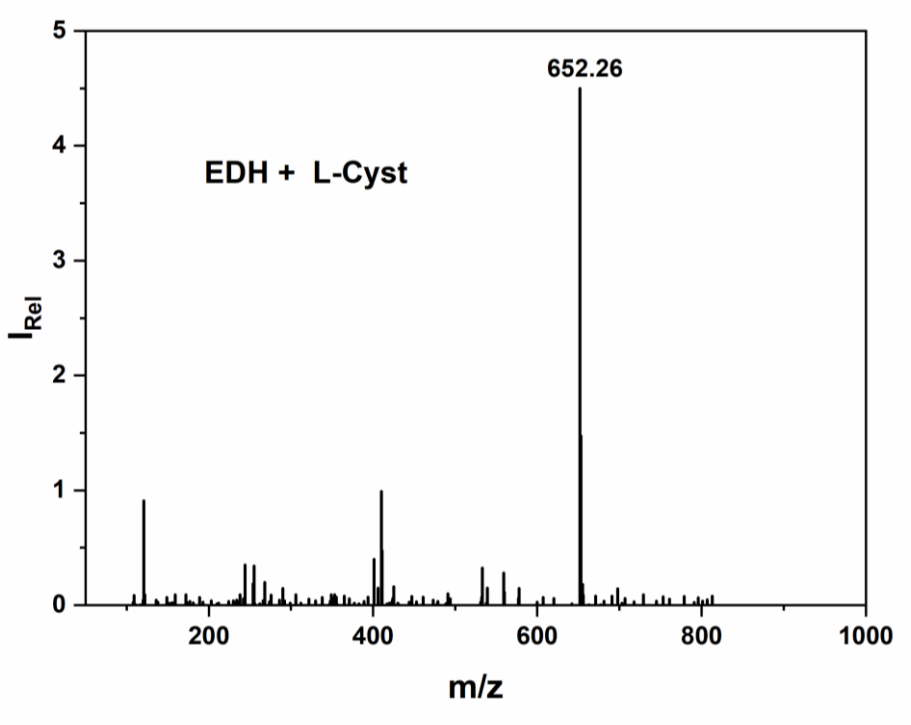

Fig S9 Mass spectrum of EDH + 2 L-Cysteine.

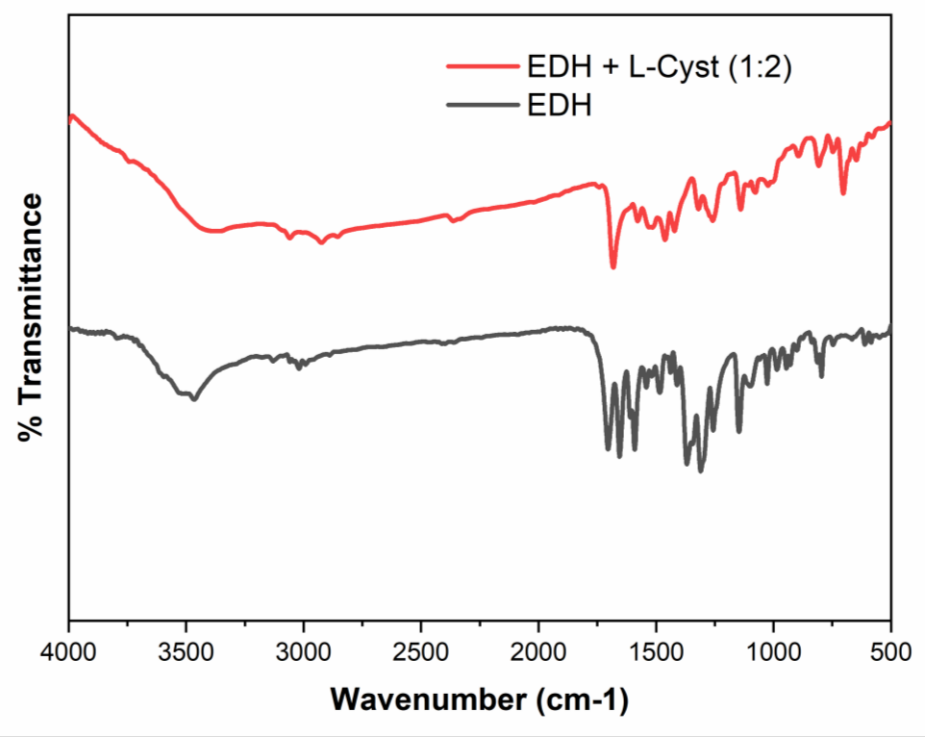

Fig S10 Mass spectrum of EDH and EDH + 2 L-Cysteine.

Table S3 Determination of L-Cys in real sample

Sample	**Added (M)**	**Found (M)**	**Recovery *(%)**	**RSD (%)**
Synthetic urine	1×10^{-6} to 5×10^{-7}	0.97×10^{-6} to 4.85×10^{-7}	98.4	3.09

References

1. Q. Zhang, Y. Gao, S. Zhang, J. Wu, H. Zhou, J. Yang, X. Tao and Y. Tian, *Dalton Transactions*, 2012, **41**, 7067-7072.
2. J. E. Murphy, M. C. Beard, A. G. Norman, S. P. Ahrenkiel, J. C. Johnson, P. Yu, O. I. Mićić, R. J. Ellingson and A. J. Nozik, *Journal of the American Chemical Society*, 2006, **128**, 3241-3247.