Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information(S.I)

FeS_2 based aerogel as a flexible low-cost substrate for rapid SERS detection of histamine in biofluids

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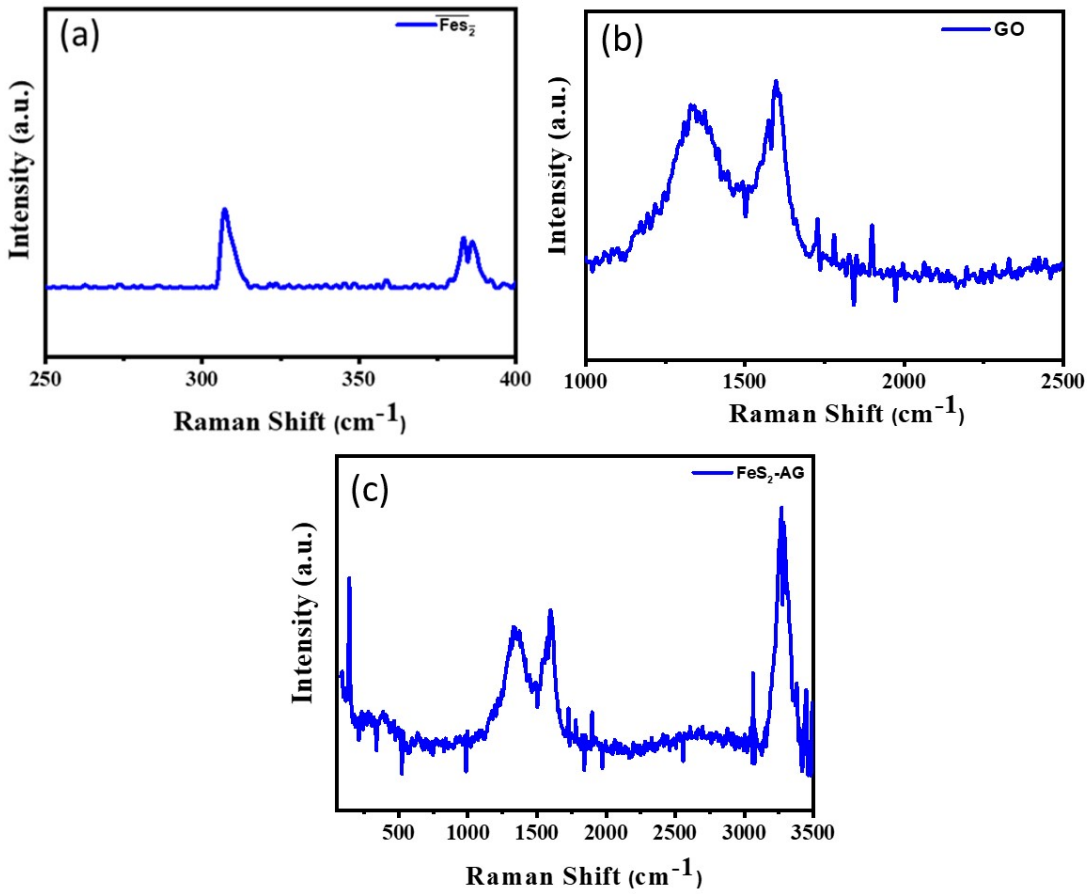
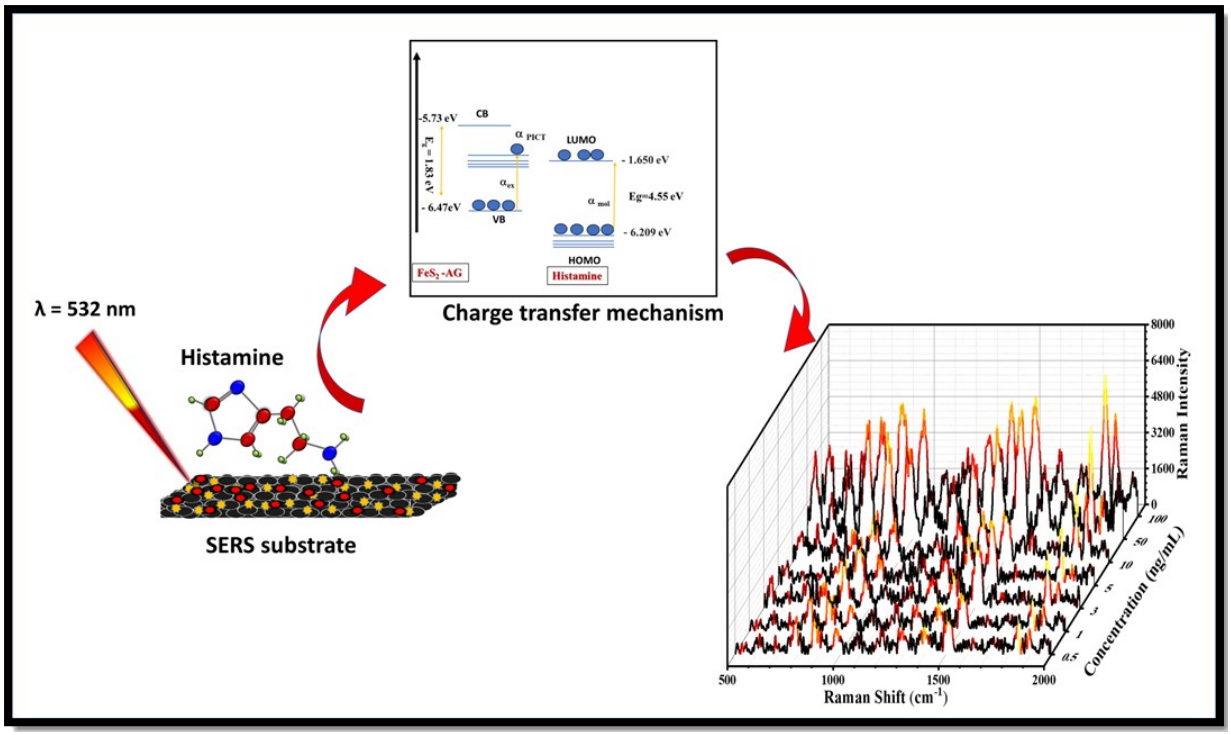


Fig. S1 Raman Spectra of (a) FeS_2 (b) GO (c) FeS_2- AG

Fig.S1 (a) depicts the Raman spectra of FeS_2 . The Raman spectrum of FeS_2 typically shows several distinct bands that can be attributed to the vibrational modes of the molecule. One of the most prominent peaks in the Raman spectrum of FeS_2 occurs at around 370 cm^{-1}, and is typically attributed to the Fe-S stretching mode, respectively. Fig. S1 (b) represents the Raman spectra of GO. One of the most well-known features of the Raman spectra of GO is the D-band, which is located at around 1350 cm^{-1}. This peak arises from the breathing mode of sp2 carbon atoms in the GO lattice that have been disrupted by the introduction of sp3 carbon atoms or defects. Another important peak in the Raman spectra of GO is the G-band, which is located at 1590 cm^{-1}. This peak arises from the stretching mode of sp2 carbon atoms in the GO lattice and is a measure of the degree of graphitization or order in the GO structure.

Fig.S1 (c) depicts the Raman spectra of FeS_2-AG. In addition to the characteristic GO peaks, there are prominent peaks corresponding to polyvinyl alcohol (PVA). The peak at 3500 cm^{-1}, corresponds to the presence of PVA as a significant component in the sample which corresponds to the hydroxyl (-OH) stretching vibrations of the PVA polymer. The hydroxyl (-OH) group in PVA exhibits characteristic vibrational modes, and one of these modes is the stretching vibration. When the PVA polymer is excited by the incident laser light, the -OH groups vibrate at specific frequencies. These vibrations result in the absorption or scattering of light at corresponding wavelengths, which can be observed in the Raman spectrum. This peak confirms the significant presence of PVA in the sample, likely as a component of the FeS_2-AG aerogel material.



Scheme 1: SERS-enhanced mechanism for detection of histamine.

Table S1. SERS peak assignment of MB on FeS_2 – AG

Wave number (cm^{-1})	**Raman Intensity**	**SERS Intensity with Substrate**	**Assignments**
546	-	~ 1364	υ(S-S)
619	~ 83	~ 1699	υ(CC) alicyclic chain vibrations
694		~ 1277	υ(CC) alicyclic chain vibrations

753	~ 80	~ 1584	υ(CC) alicyclic chain vibrations
793	~ 131	~ 1373	υ(C-C-C)
882		~ 2042	υ(CC) alicyclic chain vibrations
901		~ 2255	υ(C-C-C)
987	~ 196	~ 2058	υ(C-C-C)
1183	~ 118	~ 1248	υ(CC) alicyclic chain vibrations
1284	~ 305	~ 2229	υ(CC) alicyclic chain vibrations
1404	~ 77	~ 2249	δ(CH3)
1512	~ 458	~ 2210	υ(C=O)
1594	~ 214	~ 1634	υ(C=N)
1844	**~ 253**	**~ 3662**	**υ(C≅N)**
1891	~ 91	~ 3072	υ(C≅N)

Table S2 Detection of histamine in simulated blood serum samples via standard addition technique.

Concentration in blood serum (ng/ mL)	**Spiked Concentration (ng/ mL)**	**Recovered Concentration (ng/ mL)**	**RSD %**	**Recovery %**
0.5	0.5	0.466	3.45	96.55
1	0.5	1.22	0.21	100.21
2	1	2.04	10.08	89.92
3	1	3.25	0.24	100.24
4	1	3.76	2.42	97.58