

2- Borono benzoic acid functionalized silver nanocubes for the label free detection of L-Arginine and L-Cysteine with real sample applications.

Saumya Singh^a, K.K. Upadhyay^{a*}

^a Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi

*Corresponding Author

S.No.	Caption	Page No.
1.	Fig. S1 Blank studies performed in the absence of (a) AgNO ₃ , (b) 2-Formylphenylboronic acid and inset showing corresponding images.	3
2.	Fig. S2 (a) AFM image of AgNCs, (b) AFM image of AgNCs + L-Arg, (c) AFM image of AgNCs + L-Cys.	4
3.	Fig. S3 (a) EDX spectra of AgNCs, (b) EDX spectra of AgNCs + L-Arg, (c) EDX spectra AgNCs + L-Cys.	5
4.	Fig. S4 XPS spectra of AgNCs, AgNCs + L-Arg and AgNCs + L-Cys (a) XPS survey spectra, (b) High resolution B 1s spectra, (c) High resolution Ag 3d spectra, (d) High resolution O 1s spectra (e) High resolution N 1s spectra	6
5.	Fig. S5 FT-IR spectra of AgNCs, L-Arg, AgNCs+L-Arg, L-Cys, AgNCs+L-Cys.	7
6.	Table S1. Assignment of IR bands	7
7.	Fig. S6 (a) Visual response of AgNCs under different pH conditions, (b) UV-Vis spectra showing the effect of pH on AgNCs, (c) Effect of pH on 401 nm, (d) Visual response of AgNCs+L-Arg under different pH conditions, (e) UV-Vis spectra showing effect of pH on AgNCs+L-Arg, (f) The effect of pH on A ₅₂₀ /A ₄₀₁ , (g) Visual response of AgNCs + L-Cys under different pH conditions, (h) UV-Vis spectra showing effect of pH on AgNCs + L-Cys, (i) The effect of pH on A ₅₆₀ /A ₄₀₁ values.	8-9

8.	Fig. S7 UV Vis spectral response of synthesized AgNCs in the presence of different ionic concentrations of NaCl and inset showing corresponding image after 30 mins (a) 0.001 M, (b) 0.1 M, (c) 1 M, (d) 2 M, (e) Effect of ionic strength on 401 nm value.	10
9.	Table S2 Comparison with previously reported probes for the detection of L-Arg	11
10.	Table S3 Comparison with previously reported probes for the detection of L-Cys	12
11.	Fig S8. (a) Visual Response of AgNCs in matrix (A) AgNCs, (B) AgNCs+ L-Arg, (C) AgNCs+ L-Cys, (D) AgNCs+ L-Arg+ L-Cys, (E) AgNCs+ mixture of amino acid except L-Arg and L-Cys, (F) AgNCs+ mixture of L-Arg+ L-Cys, (G) AgNCs+ mixture of amino acids including L-Arg except L-Cys, (H) AgNCs +mixture of amino acids including L-Cys except L-Arg, (I) AgNCs+ mixture of amino acids+ L-Arg+ L-Cys and (b) Corresponding UV-Vis spectra	13
12.	Scheme S1. Mechanism for the synthesis of AgNCs	14
13.	Fig. S9. HRMS of AgNCs	15
13.	Fig. S10. HRMS of AgNCs after the addition of L-Cys	16
14.	Fig. S11: Raman spectrum of AgNCs	17
15.	Table S4. Raman wavenumbers (cm ⁻¹) and intensity (a.u.) and their probable assignments.	17
16.	Fig. S12 Raman spectrum of L-Arg	18
17.	Table S5. Raman and SERS wavenumbers (cm ⁻¹) and relative intensities (a.u.) and their probable assignments corresponding to Fig. 6a (Main Text).	18
18.	Fig. S13 Raman spectrum of L-Cys	19
19.	Table S6. Raman and SERS wavenumbers (cm ⁻¹) and relative intensities (a.u.) and their probable assignments corresponding to Fig. 6b (Main Text).	19
20.	Fig. S14 Visual response and corresponding UV-Vis spectra after addition of N-methyl L-Cysteine and S- Methyl L Cysteine into AgNCs.	20
21	Fig. S15 Probable mechanism for change in optical properties at very high and very low pH	21- 22

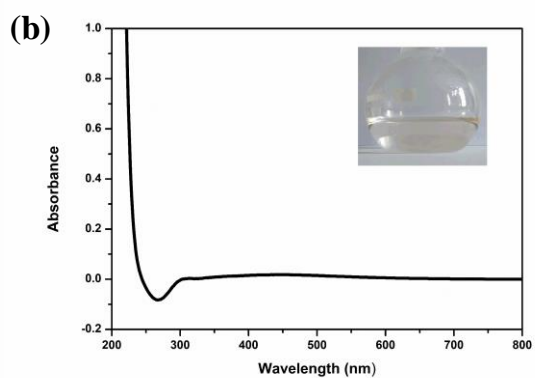
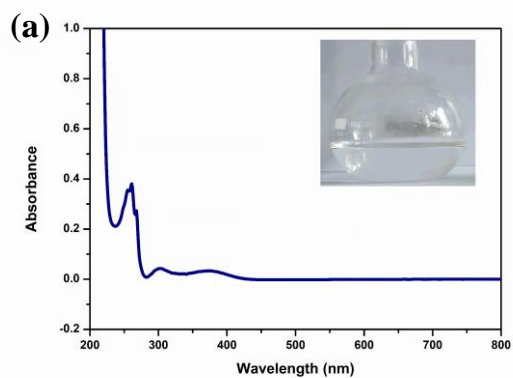


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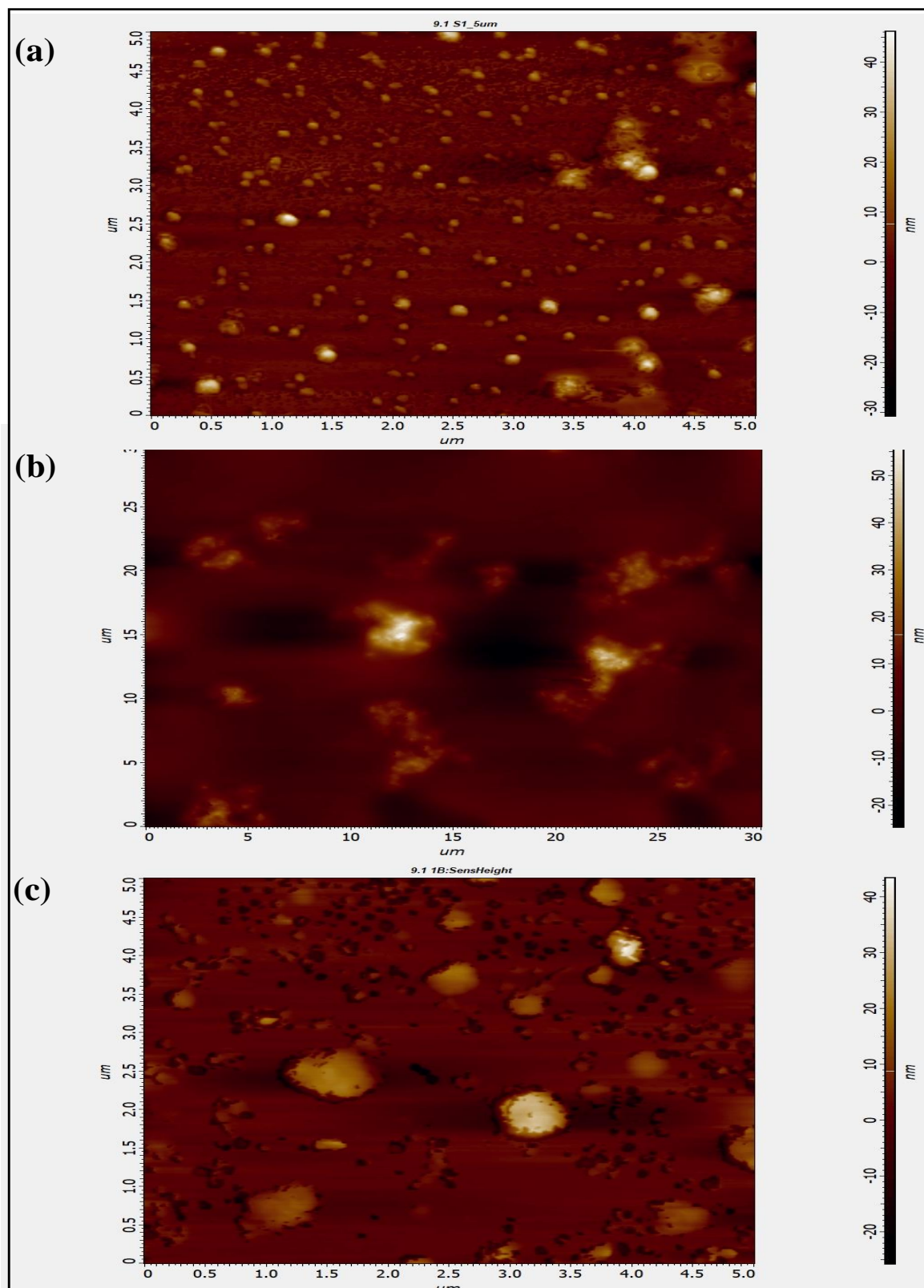


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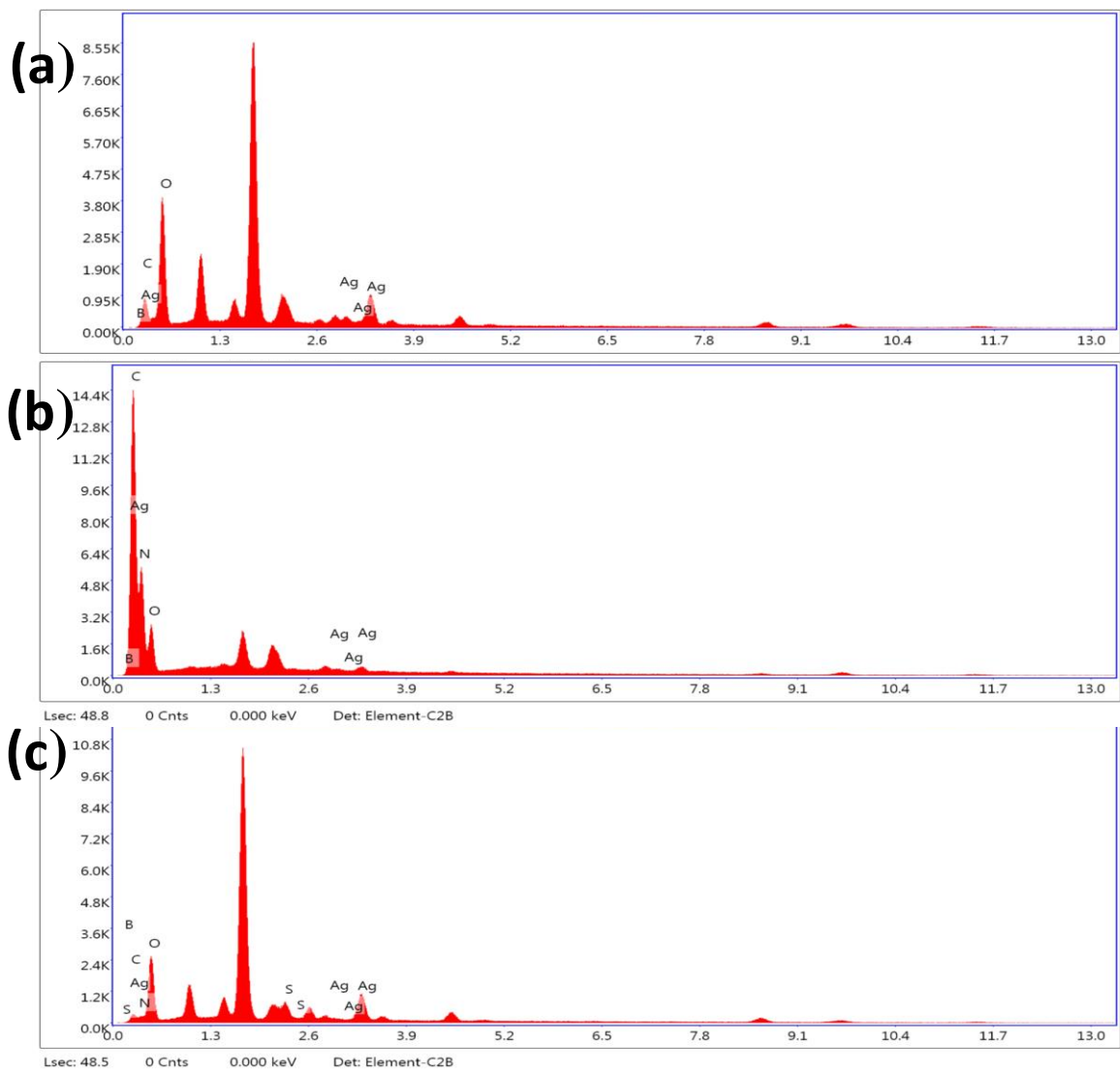


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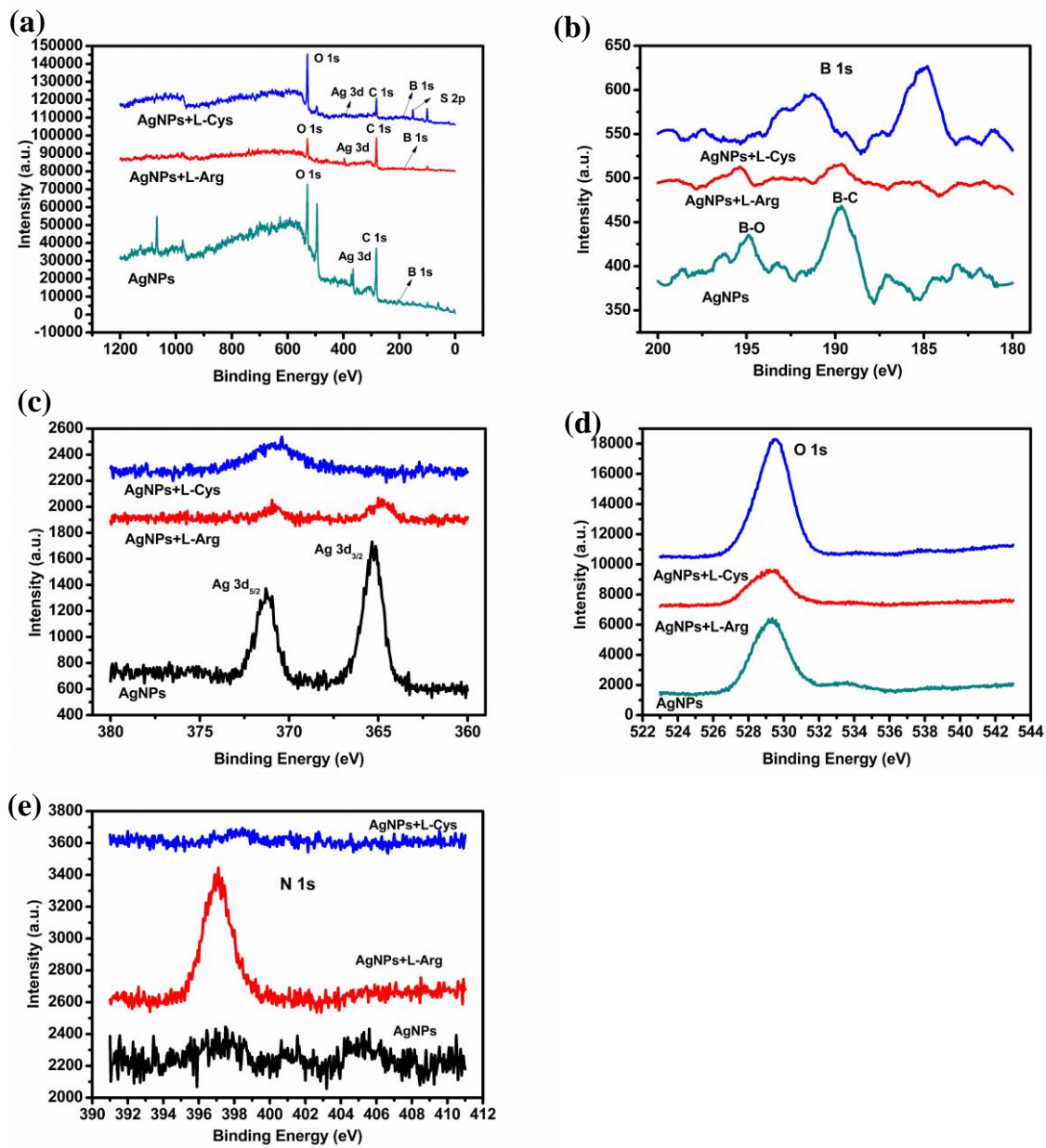


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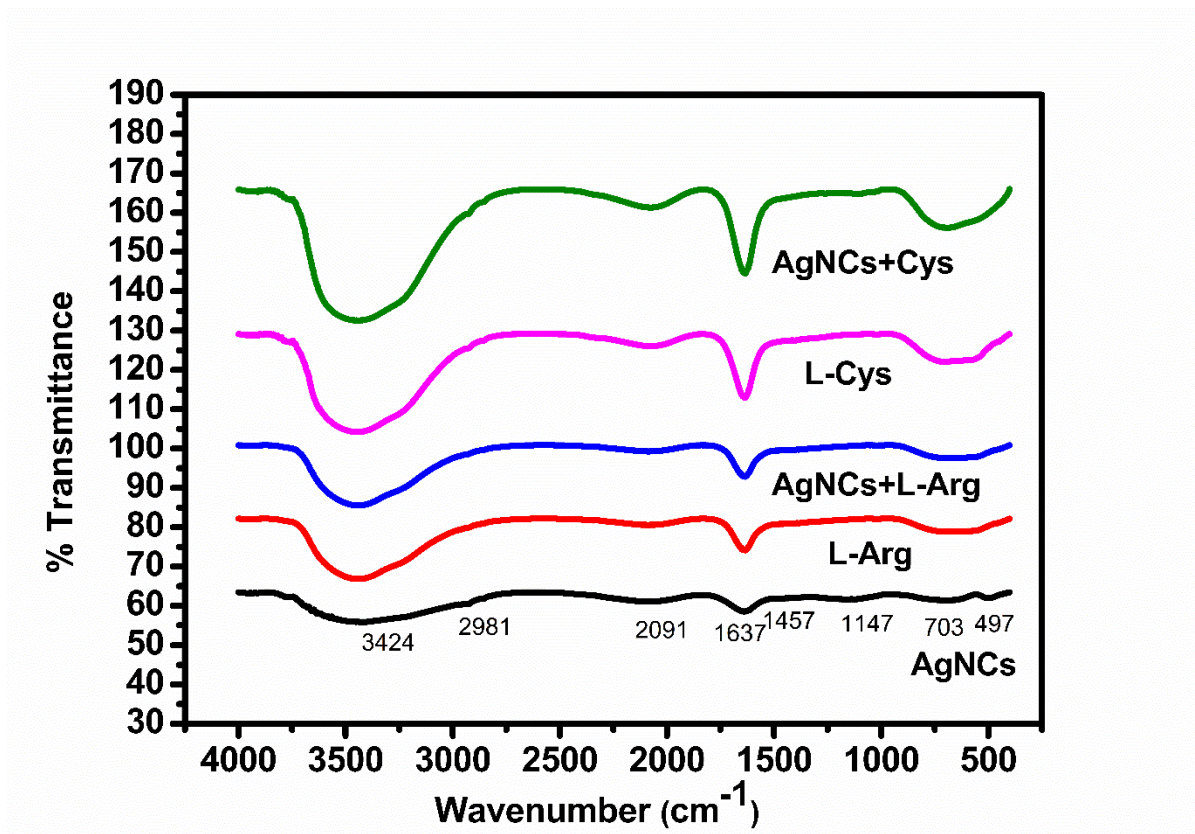


Fig. S5 FT-IR spectra of AgNCs, L- Arg, AgNCs + L-Arg, L- Cys, AgNCs + L-Cys.

Table S1: Assignment of IR bands

S.No.	Wavenumber (cm ⁻¹)	Assignment
1.	3424	O-H asymm
2.	2981	v C-H phenyl
3.	1637	Benzene ring vib.+bending vib.
4.	1457	v asymm. B-O + v asymm. C-O
5.	1147	v asymm. C-C
6.	703	C-H bending
7.	497	v asymm. Ag-O
8.	2091	Intramolecular H bond between B-OH and COO ⁻

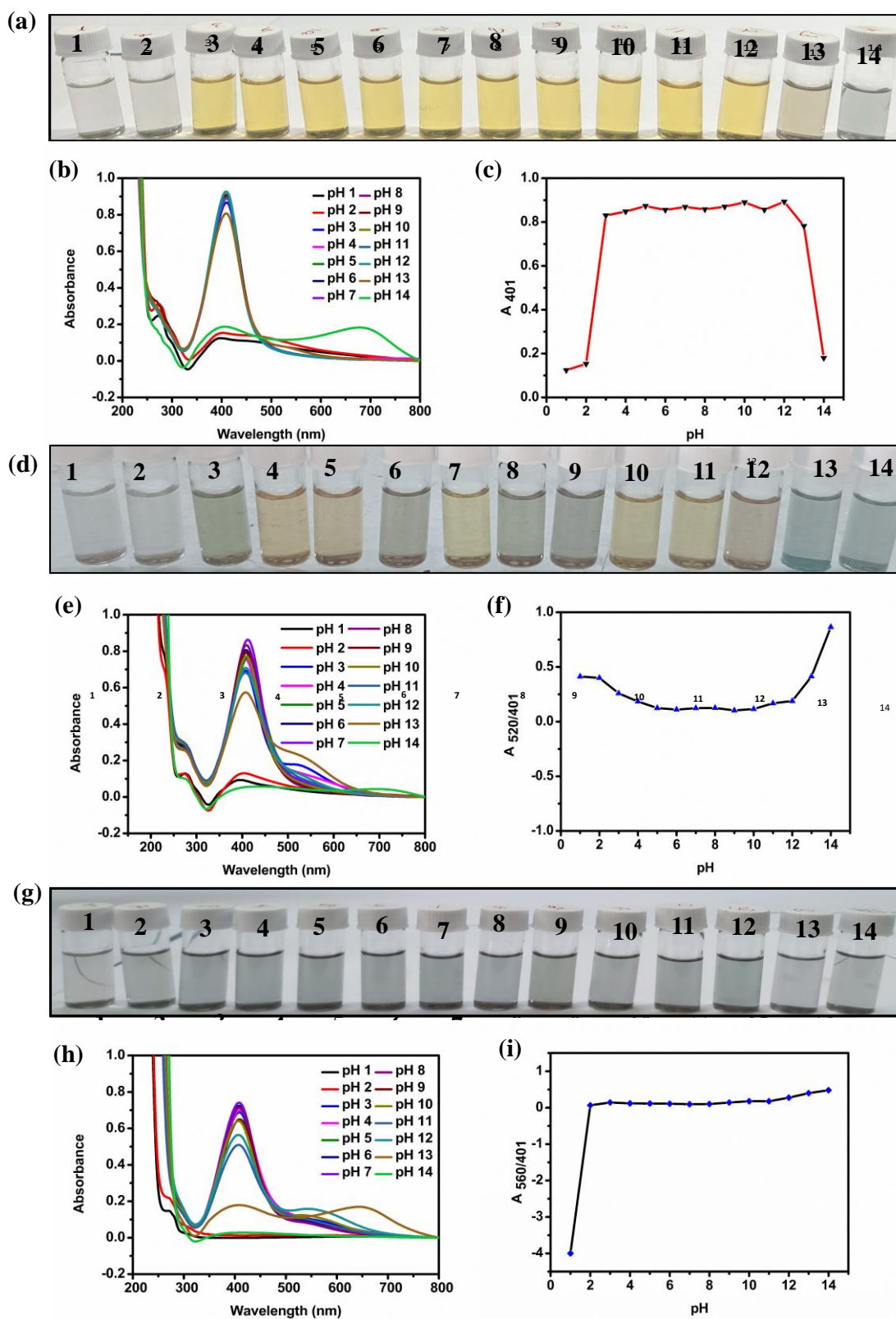


Fig. S6 (a) Visual response of AgNCs under different pH conditions, (b) UV-Vis spectra showing the effect of pH on AgNCs, (c) Effect of pH on 401 nm, (d) Visual response of AgNCs + L-Arg

under different pH conditions, (e) UV-Vis spectra showing effect of pH on AgNCs + L-Arg, (f) The effect of pH on A_{520}/A_{401} , (g) Visual response of AgNCs + L-Cys under different pH conditions, (h) UV-Vis spectra showing effect of pH on AgNCs + L-Cys, (i) The effect of pH on A_{560}/A_{401} values.

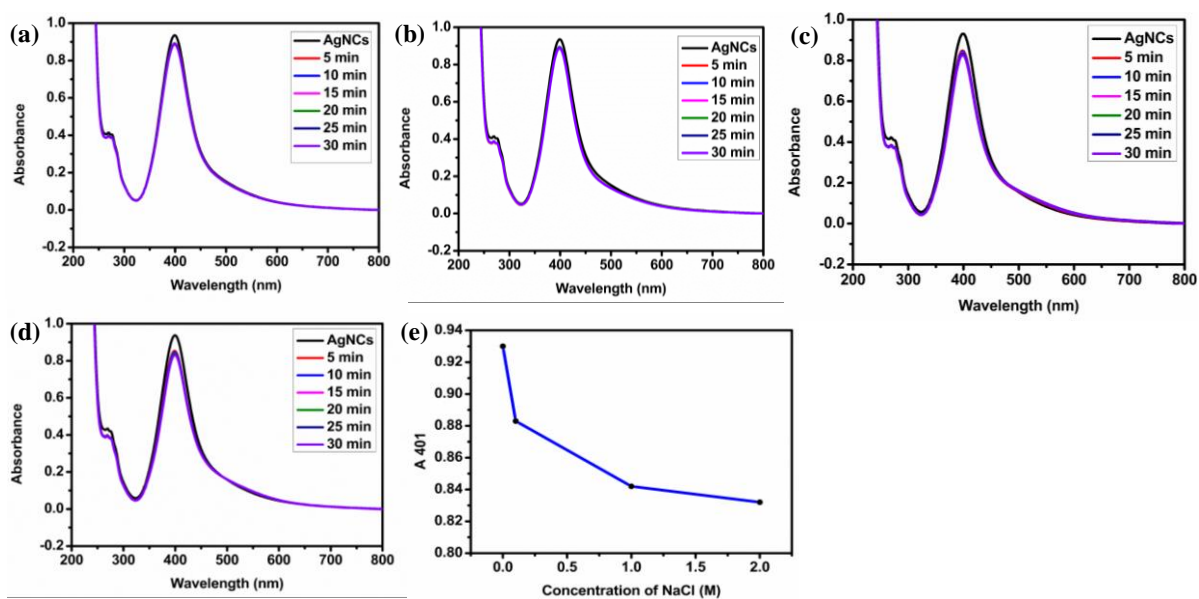


Fig. S7 UV Vis spectral response of synthesized AgNCs in the presence of different ionic concentrations of NaCl and inset showing corresponding image after 30 mins (a) 0.001 M, (b) 0.1 M, (c) 1 M, (d) 2 M, (e) Effect of ionic strength on 401 nm value.

Table S2. Comparison with previously reported probes for the detection of L-Arg

S.No.	Sensing Material	Method	LOD value	Selectivity for other analyte	Reference
1.	Carbon dots (Spherical)	Fluorescence	9.16 μ M	-	1.
2.	P-sulfonatocalix[4]arene thiol functionalized gold nanoparticles (Quasi Spherical)	Colorimetry	4 μ M	Lysine, Histidine	2.
3.	6-aza-2-thiothymine functionalized silver nanoparticles (Spherical)	Colorimetry	2.7 μ M	Spermine	3.
4.	Silver nanoparticles (Cubic)	Colorimetry	6 μ M	Cysteine	This work
5.	Carbon nano-dots (Spherical)	Fluorescence	0.26 μ M	Guanine, Lysine	4.

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Table S3. Comparison with previously reported probes for the detection of L-Cys

S.No.	Material	Method	LOD values	Selectivity for other analyte	Reference
1.	Protein coated gold nanoclusters	Fluorescence	9.87 μM	NO_3^- , Fe^{2+}	1
2.	Oligonucleotide functionalized gold nanoparticle	Colorimetry,	100 nM	-	2
3.	Cobalt sulphide nanosheets	Colorimetry	2.7 μM	-	3
4.	Fluorosurfactant capped silver nanoparticles (Spherical)	Colorimetry	0.05 μM	-	4
5.	Dextran coated silver nanoparticles (Spherical)	Colorimetry,	12 μM	-	6

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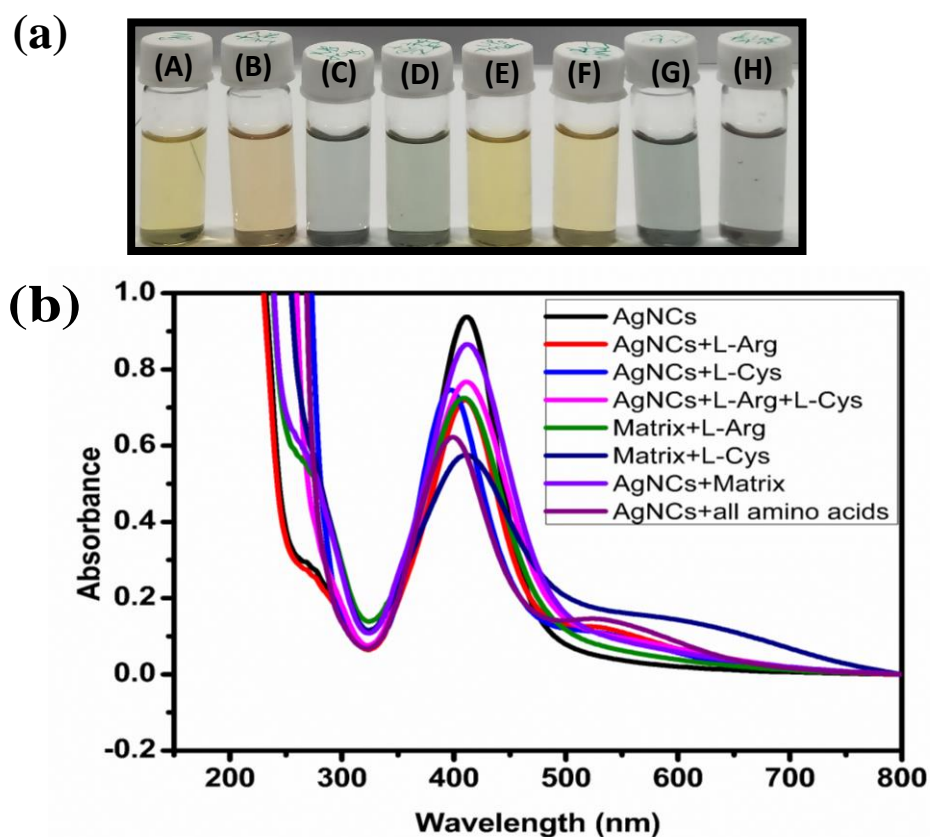
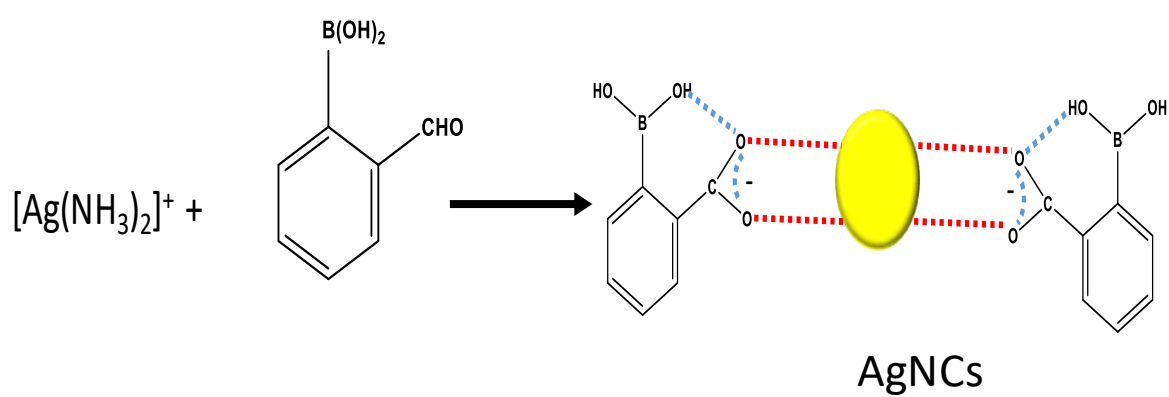
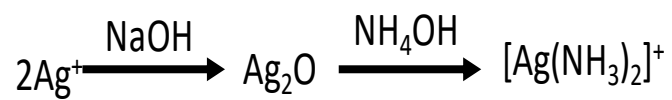


Figure S8. (a) Visual Response of AgNCs in matrix (A) AgNCs, (B) AgNCs+ L-Arg, (C) AgNCs+ L-Cys, (D) AgNCs+ L-Arg+ L-Cys, (E) AgNCs+ mixture of amino acid except L-Arg and L-Cys, (F) AgNCs+ mixture of L-Arg+ L-Cys, (G) AgNCs+ mixture of amino acids including L-Arg except L-Cys, (H) AgNCs +mixture of amino acids including L-Cys except L-Arg, (I) AgNCs+ mixture of amino acids+ L-Arg+ L-Cys and (b) Corresponding UV-Vis spectra



Scheme S1. Mechanism for the synthesis of AgNCs

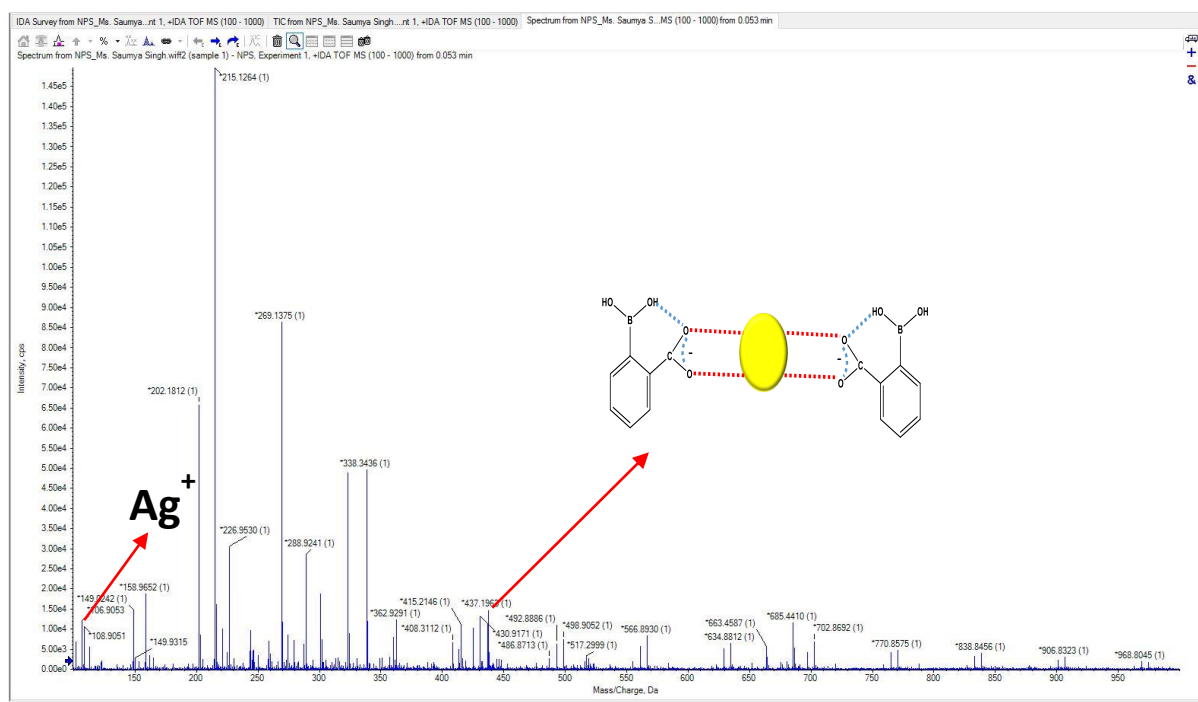


Fig S9. HRMS of AgNCs

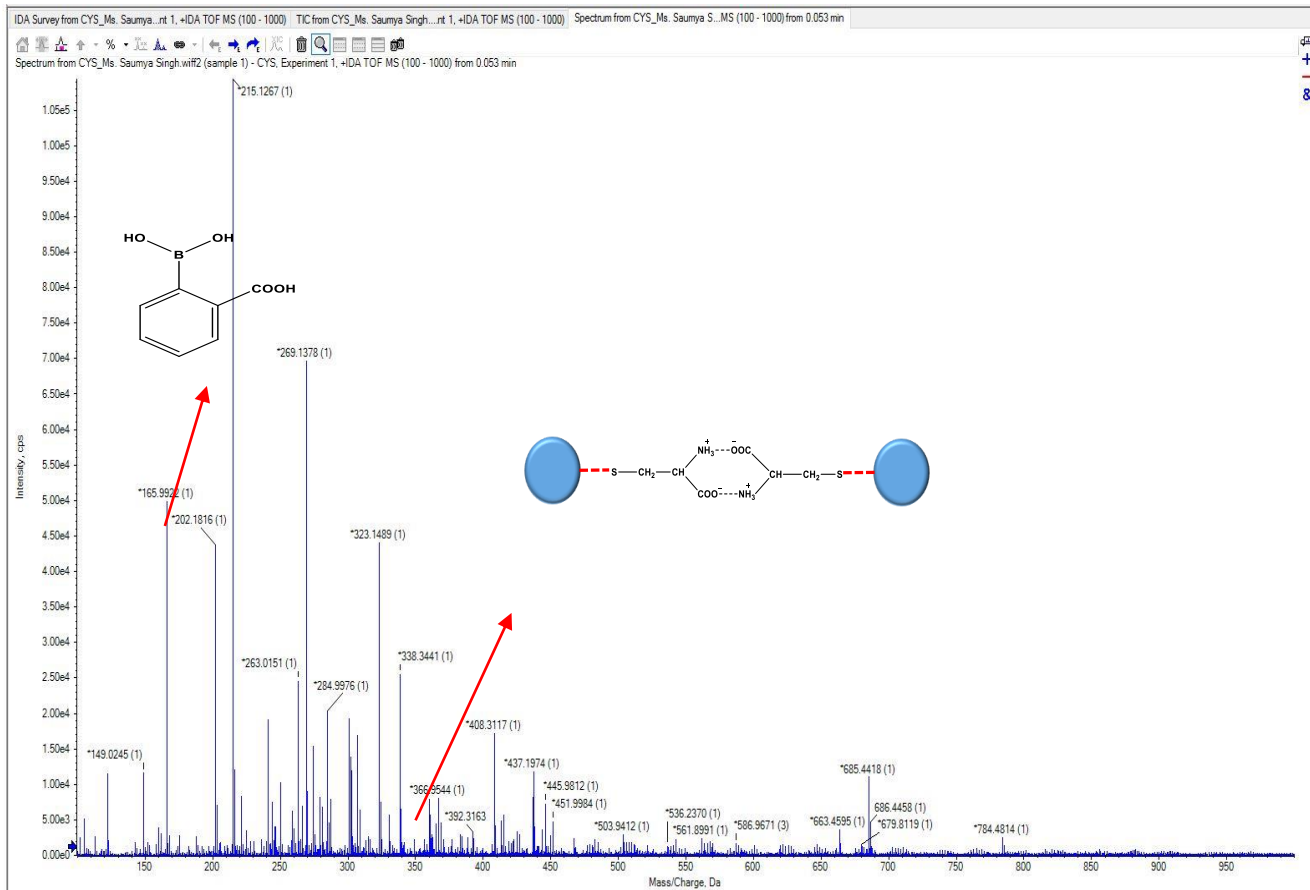


Fig. S10: HRMS of AgNCs+L-Cys

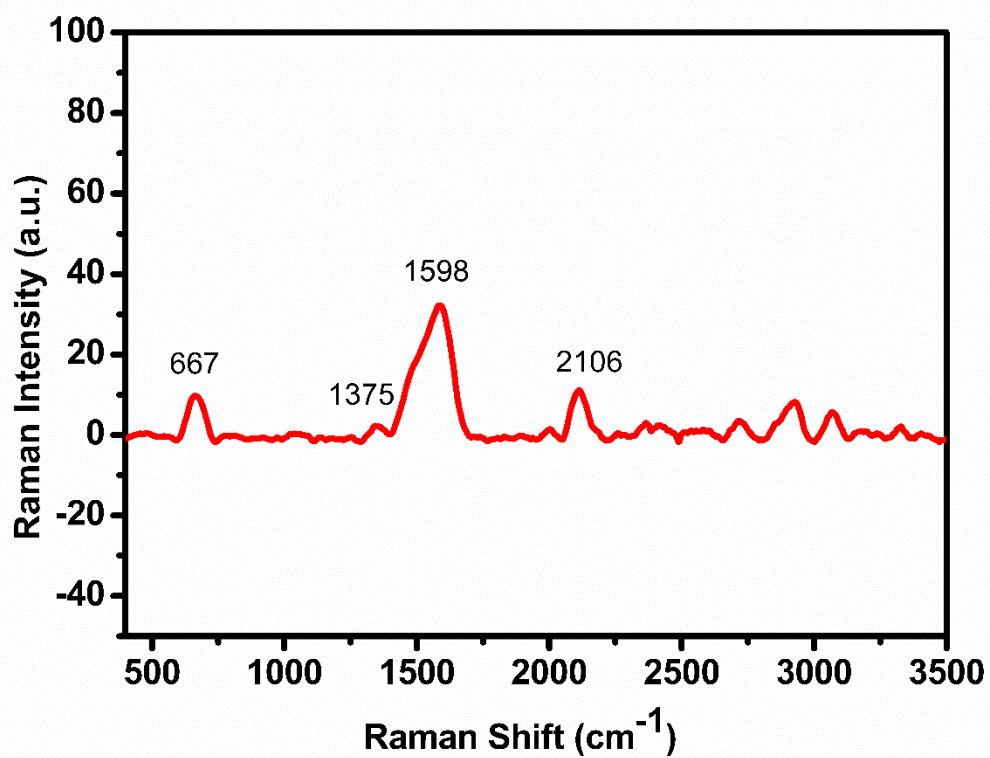


Fig. S11: Raman spectrum of AgNCs

Table S4. Raman wavenumbers (cm^{-1}) and intensity (a.u.) and their probable assignments.

Wavenumber (cm^{-1})	Intensity (a.u.)	Probable assignment
667	20	C-B-O out of plane bending
1371	36	B-C
1598	60	Aromatic C-C
2106	10	Intramolecular hydrogen bonding

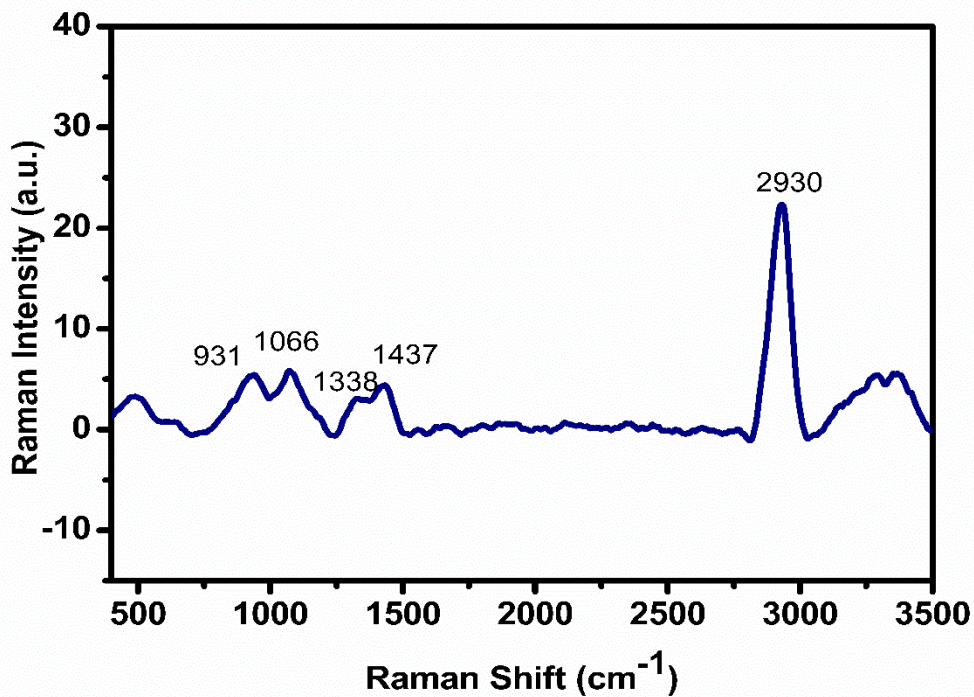


Fig. S12 Raman spectrum of L-Arg

Table S5. Raman and SERS wavenumbers (cm⁻¹) and relative intensities (a.u.) and their probable assignments corresponding to Fig. 6a (Main Text).

Raman (cm ⁻¹)	Relative Intensity (a.u.)	SERS (cm ⁻¹)	Relative Intensity (a.u.)					Most Probable Assignment
			A	B	C	D	E	
931	138	1029	207	271	382	550	689	ν C-COO-
1066	134	1122	191	259	354	517	668	ν CN
1338	127	1332	221	290	396	562	784	ω CH ₂
1437	134	1568	216	304	443	599	850	NH δ guanidium fragment
2930	157	2914	205	276	382	545	715	ν CH

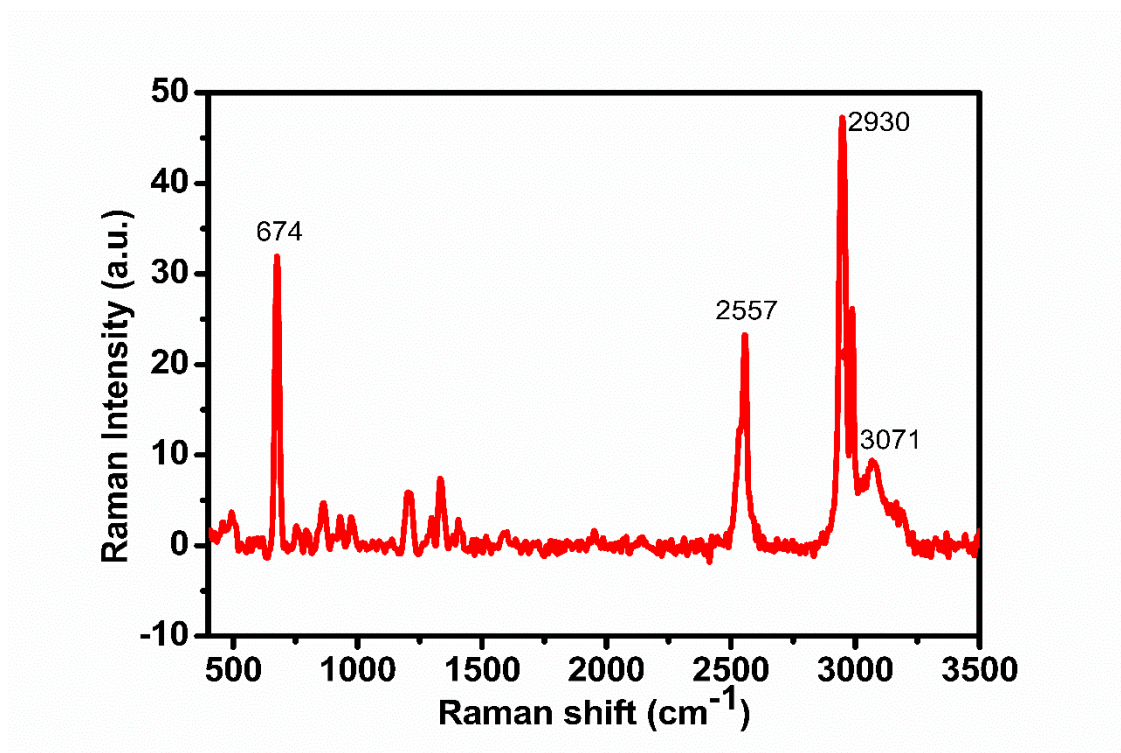


Fig. S13 Raman spectrum of L-Cys

Table S6. Raman and SERS wavenumbers (cm⁻¹) and relative intensities (a.u.) and their probable assignments corresponding to Fig. 6a (Main Text).

Raman (cm ⁻¹)	Relative Intensity (a.u.)	SERS (cm ⁻¹)	Relative Intensity (a.u.)					Most Probable Assignment
			A	B	C	D	E	
674	148	504	241	333	462	568	686	v C-S
2557	136	-	-	-	-	-	-	v S-H
2930	163	2916	246	360	462	565	698	v C-H
3071	144	2962	215	322	418	530	648	v N-H

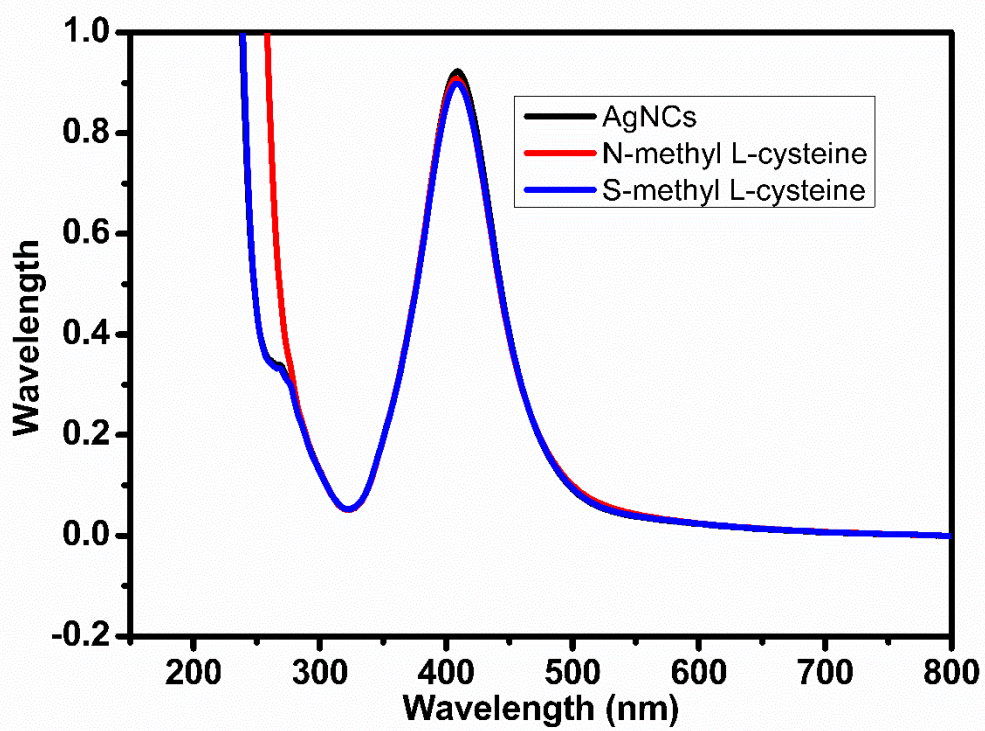
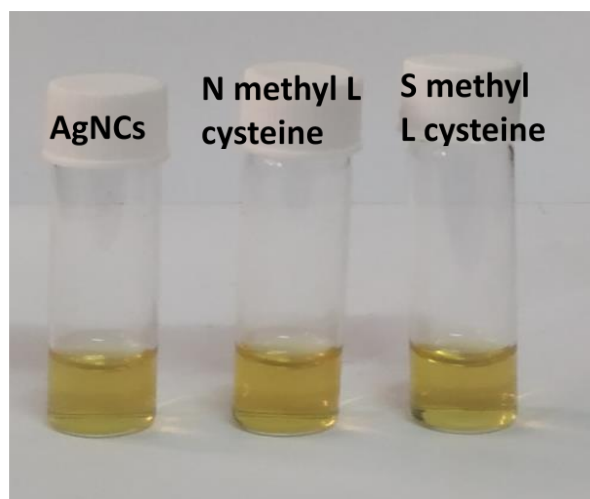
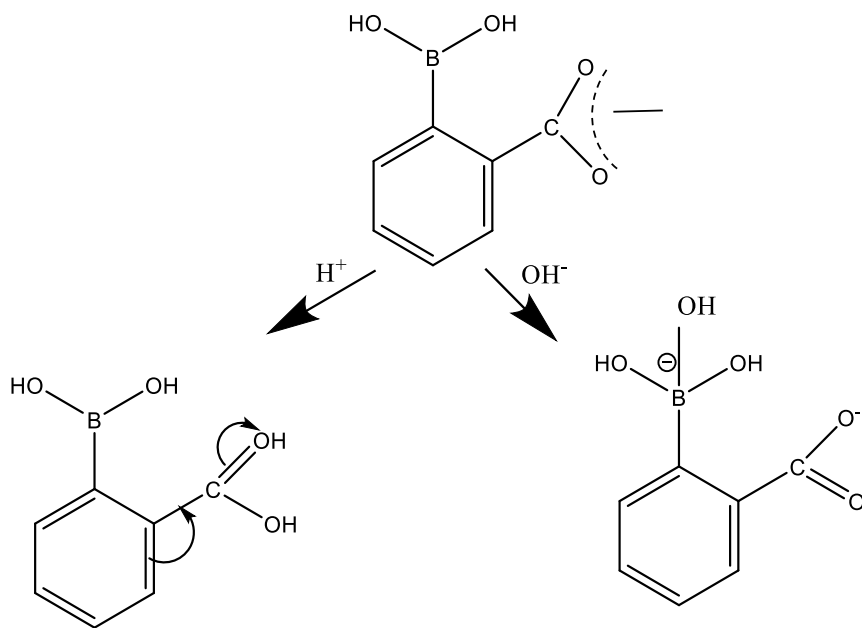


Fig. S14 Visual response and corresponding UV-Vis spectra after addition of N-methyl L-Cysteine and S- Methyl L Cysteine into AgNCs.



Destabilises the benzenoid structure
hence possibly gets removed from
AgNCs

The occurrence of one -ve charge
over B atom destabilizes the
system hence might be getting
AgNCs surface

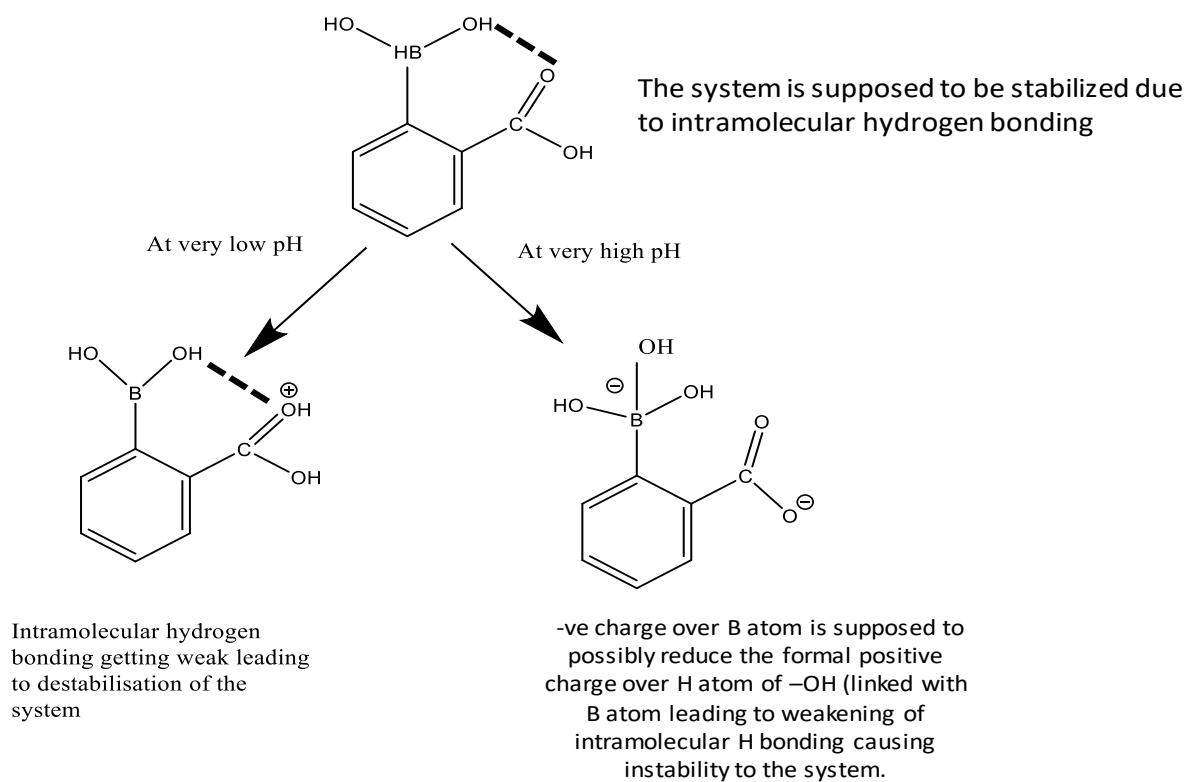


Fig. S15 Probable mechanism for change in optical properties at very high and very low pH.