Electronic Supplementary Information

Dual-emissive solid-state histidine-stabilized gold nanoclusters for applications in white-light generation

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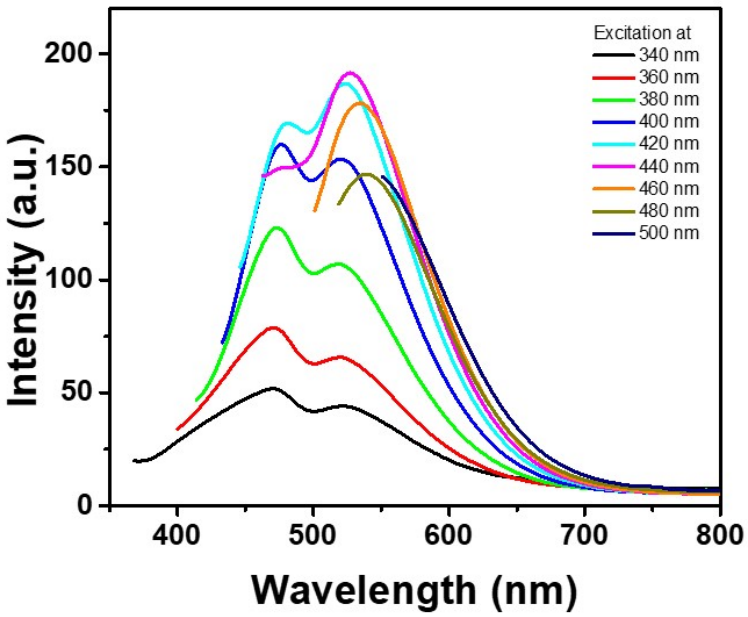

Figure S1. PL spectra of powder His-AuNCs at different excitation wavelengths.

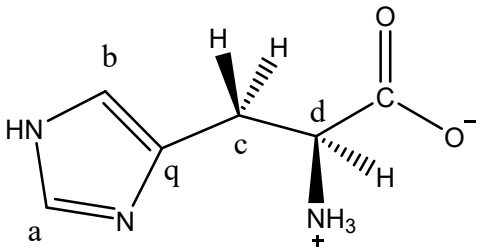

Figure S2. The L-histidine structure with the imidazole ring and the numbering used to assign the signals in ^{1}H and ^{13}C NMR spectra.

L-Histidine

^{1}H-NMR (600MHz, D_2O, δppm): 7. 56 (s, 1H, Ha), 6.87(s, 1H, Hb), 3,80(dd, 1H, J=8.01Hz, J=4.75Hz, Hd), 3.04(dd, 1H, J=0.74Hz, J=15.4Hz Hc'), 2.94(dd, 1H, J= 8.01Hz, J=15.4Hz, Hc)

^{13}C-NMR (150MHz, D_2O, δppm): 28.1Cc, 54.7Cd, 116.6Cb, 132.1Cq, 136.2Ca, 173.9 Cq(C=)O

His-AuNCs

^{1}H-NMR (600MHz, D_2O, δppm): 7.78(s, 1H, Ha), 6.97(s, 1H, Hb), 3.85(dd, 1H, J=7.8 Hz, J=5.0 Hz, Hd), 3.10(dd, 1H, J= 15.5Hz, J= 5.0Hz, Hc') 3.01(dd, 1H, J=15.5 Hz, J=7.8 Hz, Hc)

^{13}C-NMR (150MHz, D_2O, δppm): 27.6 Cc, 54.5 Cd, 116.8 Cb, 131.2 Cq, 135.8 Ca, 173.5 Cq(C=)O

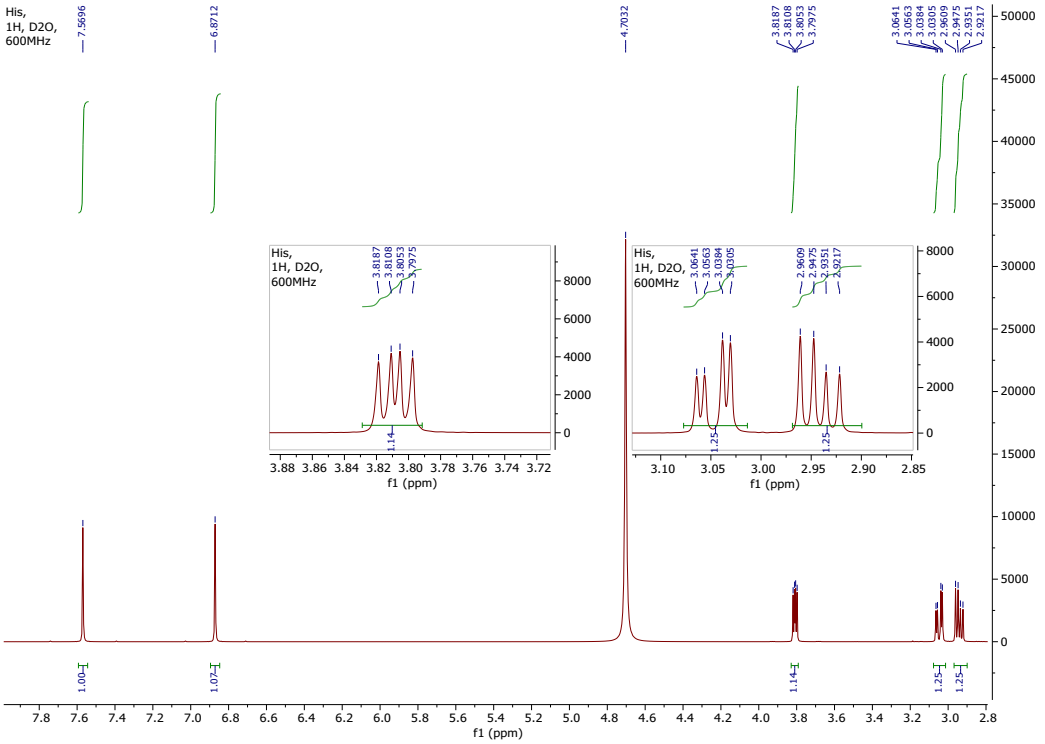

Figure S3. ^{1}H-NMR spectra of L-histidine at 600 MHz in D_2O, including the detail of aliphatic region.

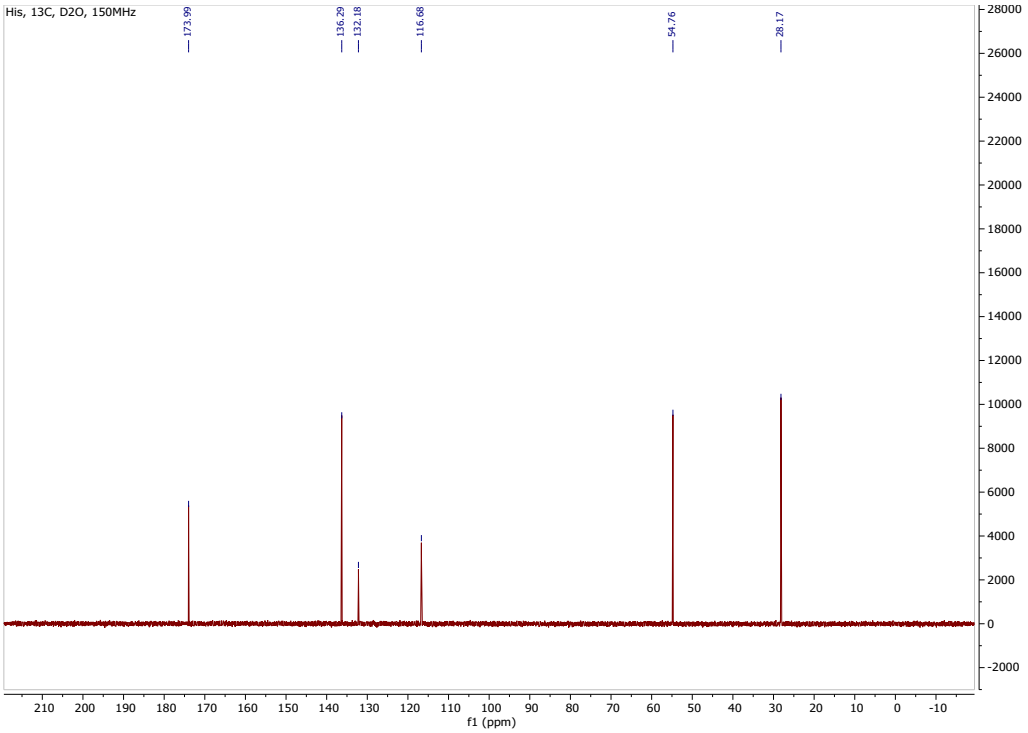

Figure S4. ^{13}C-NMR spectra of L-histidine at 150 MHz in D_2O.

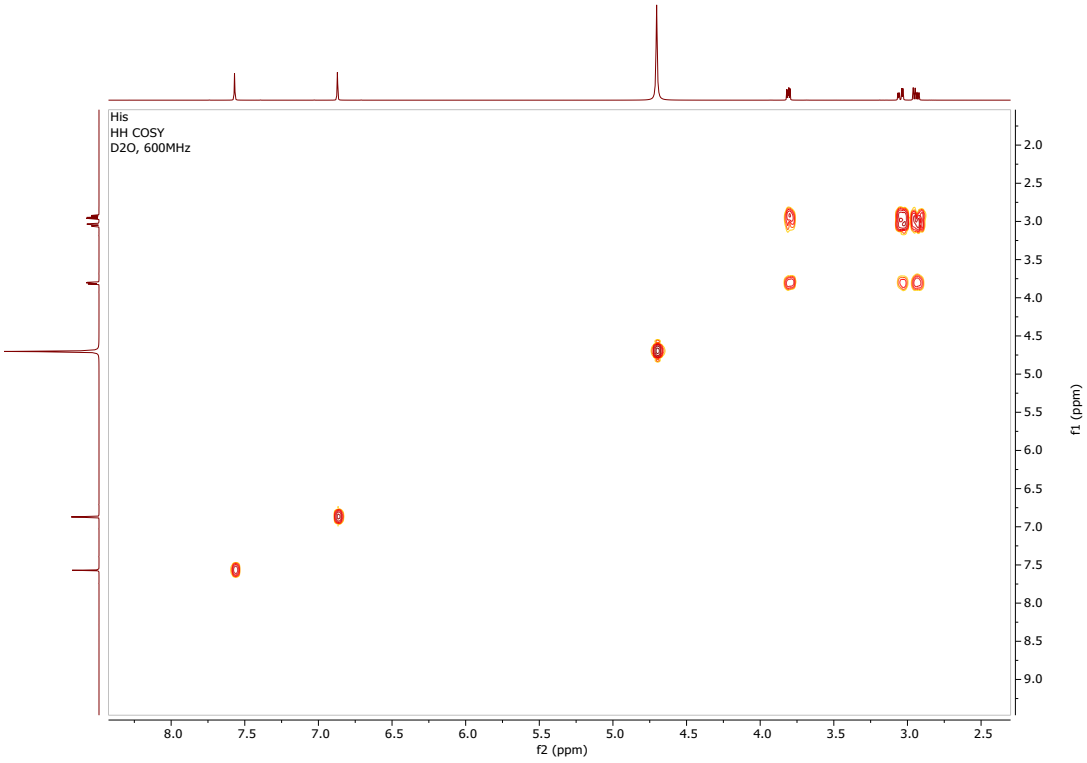

Figure S5. The ^{1}H-^{1}H COSY spectra of L-histidine.

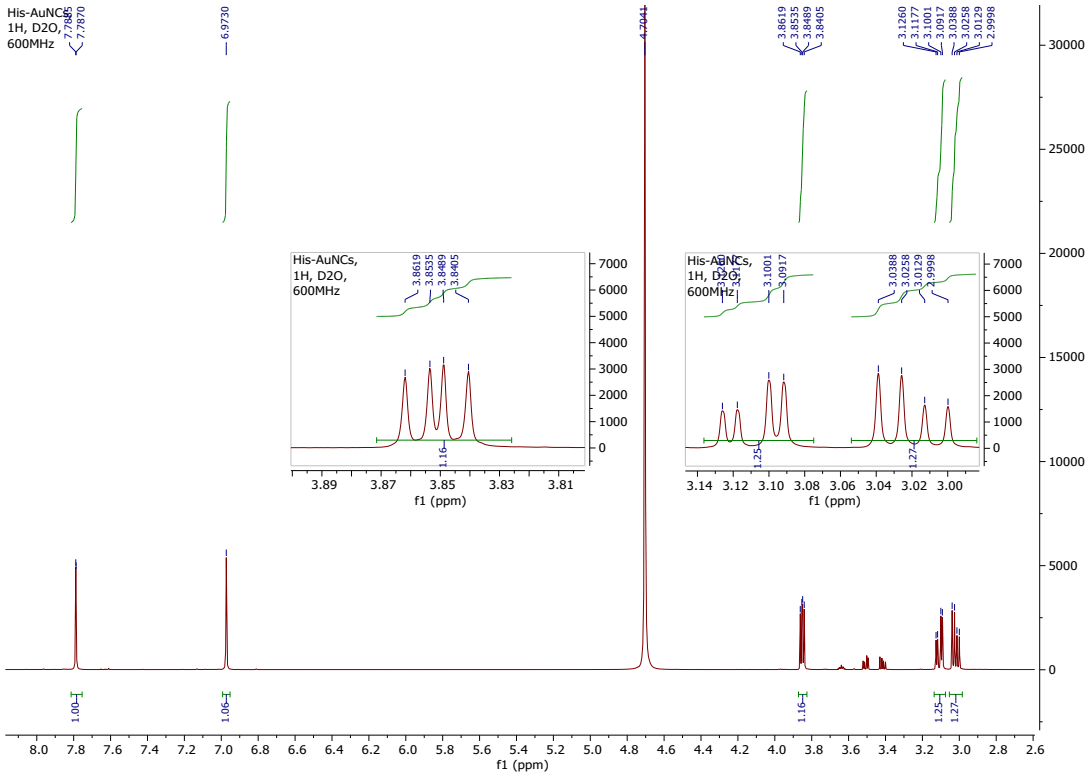

Figure S6. ^{1}H-NMR spectra of His-AuNCs at 600 MHz in D_2O, including the detail of aliphatic region.

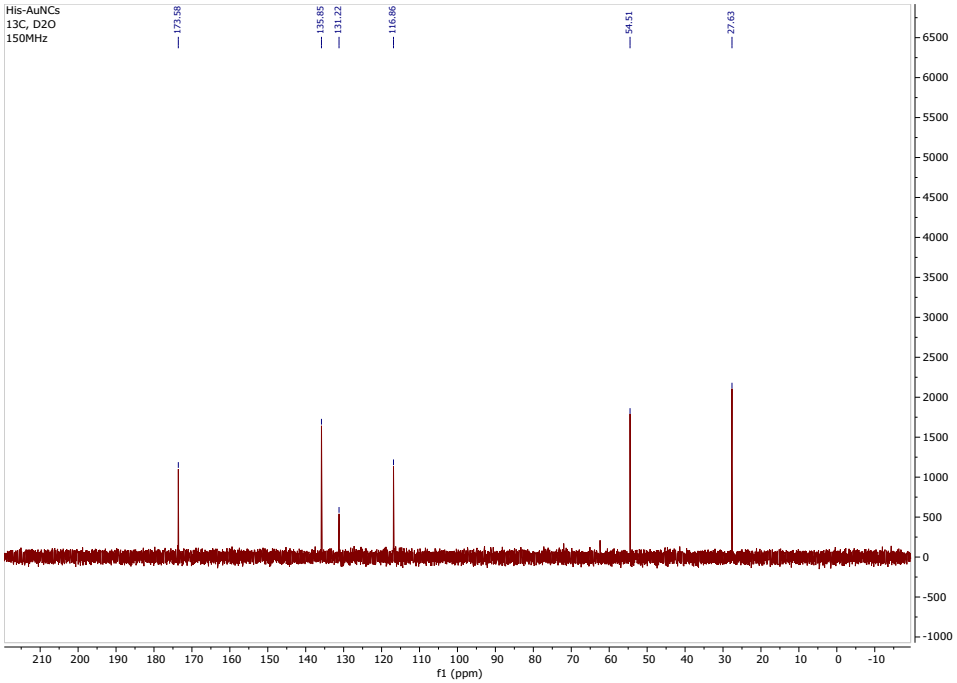

Figure S7. ^{13}C-NMR spectra of His-AuNCs at 150 MHz in D_2O.

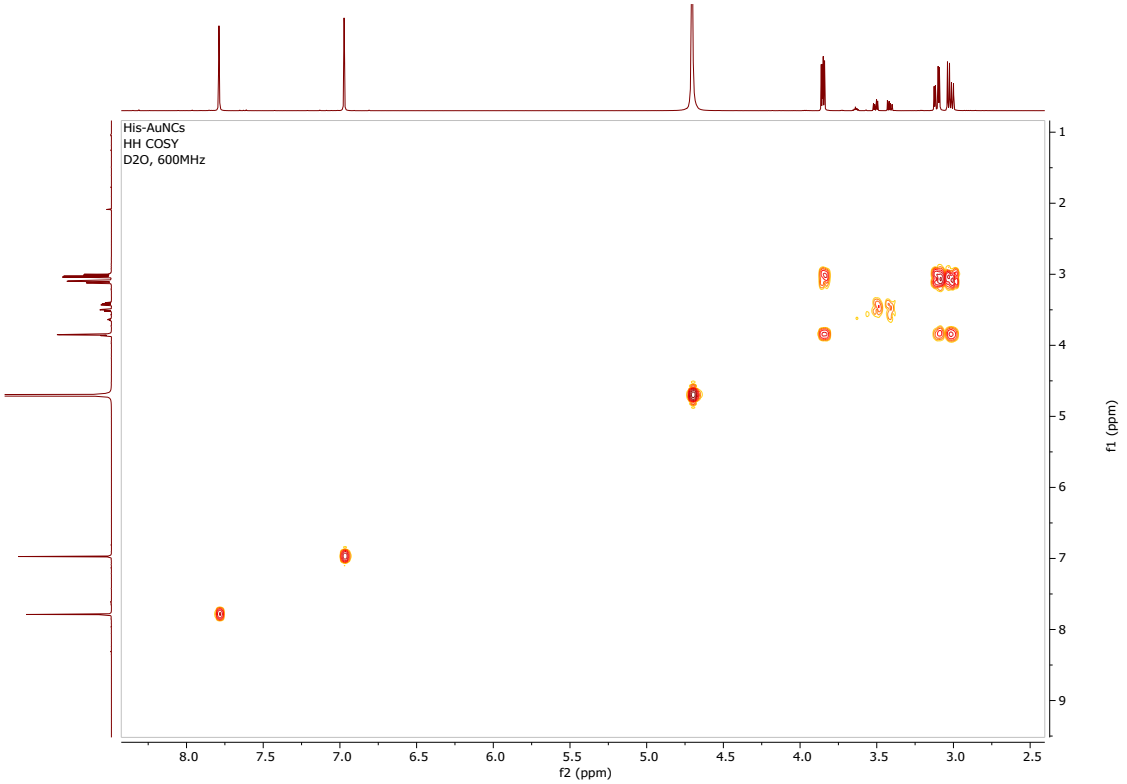

Figure S8. The ^{1}H-^{1}H COSY spectra of His-AuNCs.

Table S1. Elemental at% composition at the surface of the His and His-AuNCs samples.

Sample	at%				
	O	**C**	**N**	**Cl**	**Au**
His-AuNCs	15.1	62.4	20.3	2.1	0.1
His	17.6	64.5	17.9	-	-

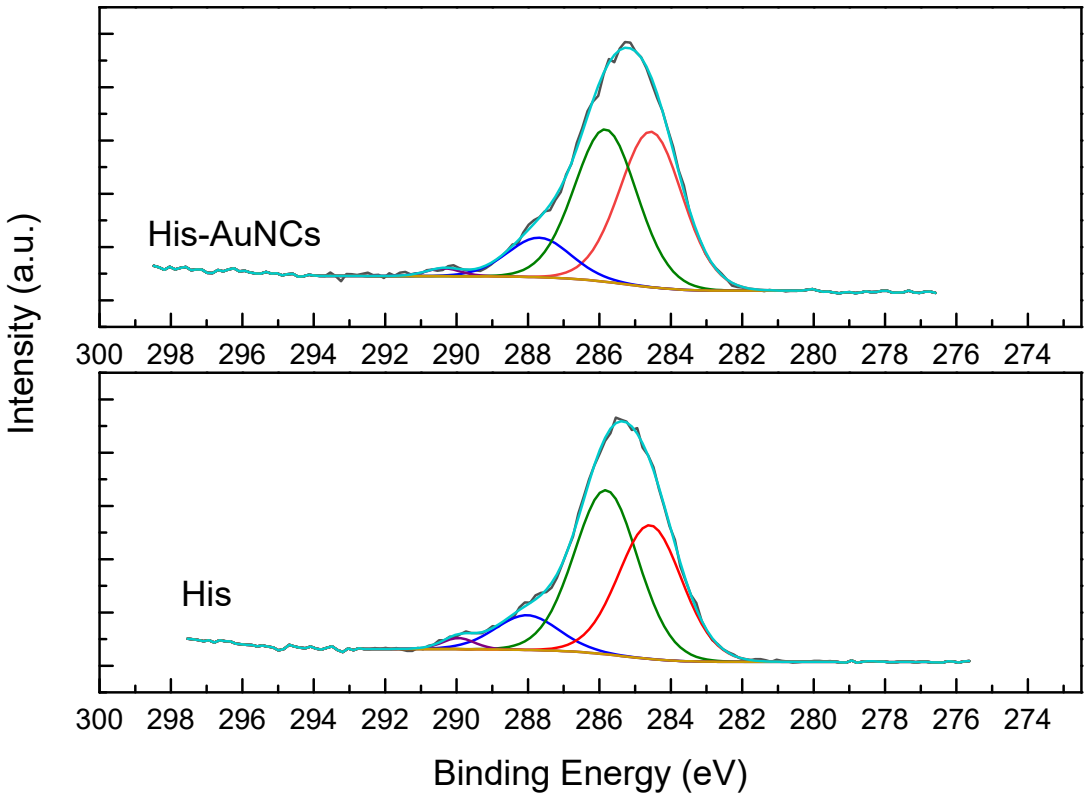

Figure S9. C1s core level spectra.

Table S2. Deconvolution of C1s spectra.

Sample/component	C-C C-H	%	C-N C-O	%	C=O	%	O=C–OH N–C=O	%
His-AuNCs	284.6	44.2	285.8	43.3	287.7	11.3	290.3	1.2
His	284.6	39.5	285.8	48.5	288	10.3	289.9	1.7

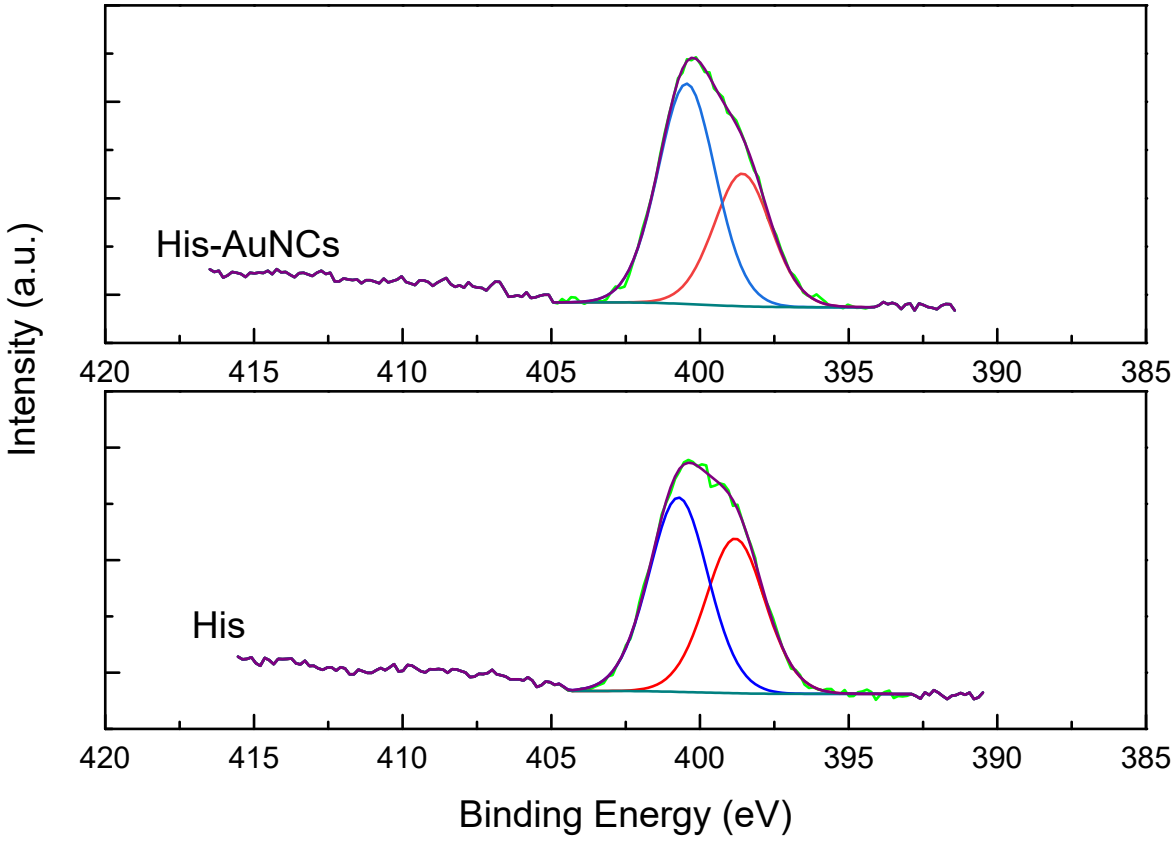

Figure S10. N1s core level spectra.

Table S3. Deconvolution of N1s spectra.

Sample/component	Imino N in IM ring	%	(-NH2) amino group C-NH-C (IM-ring)	%
His-AuNCs	398.6	37.6	400.5	62.4
His	398.8	44.3	400.7	55.7

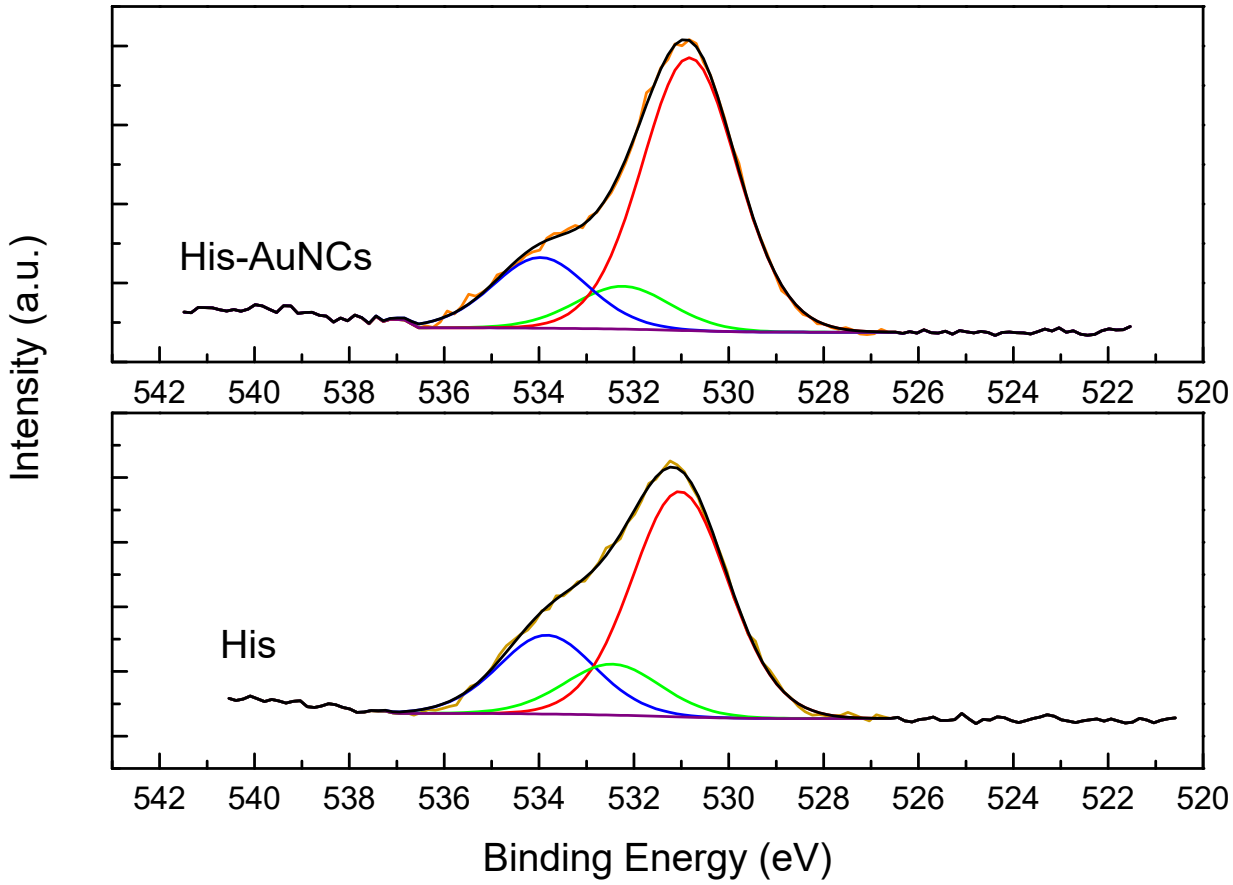

Figure S11. O1s core level spectra.

Table S4. Deconvolution of O1s spectra

Sample/component	HO-C=O O=C-N C=O	%	C-OH O=C-O	%	O=C-O C-O-C	%
His-AuNCs	530.8	70.6	532.2	11.1	533.9	18.3
His	531	63.4	532.4	14.4	533.8	22.2

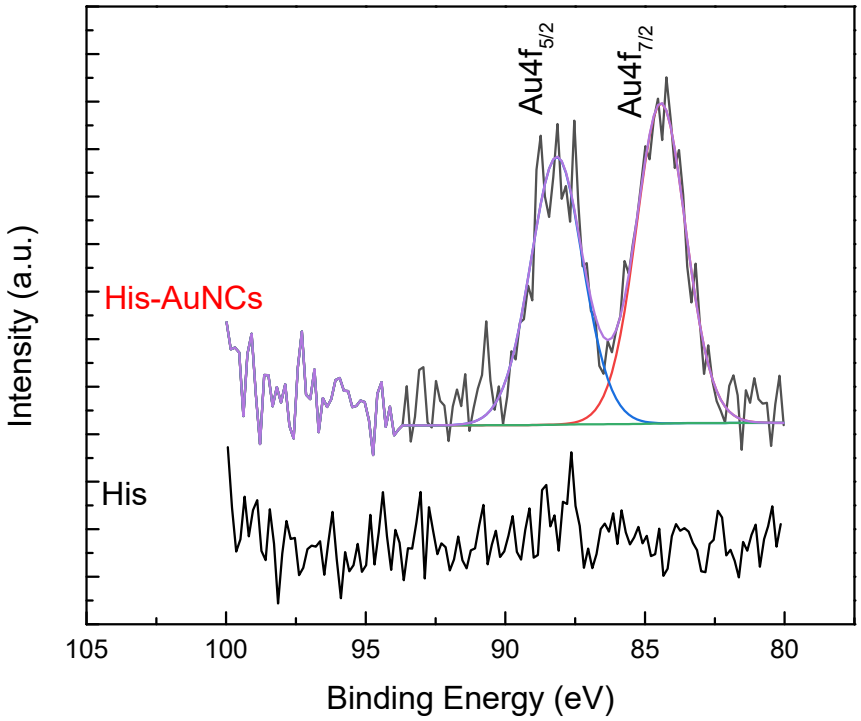

Figure S12. Au4f core level spectra.

Table S5. deconvolution of Au4f spectra

Sample/component	$Au4f_{7/2}$	%	$Au4f_{5/2}$	%
His-AuNCs	84.5	57.1	88.2	42.9
His	-	-	-	-

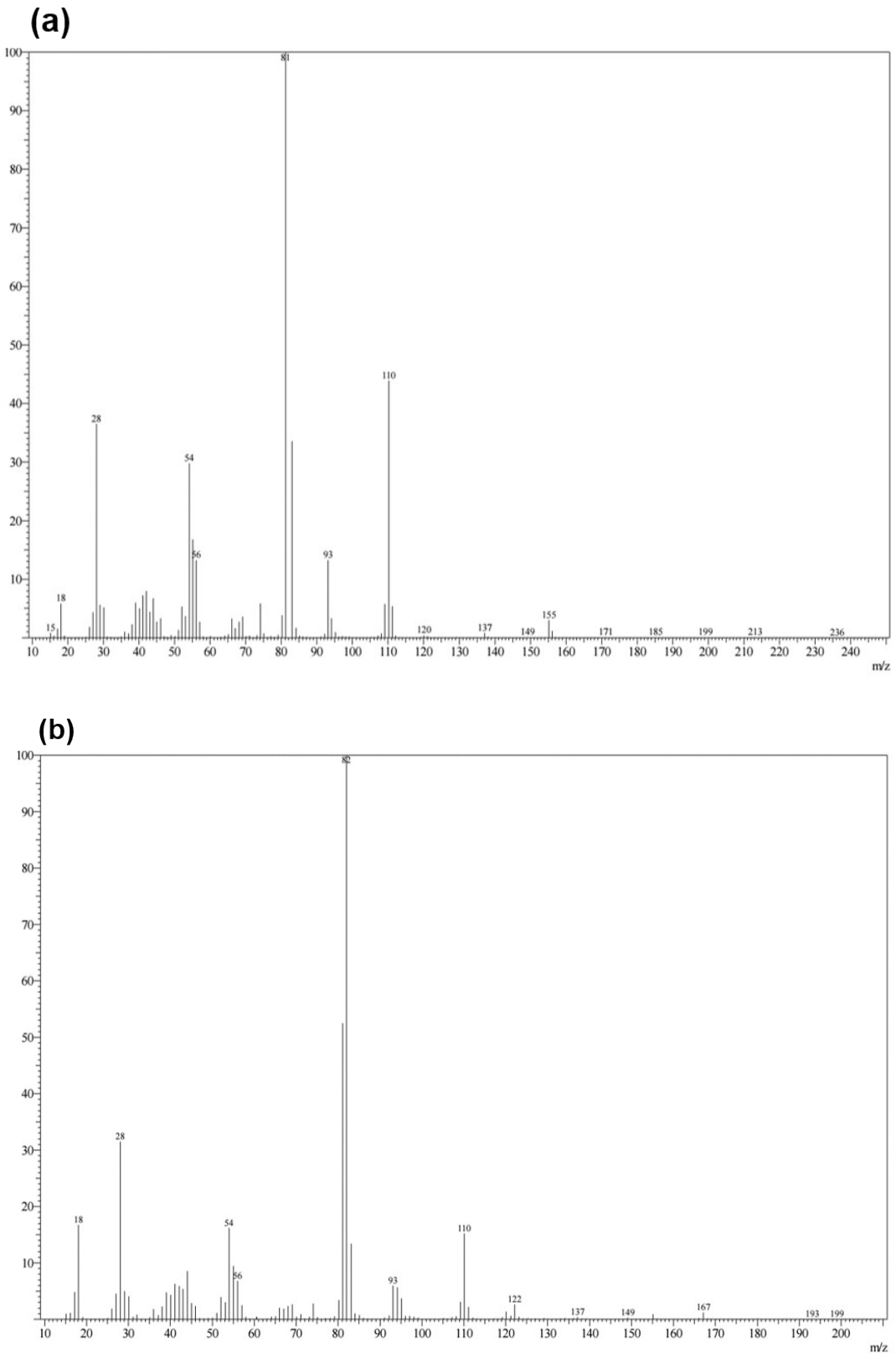

Figure S13. The EI mass spectra of His (a) and His-AuNCs (b).

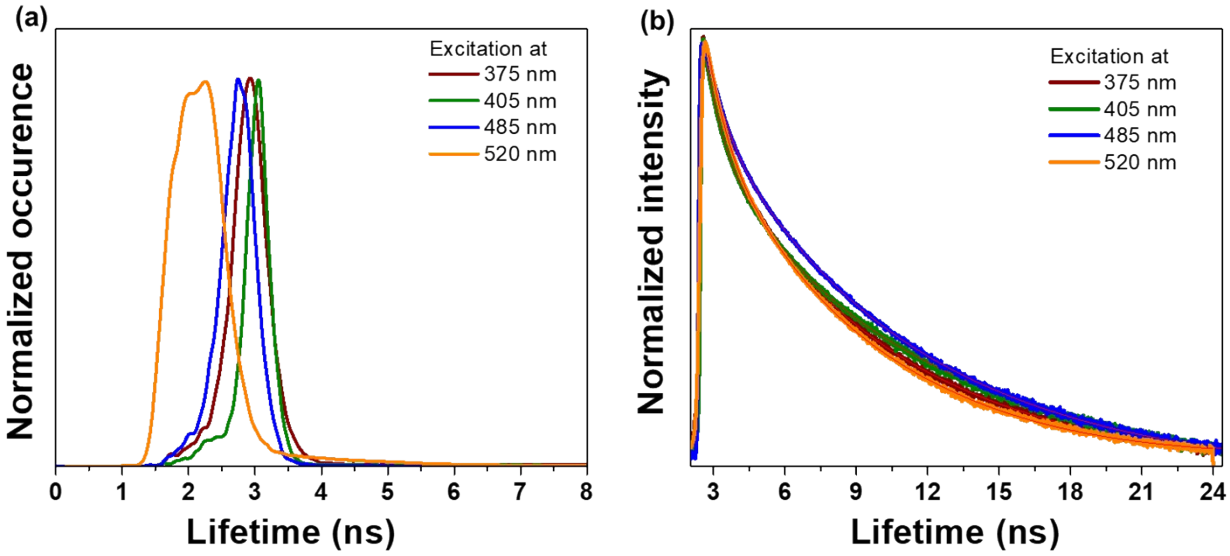

Figure S14. (a) Lifetime histograms extracted from the FLIM images recorded at different excitation wavelengths (see FLIM images in Figure 4a – bottom row). (b) Fluorescence lifetime decay curves obtained for powder His-AuNCs at different excitation wavelengths.

Table S6. The average PL lifetime obtained for His-AuNCs in solid state under different excitation wavelengths.

Excitation (nm)	**375**	**405**	**485**	**520**
Average lifetime (ns)	2.38	2.75	2.7	2.15

Average lifetime represents the intensity-weighted average lifetime calculated with the formula $\tau_{av\,int} = \frac{\sum_{1}^{n} a_i \tau_i^2}{\sum_{1}^{n} a_i \tau_i}$; τ_i and a_i are the fluorescence lifetime components and corresponding amplitudes, respectively.

Table S7. The CIE color coordinates of His-AuNCs obtained at different excitation wavelengths.

Excitation (nm)	**340**	**365**	**380**	**400**	**420**
CIE	0.39/0.35	0.38/0.34	0.37/0.34	0.37/0.34	0.36/0.33

Table S8. The CIE color coordinates of His-AuNCs after thermal treatment (λ_{exc} = 365 nm).

Temperature (°C)	**25**	**50**	**100**	**150**	**200**
CIE	0.38/0.34	0.38/0.34	0.38/0.34	0.38/0.34	0.12/0.04