Supporting information

A highly sensitive and selective acid hydrazide-based chemosensor for detection of Cu^{2+} in aqueous environment: Experimental and DFT/TDDFT study

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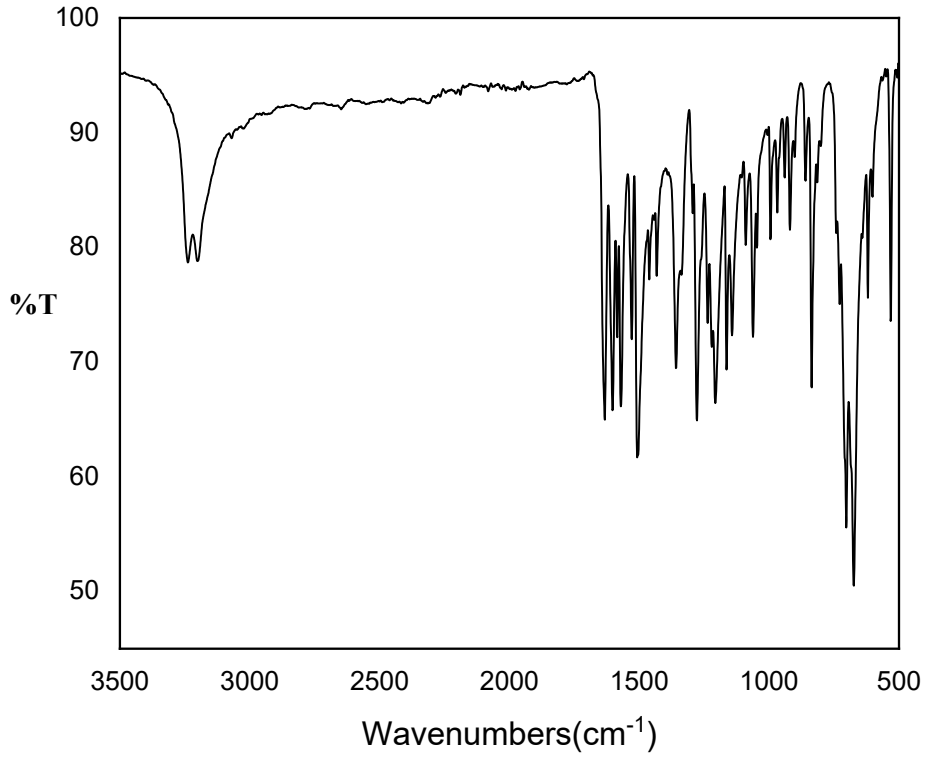

Fig. S1. FT-TR Spectrum of HP.

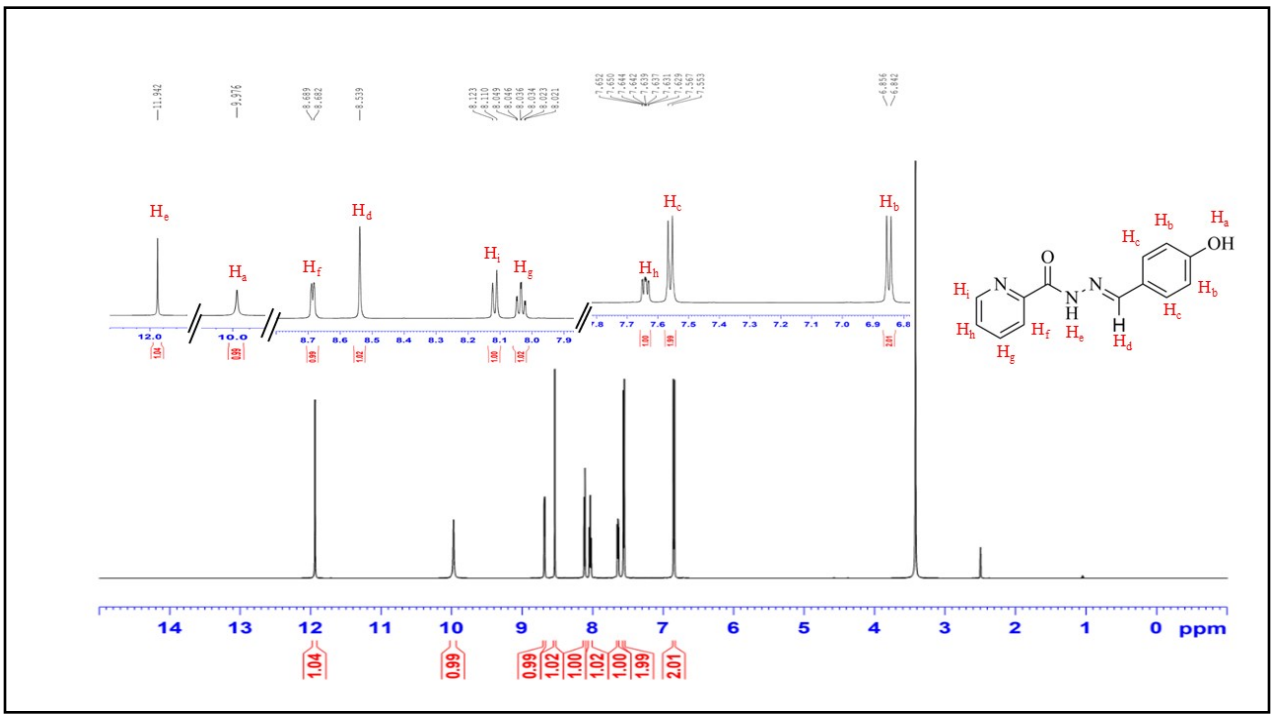

Fig. S2. ^{1}H NMR Spectrum of HP.

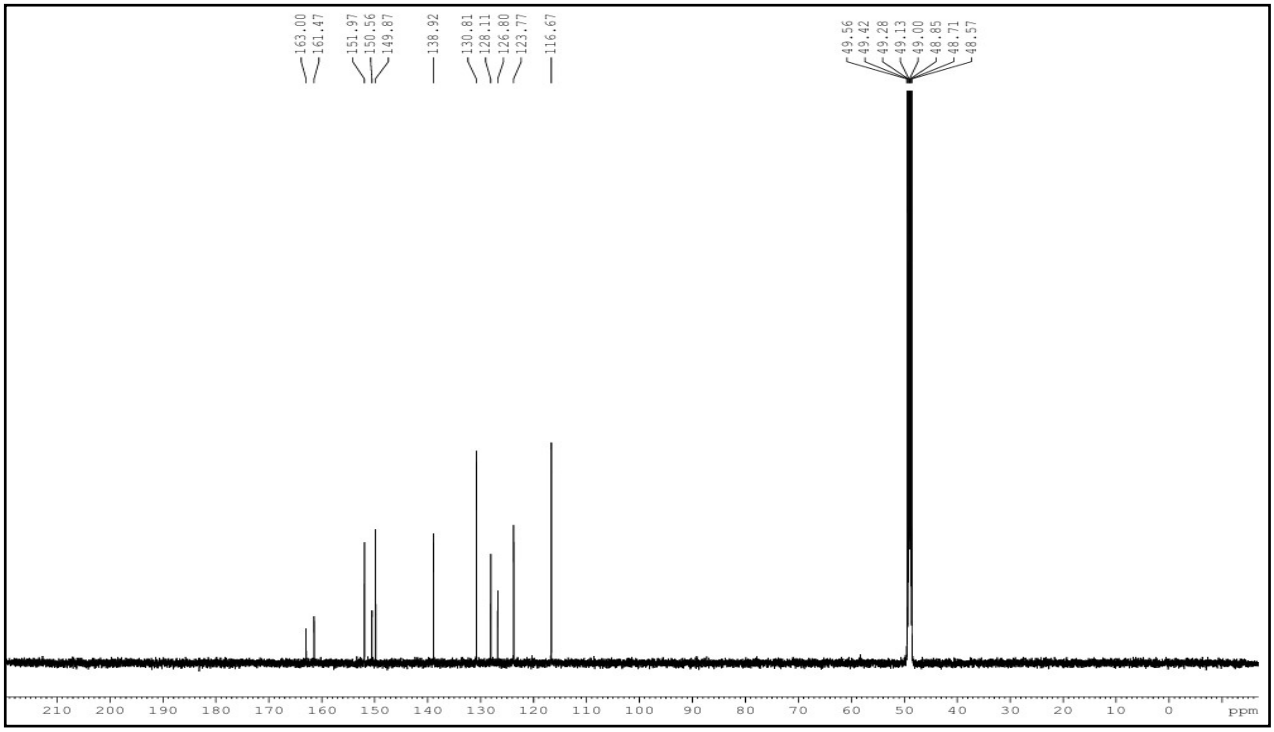

Fig. S3. ^{13}C NMR Spectrum of HP.

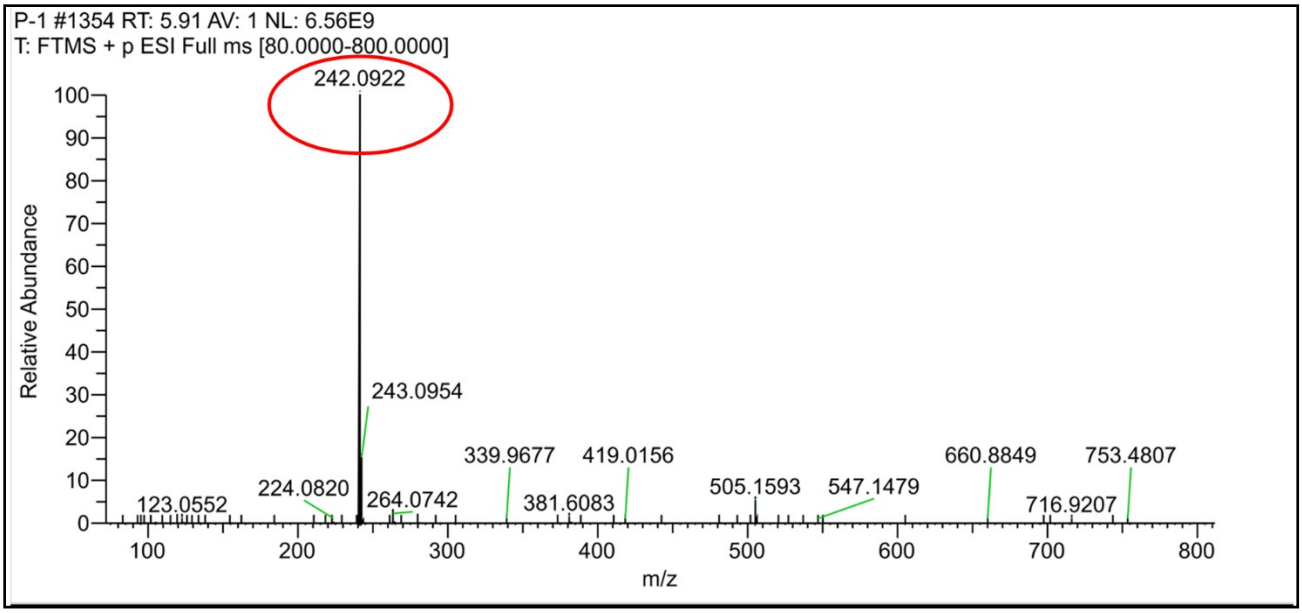

Fig. S4: HRMS spectra of HP.

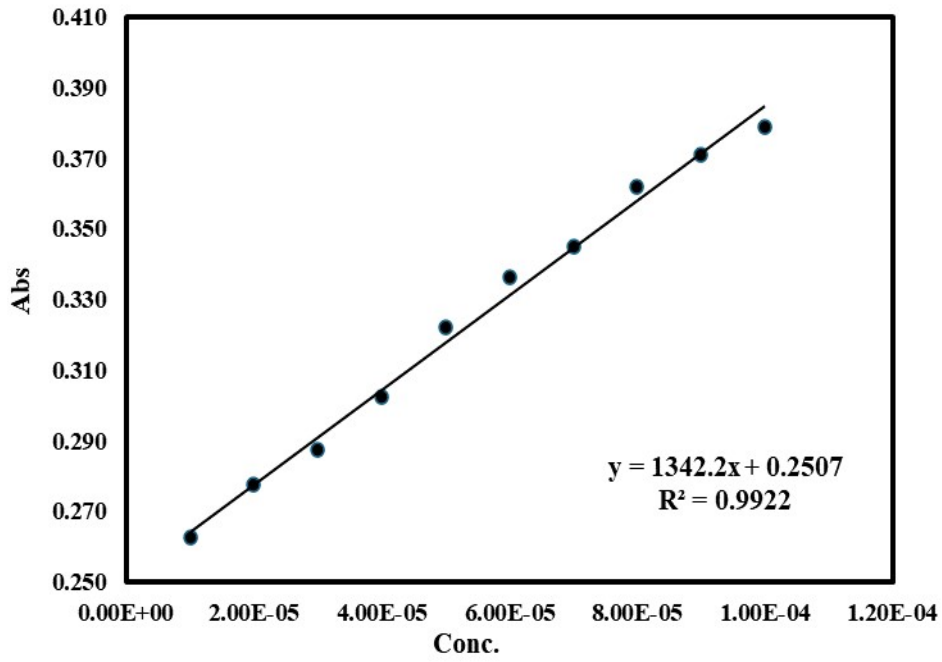

Fig. S5. Detection limit for Cu^{2+} in MeOH/H_2O (6:4 v/v, HEPES = 10 mM, pH 7.4).

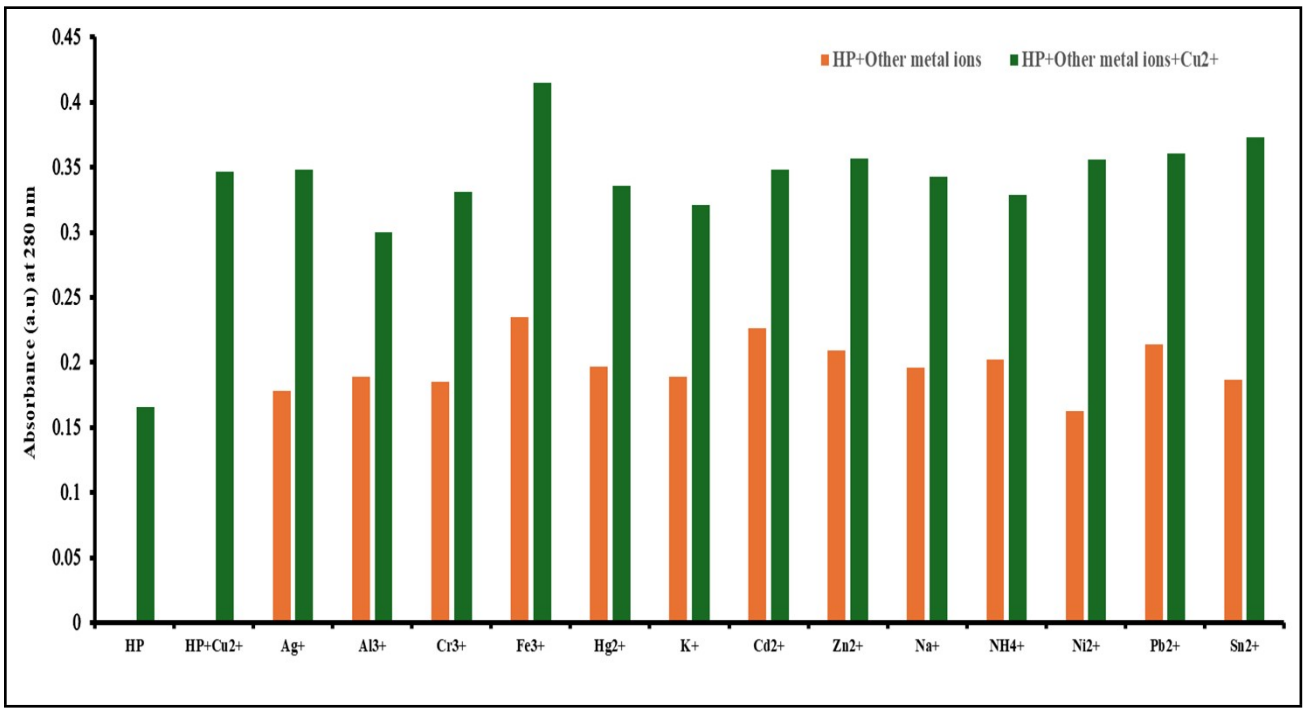

Fig. S6. UV−Vis absorption responses of probe HP with a mixture of dual metal ions (Cu^{2+} and other stated metal ions,10^{-1}M) in MeOH/H_2O (6:4 v/v, HEPES = 10 mM, pH 7.4).

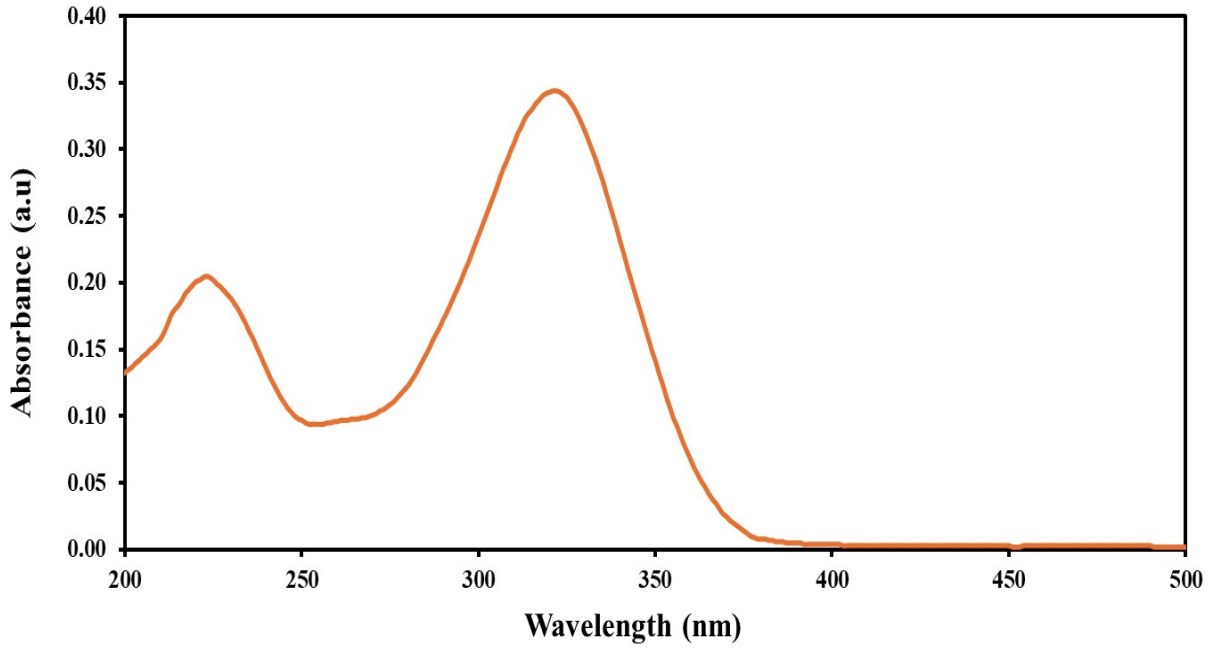

Figure S7. Base line spectra of HP.

Table S1: The DFT-optimized and ORTEP bond length values of **HP**.

Atom 1	**Atom 2**	**XRD Bond Length (A^O)**	**DFT Bond Length (A^O)**
O1	C1	1.2421(13)	1.2156
O2	C11	1.3587(12)	1.366
N1	N2	1.3868(11)	1.3769
N1	C1	1.3413(14)	1.3713
N2	C7	1.2805(14)	1.2816
N3	C2	1.3423(14)	1.3404
N3	C6	1.3363(14)	1.3343
C1	C2	1.4954(13)	1.5138
C2	C3	1.3864(15)	1.3949
C3	C4	1.3867(15)	1.3905
C4	C5	1.3794(16)	1.3926
C5	C6	1.3904(15)	1.3939
C7	C8	1.4643(13)	1.4601
C8	C9	1.3961(15)	1.4
C8	C13	1.4021(14)	1.4074
C9	C10	1.3902(14)	1.3918
C10	C11	1.3929(15)	1.3948
C11	C12	1.3980(15)	1.4001
C12	C13	1.3750(15)	1.3833

Table S2: The DFT-optimized and ORTEP angles values of **HP**.

Atom	**Atom**	**Atom**	**XRD Angle°**	**DFT Angle°**
C1	N1	N2	117.73(9)	118.23
C7	N2	N1	116.47(9)	116.77
C6	N3	C2	116.90(9)	118.05
O1	C1	N1	122.77(9)	122.45
O1	C1	C2	120.77(9)	121.17
N1	C1	C2	116.46(9)	116.21
N3	C2	C1	117.30(9)	118.14
N3	C2	C3	124.00(9)	123.12
C3	C2	C1	118.70(9)	118.73
C2	C3	C4	118.03(10)	118.33
C5	C4	C3	118.94(10)	118.9
C4	C5	C6	118.90(10)	118.51

N3	C6	C5	123.22(10)	123.07
N2	C7	C8	119.59(9)	120.51
C9	C8	C7	120.98(9)	120.69
C9	C8	C13	118.38(9)	118.38
C13	C8	C7	120.60(9)	121.23
C10	C9	C8	121.05(9)	121.11
C9	C10	C11	119.64(9)	119.64
O2	C11	C10	123.43(9)	122.76
O2	C11	C12	116.79(9)	117.23
C10	C11	C12	119.78(9)	119.999
C13	C12	C11	120.12(10)	119.97
C12	C13	C8	121.03(10)	120.88