Electronic Supplementary Information (ESI)

A highly sensitive pyridine-dicarbohydrazide based chemosensor for colorimetric recognition of Cu^{2+}, AMP^{2-}, F^- and AcO^- ions

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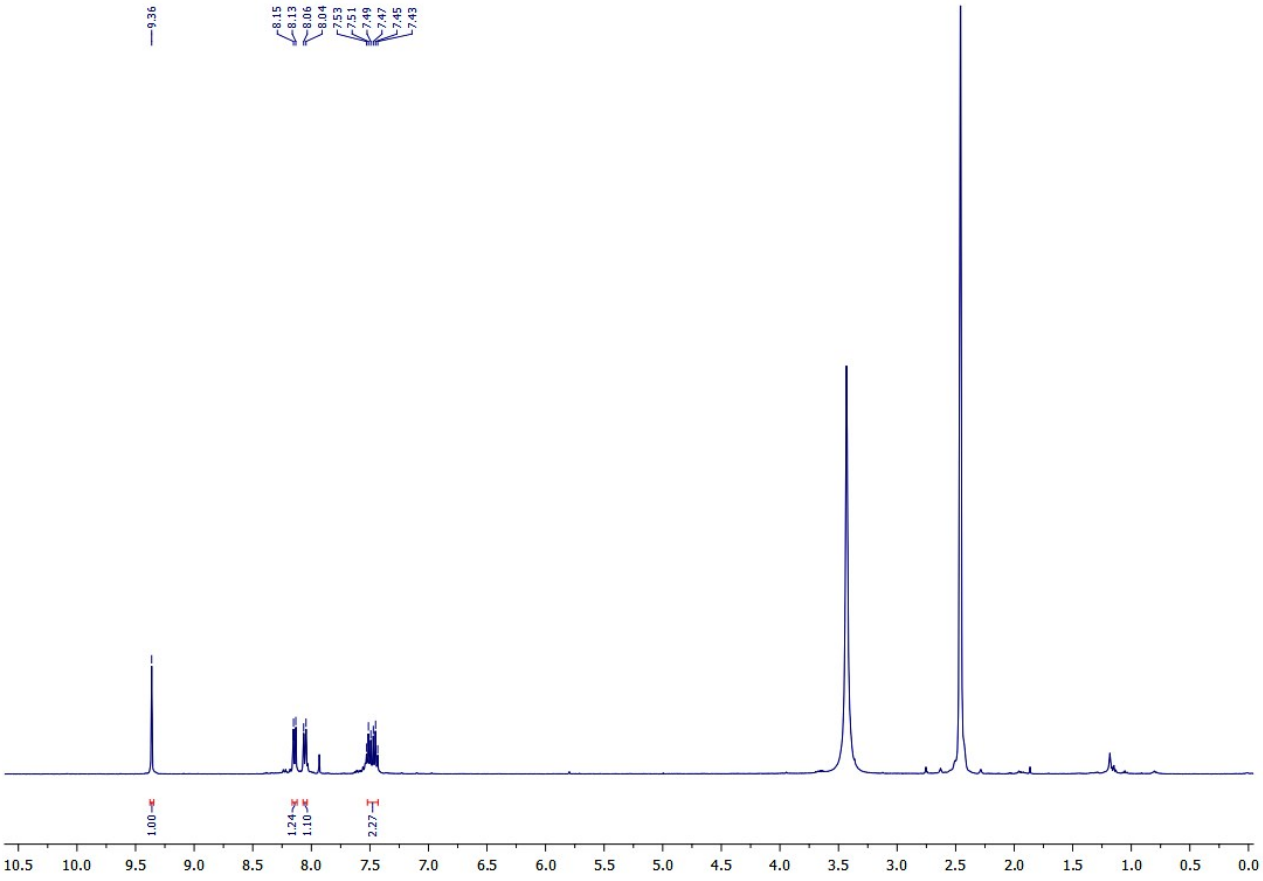


Fig. S1 ^{1}H NMR spectrum of compound **1** in DMSO-d_6.

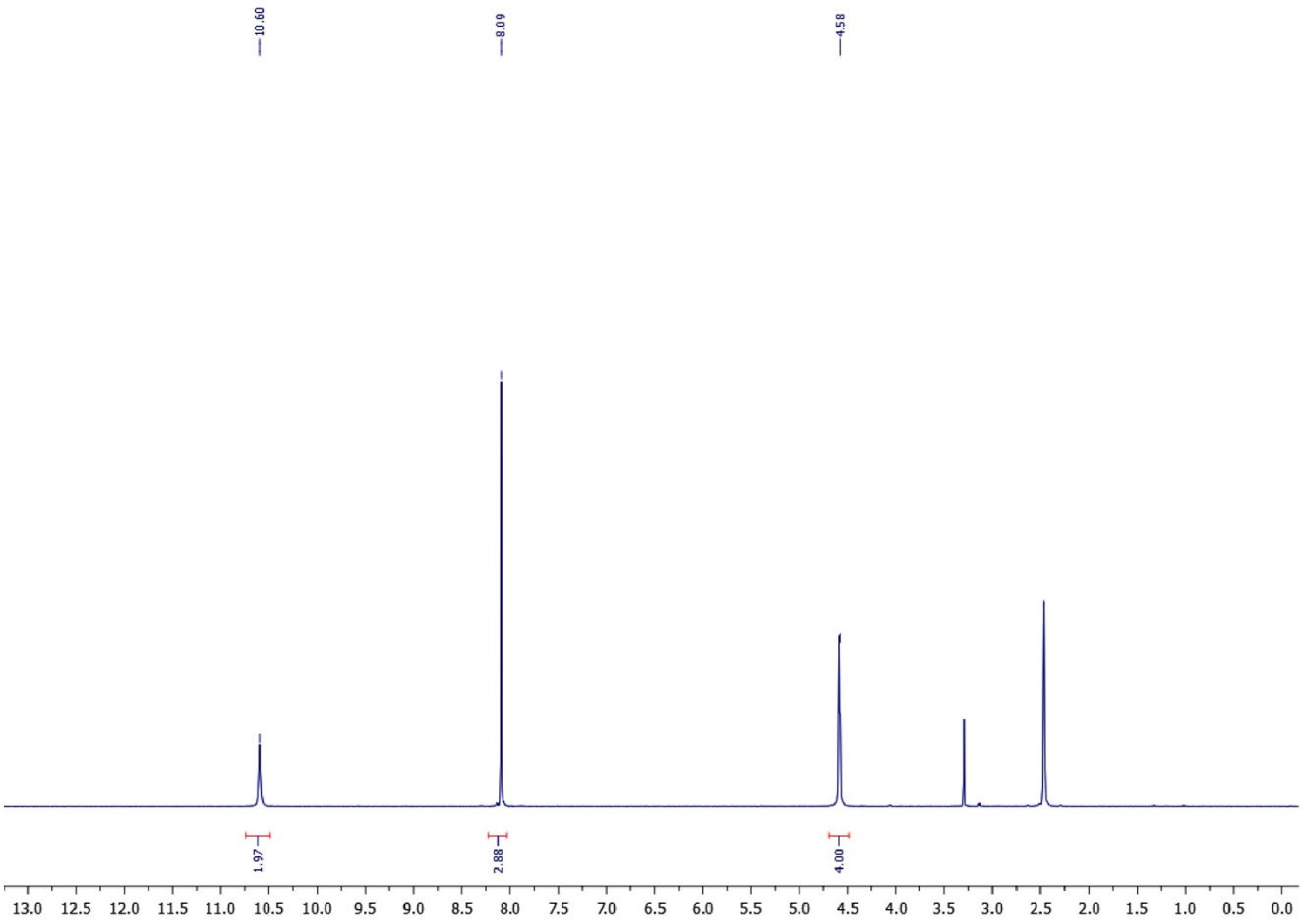


Fig. S2 ^{1}H NMR spectrum of compound **2** in DMSO-d_6.

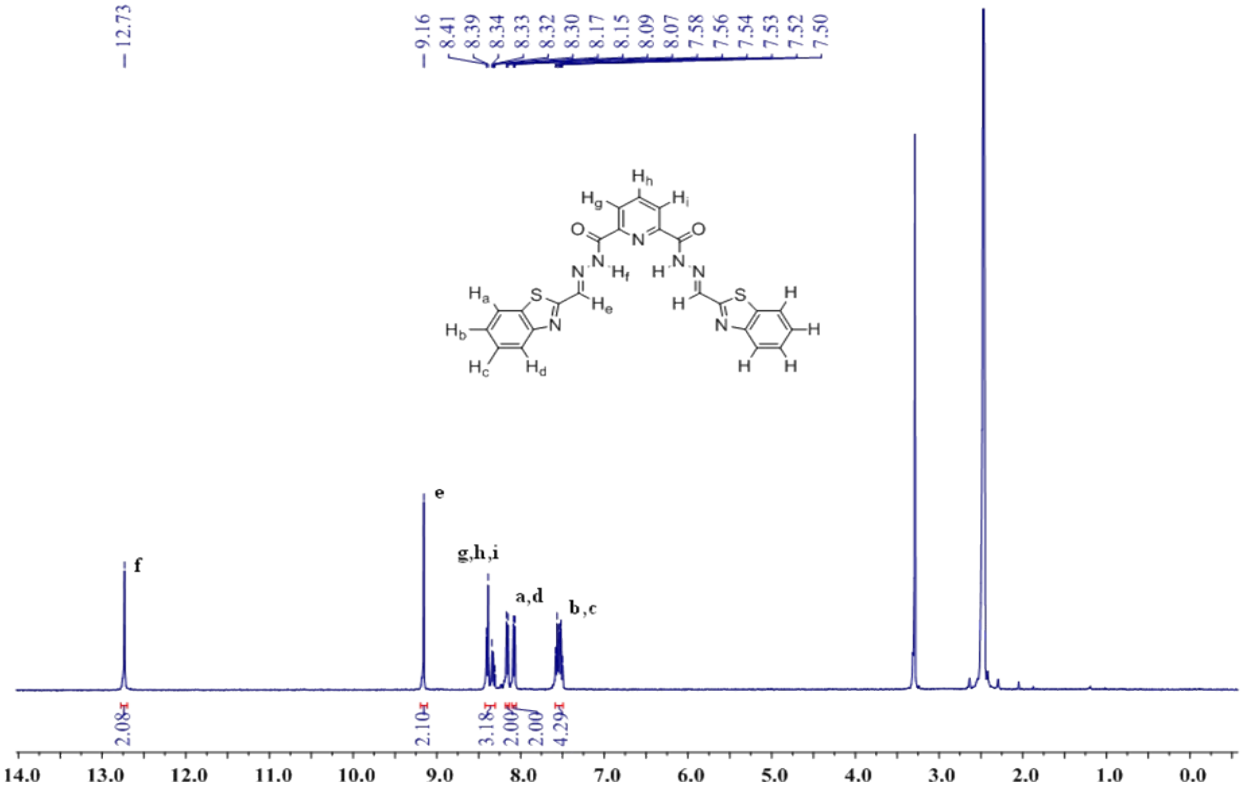


Fig. S3 ^{1}H NMR spectrum of compound **L1** in DMSO-d_6.

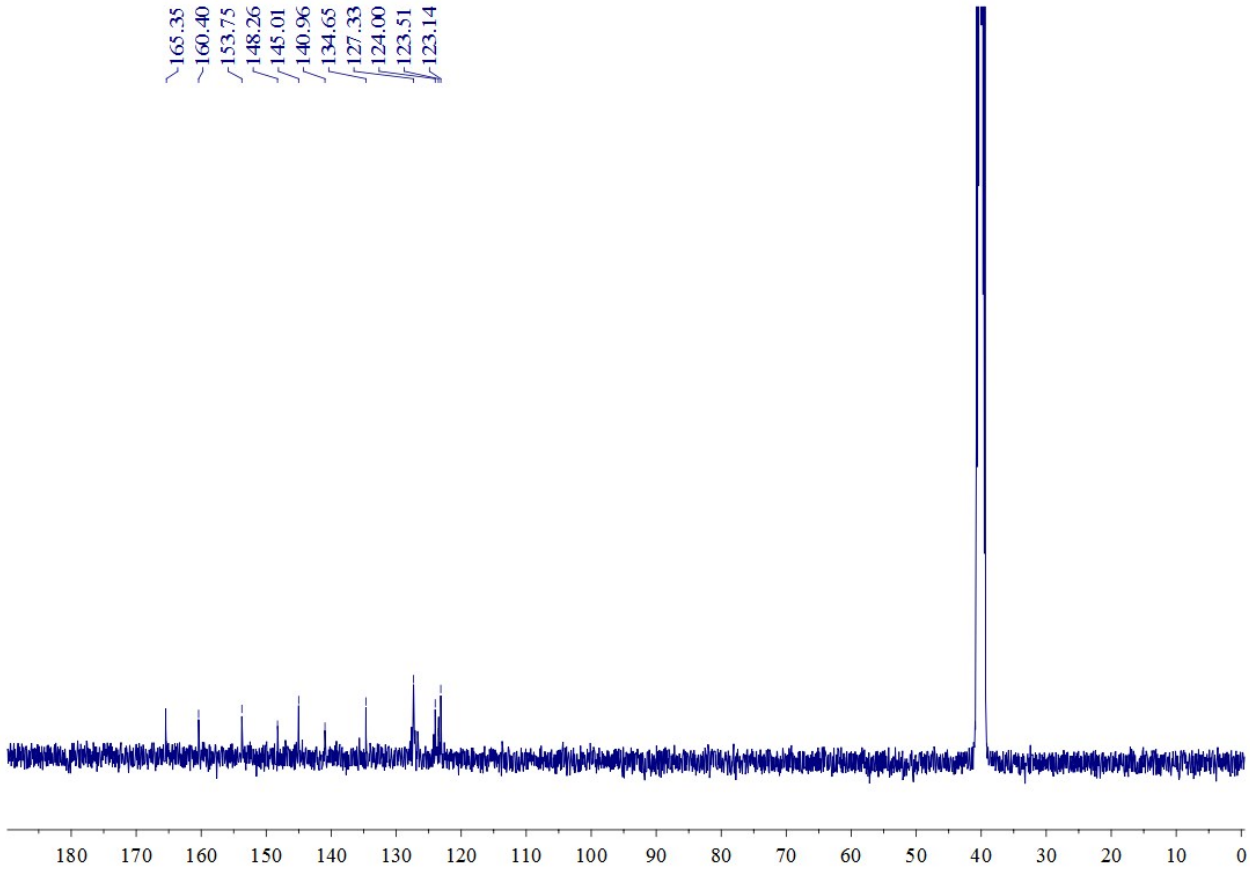


Fig. S4 ^{13}C NMR spectrum of compound **L1** in DMSO-d_6.

Sample Name	HJ41	**Position**		**Instrument Name**	Instrument 1
User Name		**Inj Vol**	0	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	RH219_HJ41.d
ACQ Method	MS-Service.m	**Comment**	in MeOH	**Acquired Time**	2/19/2018 10:58:48 AM (UTC+01:00)

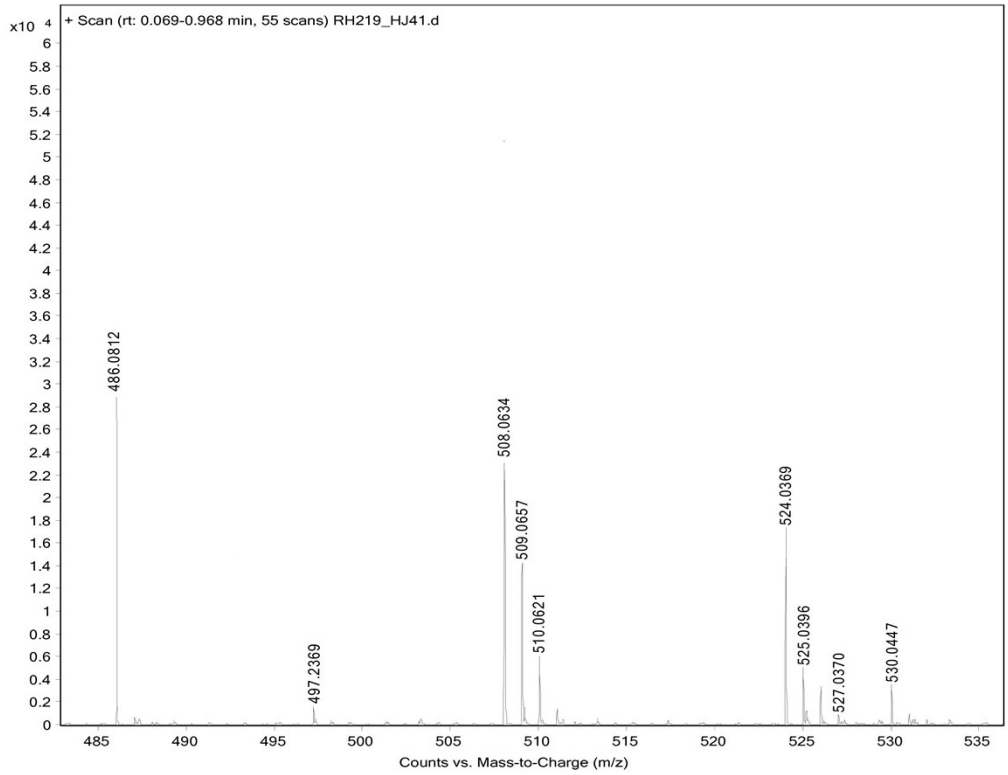


Fig. S5 HRMS of compound **L1**.

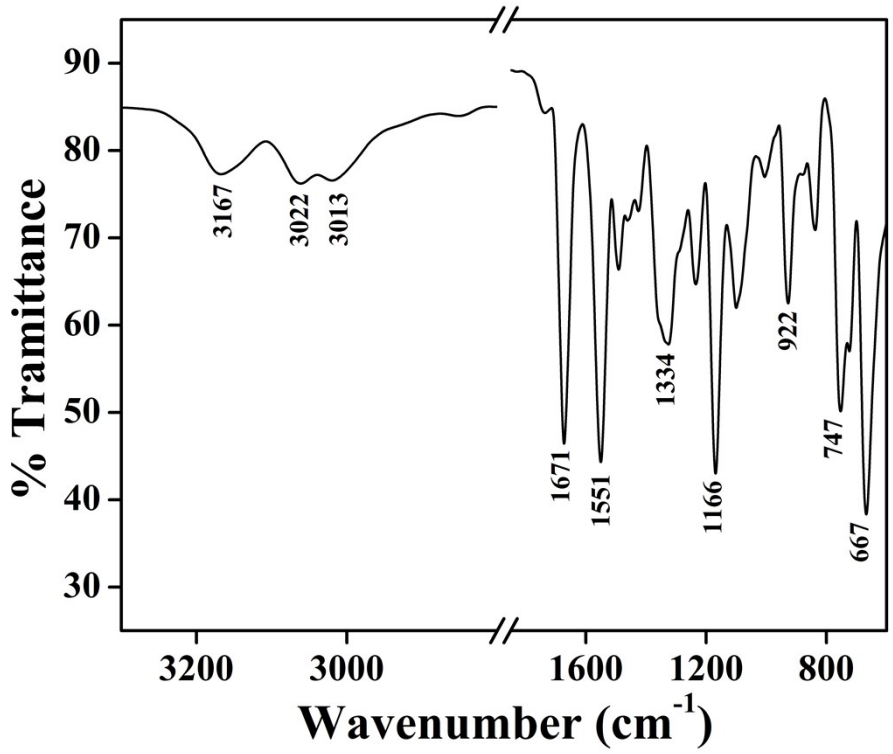


Fig. S6 FT-IR spectrum of compound **L1**.

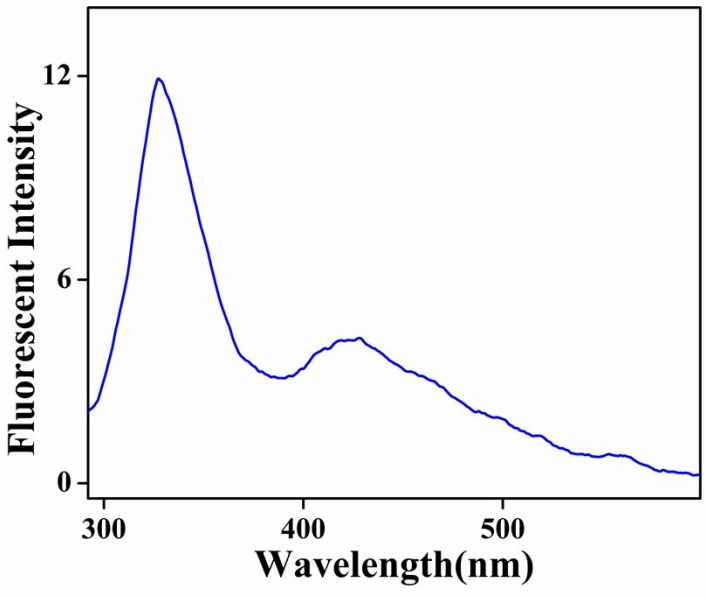


Fig. S7 Fluorescence spectra of **L1** on excitation at 270 nm.

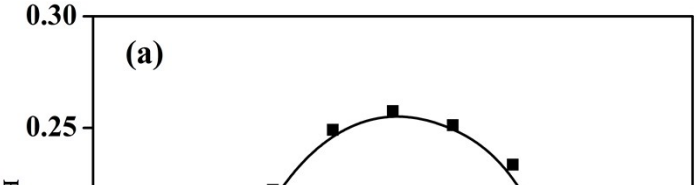


Fig. S8 Job's Plot for **L1** with (a) AcO^- and (b) F^- in DMSO showing 1:1 stoichiometry.

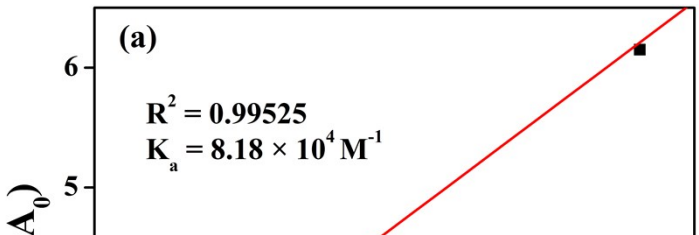


Fig. S9 Benesi-Hildebrand Plot for UV-Vis titration of **L1** with (a) AcO^- and (b) F^- showing 1:1 binding stoichiometry.

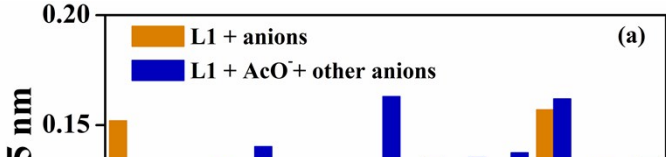


Fig. S10 Absorption response of **L1** (10 μM, DMSO/H_2O, 8:2, v/v) for (a) Acetate and (b) Fluoride at the wavelength of 405 nm in presence of various anions.

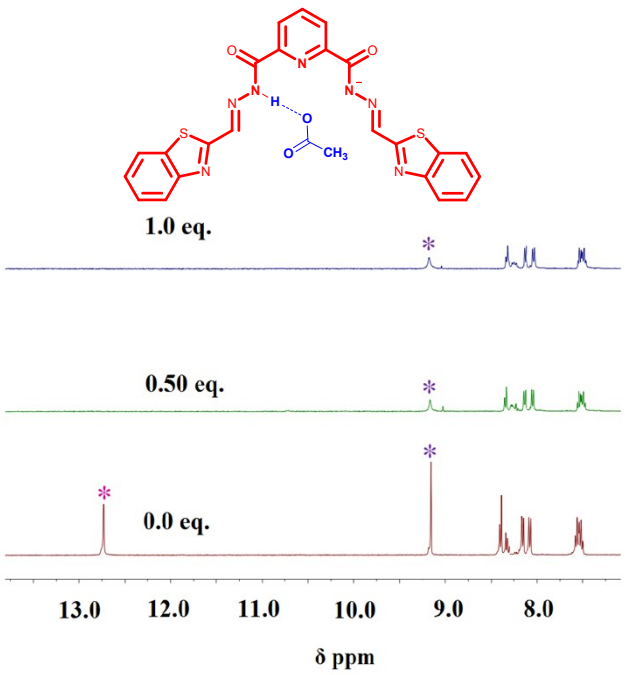
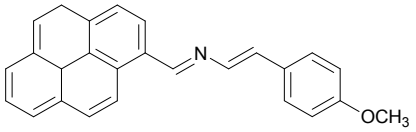
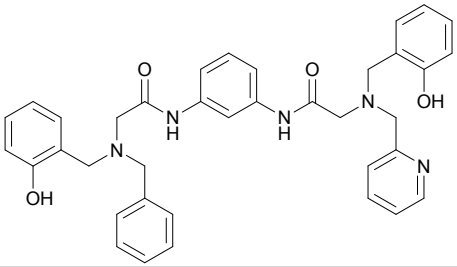
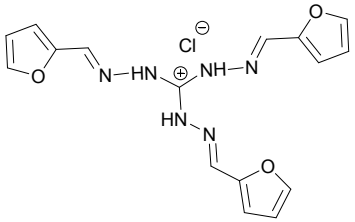
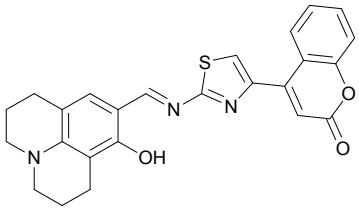
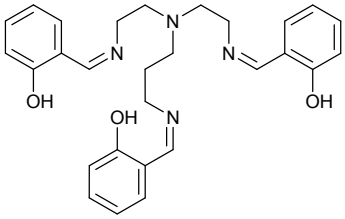
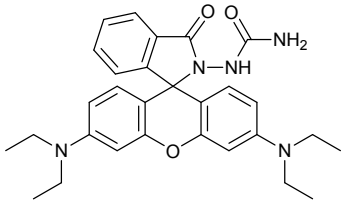


Fig. S11 Stack plot of ^{1}H NMR spectra of compound **L1** in presence of NaAc (0-1.0 equiv.) recorded in DMSO-d_6 along with the possible structure of complex of **L1** with acetate.

Table. S1 The sensing abilities of receptors (reported in literature) for Cu^{2+} ion along with chemosensor **L1**.

S.No.	Chemosensor	Cu^{2+}detection limit (in μM)	Method Of detection	Reference
1.		4.58	Fluorescence and Naked eye	S1
2.		2.98	Naked eye	S2
3.		2.7	Naked eye	S3
4.		1.53	Fluorescence	S4
5.		1.5	Naked eye	S5
6.		0.16	Fluorescence and Naked eye	S6

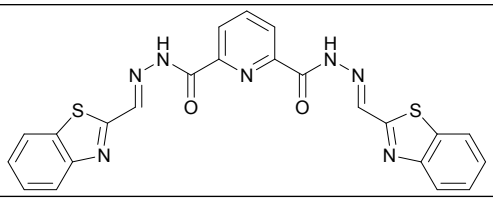
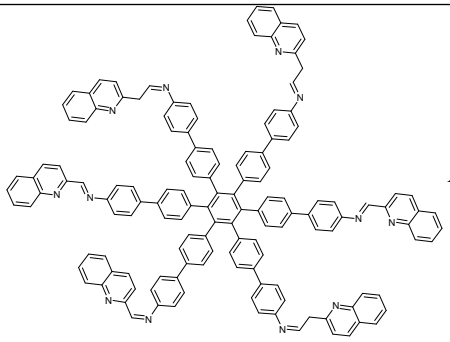
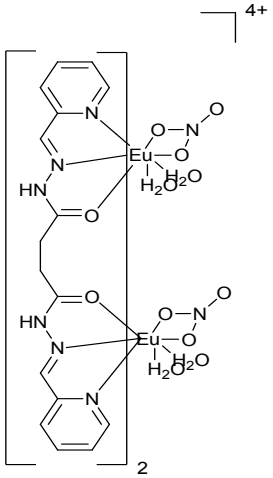
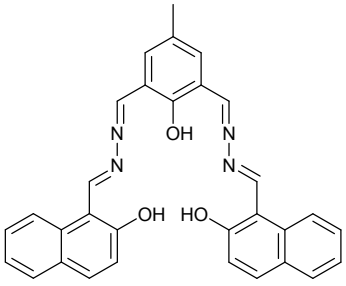
7.		**0.12**	**Naked eye**	**Our Work**

Table. S2 Response time of various chemosensors reported in literature.

S.No.	Chemosensor	Response Time (s)	Reference
1.	Fluorescein hydrazide	7200	S7
2.	Fluorescein derivative	120	S8
3.	Ninhydrin-quinoxaline derivative	60	S9
4.	Phenanthro-imidazole derivative	10	S10
5.	**Pyridine-dicarbohydrazide based sensor**	**5**	**Our work**

Table. S3 The sensing abilities of receptors (reported in literature) for AMP^{2-} , F^- and AcO^- ions along with chemosensor **L1**.

S.No	Chemosensor	Anions Detected	Limit Of Detection (in μM)	Method Of detection	Reference
1.		AMP^{2-}	0.9	Fluorescence	S11
2.		AMP^{2-}	2.0	Luminiscence	S12
3.		AcO^-	11	Naked-eye and Fluorescence	S13

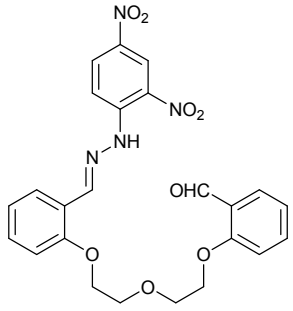
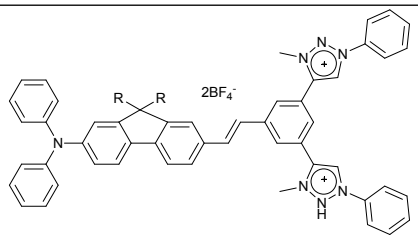
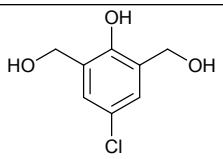
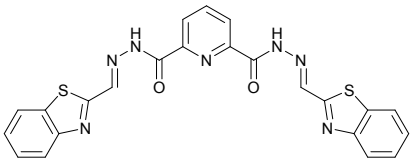
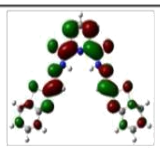
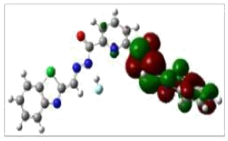
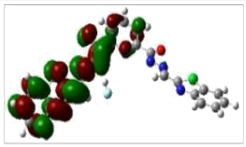
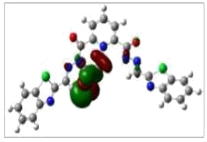
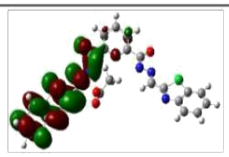
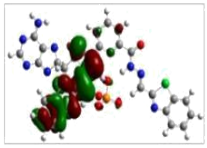
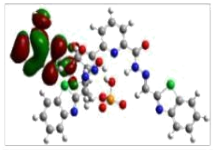
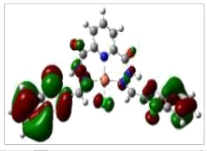
4.		AcO^-	3	Naked-eye	S14
5.		F^-	100	Fluorescence	S15
6.		F^-	1.7	Naked-eye and Fluorescence	S16
7.		**F^-** **AcO^-** **AMP^{2-}**	**1.4** **1.4** **0.08**	**Naked-eye**	**Our work**

Table.S4 Energy gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), $\Delta E_{H\text{-}L}$ of free ligand (**L1**), and its complexes with F^-, CH_3COO^-, AMP^{2-} and Cu^{2+}.

Compound	HOMO	LUMO	$\Delta E_{H\text{-}L}$ (eV)
Ligand			4.11
F^- based Complex			2.89
CH_3COO^- based complex			2.51
AMP^{2-} based complex			1.45
Cu^{2+} based complex			2.37

Reference

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