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Solvent effect on the neutral chiral supramolecular assemblies and their distinct receptor behaviour towards anions

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Supplementary Information

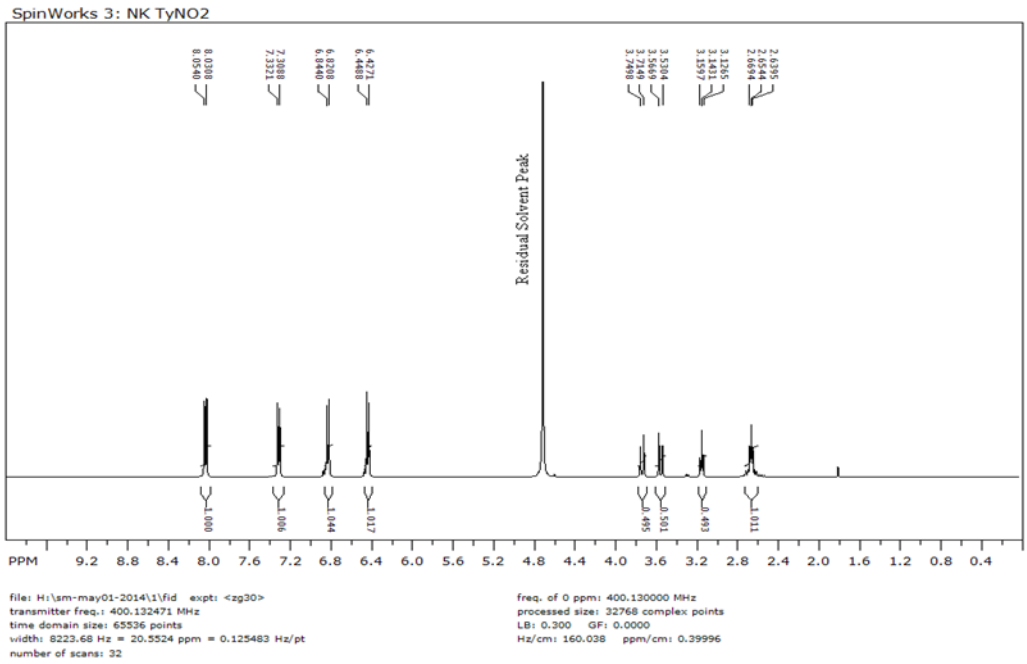


Fig. S1 ^{1}H NMR spectrum of H_2Tyr-4-nitro.

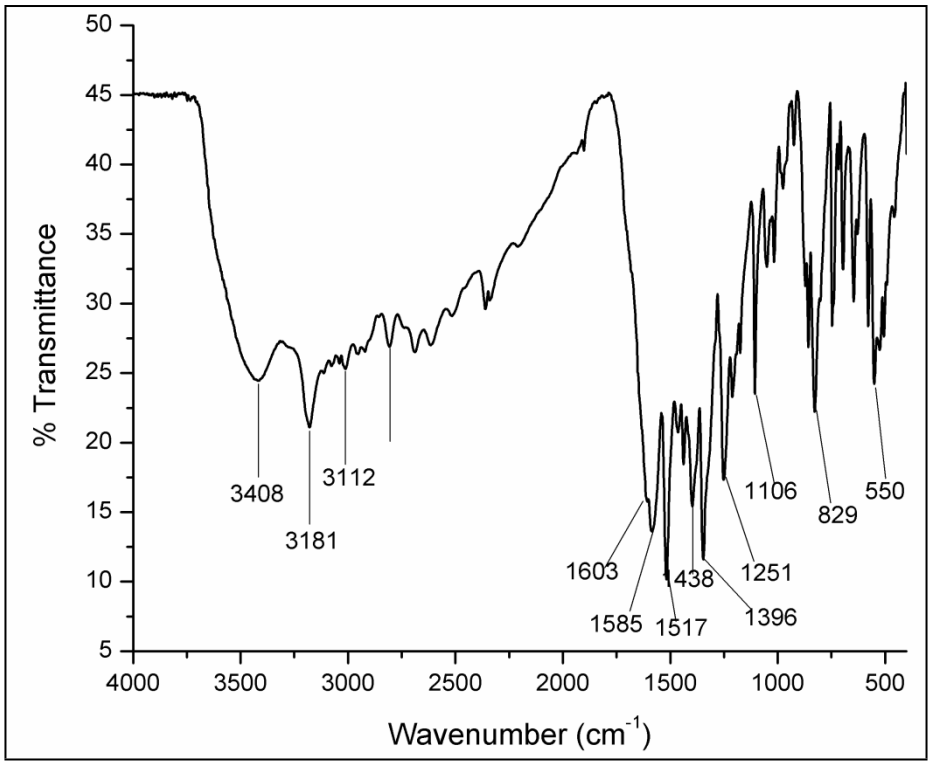


Fig. S2 FTIR spectrum of H_2Tyr-4-nitro.

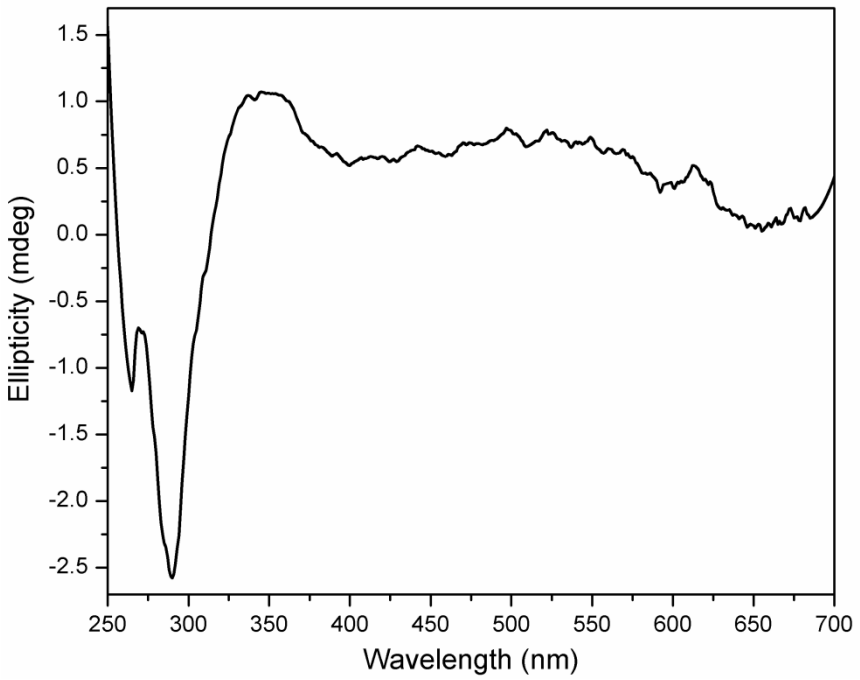


Fig. S3 CD Spectrum of H_2Tyr-4-Nitro in DMSO (in the range of 250-700nm).

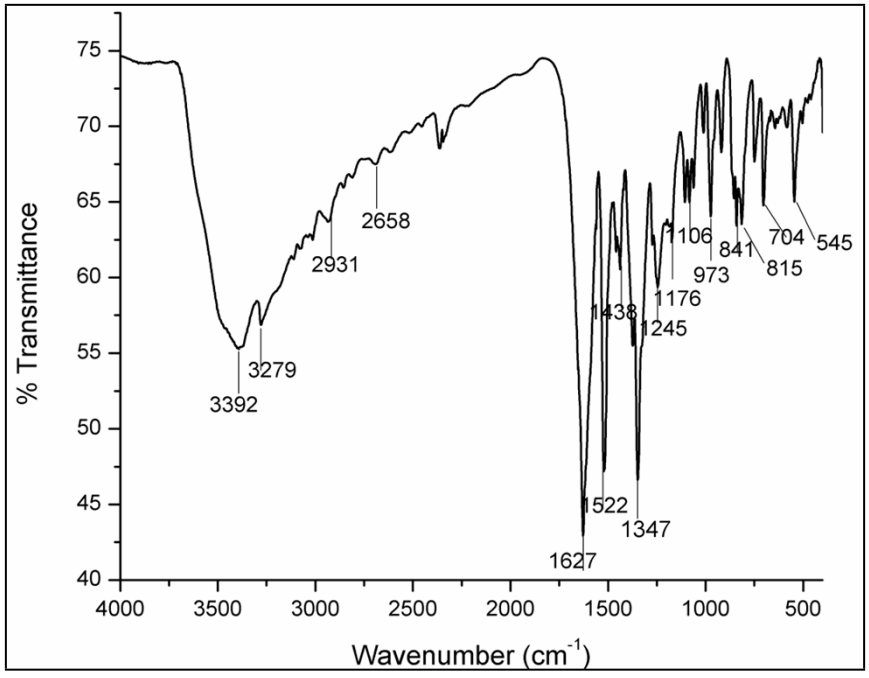


Fig. S4 FTIR spectrum of **1**.

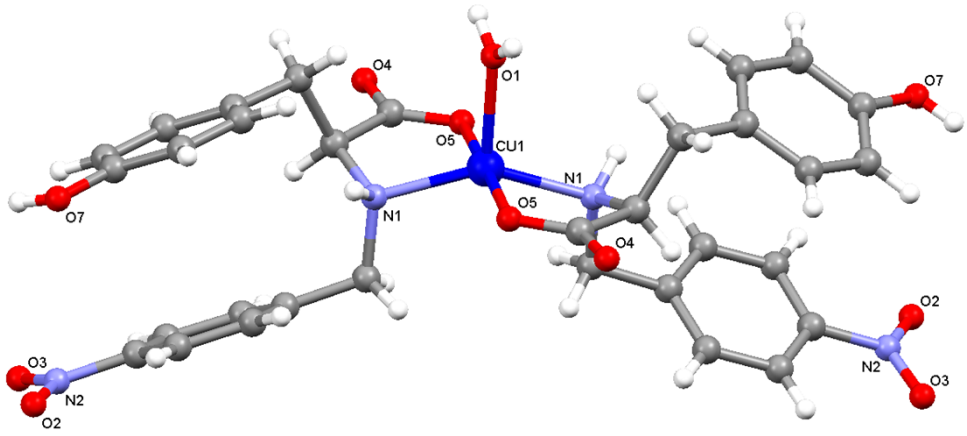


Fig. S5 Asymmetric unit of **1a** (DMSO molecules are omitted for clarity).

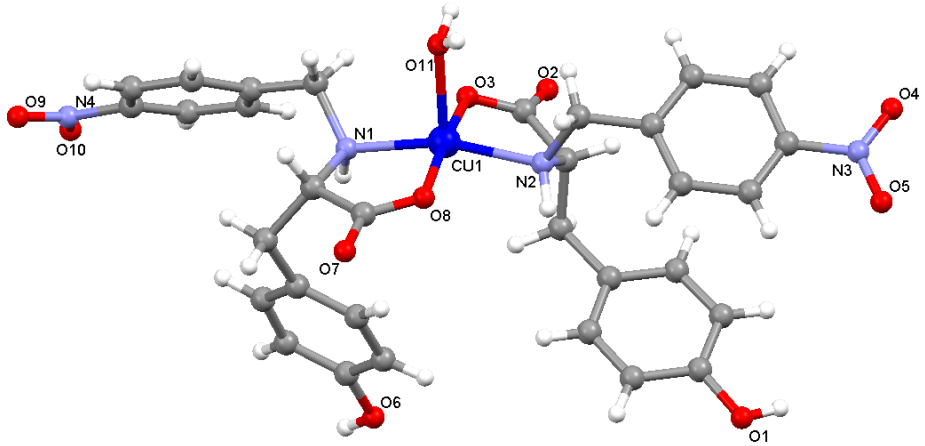


Fig. S6 Asymmetric unit of **1b** (Methanol molecules are omitted for clarity).

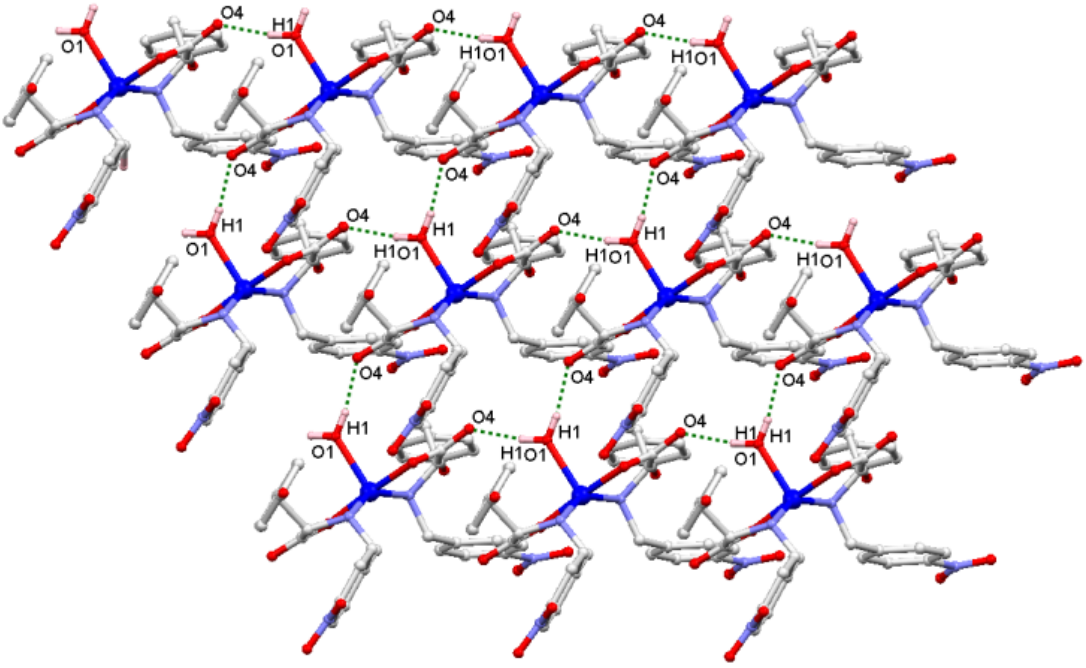


Fig. S7 2D supramolecular ensemble in **1a.**

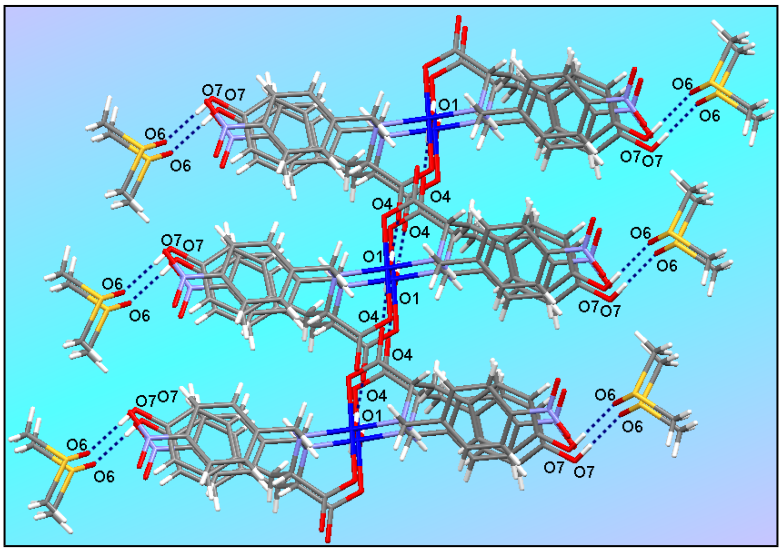


Fig. S8 Interaction of the DMSO molecules with the supramolecular array in **1a**.

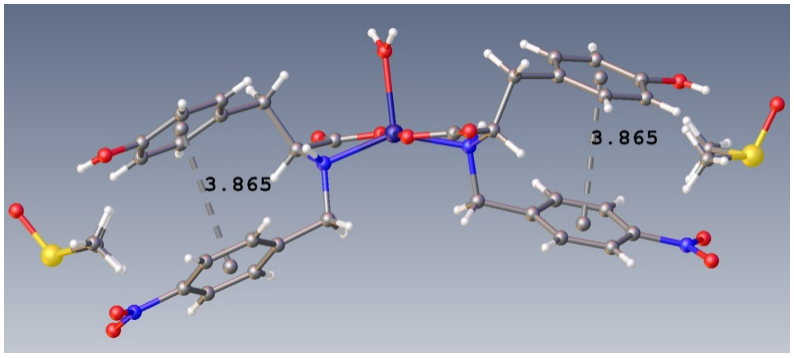
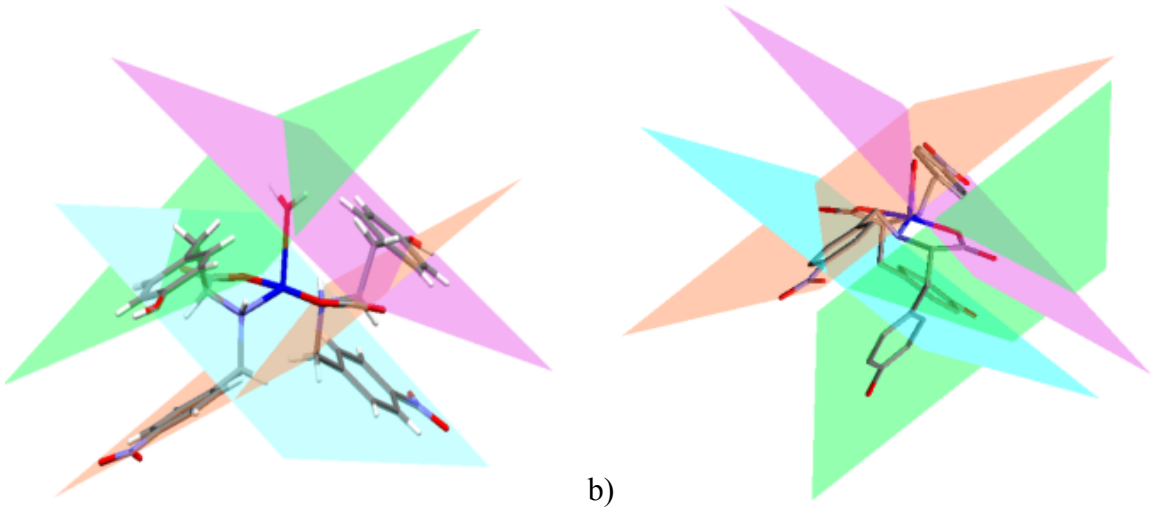


Fig. S9 Intramolecular π–π interactions in **1a**.



a) b)

Fig. S10 Parallel (a) and anti-parallel (b) planes containing aromatic rings of the ligand in **1a** and **1b**, respectively.

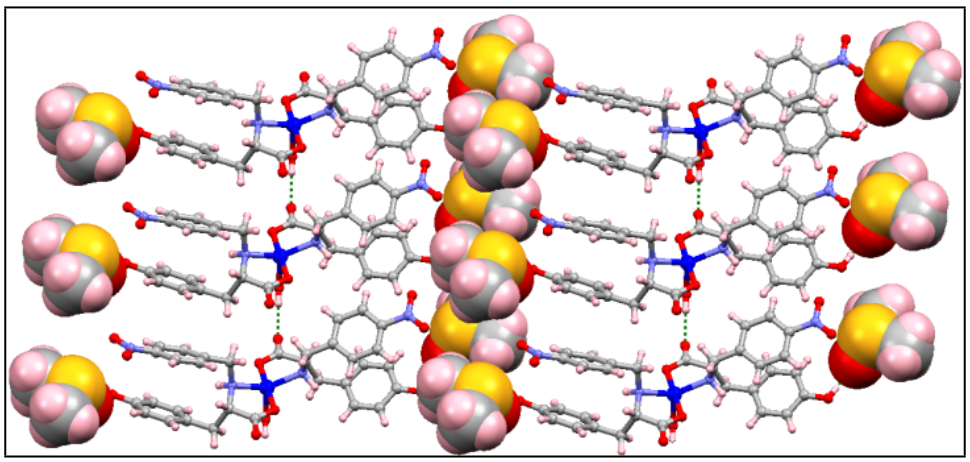


Fig. S11 Encapsulation of the DMSO cluster within the supramolecular array in **1a.**

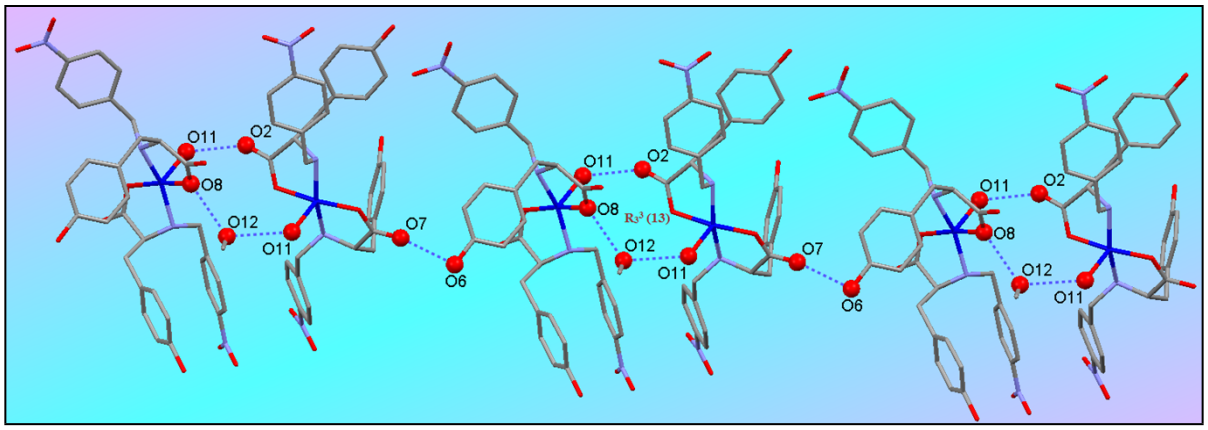


Fig. S12 1D supramolecular chain in **1b**.

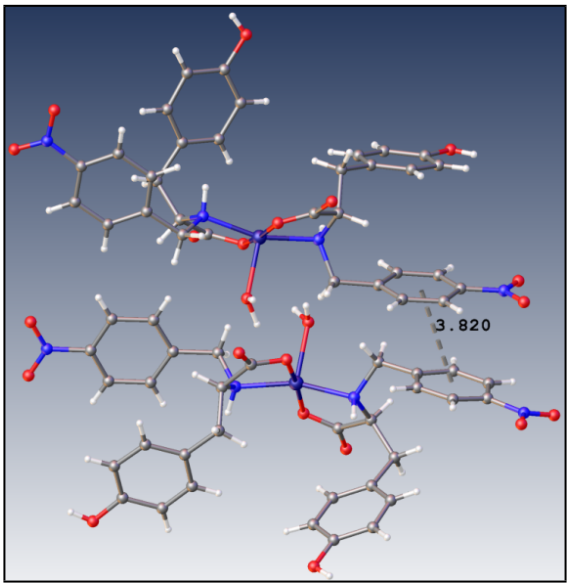


Fig. S13 Intermolecular π–π interactions in **1b**.

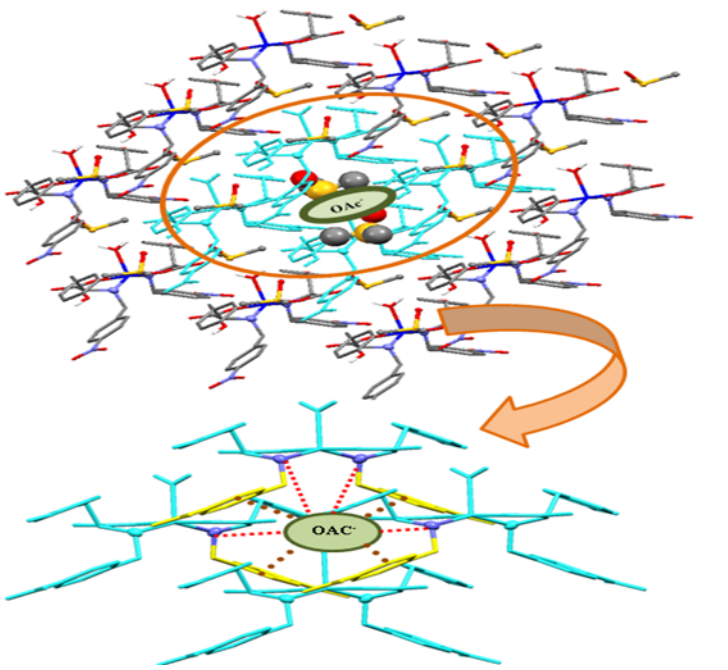


Fig. S14. Schematic representation of interactions of OAc^- with **1a**.

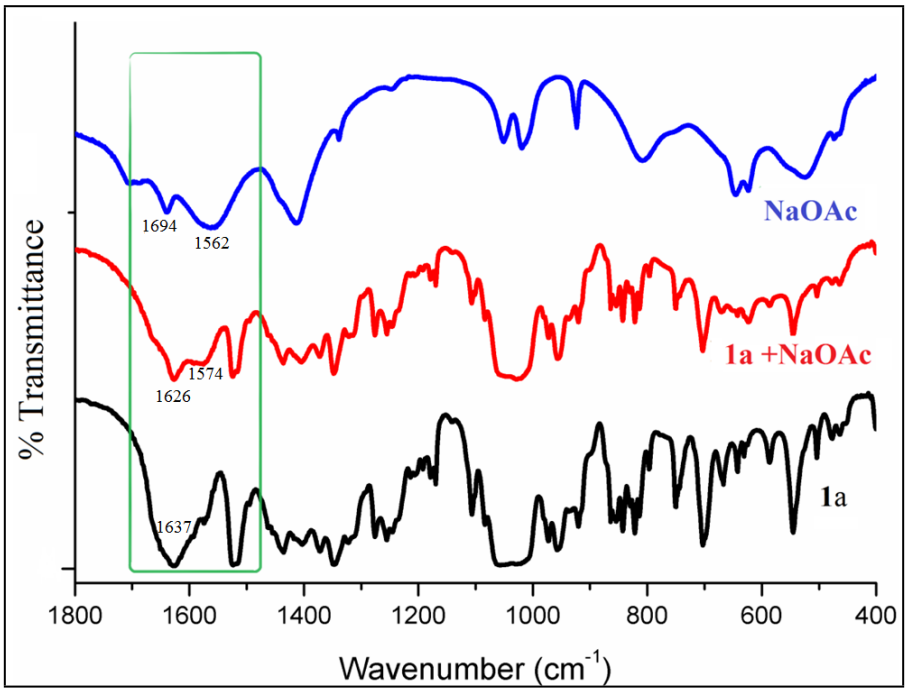


Fig. S15 Comparison of FTIR spectra of NaOAc, **1a**, and **1a** + 0.5 eqv NaOAc.

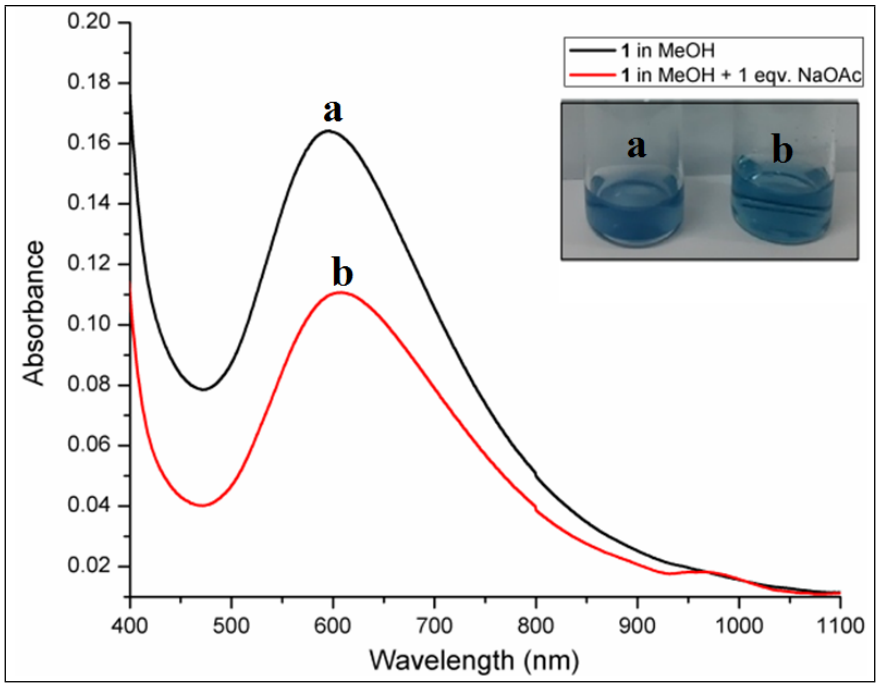


Fig. S16 Effect of NaOAc on the absorption spectra of **1b** in methanol**.**

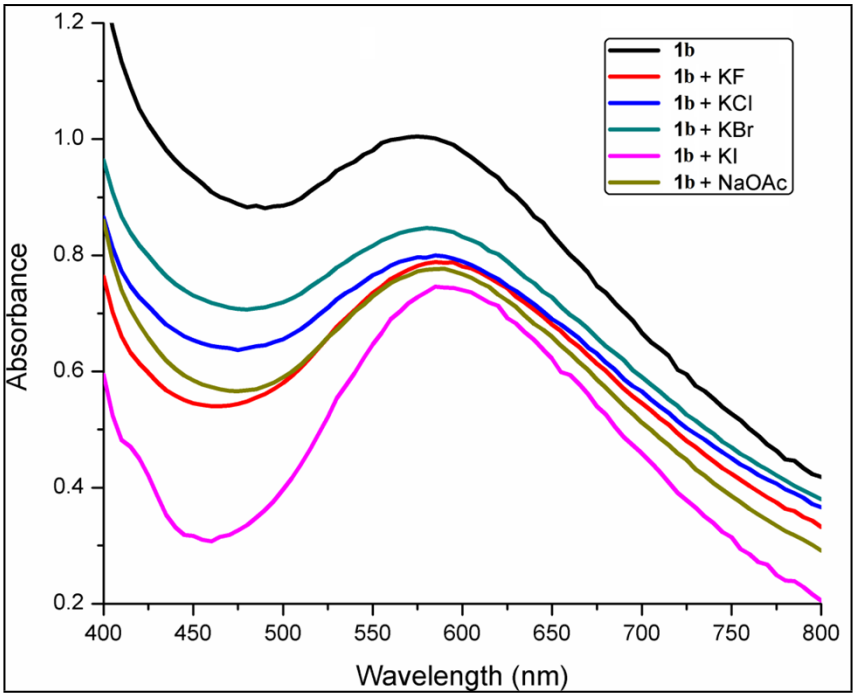


Fig. S17 Effect of anions on the absorption spectra of **1b** in methanol.

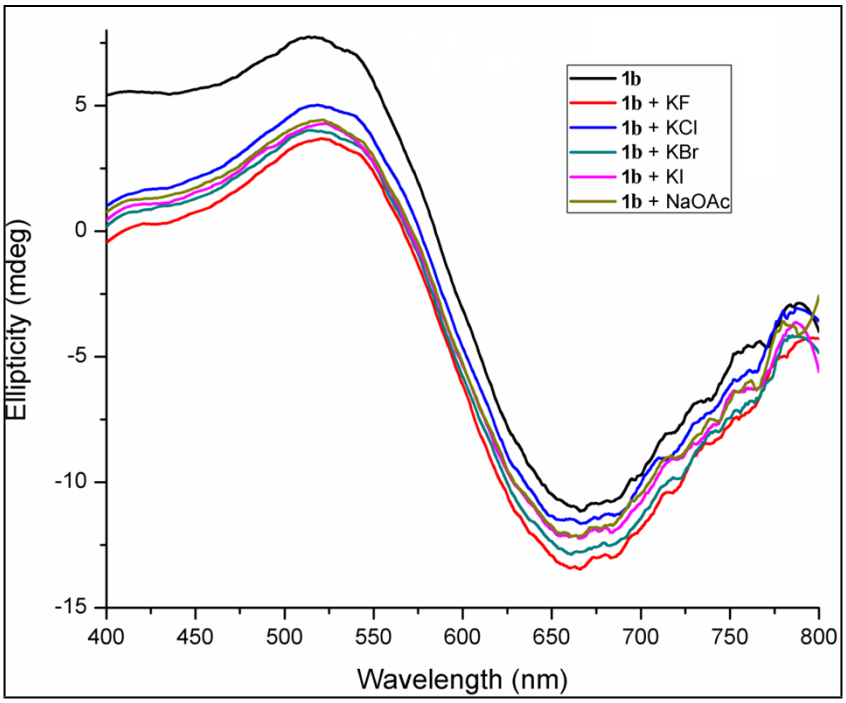


Fig. S18 Effect of anions on the CD spectra of **1b** in methanol.

Table S1. Selected Bond Lengths (Å) and Bond Angles (degrees) for **1a** and **1b**.

Bond Lengths

1a

Cu1-O5	1.919(3)	Cu1-O5	1.919(3)
Cu1-N1	2.022(4)	Cu1-N1	2.022(4)
Cu1-O1	2.183(6)		

1b

Cu1-O8	1.933(5)	Cu1-O3	1.955(6)
Cu1-N1	2.021(6)	Cu1-N2	2.034(6)
Cu1-O11	2.197(5)		

Bond Angles

1a

O5-Cu1-O5	176.8(3)	O5-Cu1-N1	84.40(13)
O5-Cu1-N1	94.68(13)	O5-Cu1-N1	94.68(13)
O5-Cu1-N1	84.40(13)	N1-Cu1-N1	147.2(2)
O5-Cu1-O1	91.61(15)	O5-Cu1-O1	91.61(15)
N1-Cu1-O1	106.39(11)	N1-Cu1-O1	106.39(11)
C14-O5-Cu1	115.2(2)	C15-N1-Cu1	106.8(2)
C7-N1-Cu1	109.3(3)		

1b

O8-Cu1-O3	171.8(2)	O8-Cu1-N1	84.7(2)
O3-Cu1-N1	95.3(2)	O8-Cu1-N2	92.8(2)
O3-Cu1-N2	84.6(2)	N1-Cu1-N2	161.4(2)
O8-Cu1-O11	99.4(3)	O3-Cu1-O11	88.7(3)
N1-Cu1-O11	95.8(2)	N2-Cu1-O11	102.8(2)
C25-O8-Cu1	116.5(5)	C24-N1-Cu1	109.8(4)
C26-N1-Cu1	112.8(5)	C9-O3-Cu1	114.2(5)

Table S2. Hydrogen Bonding Parameters for **1a** and **1b**.

D-H..A	r(D-H) (Å)	r(H..A) (Å)	r(D..A) (Å)	∠D-H..A (°)	Symmetry
1a					
O1-H1..O4	0.84	1.89	2.734(6)	171	1/2-x,1/2+y,1-z
O7-H7..O6	0.82	1.83	2.650(6)	176	1-x,y,-z
C7-H7B..O4	0.97	2.34	3.299(6)	168	1/2+x,-1/2+y,z
C18-H18B..O(6)	0.96	2.59	3.401(9)	143	1/2-x,-1/2+y,-z
1b					
O6-H6..O7	0.82	2.03	2.810(7)	158	2-x,1/2+y,1-z
O1-H1A..O2	0.82	1.90	2.692(8)	163	1-x,-1/2+y,-z
O11-H11B..O12	0.85	1.96	2.781(8)	164	1+x,y,-1+z
O11-H11A..O2	0.84	1.88	2.631(7)	147	2-x,-1/2+y,-z
O12-H12A..O8	0.82	2.23	2.749(7)	152	1-x,1/2+y,1-z
C18-H18..O7	0.93	2.57	3.270(9)	132	2-x,1/2+y,1-z
C8-H8..O1	0.98	2.55	3.296(9)	133	1-x,1/2+y,-z
C3-H3.. O7	0.93	2.51	3.431(10)	168	2-x,1/2+y,-z
C34-H34B..O5	0.96	2.48	3.420(14)	167	x,y,1+z