Supporting information

Intrinsic Structural Features of Coordination Polymers Make Impact on Dye Selectivity

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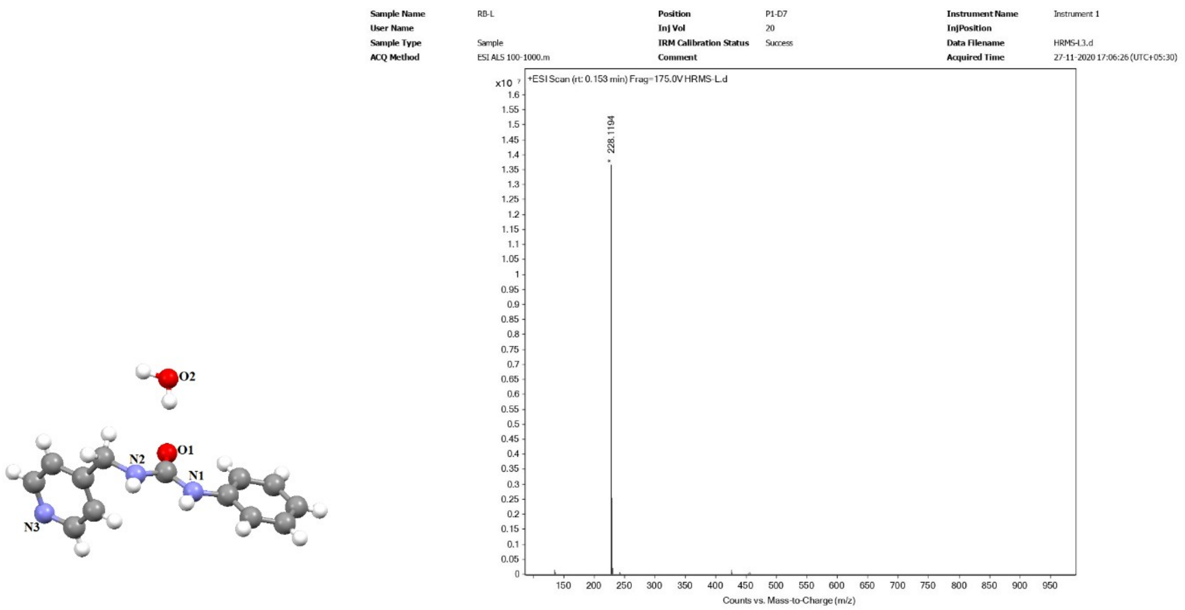


(a) (b)

Figure 1S: (a) The structure of 1-phenyl-3-((pyridin-4-yl)methyl)urea monohydrate; (b) ESI-mass of 1-phenyl-3-((pyridin-4-yl)methyl)urea.

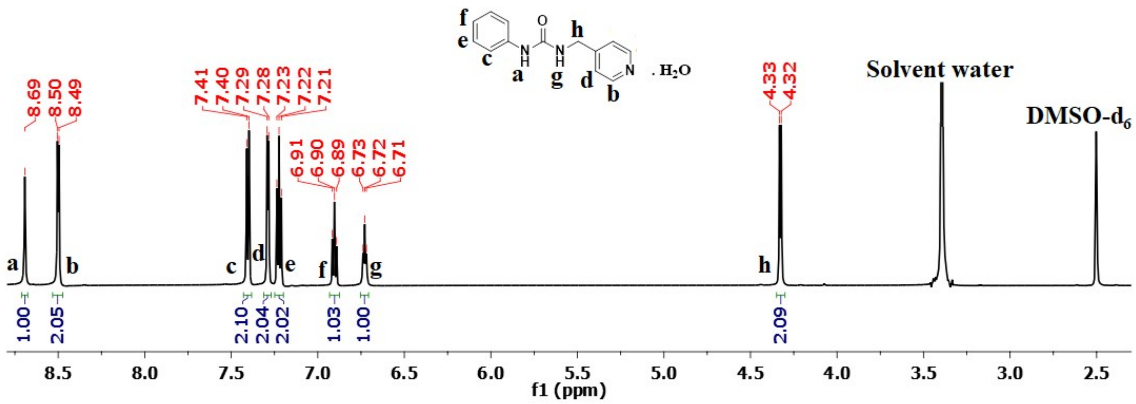
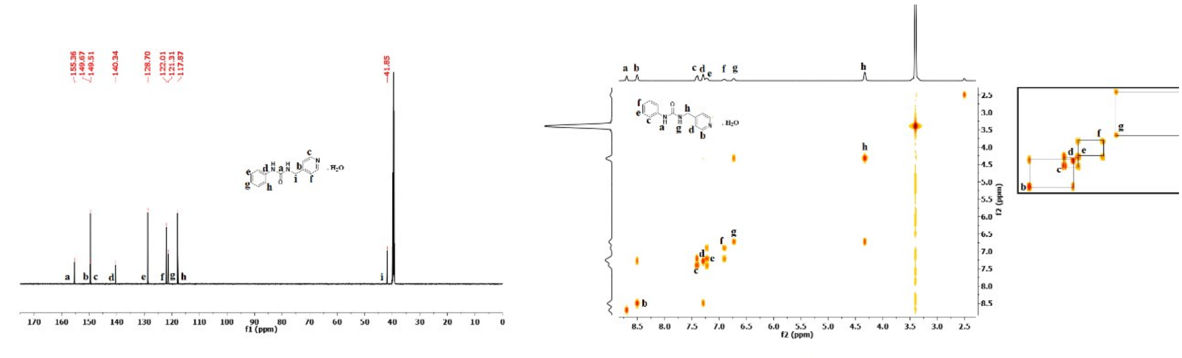


Figure 2S: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of L.H_2O.



(a) (b)

Figure 3S: (a) ^{13}C-NMR (150 MHz, DMSO-d_6) spectrum (b) 2D HOMO-COSY ^{1}H-NMR spectra (600 MHz, DMSO-d_6) of L.H_2O.

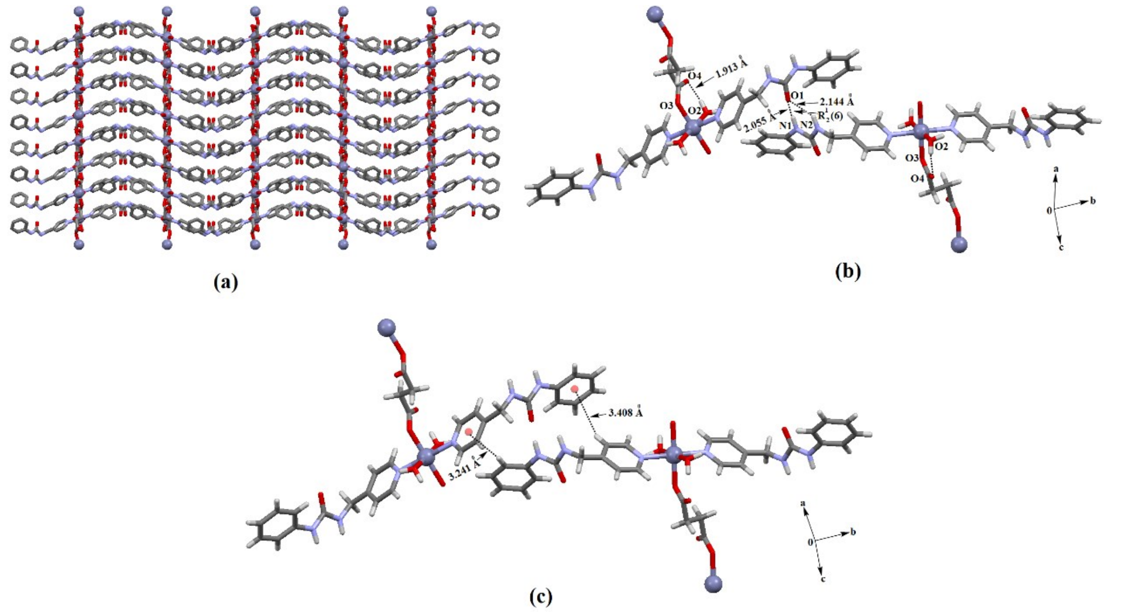
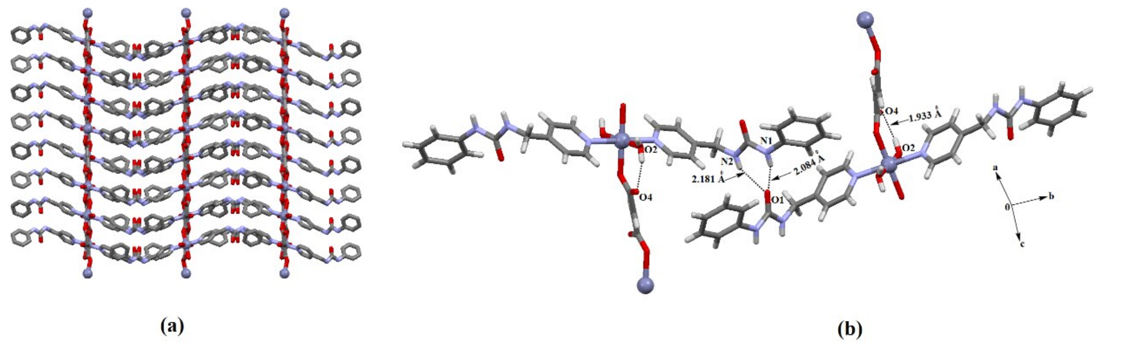
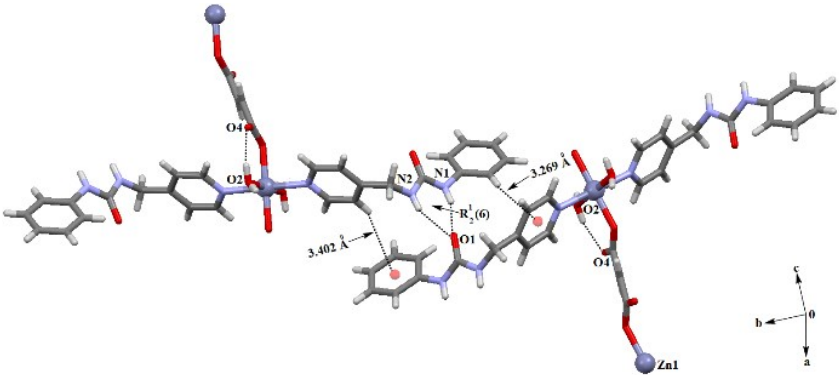


Figure 4S: Hydrogen bonded self-assembly of **CP4** (a) packing diagram along a-axis, (b) showing N1-H-O1, N2-H-O1, O2-H-O4 hydrogen bonds, (c) C-H-π interactions.





(c)

Figure 5S: Hydrogen bonded self-assembly of **CP5** (a) packing diagram along a-axis, (b) showing N1-H-O1, N2-H-O1, O2-H-O4 hydrogen bonds, (c) C-H-π interactions.

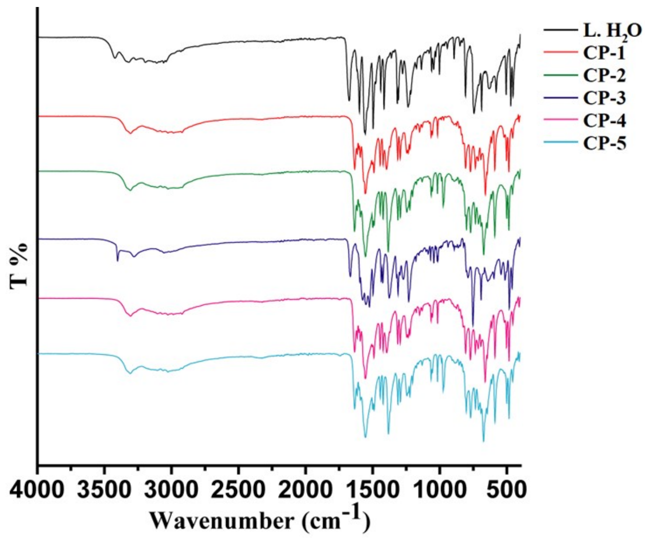
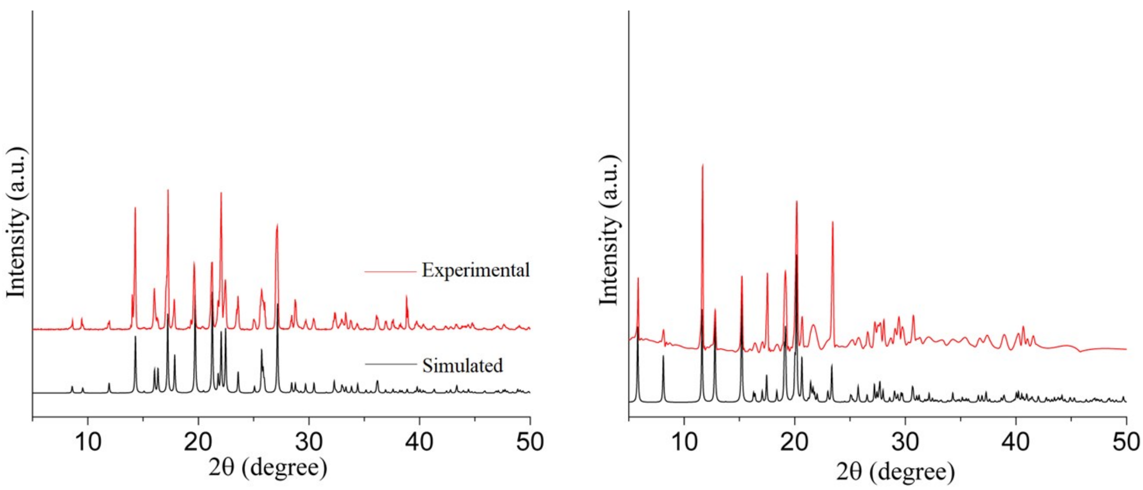


Figure 6S: IR-spectra of the solid samples of the ligand and coordination polymers **CP1**, **CP2**, **CP3**, **CP4** and **CP5**.



(a)

(b)

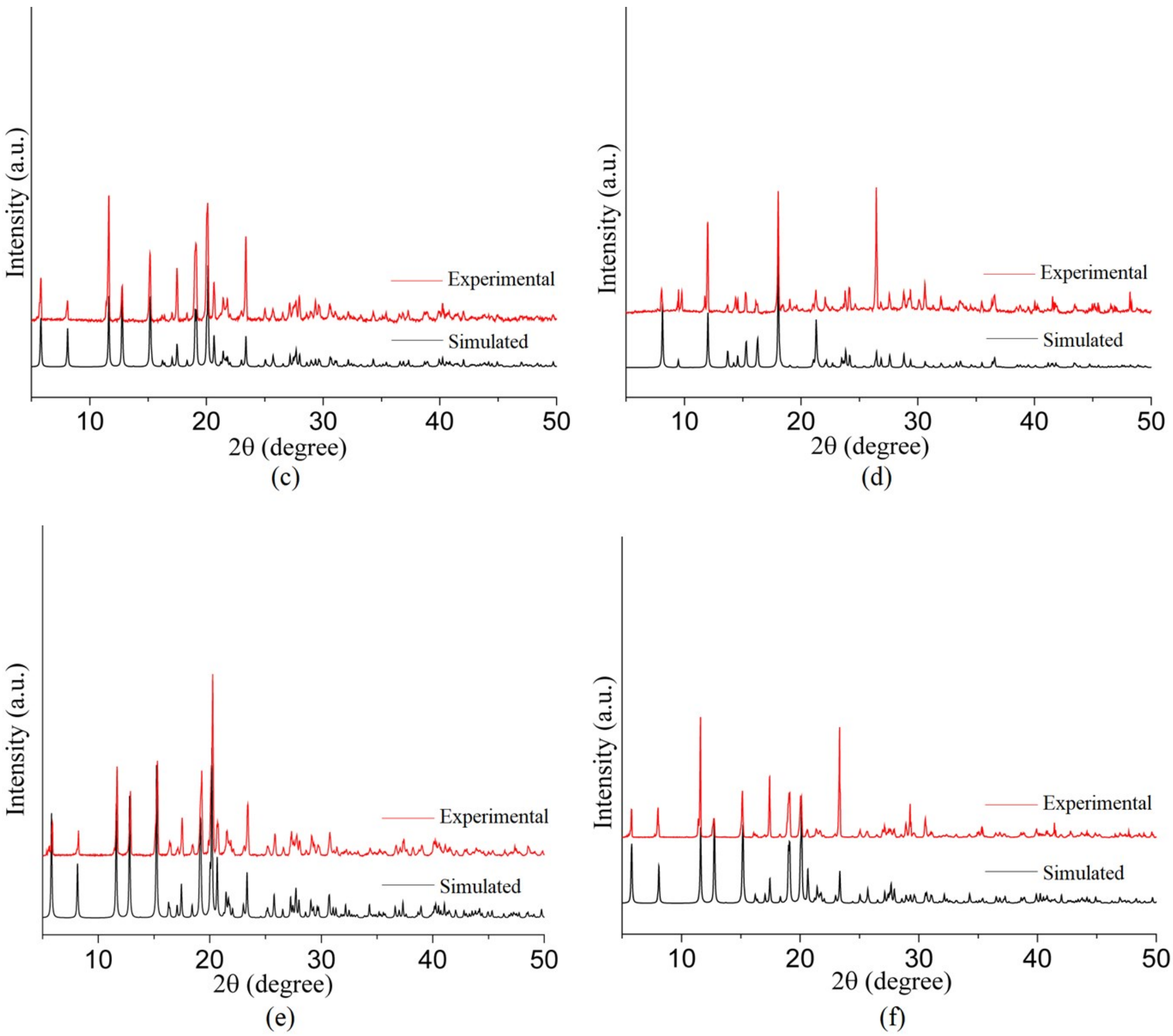
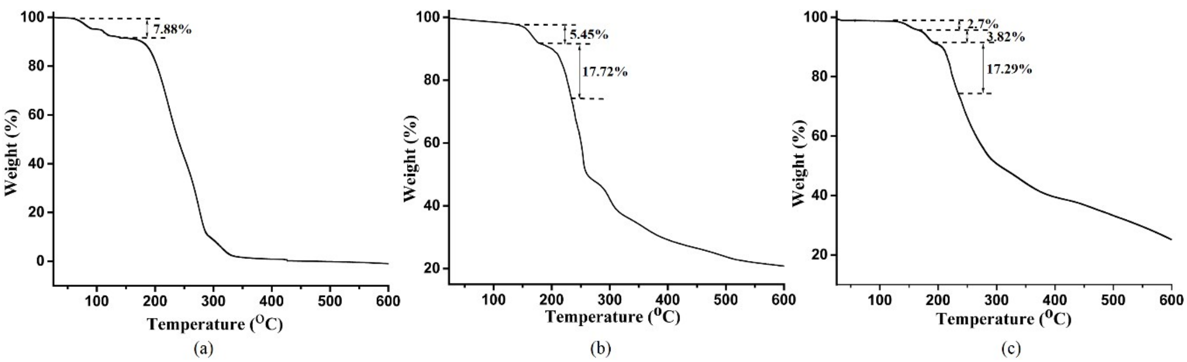


Figure 7S: PXRD patterns of (a) **L.H_2O**, (b) **CP1**, (c) **CP2**, (d) **CP3**, (e) **CP4** and (f) **CP5**. Simulated patterns generated from crystallographic information files (Red = Experimental, Black = Simulated).



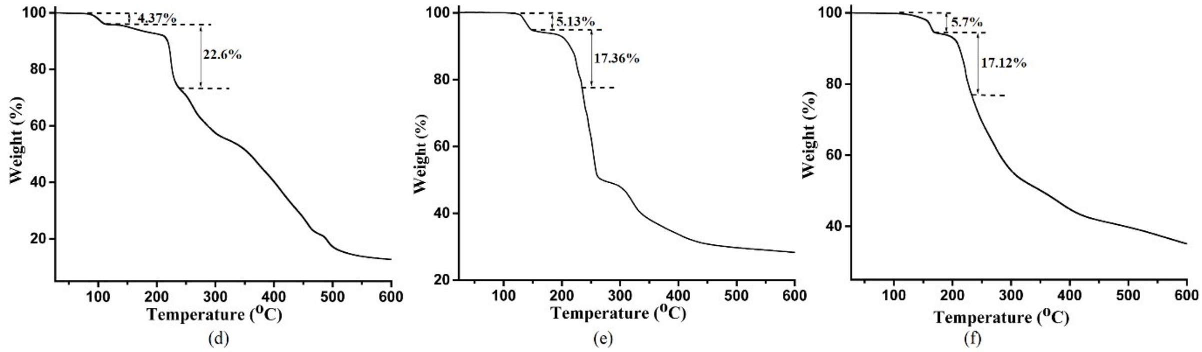


Figure 8S: Thermogram of (a) **L·H_2O**, (b) **CP1** (c) **CP2** (d) **CP3** (e) **CP4** (f) **CP5** (heating rate 10^0C/min under nitrogen atmosphere).

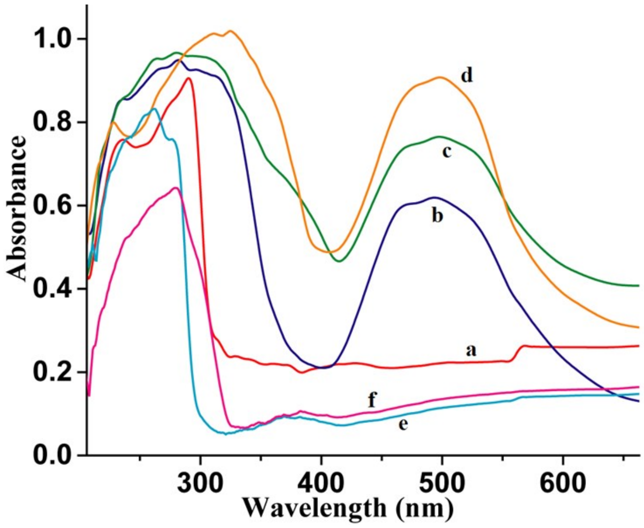


Figure 9S: UV-Vis spectra solid samples of (a) **L.H_2O** (λ_{max} = 291 nm), (b) **CP1** (λ_{max} = 282 nm, 494 nm), (c) **CP2** (λ_{max} = 282 nm, 498 nm), (d) **CP3** (λ_{max} = 324 nm, 498 nm), (e) **CP4** (λ_{max} = 262 nm, 368 nm), (f) **CP5** (λ_{max} = 281 nm, 384 nm).

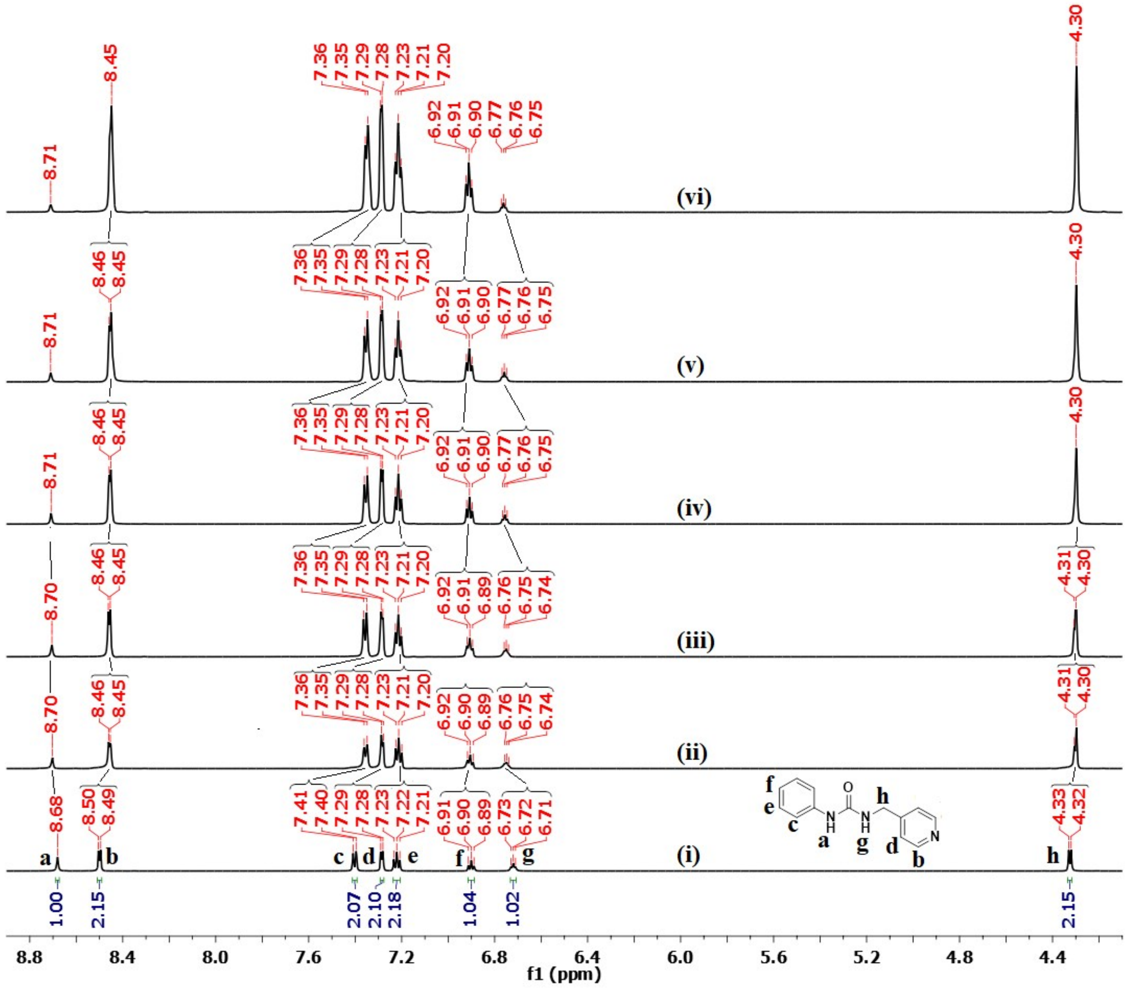
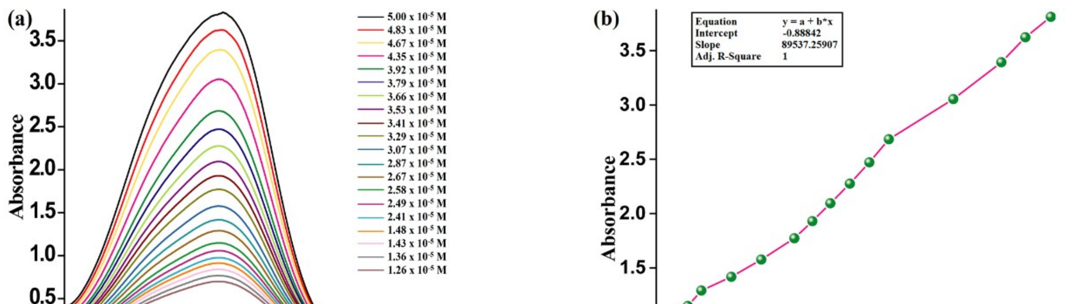


Figure 10S: ^{1}-HNMR (600 MHz) spectra of **L** in (i) DMSO-d_6 and with different fractions of D_2O (ii) 10% (iii) 30% (iv) 60% (v) 70% (vi) 90%.



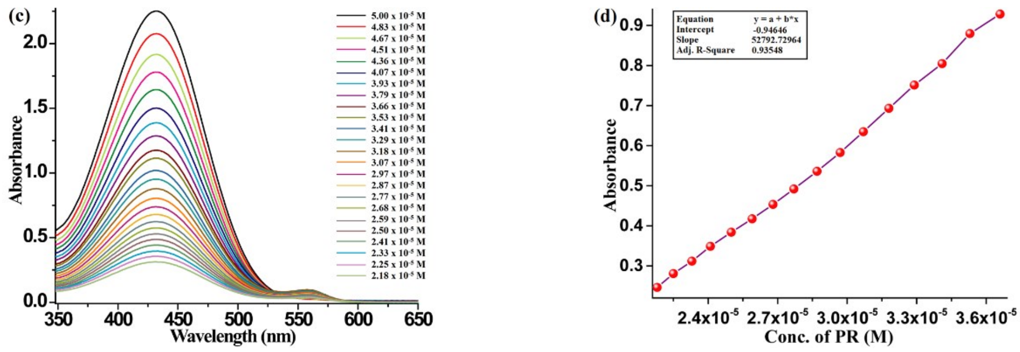


Figure 11S: Calibration plots for Methyl orange (λ_{max}= 464 nm) and Phenol red (λ_{max}= 432 nm) (a, c) by UV-Vis spectra in an aqueous solution and their fitting of absorbance vs concentration of respective dye values (b, d) respectively.

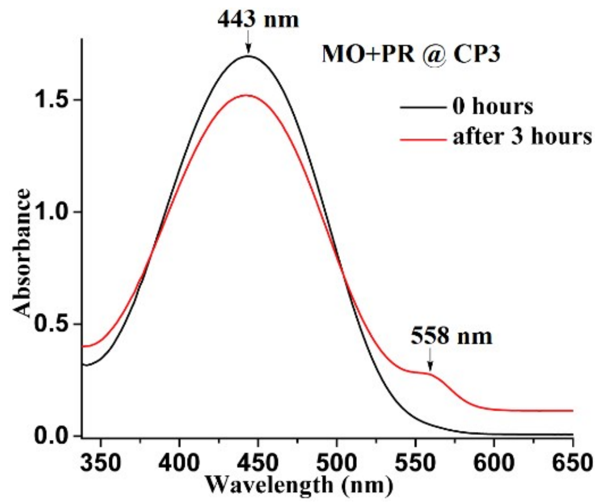


Figure 12S: Dye adsorption with a mixture of MO and PR by **CP3** after 3 hours.

Table 1S: The absorbance and removal of dyes by coordination polymers:

Coordination polymer (CP)	**Amount of Methyl orange dye adsorbed (q_e, mg g^{-1})**
CP1	1.320
CP2	1.369
CP3	1.986
CP4	0.867
CP5	0.731
CP6	1.309

Coordination polymer (CP)	**Amount of Phenol Red dye adsorbed (q_e, mg g^{-1})**
CP1	0.632
CP2	0.714
CP3	0.100

CP4	0.378
CP5	0.194
CP6	0.289

Coordination polymer (CP)	**Removal percentage of Methyl orange dye (%)**
CP1	48.4
CP2	50.2
CP3	72.83
CP4	31.8
CP5	26.8
CP6	48

Coordination polymer (CP)	**Removal percentage of Phenol Red dye (%)**
CP1	21.4
CP2	24.2
CP3	3.4
CP4	12.8
CP5	6.6
CP6	9.8

Table 2S: Hydrogen bond parameters of ligand and coordination polymers **1-5**.

Compound	D-H···A	d_{D-H} (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	∠D-H···A (°)
L.H_2O	N(1)-H(1A) ···O(2) [x,y,z]	0.93 (5)	2.01 (5)	2.924 (5)	166 (4)
	N(2) -H(2A) …O(2) [x,y,z]	0.83 (5)	2.29 (5)	2.980 (5)	141 (5)
	O(2) -H(2B) …O(1) [1/2+x,1/2-y,z]	0.87 (5)	1.95 (5)	2.819 (5)	174 (4)
	O(2) -H(2C) …N(3) [1/2-x,1/2+y,-1/2+z]	0.98 (7)	1.91 (7)	2.876 (5)	169 (6)
	C(5)-H(5)…O(1) [x,y,z]	0.929	2.290	2.887 (6)	121
	C(10)-H(10)…N(2) [x,y,z]	0.93	2.541	2.873 (5)	101
	C(12)-H(12)…O(1) [-x,-y,-1/2+z]	0.929	4.774	4.892 (6)	92
CP1	N(1)-H(1A) ···O(1) [x,1/2-y,-1/2+z]	0.85 (2)	2.03 (2)	2.835 (4)	160 (3)
	N(2)-H(2A) ···O(1) [x,1/2-y,-1/2+z]	0.84 (4)	2.12 (4)	2.876 (3)	149 (4)
	O(2)-H(2B) ···O(4) [1/2-x,y,1/2+z]	0.820	1.870	2.674 (3)	166
	O(2)-H(2C) ···O(4) [x,y,z]	0.84 (3)	1.89 (3)	2.675 (3)	156 (3)
	C(10)-H(10) ···N(2) [x,y,z]	0.929	2.603	2.906 (4)	100
CP2	N(1) -H(1A) ···O(1) [1/2-x,y,1/2+z]	0.82 (4)	2.05 (4)	2.829 (3)	158(4)
	N(2) -H(2A) ···O(1) [1/2-x,y,1/2+z]	0.85 (4)	2.10 (4)	2.870 (3)	151 (4)
	O(2) -H(2B) ···O(4) [x,y,z]	0.821	1.935	2.688 (3)	152
	O(2) -H(2C) …O(4) [x, 1/2-y,-1/2+z]	0.82 (5)	1.84 (5)	2.662 (3)	178 (5)
	C(10) -H(10) …N(2) [x,y,z]	0.929	2.565	2.878 (5)	100
CP3	N(1) -H(1A) [x,y,z]	0.81 (2)	-	-	-
	N(2) -H(2A) ···O(4) [-1/2+x,3/2-y,-1/2+z]	0.83 (2)	2.10 (2)	2.922 (2)	167 (2)
	O(2) -H(2B) ···O(1) [x, 1+y, z]	0.820	2.034	2.753 (2)	146
	O(2) -H(2C) …O(4) [1-x,2-y,1-z]	0.82 (2)	1.86 (2)	2.669 (2)	166 (2)
	C(5) –H(5) …O(1) [x,y,z]	0.931	2.263	2.863 (4)	121
	C(8) –H(8A) …(O1) [x,y,z]	0.970	2.449	2.784 (2)	100
	C(10) –H(10) …N(2) [x,y,z]	0.931	2.586	2.904 (2)	101

CP4	N(1)-H(1A) ···O(1) [x,1/2-y,-1/2+z]	0.860	2.058	2.830 (3)	149
	N(2)-H(2A) ···O(1) [x,1/2-y,-1/2+z]	0.860	2.143	2.874 (3)	143
	O(2)-H(2B) ···O(4) [1-x,-y,1-z]	0.850	1.907	2.676 (3)	150
	O(2)-H(2C) [x,y,z]	1.008	-	-	-
	C(10)-H(10) ···N(2) [x,y,z]	0.930	2.585	2.891 (3)	100
CP5	N(1)-H(1A) ···O(1) [x,1/2-y,-1/2+z]	0.79 (4)	2.08 (4)	2.834 (3)	157 (3)
	N(2) -H(2A) …O(1) [x,1/2-y,-1/2+z]	0.77 (3)	2.18 (3)	2.870 (3)	149 (3)
	O(2)-H(2B)…O(4) [x,y,z]	0.820	1.933	2.685 (3)	152
	O(2)-H(2C)…O(4) [3/2-x,y,1/2+z]	0.79 (4)	1.87 (4)	2.668 (2)	176 (4)
	C(10)-H(10)…N(2) [x,y,z]	0.930	2.566	2.878 (4)	100