Supporting Information：Metalo-hydrogen bonded organic frameworks with nitrogen tridentate ligands: Exploring Inclusion and dyes adsorption properties

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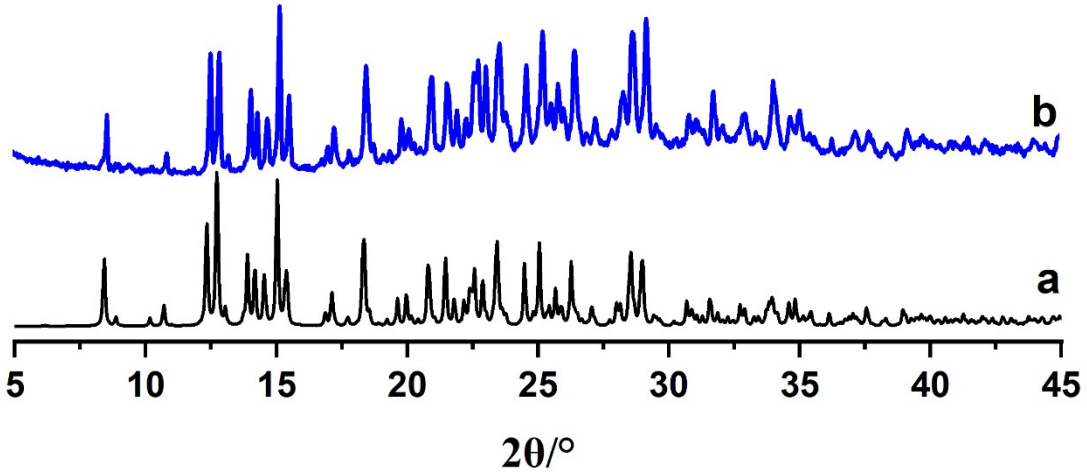

Figure S1. Experimental PXRD patterns of salt of **1**: (a) Simulated PXRD from single crystal salt of **1**; (b) Experimental PXRD from single crystal salt of **1**.

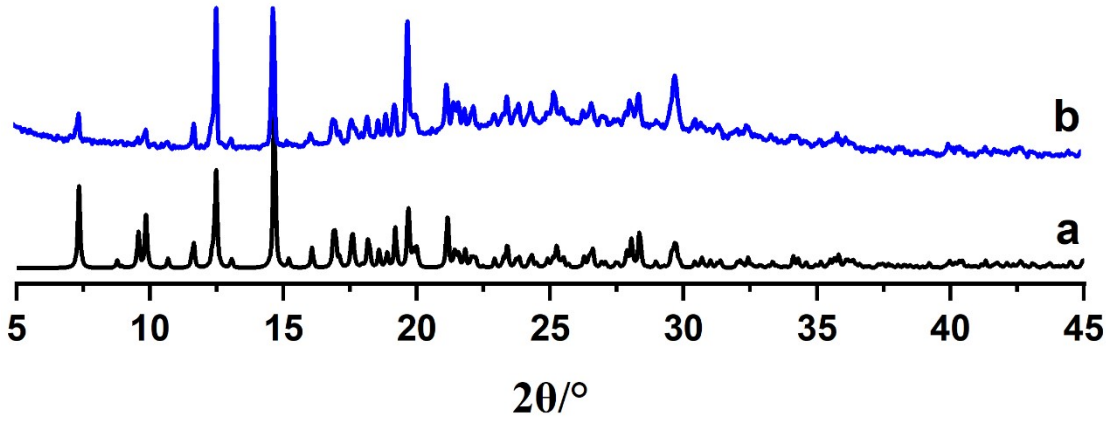

Figure S2. Experimental PXRD patterns of salt of **2**: (a) Simulated PXRD from single crystal salt of **2**; (b) Experimental PXRD from single crystal salt of **2**.

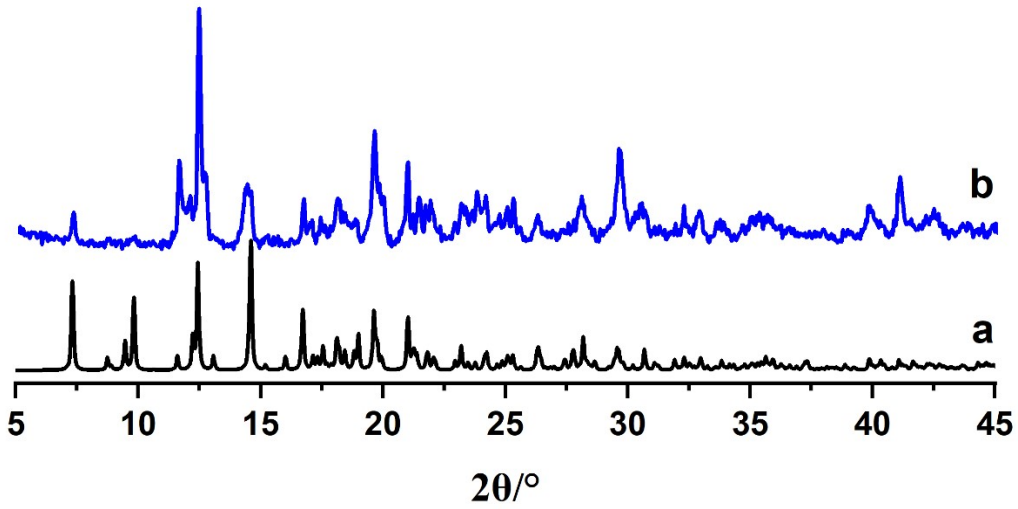

Figure S3. Experimental PXRD patterns of salt of **3**: (a) Simulated PXRD from single crystal salt of **3**; (b) Experimental PXRD from single crystal salt of **3**.

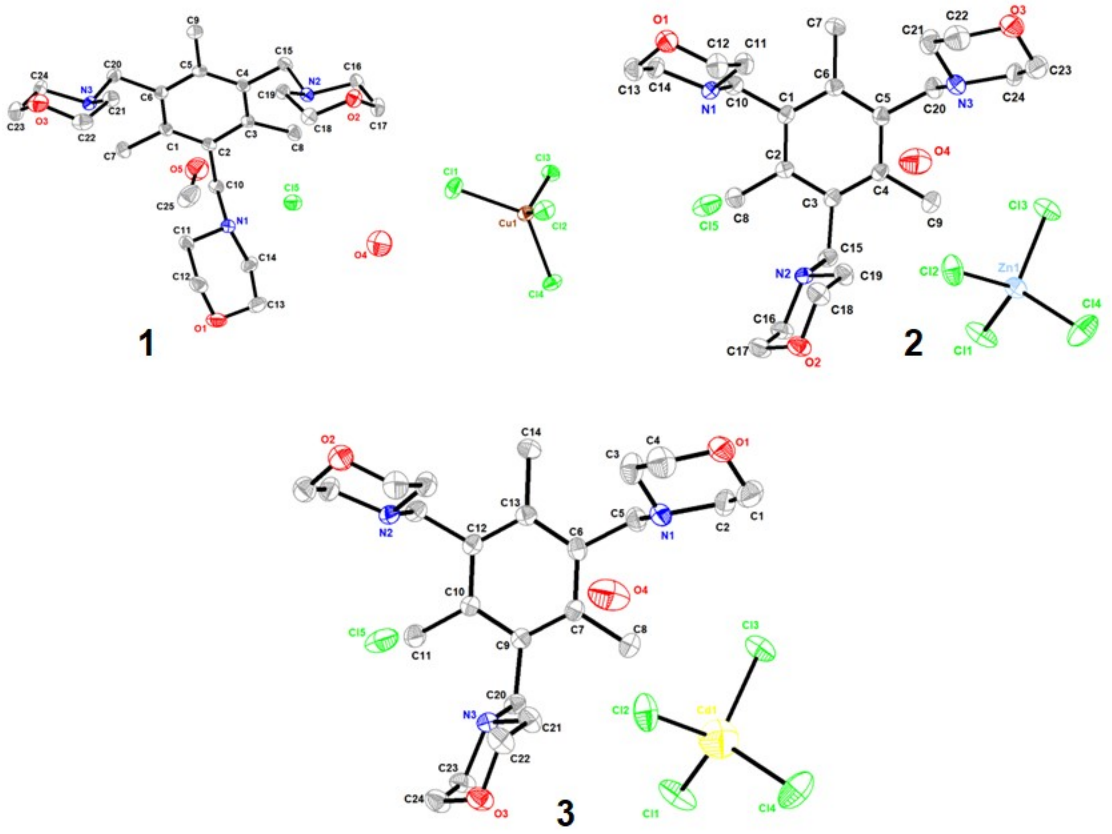

Figure S4. The asymmetric units of **1–3**. Thermal ellipsoids are set at 30% probability level. All the hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structural refinement parameters for **1**–**3**.

Crystal	**1**	**2**	**3**
Empirical formula	$C_{25}H_{48}Cl_5CuN_3O_5$	$C_{24}H_{44}Cl_5N_3O_4Zn$	$C_{24}H_{44}Cl_5CdN_3O_4$
Formula weight	711.45	681.24	728.27
Temperature (K)	293	293	293
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	$P2_1/n$
Z	4	4	4
a (Å)	14.361(2)	10.9164(4)	11.0149(7)
b (Å)	13.865(2)	19.7454(8)	19.8174(13)
c (Å)	16.142(3)	15.8657(6)	15.8532(10)
α (deg)	90	90	90
β (deg)	94.825(5)	106.713(1)	106.045(2)
γ (deg)	90	90	90
V (Å^3)	3202.7(9)	3275.4(2)	3325.7(4)
D_x (Mg.cm^{-3})	1.475	1.382	1.454
μ (mm^{-1})	1.138	1.190	1.090
F (000)	1492	1424	1496
R_{int}	0.0636	0.0626	0.0309
Total reflns	37912	44126	28597
Unique reflns	4736	4046	4626
s	1.032	1.022	1.040
R_1	0.0372	0.0548	0.0489
wR_2	0.1028	0.1580	0.1387
CCDC number	2393652	2393653	2393654

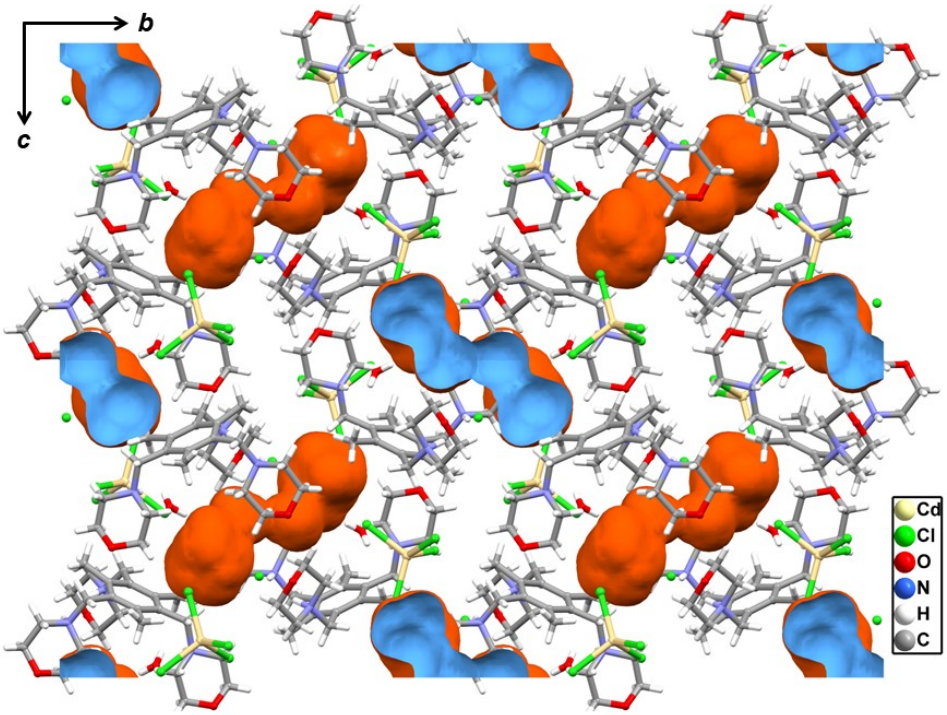

Figure S5. The voids in **3** viewed along the a-crystallographic axis. Disorder part of water molecule is omitted for clarity.

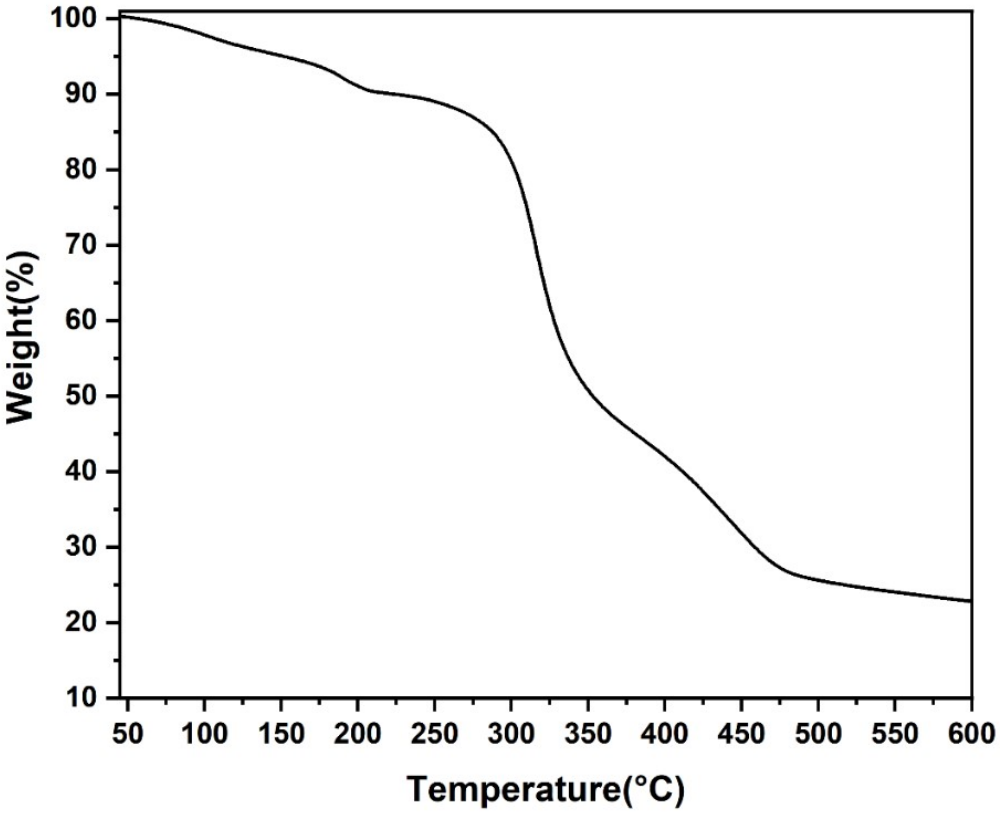

Figure S6. TGA curve of **1**.

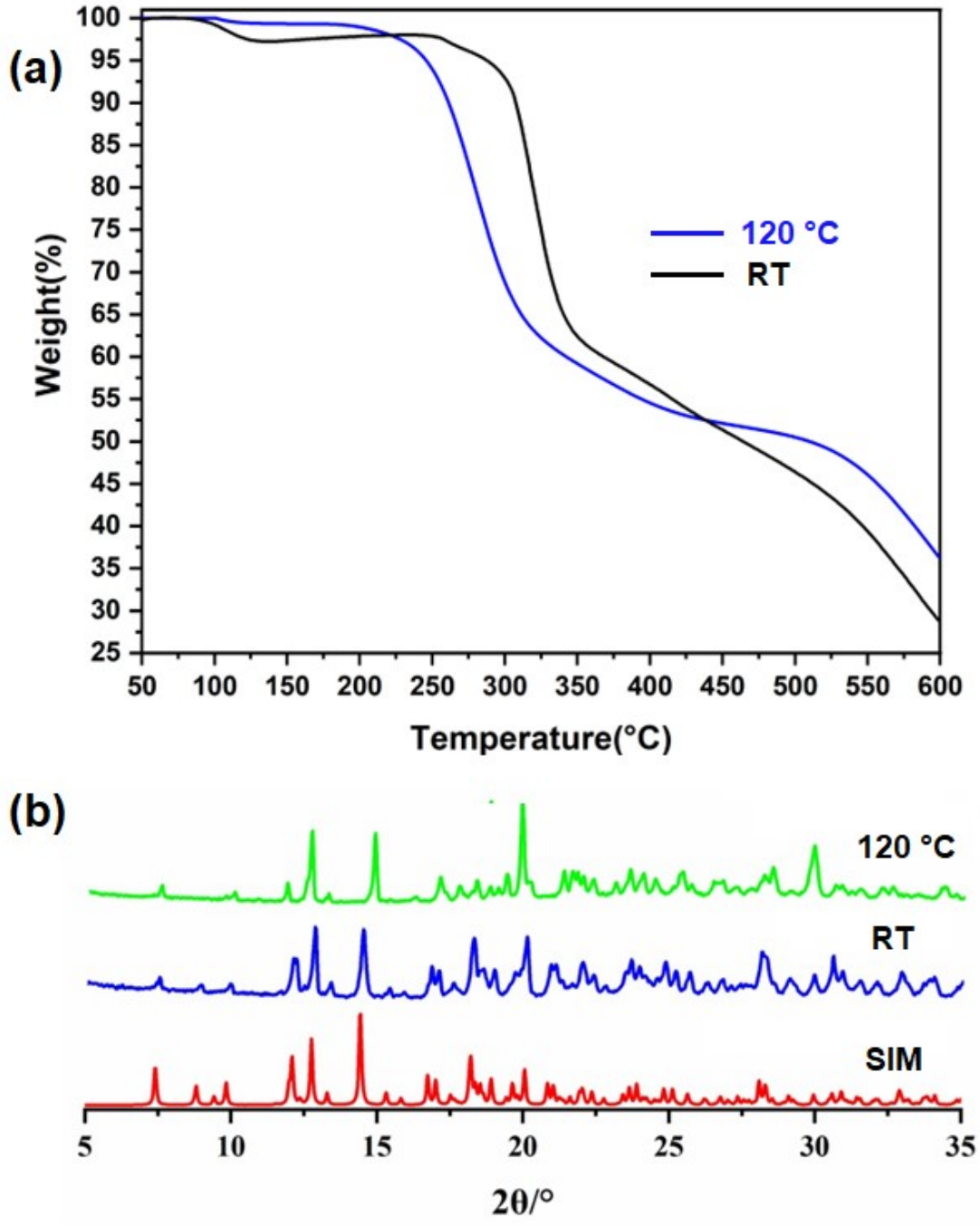

Figure S7. (a) TG plots of **3** (black line) at room temperature and after being heated to 120 °C (blue line); (b) PXRD patterns of the sample at RT (blue) and 120 °C (green), and the simulated PXRD patterns of crystal **3** (red).

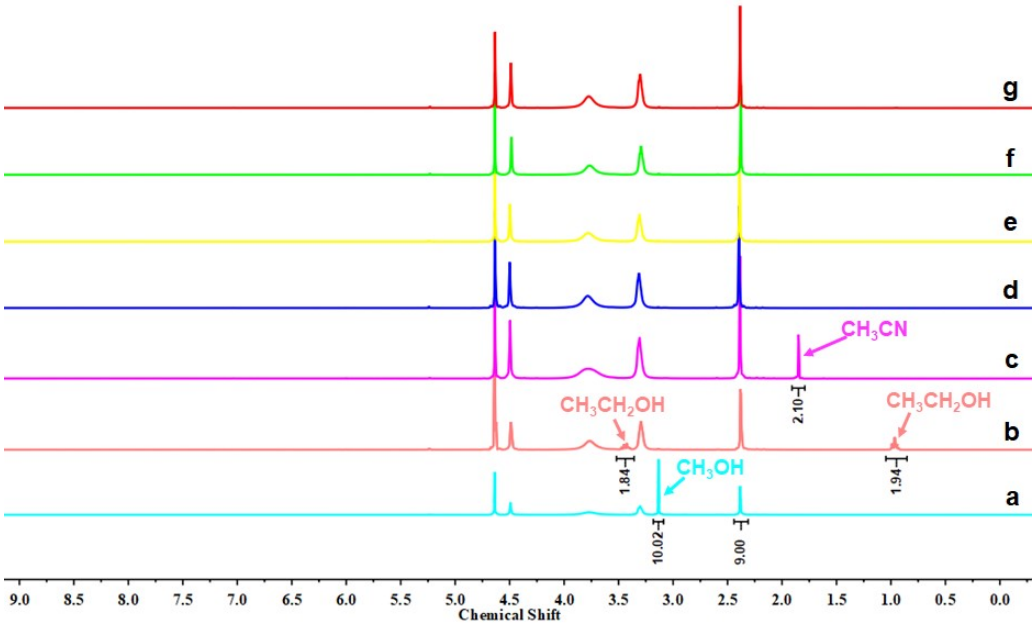

Figure S8. ^{1}H NMR spectra of the heated host frameworks **3** dipped into MeOH (a), EtOH (b), CH_3CN (c), DCM (d), THF (e), EA (f) and *i*-PrOH (g) for 24 hours respectively.

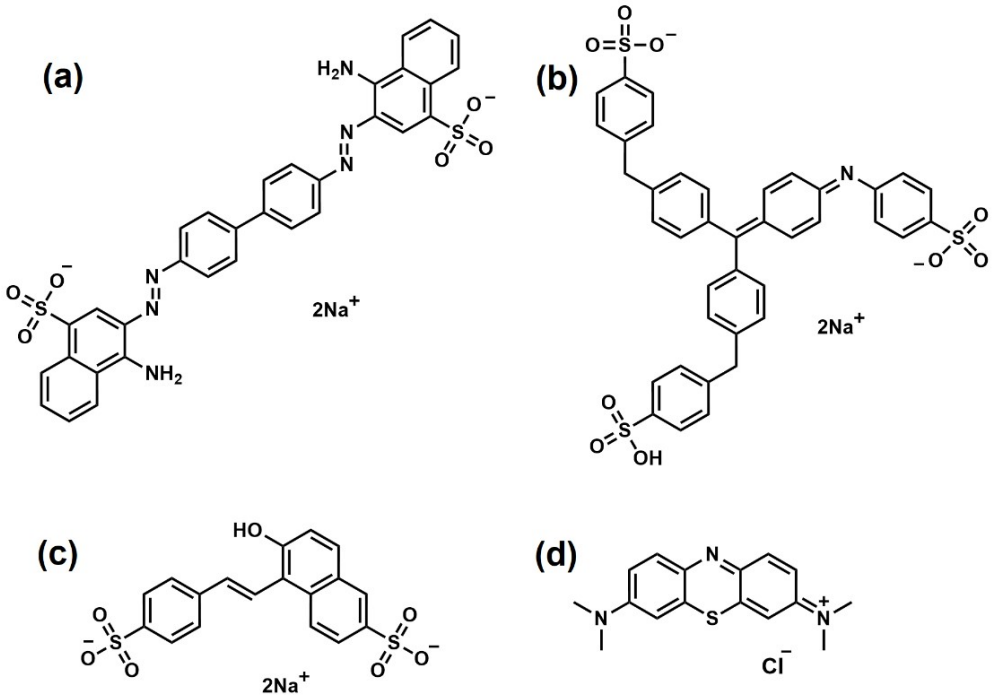

Figure S9. The chemical structure of (a) CR, (b) MB, (c) SY and (d) MTB.

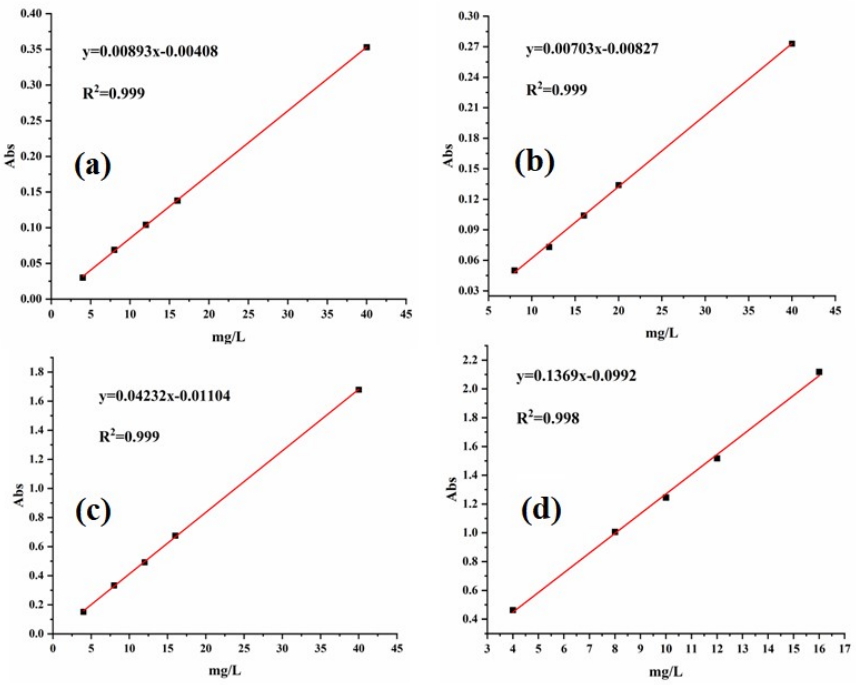

Figure S10. The calibration curve of (a) CR, (b) MB, (c) SY and (d) MTB in methanol solutions.

Table S2. The adsorption capacity of CR, MB and SY onto adsorbents MOHFs **2** and **3** with repeated experiments.

Dye	Adsorption capacity (mg/g)					Mean	Standard error
Congo red (CR)	MHOF **2**	37.2	36.5	36.6	35.2	36.4	0.421
	MHOF **3**	35.6	32.9	34.8	35.3	34.7	0.606
Methyl blue (MB)	MHOF **2**	33.6	32.2	33.4	31.2	32.6	0.560
	MHOF **3**	32.4	32.0	31.1	30.0	31.4	0.533
Sunset yellow (SY)	MHOF **2**	31.6	31.1	30.9	32.5	31.5	0.357
	MHOF 3	30.0	29.2	31.8	28.9	30.0	0.651

Table S3. Comparison of the maximum adsorption capacity of CR onto various adsorbents.

Adsorbent	Adsorption capacity (mg/g)	Ref.
MHOFs **2**	36.4	This work
MHOFs **3**	34.7	This work
Activated carbon from coir pith	6.72	42
Single-crystalline NiO nanosheets	36.1	43
Zeolite (Clay materials)	3.77	44
Kaolin	5.44	45
$[La(L)Cl(H_2O)_2]_n$	1428	46
$\{[Nd(L)Cl(H_2O)_3]\cdot 2H_2O\}_n$	433	46
$\{[Pr_2(L)_2Cl_2(H_2O)_6]\cdot H_2O\}_n$	319	46
Co-MOF	974.86	47
$[Ni_2F_2(4,4'\text{-bipy})_2(H_2O)_2](VO_3)_2.8H_2O$	242.1	48

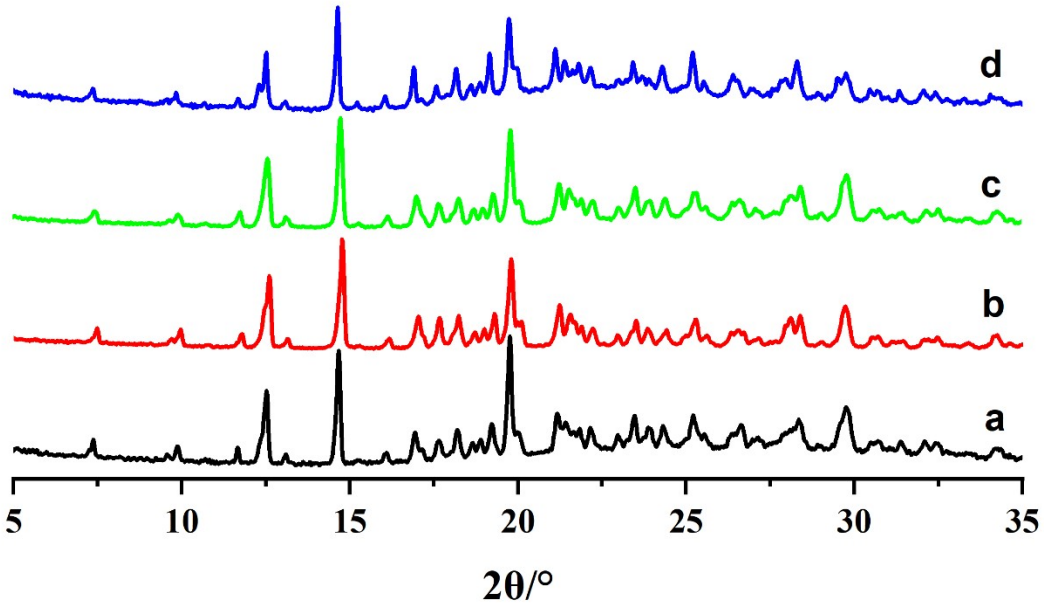

Figure S11. PXRD patterns of (a) as-synthesized **2**, (b) CR-loaded **2**, (c) MB-loaded **2** and (d) SY-loaded **2**.

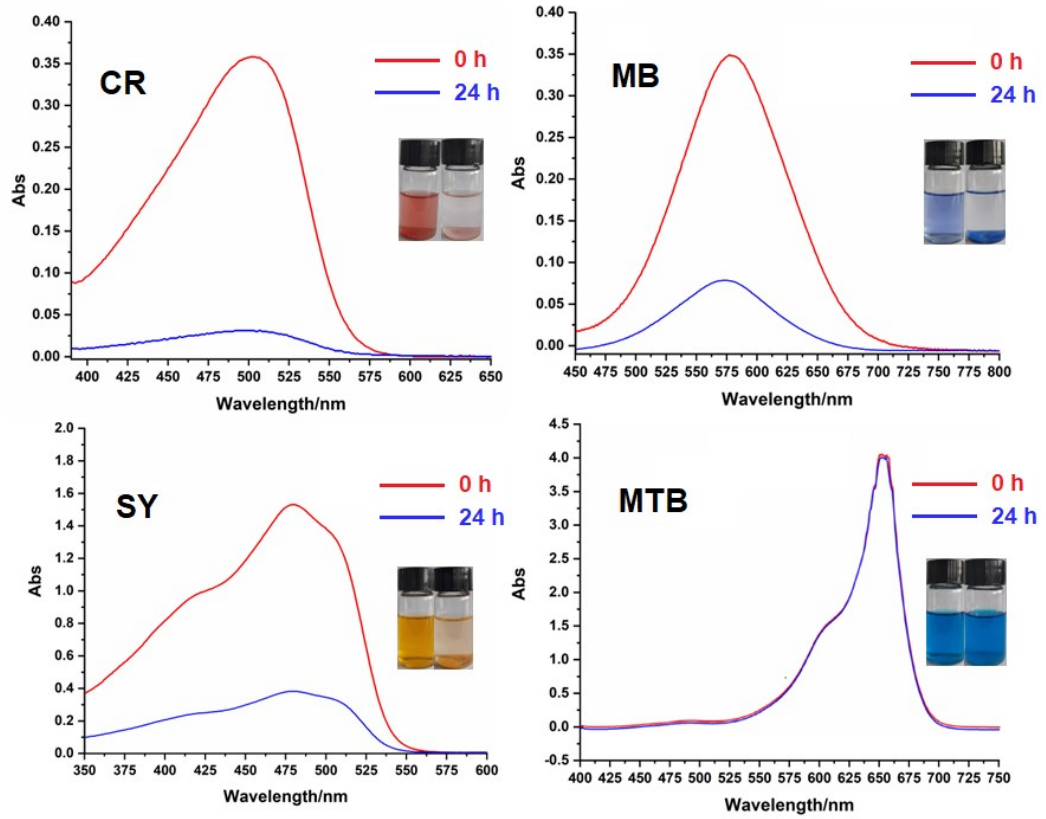

Figure S12. UV–Vis spectra of methanol solutions of CR, MB, SY and MTB during an adsorption test with heated **3** over 24 h. The inset photographs depict the color changes of the dye solutions before (left) and after the adsorption (right).

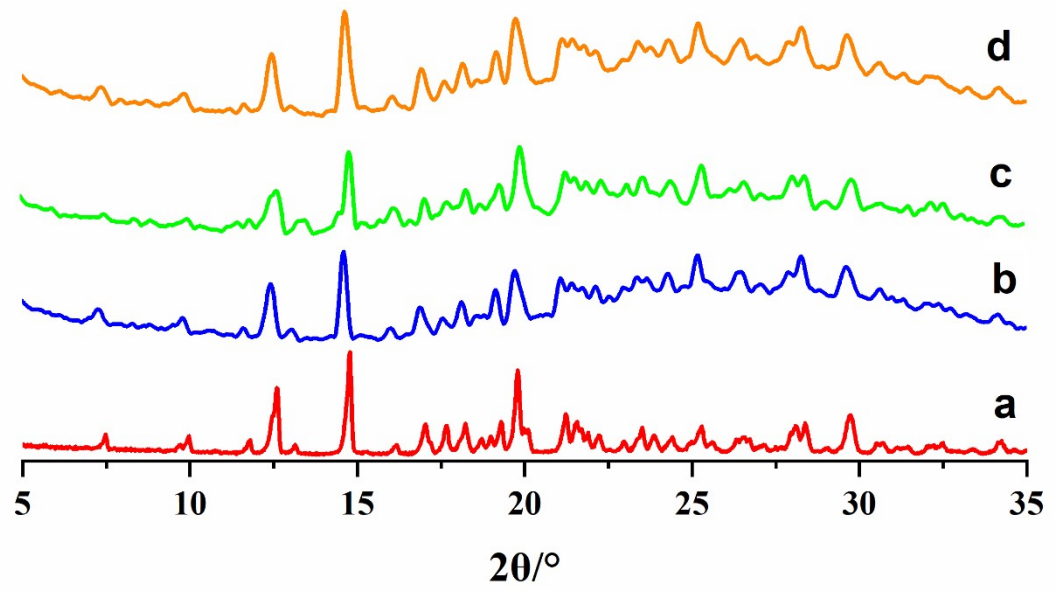

Figure S13. PXRD patterns of (a) as-synthesized **3**, (b) CR-loaded **3**, (c) MB-loaded **3** and (d) SY-loaded **3**.

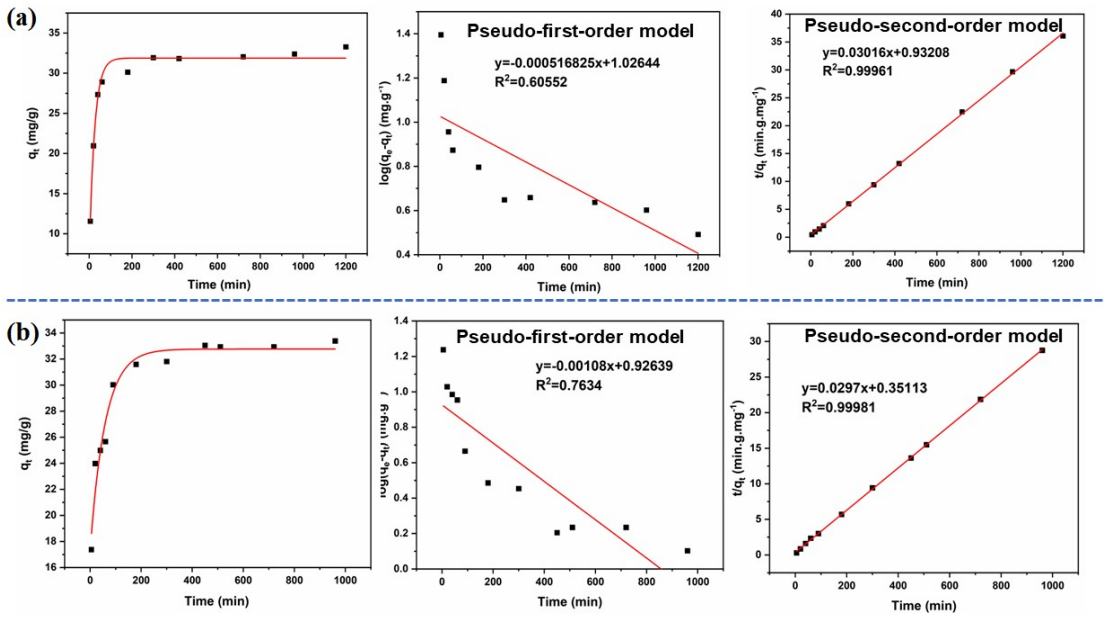

Figure S14. The variation of adsorption capacity with adsorption time for CR on samples **2** (a) and **3** (b) and fitting with pseudo-first-order and pseudo-second-order kinetic models.