Electronic Supplementary Information

Secondary-amine-functionalized isoreticular metal–organic frameworks for controllable and selective dye capture

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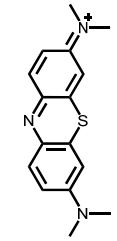
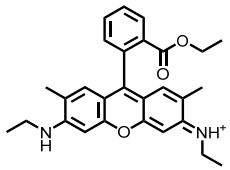
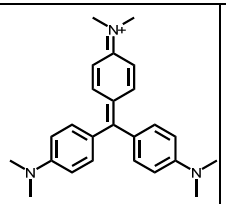
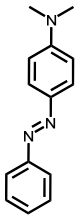
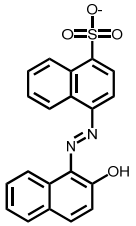
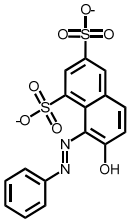
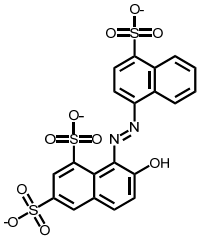
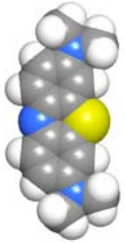
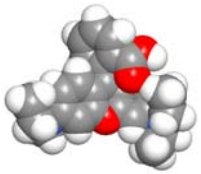
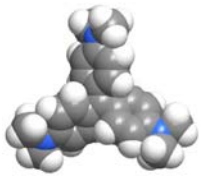
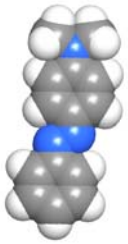
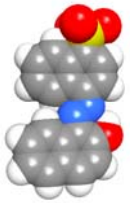
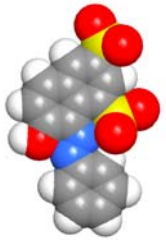
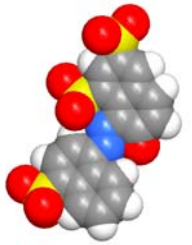
Table S1. Crystal data and structure refinements results.

Compound	ST-14	ST-15
Formula	$C_{42}H_{28}N_{10}O_8Cu_2$	$C_{42}H_{28}N_{10}O_8Zn_2$
Formula weight	927.82	931.48
Crystal system	cubic	cubic
Space group	*P*-43*n* (No.218)	*P*-43*n* (No.218)
a (Å)	27.6887(13)	28.1049(10)
V (Å^3)	21228(3)	22200(2)
Z	6	6
Crystal size (mm^3)	0.12 × 0.12 × 0.12	0.12 × 0.12 × 0.12
T (K)	173	173
λ (Å)	1.54178	1.54178
θ range (°)	2.26–42.9	3.14–43.0
Total reflections	68406	32606
Unique reflections	2572	2690
R_{int}	0.0636	0.0439
Observed Data	2572	2690
Resolution (Å)	1.10	1.10
R_1, wR_2 ($I > 2\sigma$)	0.0200, 0.0517	0.0322, 0.0810
R_1, wR_2 (all)	0.0225, 0.0535	0.0363, 0.0826
S	1.156	1.104

[a] $R_1=\sum||F_o|-|F_c||/\sum|F_o|$.

[b] $wR_2=\{\sum w[(F_o)^2-(F_c)^2]^2/\sum w[(F_o)^2]^2\}^{1/2}$

Table S2. Crystal data and structure refinements results.

Structure							
3D structure							
Name	Methylene Blue	Rhodamine B	Crystal Violet	Solvent Yellow 2	Acid Red 88	Orange G	New Coccine
Abbr	MLB	RHB	CV	SY2	AR88	OG	NC
Charge	+1	+1	+1	0	-1	-2	-3
MW.	373.90	479.01	407.98	225.30	400.383	452.37	604.47
Optimal absorption wavelength	655	547	589	405	510	499	514
Inclusion	Y	Y	Y	N	N	N	N
Dimension (10^{-10}m)	x = 4.00 y = 7.93 z =16.34	x = 6.53 y = 11.89 z = 15.55	x = 4.77 y = 12.43 z = 13.09	x = 4.5 y = 6.0 z = 15.1	x = 5.44 y = 10.27 z = 15.66	x = 5.44 y = 10.14 z = 15.64	x =5.44 y =10.48 z =17.38

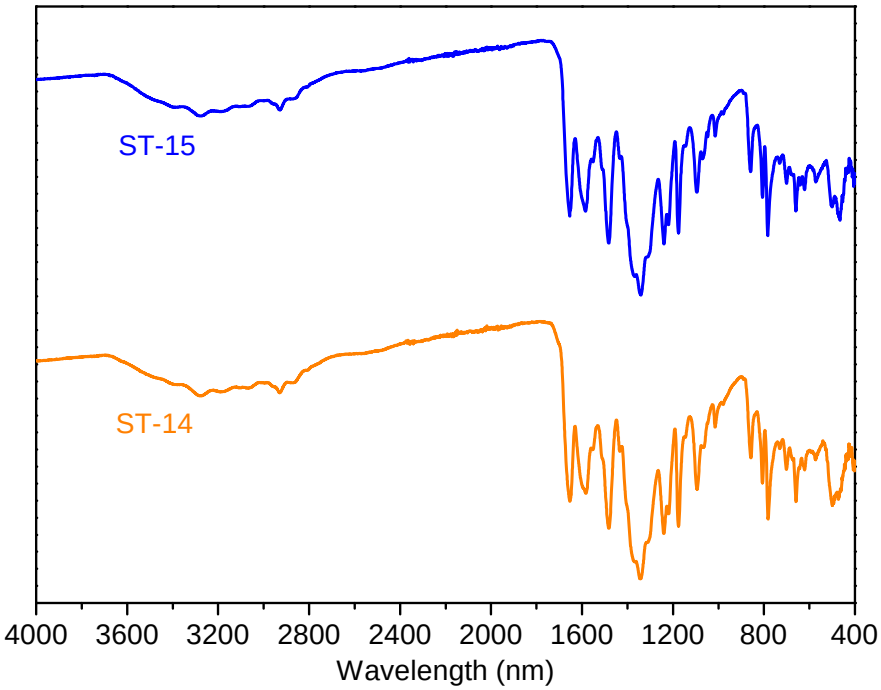


Fig. S1 IR spectra of ST-14 and ST-15.

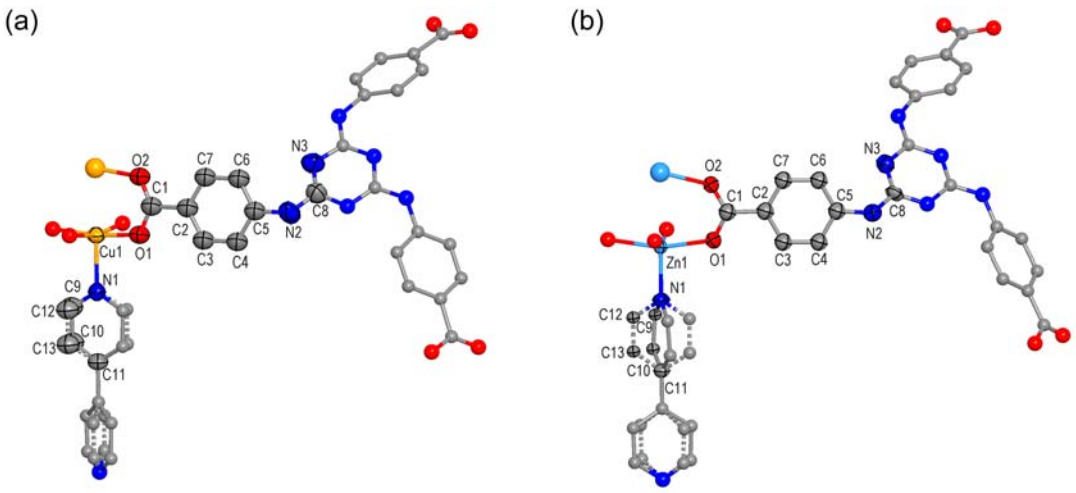


Fig. S2 Asymmetric unit in the single crystal structure of (a) ST-14 and (b) ST-15 (thermal ellipsoids with 50% probability; Carbon, grey; Nitrogen, blue; Oxygen, red; Zinc, light-blue; Copper, yellow.). Hydrogen atoms are omitted for clarity; symmetry-related atoms are not labelled and represented as spheres.

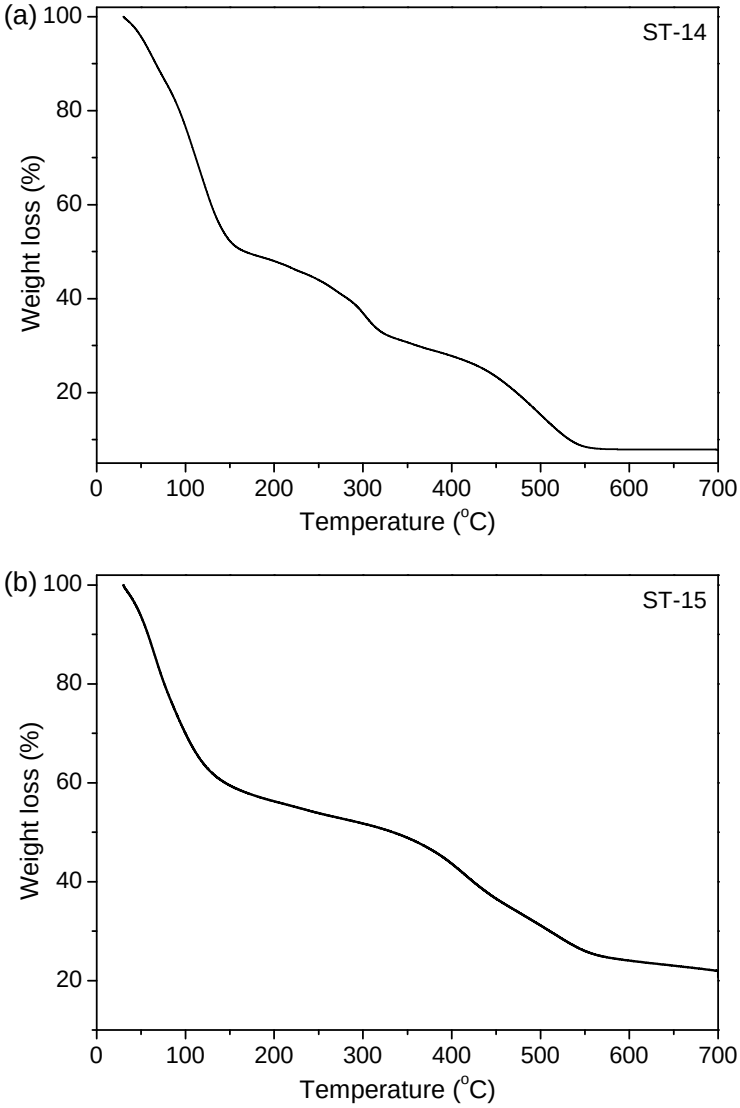


Fig. S3 TG curves of (a) ST-14 and (b) ST-15.

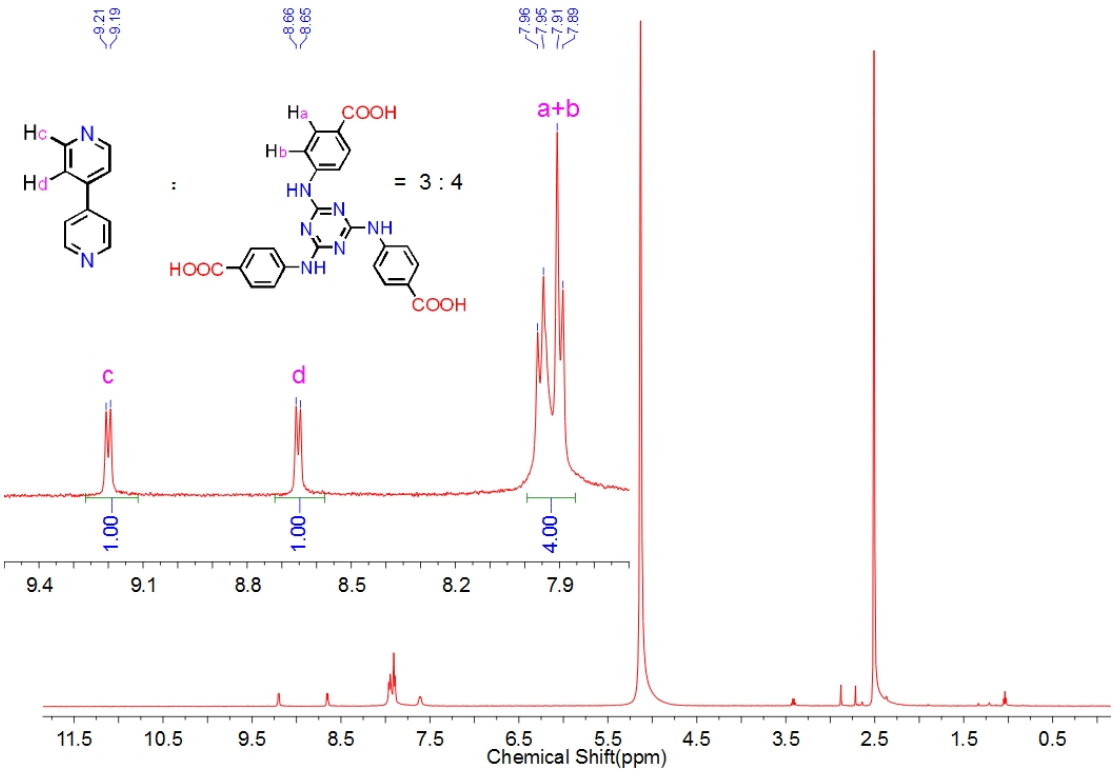


Fig. S4. ^{1}H NMR spectrum of ST-15 digested in DMSO-d_6 with DCl. Integration of the chemical shifts provides the linker molar ratio of TATAB and BPY round to 4:3, which is consistent with that of the crystallographic analysis result.

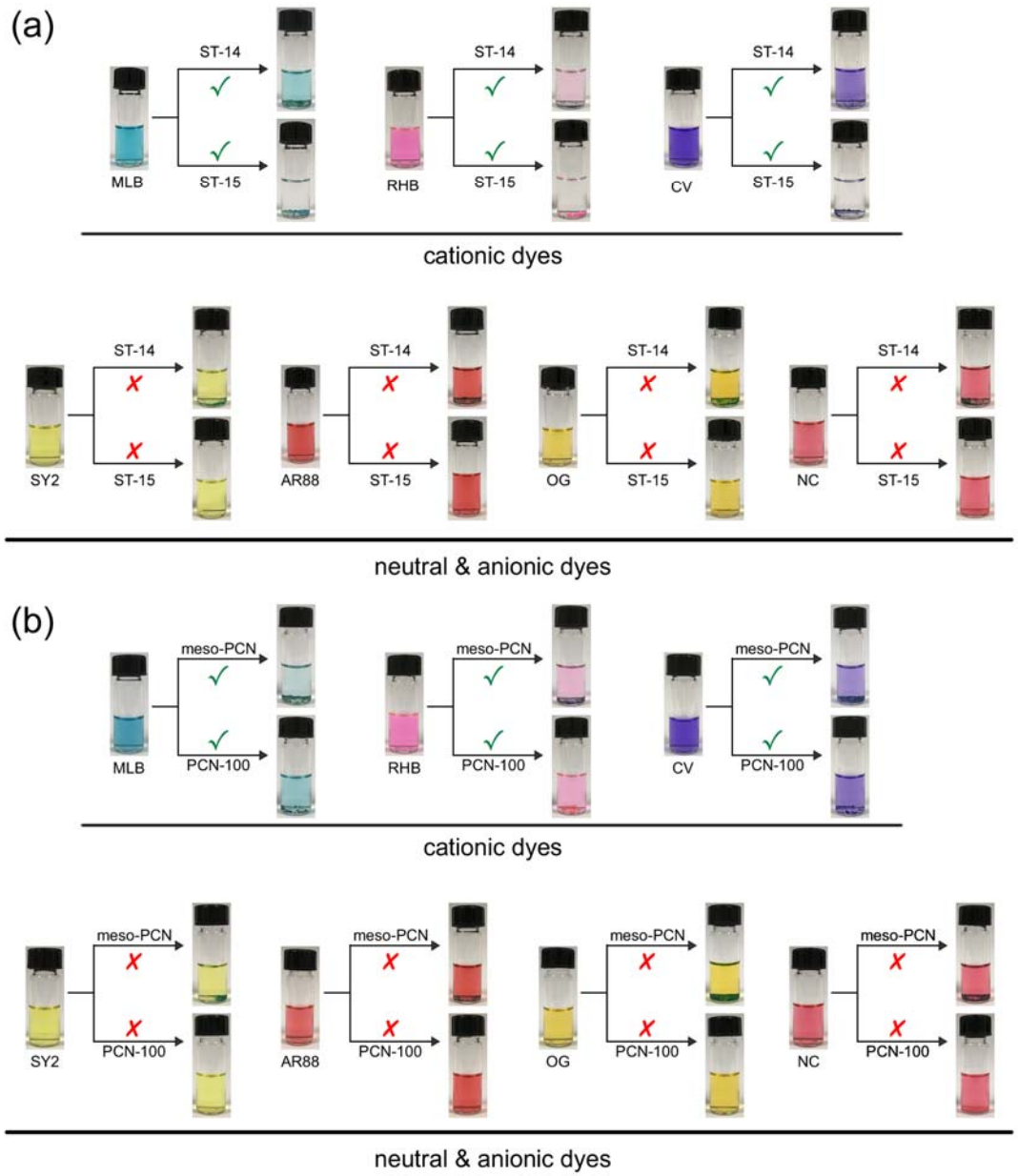


Fig. S5 Photographs of the monocomponent dye solution with the presence of (a) ST-14 and ST-15, compared with (b) other TATAB-based MOFs (meso-PCN and PCN-100).

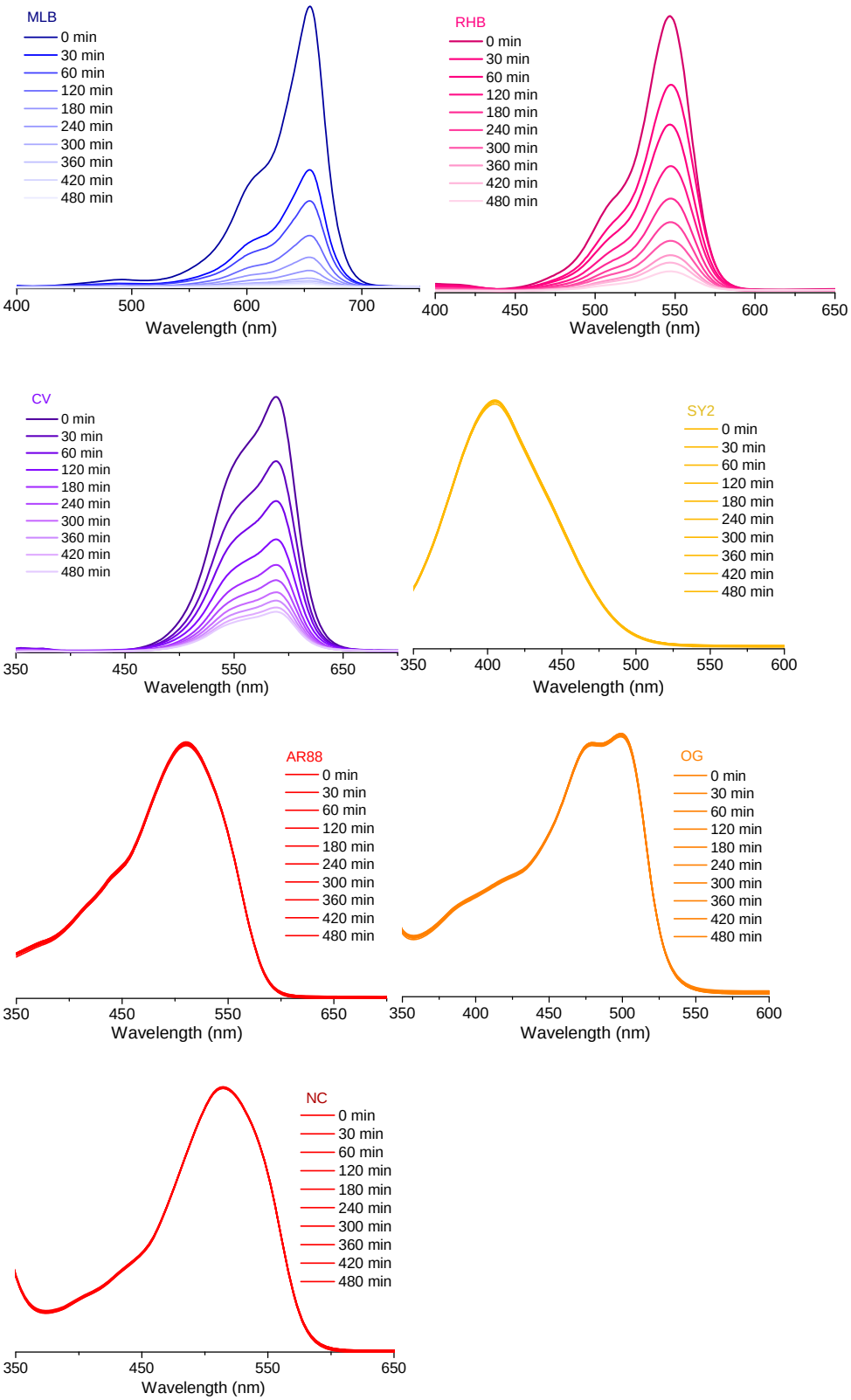


Fig. S6 UV-vis spectra changes of monocomponent dye solution with the presence of ST-15.

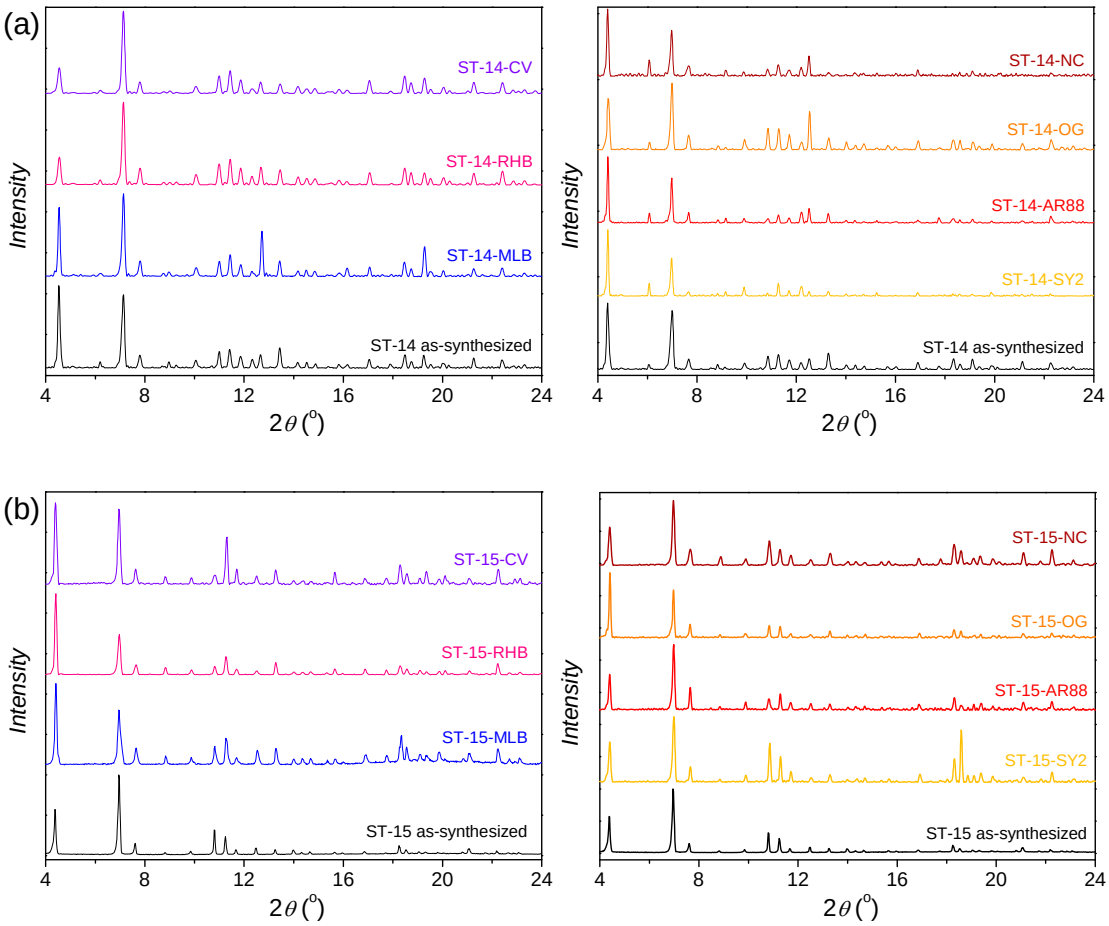


Fig.S7 Powder X-ray diffraction patterns of (a) ST-14 and (b) ST-15 after dye adsorption experiments.

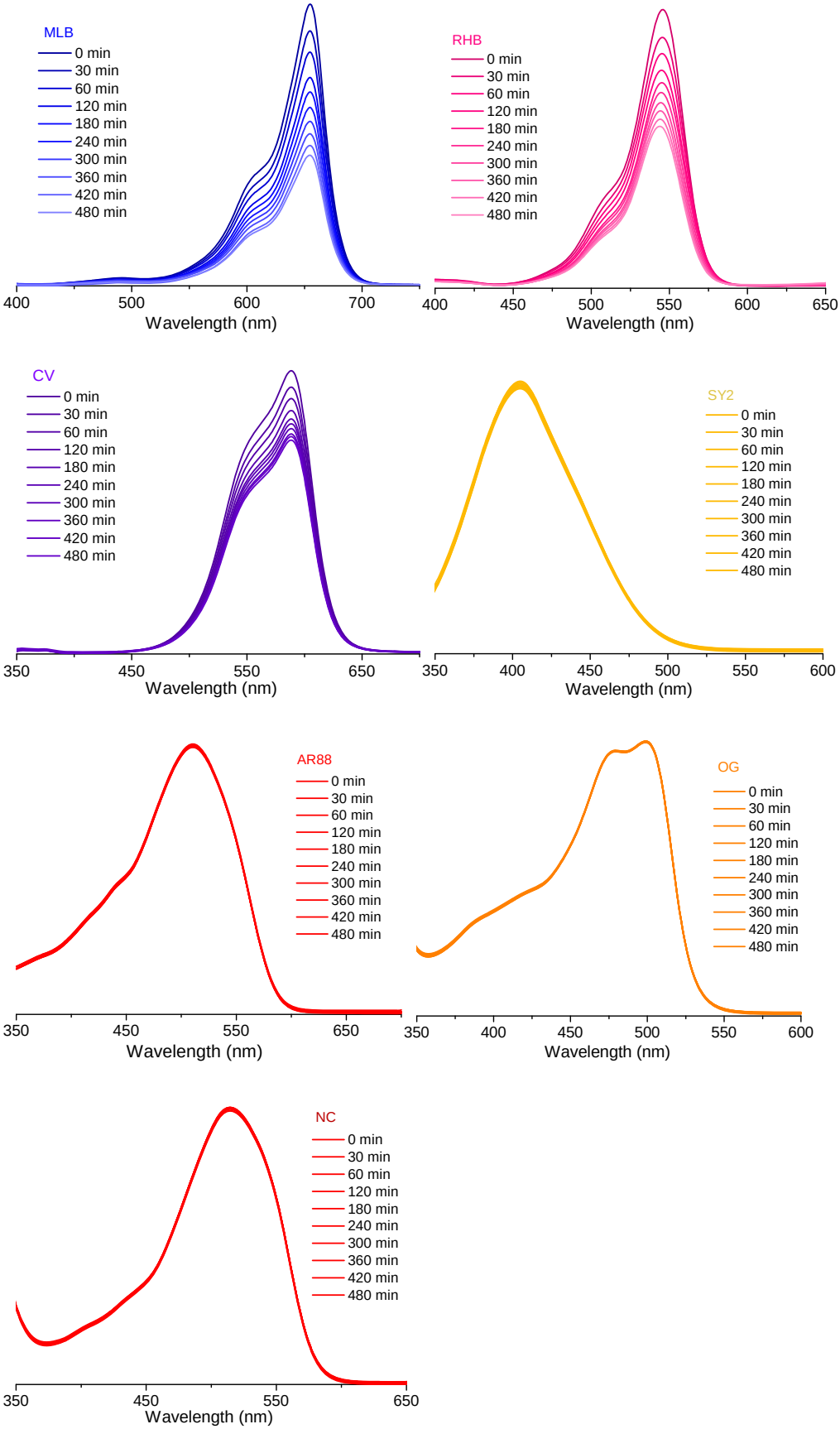


Fig. S8 UV-vis spectra changes of monocomponent dye solution with the presence of ST-14.

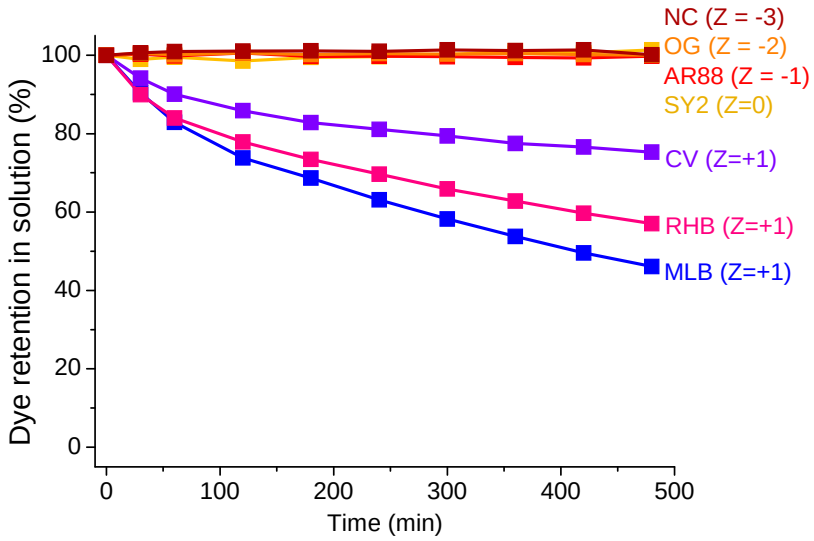


Fig. S9 Differently charged dyes contents in solution with presence of ST-14 monitored with time.

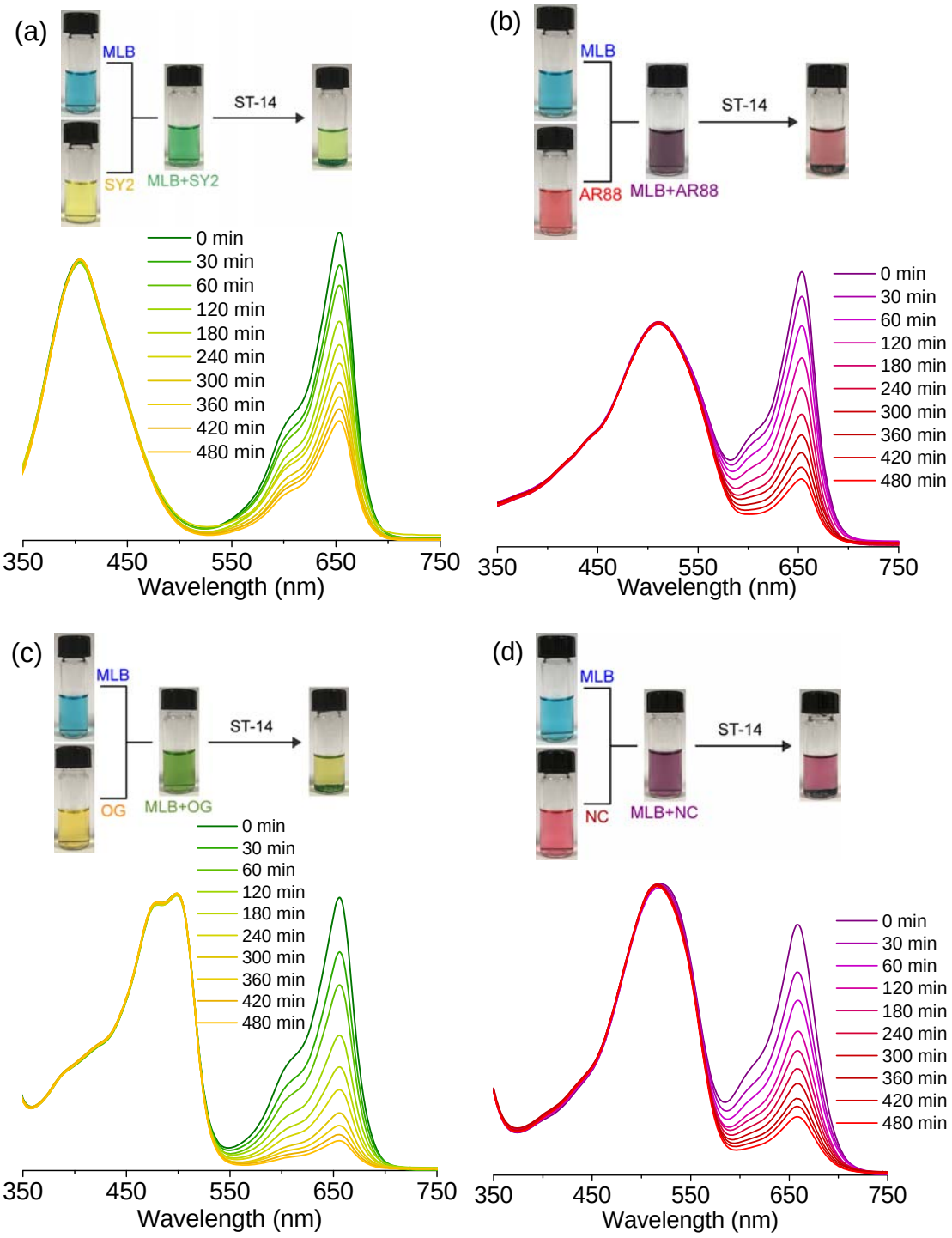


Fig. S10 UV-vis spectra changes of mixed dye solution with the presence of ST-14. The photographs show the colours of the dye solutions, their mixture before and after adsorption.

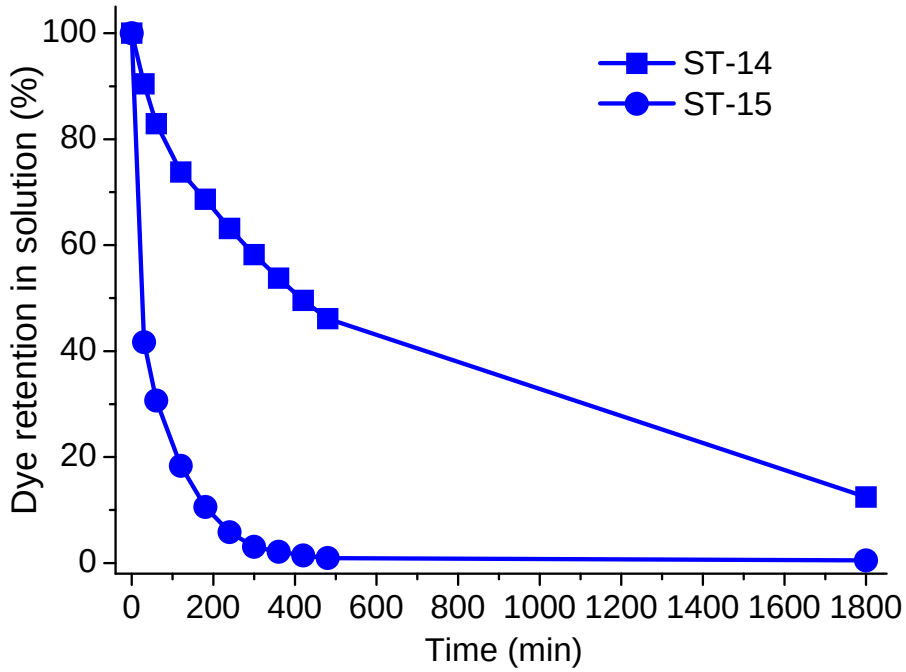


Fig. S11 MLB contents in solution with presence of ST-14 and ST-15 monitored with by 30 hours, confirming that the samples of ST-14 and ST-15 possessed similar adsorption capacity but different adsorption kinetics.

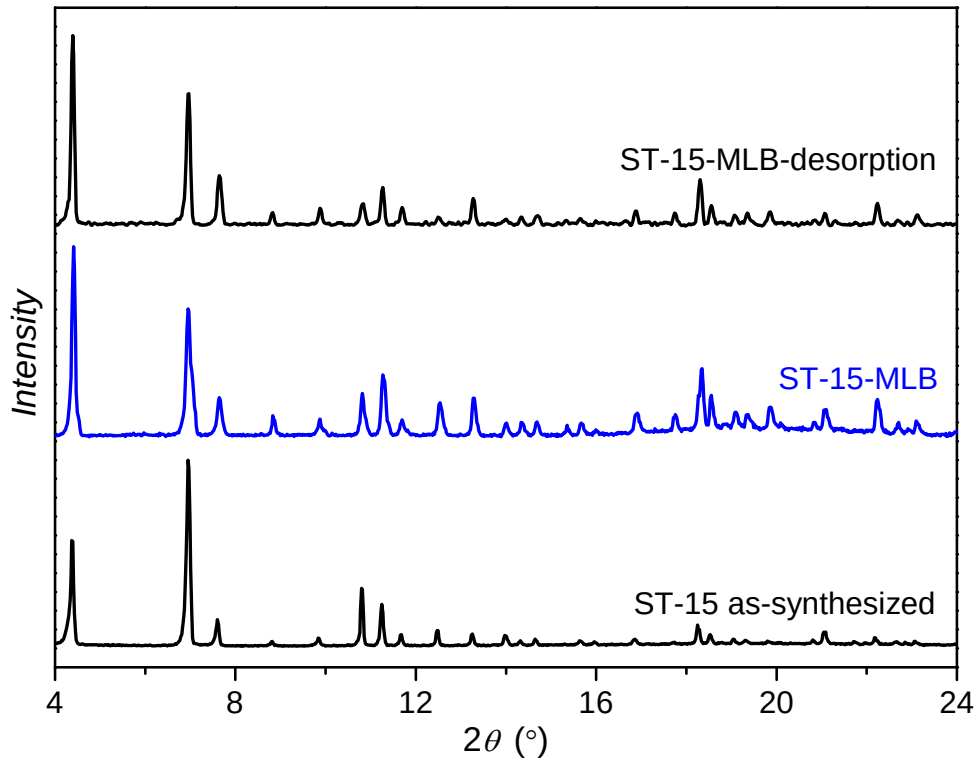


Fig.S12 Powder X-ray diffraction patterns of ST-15 after dye release experiments.