Supporting information

A Bifunctionalised Pb-Based MOF for Iodine Capture and Dyes Removal

Table S1. Selected bond lengths (Å) and bond angles (degree) for **SM-3**

Pb1-O1	2. 449 (3)
Pb1-O3	2. 477 (4)
Pb1-O4	2. 704 (4)
Pb1-N1	2. 676 (4)
Pb1-N4	2. 592 (4)
O3-Pb1-O1	79. 74 (12)
O4-Pb1-O1	114. 60 (12)
O4-Pb1-O3	49. 18 (11)
N1-Pb1-O1	138. 21 (11)
N1-Pb1-O3	84. 11 (11)
N4-Pb1-O4	80. 88 (11)
N4-Pb1-O1	76. 65 (12)
N4-Pb1-O3	77. 84 (12)
N4-Pb1-O4	118. 37 (12)
N4-Pb1-N1	62. 32 (12)

Table S2: Comparison of structural properties of Pb-crystals with **SM-3**.

Synthesized Pb-crystals	**Bond Distances**	**Geometry**	**Anagostic interactions**	**Dimensions**	**Ref.**
$[Pb(mip)(1,4\text{-}NDC)]_n$	Pb–O = 2.465(3)-2.693(3)Å, Pb–N = 2.464(3)-2.554(3)Å, Pb-Pb = 11.5400 Å	Pentagonal bipyramidal	Absent	2-D	36
$[Pb_2(pzp)_2(adip)(NO_3)_2]$	Pb–O = 2.412(4)-2.693(3)Å, Pb–N= 2.615(4)-2.557(4) Å	Pentagonal bipyramidal	Absent	2-D	37
[Pb(pzp)(glu)]	Pb–O= 2.592(4)-2.586(4)Å, Pb–N= 2.747(4)-2.691(4) Å	Distorted pentagonal bipyramidal	Absent	2-D	37

[Pb(pzp)(chdc)]·[Pb (pzp)-(chdc)]· pzp ·H_2O	Pb–O= 2.360(7)-2.481(7)Å Pb–N= 2.700(8)-2.718(8) Å	Octahedral	Absent	2-D	37
[Pb_2(ndc)$_2$(pzp)$_2$(H_2 O)]· 0.5H_2O	Pb–O= 2.714(4)-2.729(4) Å Pb–N= 2.624(4)-2.644(4) Å Pb-Pb= 4.333 Å	Octahedral	Absent	3-D	37
[Pb(pzp)(1,3-bdc)(H_2O)$_{0.5}$]	Pb–O= 2.382(4)-2.482(4) Å PbN=2.504(5)-2.671(5)Å	Pentagonal bipyramidal	Absent	2-D	37
[Pb(ptc)(1,4-bdc)]· 0.75H_2O	Pb–O= 2.551(4)-2.510(4) Å Pb-N= 2.651(4)-2.558(5) Å	Octahedral	Absent	2-D	37
[Pb($C_8H_4O_4$)($C_{24}H_{16}N_2$)]n	Pb-O=2.503 (4)- 2.663 (4) Å Pb-N= 2.686 (4)- 2.677 (4) Å	Octahedral	Absent	2-D	38
[Pb_2($C_{12}H_6O_4$)$_2$($C_{10}H_8N_2$)]$_n$	Pb-O=2.418 (4) Å Pb-N= 2.841 (4) Pb-N= 2.678 (7)- 2.630(6)	Pentagonal bipyramidal	Absent	3-D	39
[Pb_2($C_{12}H_6O_4$)$_2$($C_{12}H_8N_2$)]$_n$	Pb-O=2.464 (4)-2.756 (4) Å Pb-N=2.622(4)-2.701(4)Å	Octahedral	Absent	3-D	40
[Pb(1,4-bdc)(MOPIP)]$_n$	Pb-Pb=11.4210(24) Å	Octahedral	Absent	1-D	41
[Pb_2(1,4-bdc)$_2$(dpdp)$_2$].H_2O	Average Pb-O = 2.550 Å	Pentagonal bipyramidal	Absent	3-D	42
[Pb(bdc)(dma)]	Pb-O= 2.440(4)–2.699(4) Å	Tetragonal bipyramidal	Absent	3-D	43
SM-3	Pb-O= 2.449(3) to 2.704(4) Å Pb-N= 2.592(4) to 2.676(4) Å. Pb-Pb= 4.355 Å	Distorted square antiprismatic	Present	2-D	**This work**

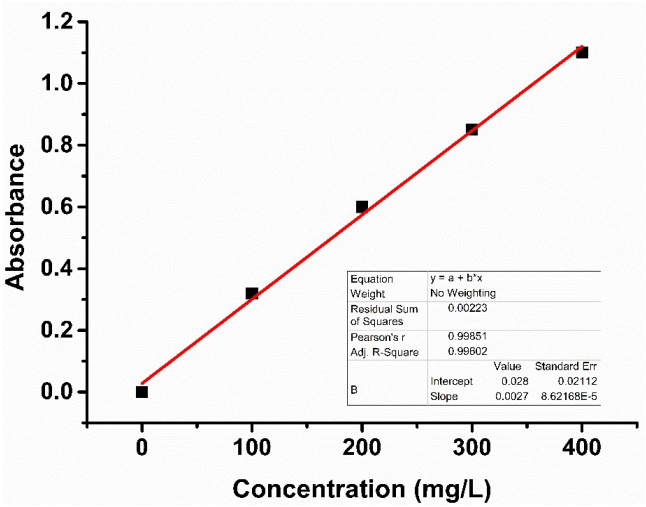

Fig. S1. Calibration plot of iodine in a cyclohexane solution via a UV−vis spectrum.

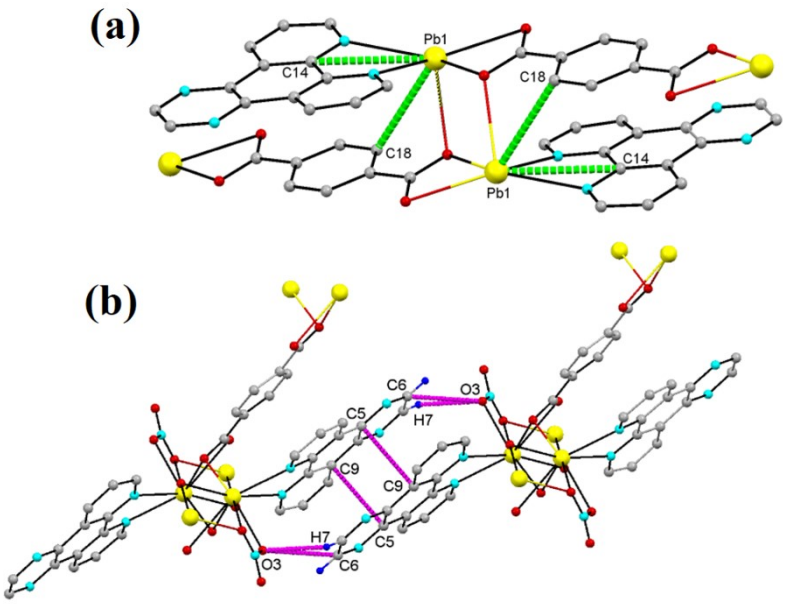

Fig. S2. Stability provided due to (a) Pb⋯ π interactions, (b) hydrogen bonding O3⋯H7-C7, C-H⋯O and π-π stacking interactions in **SM-3**.

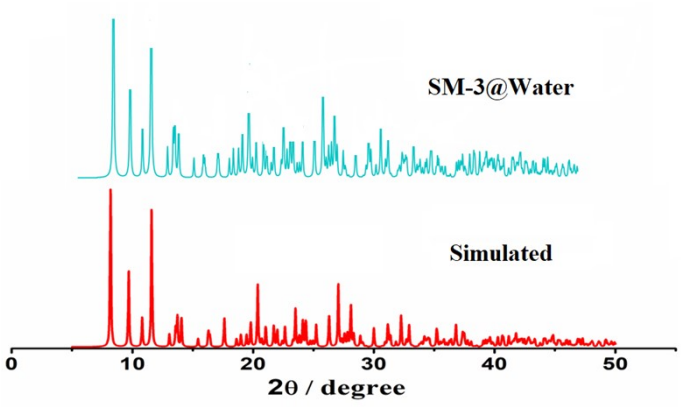

Fig. S3. PXRD pattern of synthesized **SM-3** before and after immersing in water for 24 h.

Table S3. Parameters for first and second-order kinetic models for adsorption studies of Iodine.

Model	Parameters	Values
Pseudo first order	K_1 (min^{-1}) q_e (cal.)(mg/g) q_e (Exp.)(mg/g) R^2	0.552 1148.15 350.06 0.870
Pseudo second order	K_2 (min^{-1}) q_e (cal.)(mg/g) q_e (Exp.)(mg/g) R^2	0.003 455.55 350.06 0.997

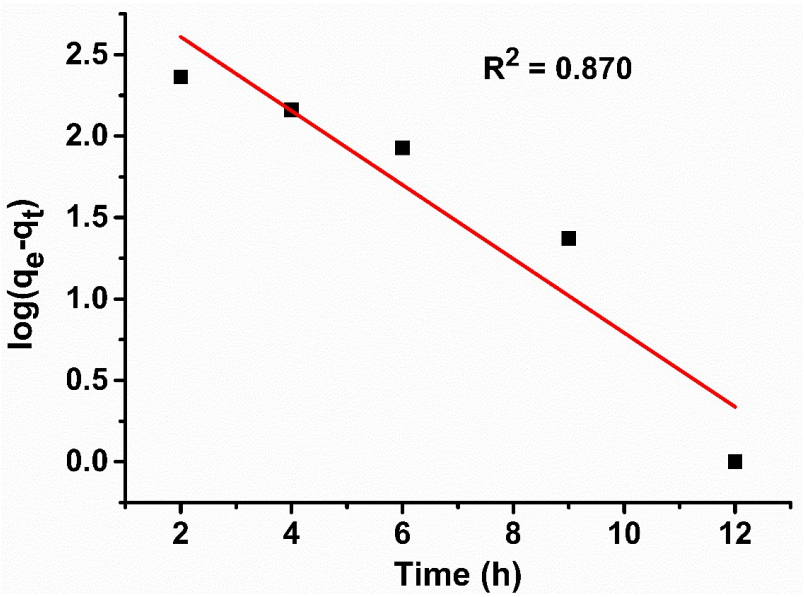

Fig. S4. Pseudo-first-order kinetics for the adsorption process of iodine by **SM-3** in cyclohexane solution.

Table S4. Adsorption isotherm constants of **SM-3** MOF for iodine adsorption.

Langmuir			**Freundlich**		
K_L	q_m *(mg/g)*	R_L^2	K_F	*1/n*	R_F^2
0.032	293.43	0.995	41.52	2.46	0.965

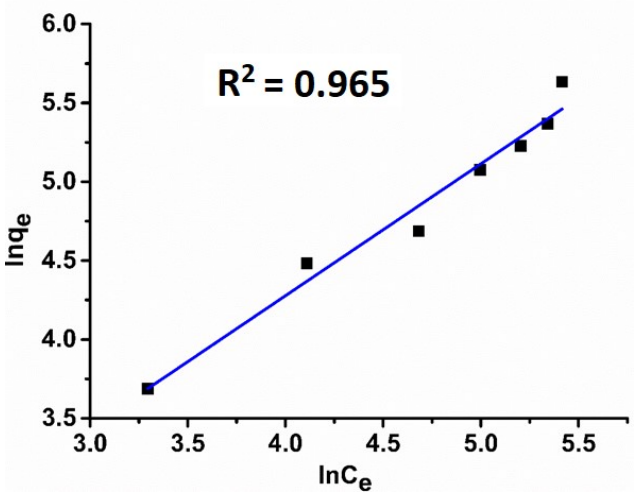

Fig. S5. Freundlich isotherm model for the adsorption of iodine on **SM-3.**

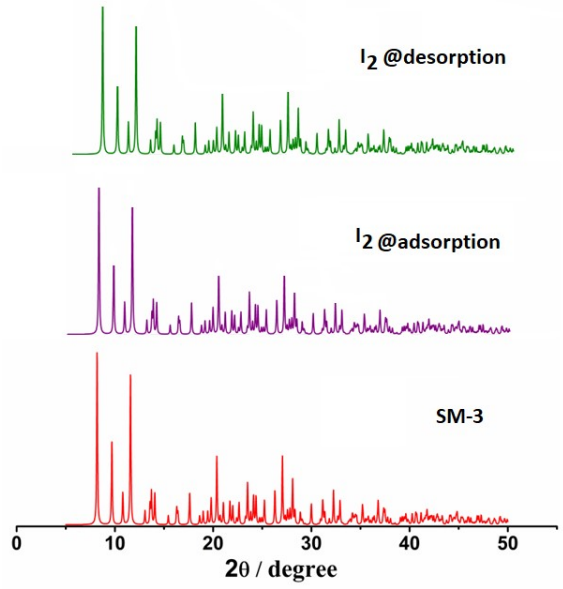

Fig. S6. PXRD pattern of synthesized **SM-3** and after iodine adsorption and desorption.

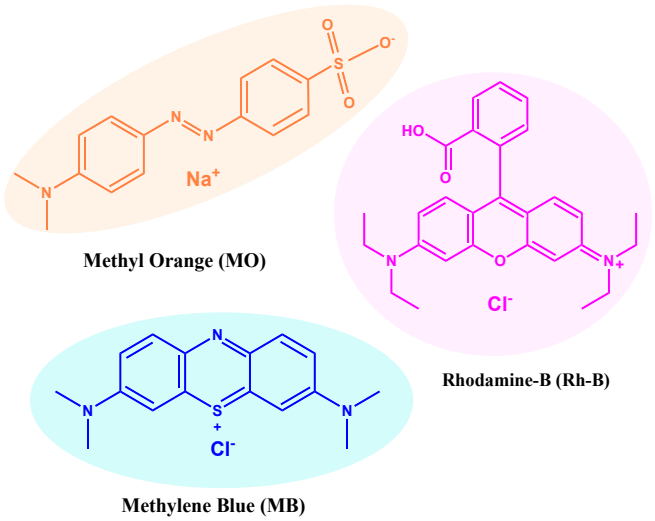

Fig. S7 Chemical structures of cationic and anionic dyes used in the experiments.

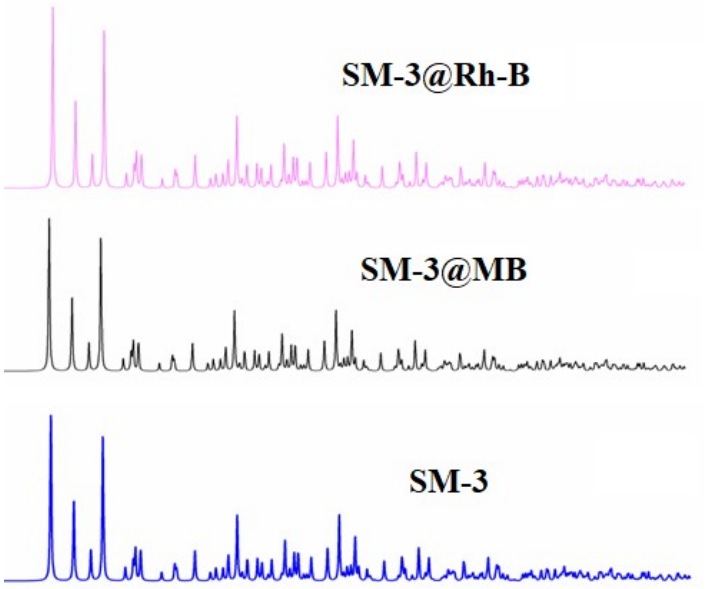

Fig. S8. PXRD pattern of synthesized **SM-3** and after adsorption of MB and Rh-B.

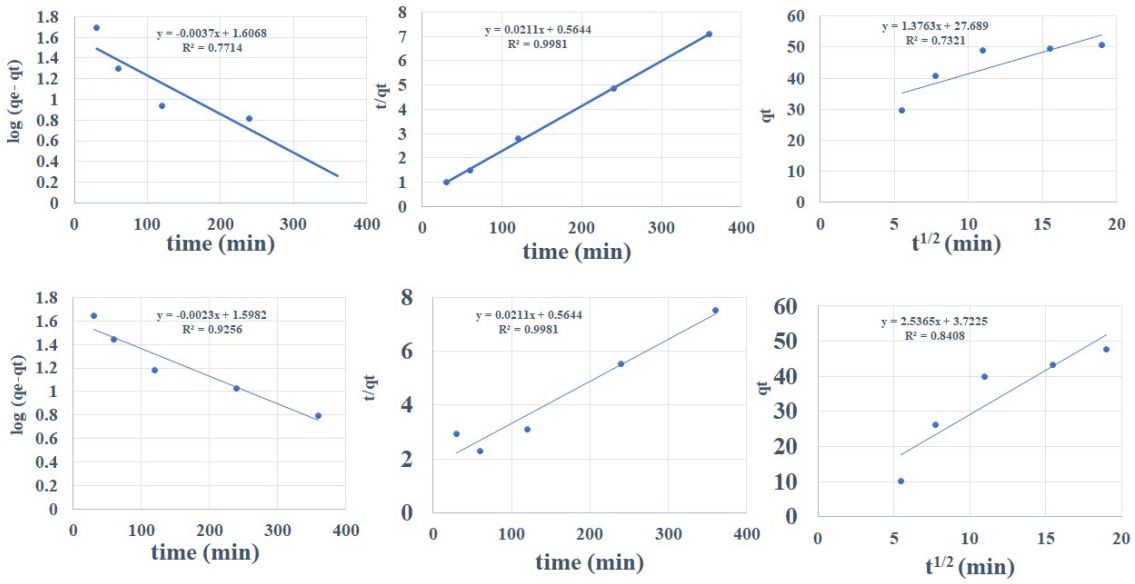

Fig. S9. The adsorption of MB and Rh-B onto **SM-3** using pseudo-first-order **(a)**, pseudo-second-order **(b)** and intra particle **(c)** kinetics models.

Table S5. Summary of maximum adsorption capacities (q_{max}) of various commercial adsorbent towards MB and/or Rh-B.

Adsorbent	Dye	Possible Mechanism	Removal Efficiency	Ref.
Apricot stones and commercial activated carbon106	MB	Chemisorption	36.68 mg/g	102
Red Oak (Quercus rubra)	MB	Chemisorption	97.18%	103
Rice husk	Rh-B	Chemisorption	478.5 mg/g	104
Coconut leaves	MB	Chemisorption	149.3 mg/g	105
Lemon peels	MB	Chemisorption	841.37 mg/g	106
Carbonaceous slurry waste	RhB	Physiosorption	91.1 mg/g	107
Platanusorientalis leaf	MB	-	114.94 mg/g	108
Coal fly ash	MB	-	85%	109
SM-3	MB, Rh-B	Electrostatic interaction. Cation- π, π–π interaction	90%, 92%	**This work**

Table S6. Determination of zeta potential of **SM-3** at varying pH.

pH	Zeta Potential (mV)
2	0.23
3	0.22
4	0.23
5	0.22
6	0.00
7	-0.23
8	-0.30
9	-0.32
10	-0.33
11	-0.33
12	-0.32

Table S7. Parameters for different kinetic models for adsorption studies of MB and Rh-B.

Model	Parameters	MB	Rh-B
Pseudo first order	K_1 (min^{-1})	0.00016	0.0052
	q_e (Cal.) (mg/g)	40.43	39.64
	qe (Exp.) (mg/g)	49.47	53.91
	R^2	0.7714	0.92
Pseudo second order	K_2 (g mg^{-1} min^{-1})	0.0007	0.0007
	q_e (Cal.) (mg/g)	50.66	47.39
	q_e (Exp.) (mg/g)	49.47	53.91
	R^2	0.99	0.99
Intraparticle Diffusion	K_3 (mg g^{-1} $min^{-1/2}$)	1.37	5.71
	C	27.68	6.98
	R^2	0.7321	0.423