Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Thioether-Based Recyclable Metal Organic Frameworks for Selective and Efficient Removal of Hg^{2+} from Water

Kan Li [a], Jing-jing Li [a], Ni Zhao [a], Ting-ting Xie [a], Bin Di [*a,b], Li-li Xu [*a,b]

[a] Jiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, Nanjing 210009, China.

[b] Key Laboratory of Drug Quality Control and Pharmacovigilance, Ministry of Education, China Pharmaceutical University, Nanjing 210009, China.

*Corresponding authors: dibin@cpu.edu.cn (B.D.); 1620174420@cpu.edu.cn (L.L.X.)

Table of Contents

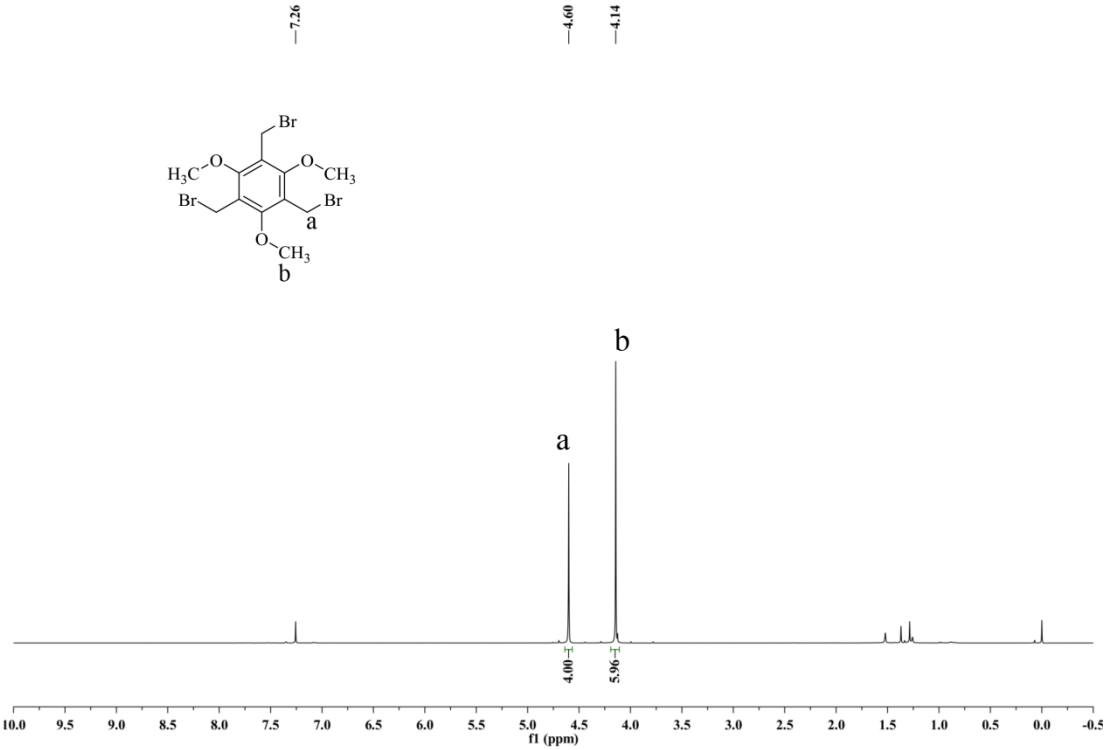

Fig. S1 ^{1}H NMR spectra of 1,3,5-tris(bromomethyl)-2,4,6-trimethoxybenzene

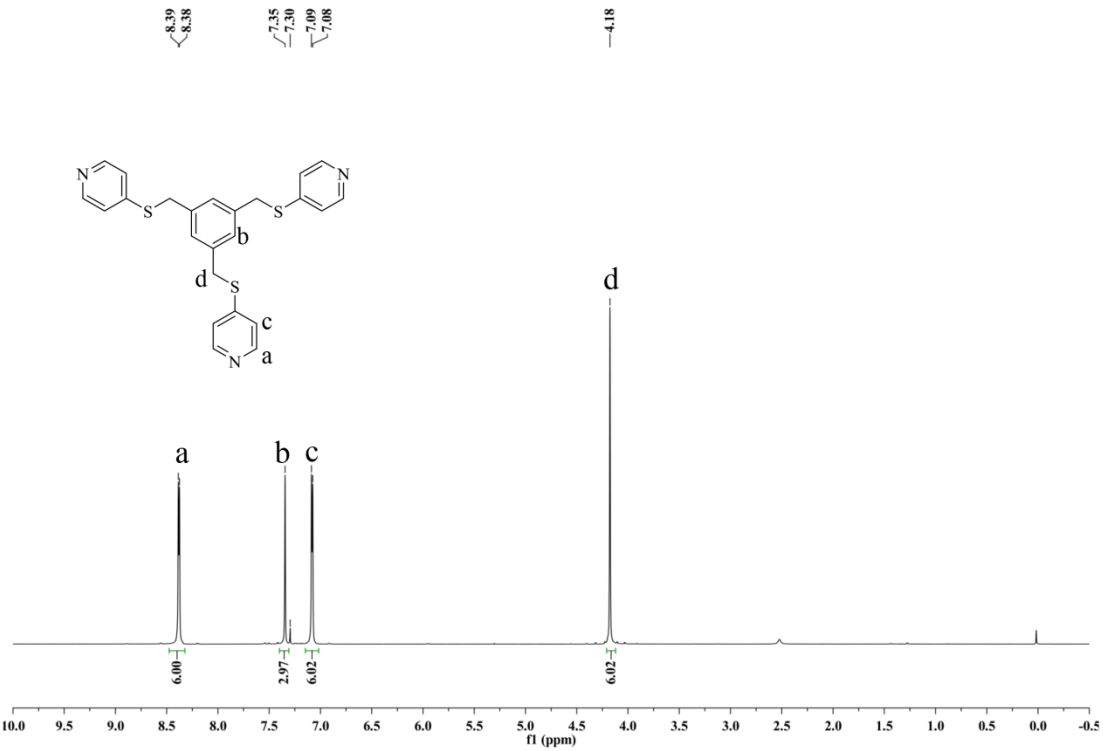

Fig. S2 ^{1}H NMR spectra of 1,3,5-tris((pyridin-4-ylthio)methyl)benzene (*L*$_1$)

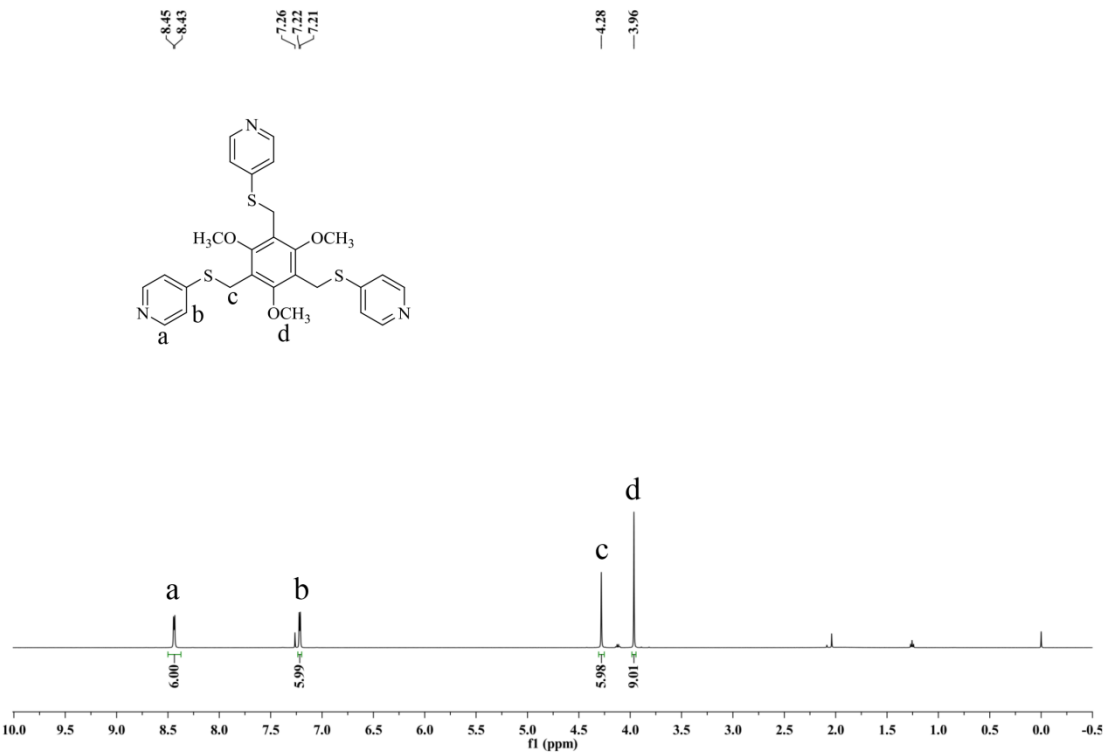

Fig. S3 ^{1}H NMR spectra of 2,4,6-trimethoxy-1,3,5-tris((pyridin-4-ylthio)methyl)benzene (L_2)

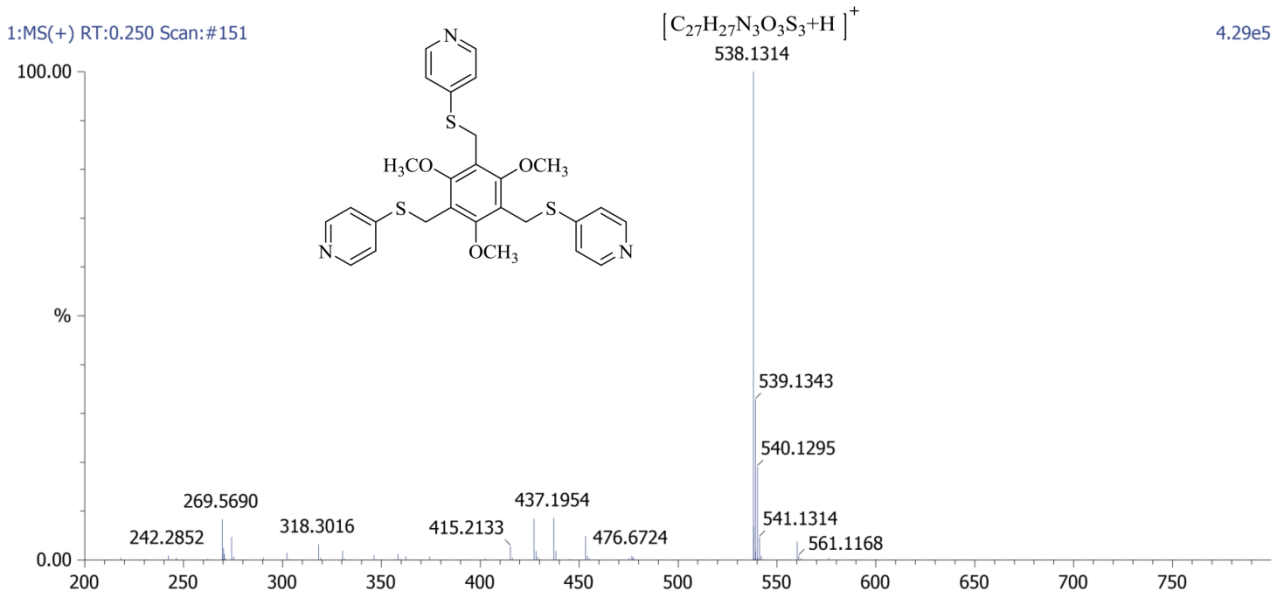

Fig. S4 HRMS of 2,4,6-trimethoxy-1,3,5-tris((pyridin-4-ylthio)methyl)benzene (L_2)

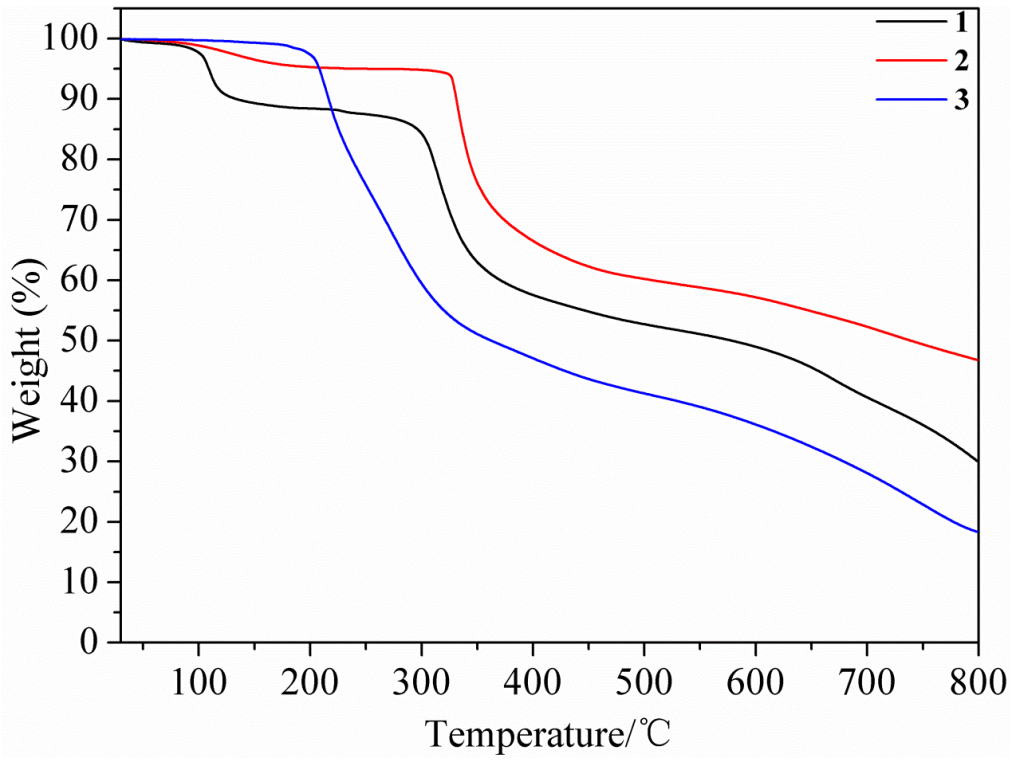

Fig. S5 Thermogravimetric curves of MOFs **1**-**3**

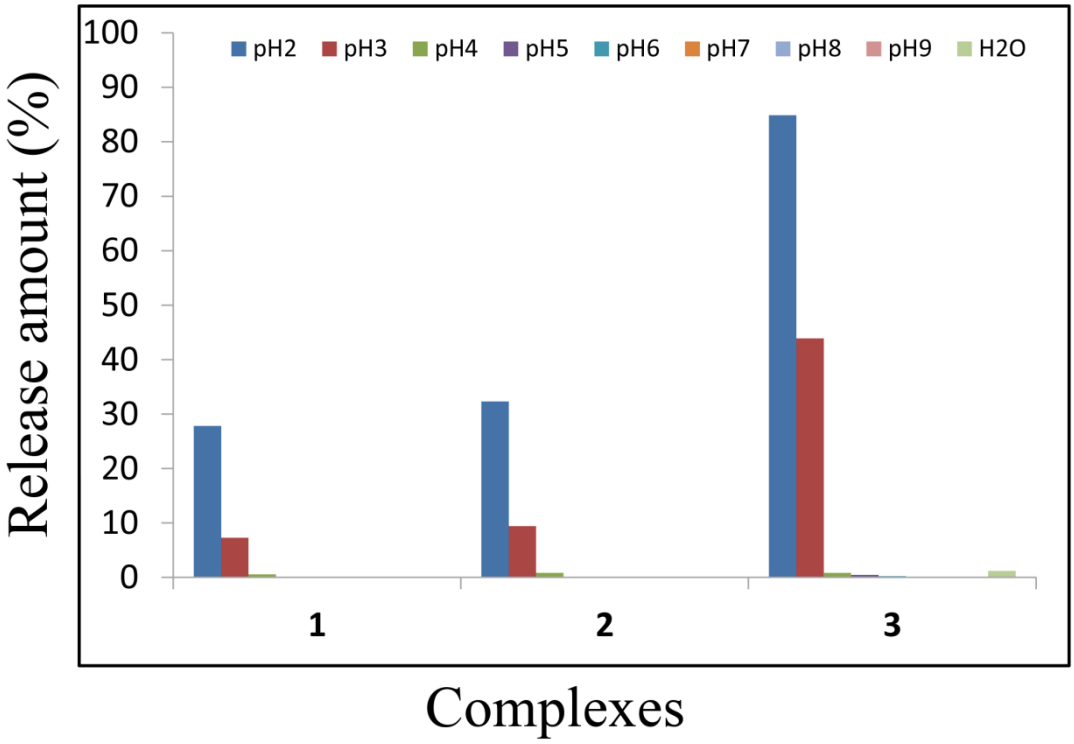

Fig. S6 The amount of metal ions released by MOFs **1**-**3** in different solutions

Table S1. Selected bond distances (Å) and angles (°) for complexes **1**-**3**

1					
Zn1–Cl1	2.2440(11)	Zn1–Cl2	2.2114(12)		
Zn1–N1	2.037(3)	Zn1–N3	2.029(3)		
Cl2–Zn1–Cl1	121.02(5)	N1–Zn1–Cl1	105.02(9)	N1–Zn1–Cl2	105.47(9)
N3–Zn1–Cl1	108.31(10)	N3–Zn1–Cl2	108.44(10)	N3–Zn1–N1	107.90(13)
2					
I1–Cu2	2.656(2)	I1–Cu1	2.624(3)	I1–O2	2.09(2)
I1–O3	2.37(2)	I2–Cu2	2.577(2)	I2–Cu1	3.065(3)
I2–O1	2.34(2)	I2–Cu3	2.2325(10)	I3–Cu2	2.960(3)
I3–Cu1	2.571(2)	I3–Cu3	2.3154(10)	I3–O4	2.00(2)
Cu2–Cu1	2.408(3)	Cu2–N3	1.975(12)	Cu1–N1	1.954(13)
Cu1–Cu3	2.548(2)				
Cu1–I1–Cu2	54.26(7)	O2–I1–Cu2	77.4(6)	O2–I1–Cu1	106.6(6)
O2–I1–O3	177.3(8)	O3–I1–Cu2	101.2(5)	O3–I1–Cu1	74.2(5)
Cu2–I2–Cu1	49.61(6)	O1–I2–Cu1	147.7(6)	Cu3–I2–Cu1	54.82(4)
Cu3–I2–O1	139.2(5)	Cu1–I3–Cu2	51.02(6)	Cu3–I3–Cu1	62.61(6)
O4–I3–Cu2	156.7(7)	O4–I3–Cu1	125.2(6)	I1–Cu2–I3	99.62(7)
I2–Cu2–I1	109.99(8)	I2–Cu2–I3	99.68(8)	Cu1–Cu2–I1	62.19(8)
Cu1–Cu2–I2	75.81(9)	Cu1–Cu2–I3	56.11(7)	N3–Cu2–I1	116.7(4)
N3–Cu2–I2	119.3(4)	N3–Cu2–I3	108.0(4)	N3–Cu2–Cu1	161.4(4)
I1–Cu1–I2	97.48(7)	I3–Cu1–I1	111.52(8)	I3–Cu1–I2	97.14(8)
Cu2–Cu1–I1	63.55(8)	Cu2–Cu1–I2	54.58(7)	Cu2–Cu1–I3	72.87(8)
N1–Cu1–I1	119.5(4)	N1–Cu1–I2	107.6(4)	N1–Cu1–I3	118.3(4)
N1–Cu1–Cu2	161.5(4)	N1–Cu1–Cu3	137.4(4)	Cu3–Cu1–I1	99.09(7)
Cu3–Cu1–I2	45.73(5)	Cu3–Cu1–I3	53.78(5)		
3					
Br01–Cu03	2.541(5)	Br02–Cu03	2.442(2)	Cu03–N1	2.015(12)
Cu03–N2	2.037(11)	Cu03–N3	2.101(12)	Cu03–Br	2.99(4)
Br02–Cu03–Br01	120.81(13)	Br02–Cu03–Br	114.4(5)	N1–Cu03–Br01	95.6(4)
N1–Cu03–Br02	90.4(3)	N1–Cu03–N2	171.4(5)	N1–Cu03–N3	83.2(5)
N1–Cu03–Br	92.0(5)	N2–Cu03–Br01	91.8(4)	N2–Cu03–Br02	89.5(3)
N2–Cu03–N3	90.6(4)	N2–Cu03–Br	95.9(5)	N3–Cu03–Br01	105.7(4)
N3–Cu03–Br02	133.4(3)	N3–Cu03–Br	111.8(6)		