Supporting Information for

Reversible adsorption and separation of volatile aromatics based on a porous Cd(II)-MOF

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1. ORTEP figures of 2-6

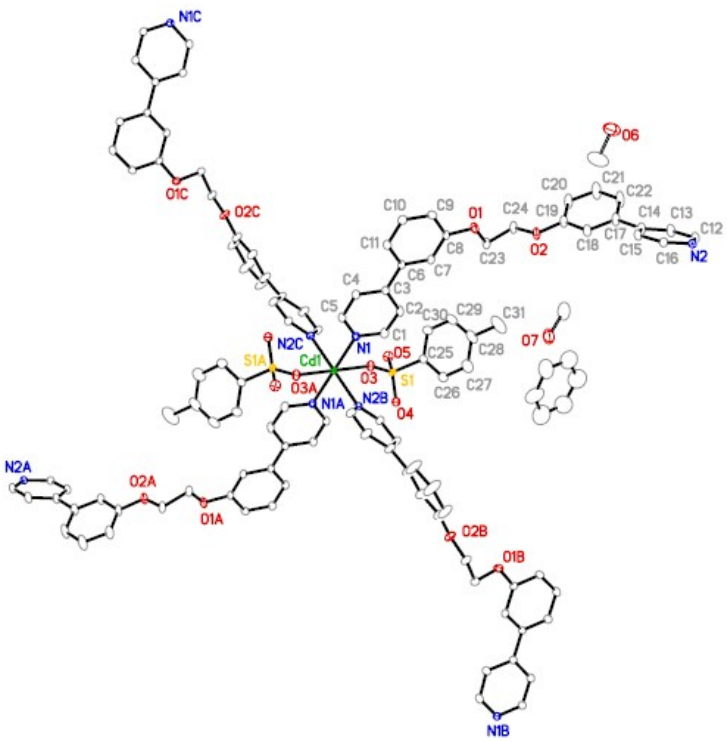


Fig. S1 The ORTEP of **2** (Displacement of ellipsoids are drawn at the 30% probability level).

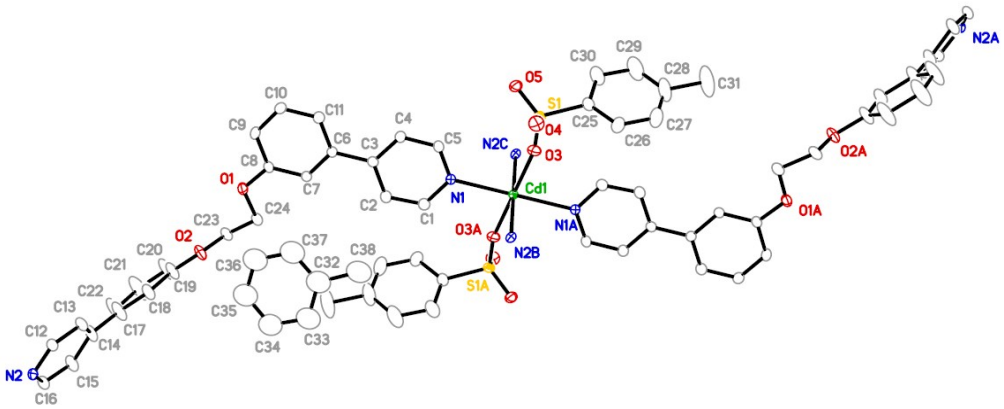


Fig. S2 The ORTEP of **3** (Displacement of ellipsoids are drawn at the 30% probability level).

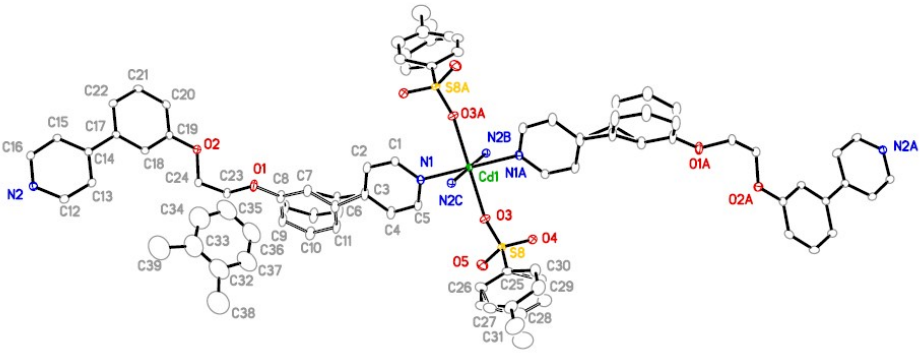


Fig. S3 The ORTEP of **4** (Displacement of ellipsoids are drawn at the 30% probability level).

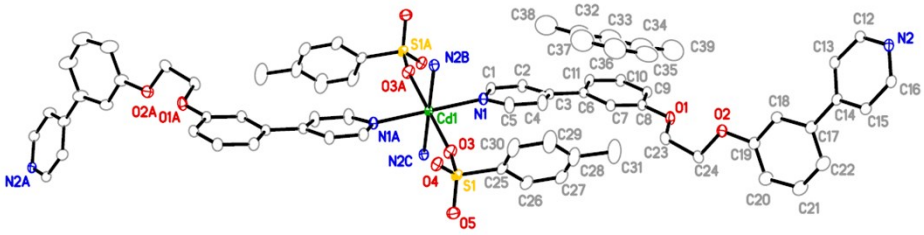


Fig. S4 The ORTEP of **5** (Displacement of ellipsoids are drawn at the 30% probability level).

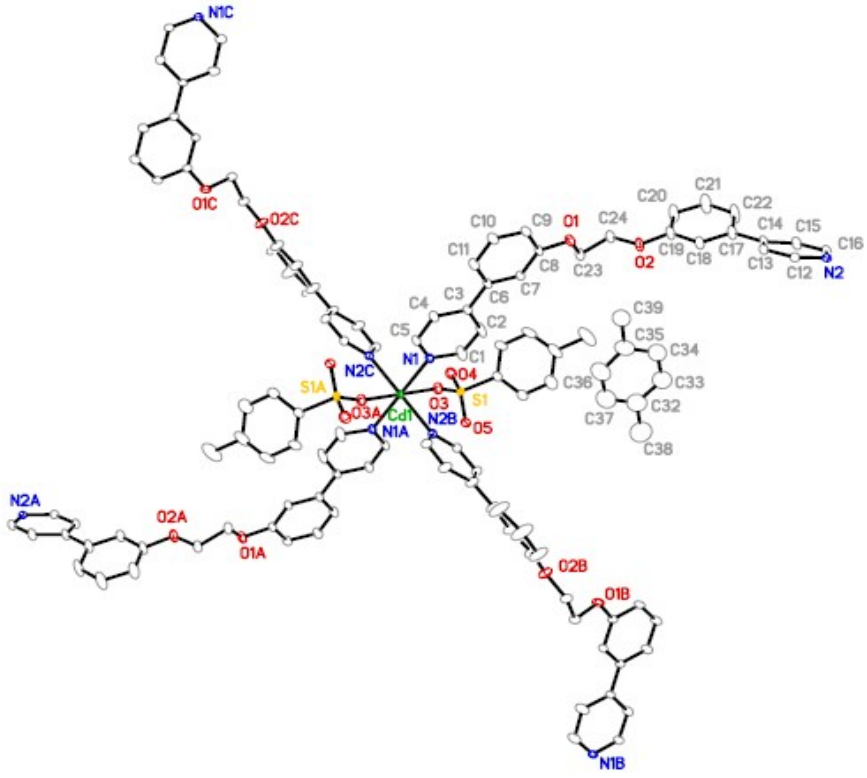


Fig. S5 The ORTEP of **6** (Displacement of ellipsoids are drawn at the 30% probability level).

2. ^{1}H NMR spectra

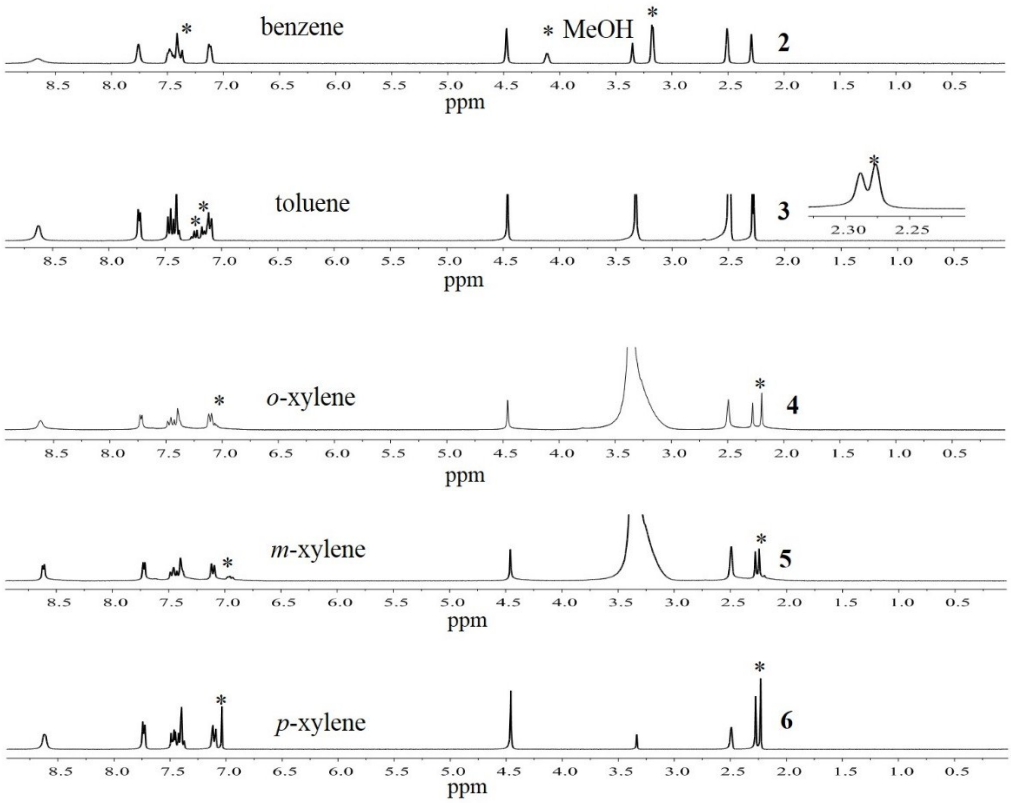
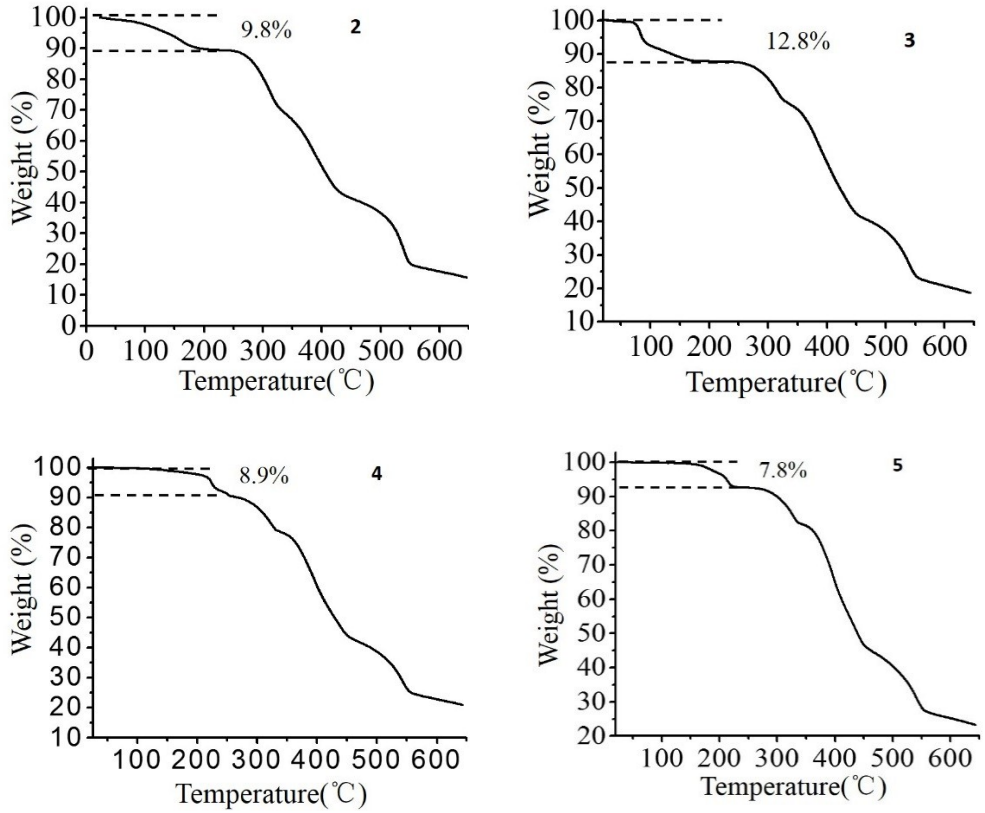


Fig. S6 ^{1}H NMR (DMSO-d^{6}) spectra of **2-6**. The peaks corresponding to the encapsulated aromatic molecules are marked with asterisks.

3. TGA traces



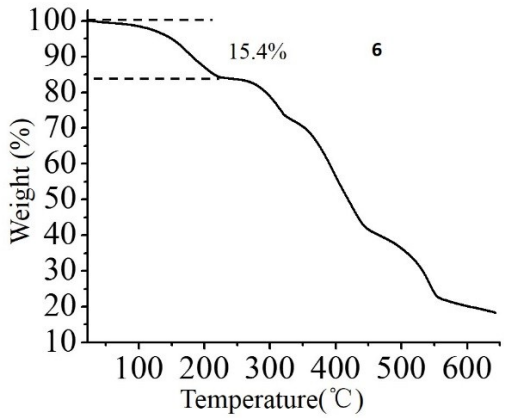


Fig. S7 TGA traces of **2** (calculated 9.3%), **3** (calculated 13.4%), **4** (calculated 8.2%) and **5** (calculated 8.2%) and **6** (calculated 15.1%).

4. XRPD patterns

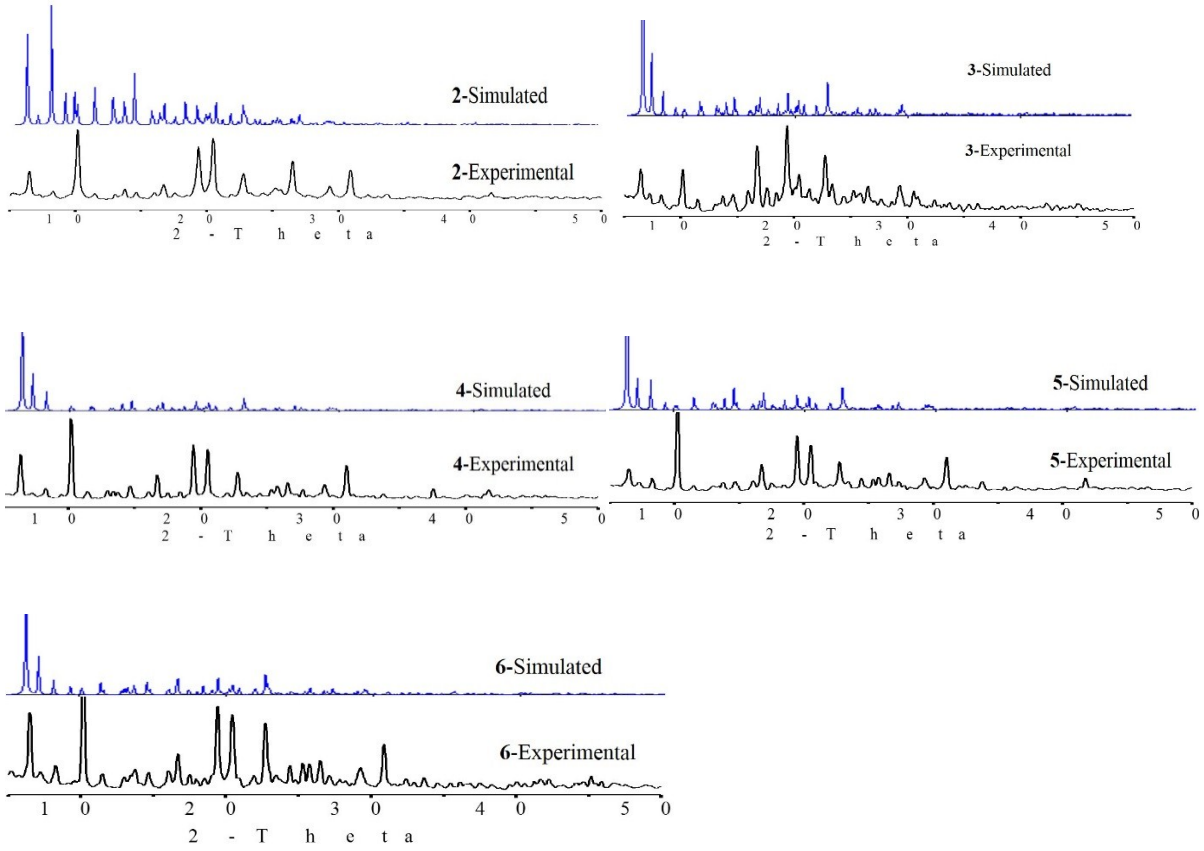


Fig. S8 Simulated and measured XRPD patterns of **2**-**6**.

5. VOCs adsorption amount vs time

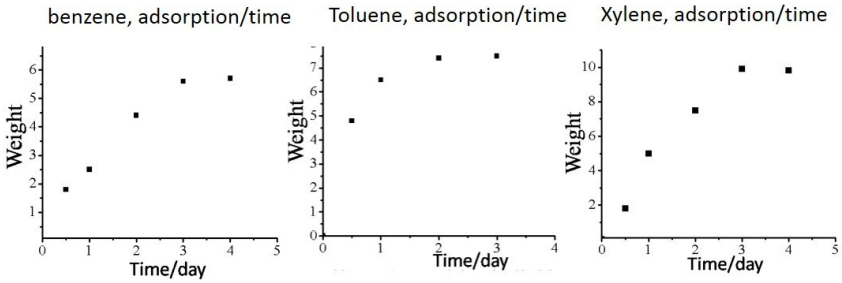


Fig. S9 Adsorption amount of VOCs vs time (day).

6. ^{1}H NMR spectra after extraction by acetone

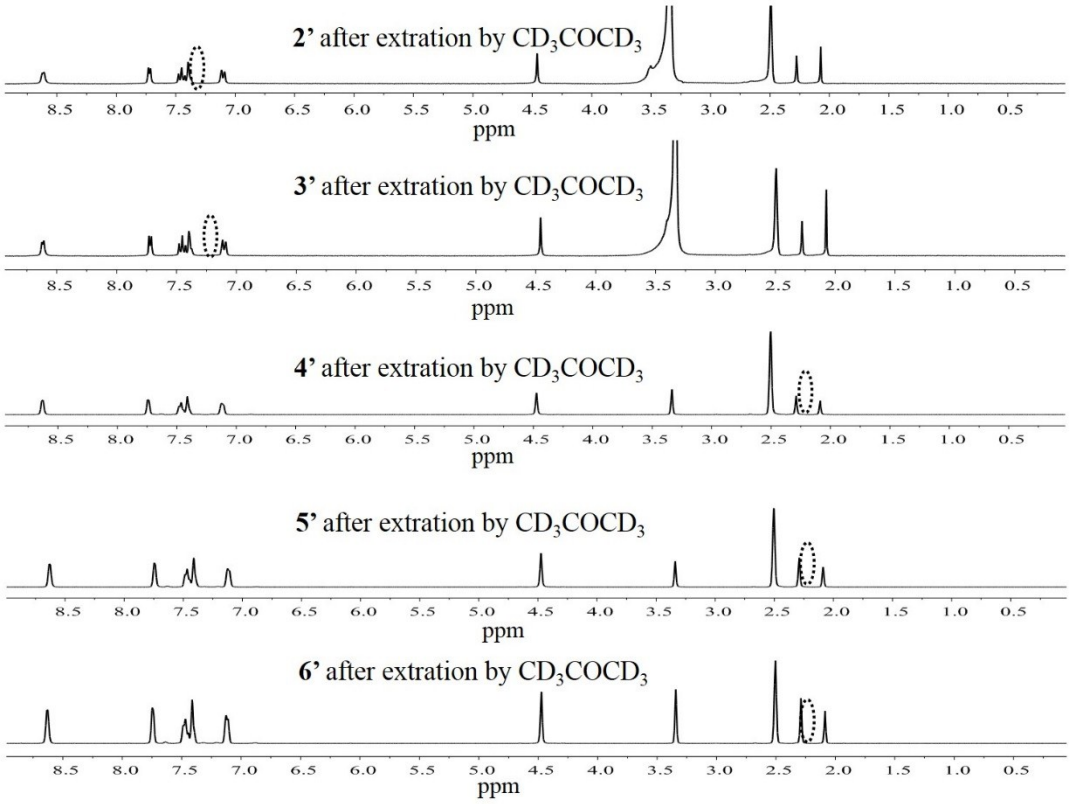


Fig. S10 ^{1}H NMR spectra of **2'-6'** after extraction by acetone.

7. XRPD patterns of 2'-6'

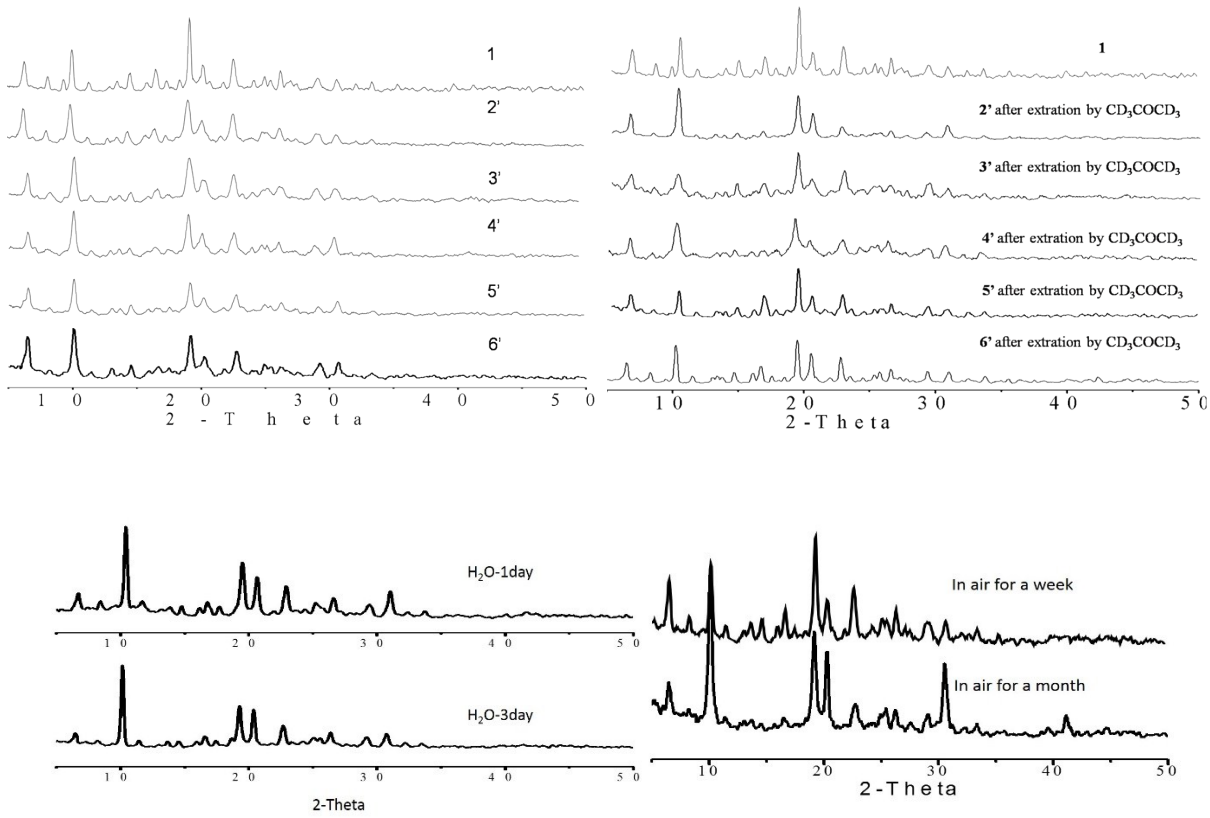


Fig. S11 The PXRD patterns of **1** and **2'**-**6'** (top left), and the PXRD patterns of **1** and **2'**-**6'** after acetone extraction (top right). The stability of **1'** in water (bottom left) and air (bottom right).

8. Vapor separation

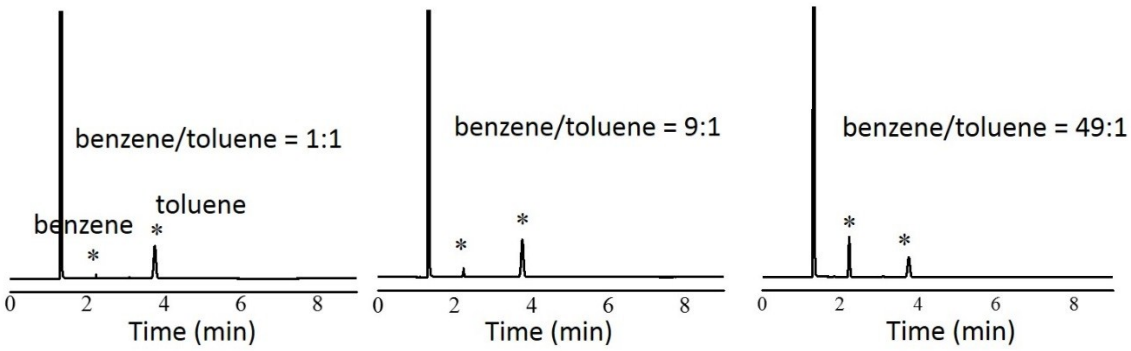


Fig. S12. GC analysis for acetone extract of **1'** from benzene/toluene mixed vapor with molar ratios of 1/1, 9/1 and 49/1.

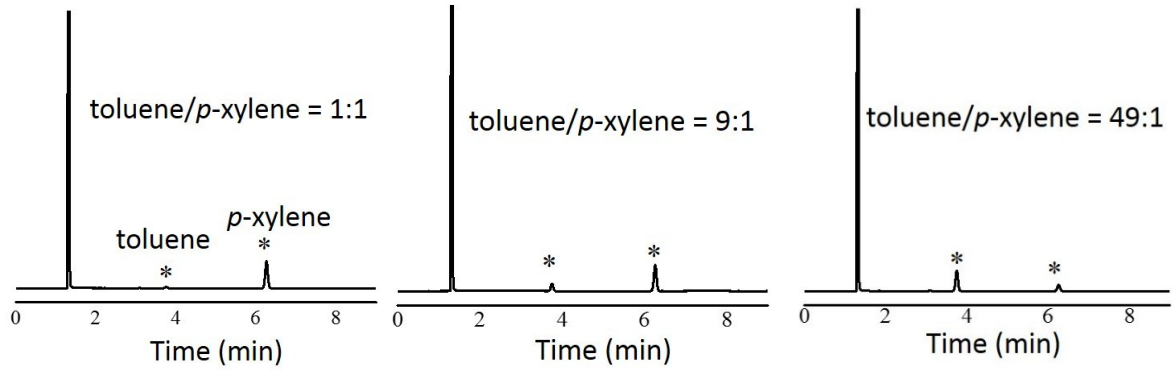
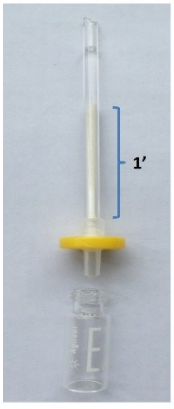


Fig. S13. GC analysis for acetone extract of **1'** from toluene/*p*-xylene mixed vapor with molar ratios of 1/1, 9/1 and 49/1.

9. Kinetic separation of toluene/*p*-xylene based on a MOF-packed column



THF as eluent

No.	GC area ratio of toluene/*p*-xylene	Ratio of toluene/*p*-xylene
1	0.4046/1.2267	1:3.03
2	45.4949/39.0688	1:0.86
3	14.5146/19.1681	1:1.31
4	6.5517/8.9732	1:1.36
5	4.6340/5.9051	1:1.27

CH_2Cl_2 as eluent

No.	GC area ratio of toluene/*p*-xylene	Ratio of toluene/*p*-xylene
1	16.6931/15.0444	1:0.90
2	5.1232/6.1841	1:1.21
3	1.3017/1.6736	1:1.29
4	0.1279/0.1479	1:1.6

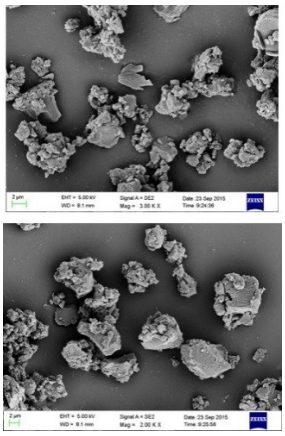


Fig. S14. Kinetic separation: column inner diameter is 2 mm, column length is 7.5 cm, MOF-packed length is 4.8 cm. The diameters of MOF particles are 2-8 μm (SEM image, right). The column was run under pressure by syringe, and every three drops of eluent solution were collected as individual sample for GC analysis.

10. Selected bond lengths and angles for 2-6

Table S1. Interatomic Distances (Å) and Bond Angles (°) for **2**.

Cd(1)-O(3)	2.295(2)	Cd(1)-N(2)#2	2.319(3)
Cd(1)-N(1)	2.326(3)		
O(3)-Cd(1)-N(2)#2	88.57(9)	O(3)-Cd(1)-N(1)#1	90.96(9)
O(3)-Cd(1)-N(1)	89.04(9)	O(3)-Cd(1)-N(2)#3	91.43(9)
N(2)#2-Cd(1)-N(1)	91.93(9)	N(2)#3-Cd(1)-N(1)	88.07(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+5/2,-z #2 -1/2,-y+3/2,z-1/2 #3 -x+1,y+1,-z+1/2

Table S2. Interatomic Distances (Å) and Bond Angles (°) for **3**.

Cd(1)-O(3)	2.286(3)	Cd(1)-N(2)#2	2.322(3)
Cd(1)-N(1)	2.330(3)		
O(3)-Cd(1)-N(2)#2	90.77(10)	O(3)-Cd(1)-N(2)#3	89.23(10)
O(3)-Cd(1)-N(1)	90.58(10)	N(2)#2-Cd(1)-N(1)	91.22(10)
N(2)#3-Cd(1)-N(1)	88.78(10)	O(3)-Cd(1)-N(1)#1	89.42(10)
N(2)#2-Cd(1)-N(1)#1	88.78(10)	N(2)#3-Cd(1)-N(1)#1	91.22(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+1/2,-z+1 #2 x-1/2,-y+3/2,z-1/2 #3 -x+1,y-1,-z+3/2

Table S3. Interatomic Distances (Å) and Bond Angles (°) for **4**.

Cd(1)-O(3)	2.287(2)	Cd(1)-N(2)#2	2.324(2)
Cd(1)-N(1)	2.327(2)		
O(3)-Cd(1)-N(2)#2	89.05(8)	O(3)-Cd(1)-N(2)#3	90.95(8)
O(3)-Cd(1)-N(1)	89.22(8)	N(2)#2-Cd(1)-N(1)	91.97(8)
N(2)#3-Cd(1)-N(1)	88.03(8)	O(3)-Cd(1)-N(1)#1	90.78(8)
N(2)#2-Cd(1)-N(1)#1	88.03(8)	N(2)#3-Cd(1)-N(1)#1	91.97(8)

#1 -x+1/2,-y+1/2,-z+1 #2 x-1/2,-y+3/2,z-1/2 #3 -x+1,y-1,-z+3/2

Table S4. Interatomic Distances (Å) and Bond Angles (°) for **5**.

Cd(1)-O(3)	2.284(3)	Cd(1)-N(2)#2	2.322(3)
Cd(1)-N(1)	2.329(3)		
O(3)-Cd(1)-N(2)#2	89.18(11)	O(3)-Cd(1)-N(2)#3	90.82(11)
O(3)-Cd(1)-N(1)	89.25(11)	N(2)#2-Cd(1)-N(1)	91.59(11)
N(2)#3-Cd(1)-N(1)	88.41(11)	O(3)-Cd(1)-N(1)#1	90.75(11)
N(2)#2-Cd(1)-N(1)#1	88.41(11)	N(2)#3-Cd(1)-N(1)#1	91.59(11)

#1 -x+1/2,-y+5/2,-z+1 #2 x-1/2,-y+3/2,z-1/2 #3 -x+1,y+1,-z+3/2

Table S5. Interatomic Distances (Å) and Bond Angles (°) for **6**.

Cd(1)-O(3)	2.281(3)	Cd(1)-N(1)	2.322(3)
Cd(1)-N(2)#2	2.331(3)		
O(3)-Cd(1)-N(1)	89.85(11)	O(3)-Cd(1)-N(1)#1	90.15(11)
O(3)-Cd(1)-N(2)#2	89.05(12)	N(1)-Cd(1)-N(2)#2	91.51(12)
N(1)#1-Cd(1)-N(2)#2	88.49(12)	O(3)-Cd(1)-N(2)#3	90.95(12)
N(1)-Cd(1)-N(2)#3	88.49(12)	N(1)#1-Cd(1)-N(2)#3	91.51(12)

#1 -x+1/2,-y+3/2,-z+1 #2 x-1/2,-y+1/2,z-1/2 #3 -x+1,y+1,-z+3/2