Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Construction of MOF-74 Analogues through Pre-Installation of Functional Ligands: Efficient Directional Functionalization and Properties

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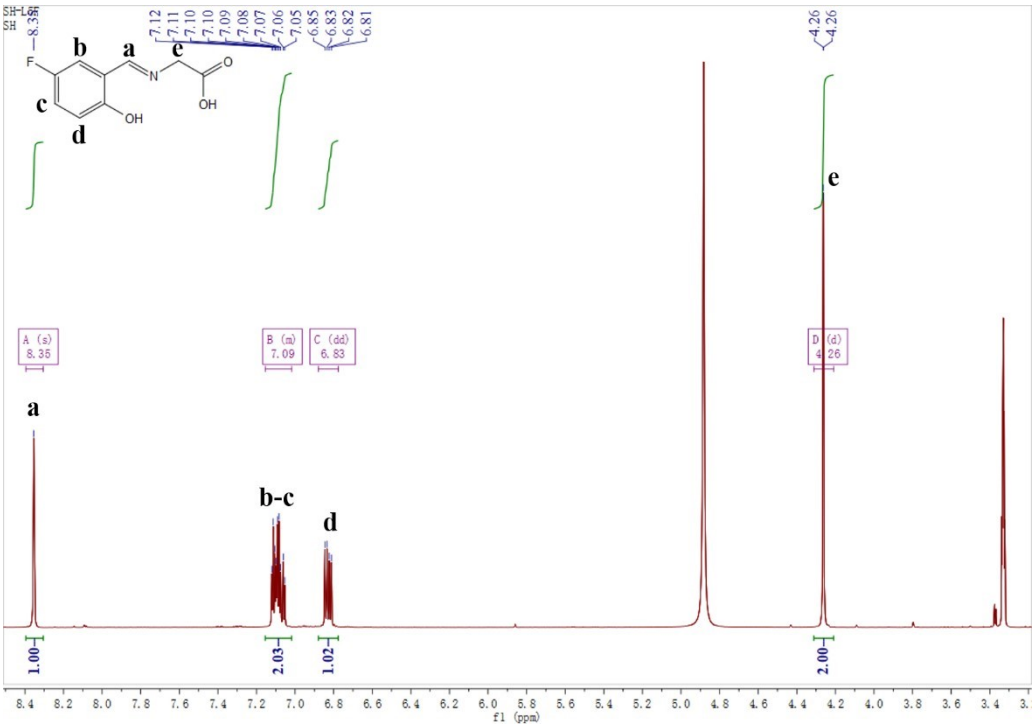

Fig. S1 NMR spectrum of L[1]

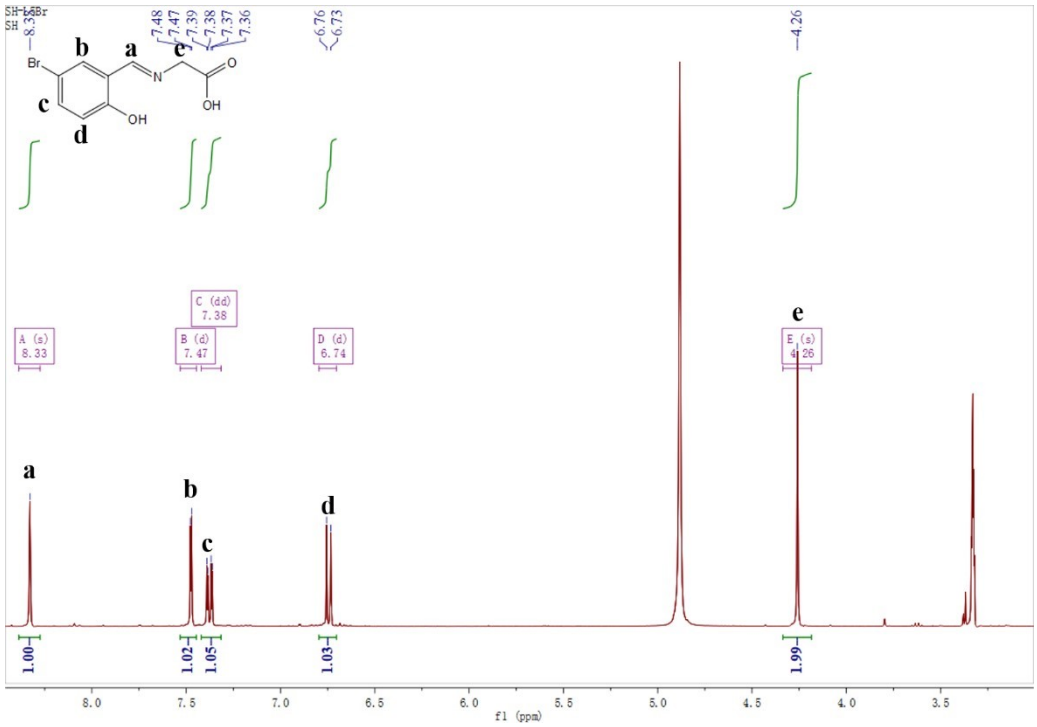

Fig. S2 NMR spectrum of L^3

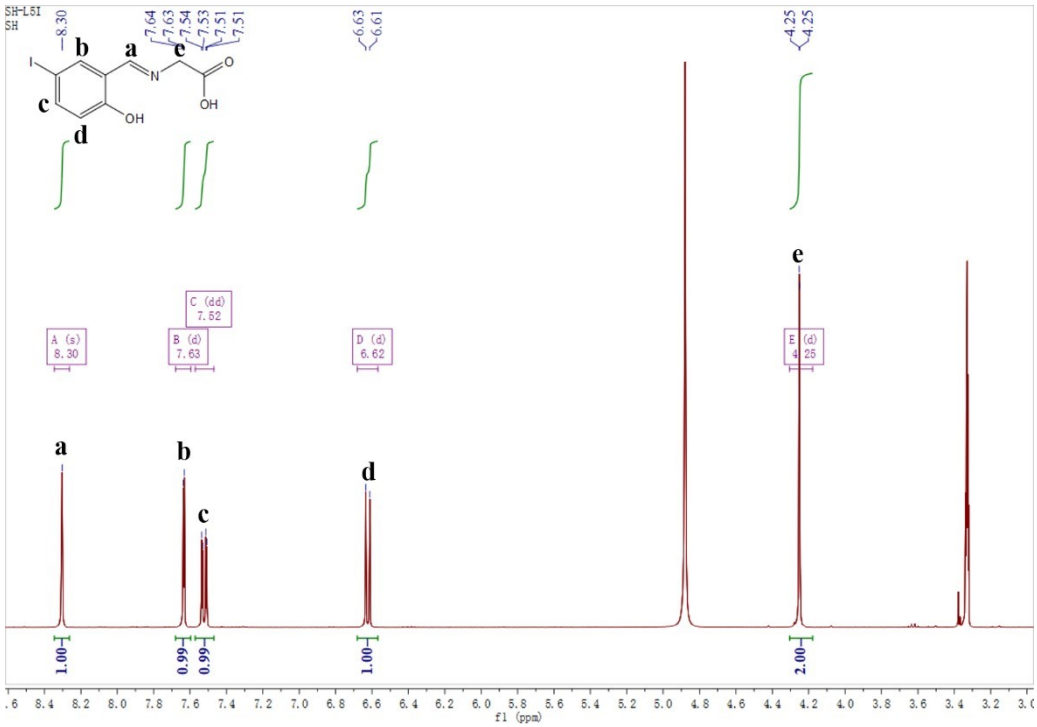

Fig. S3 NMR spectrum of L^4

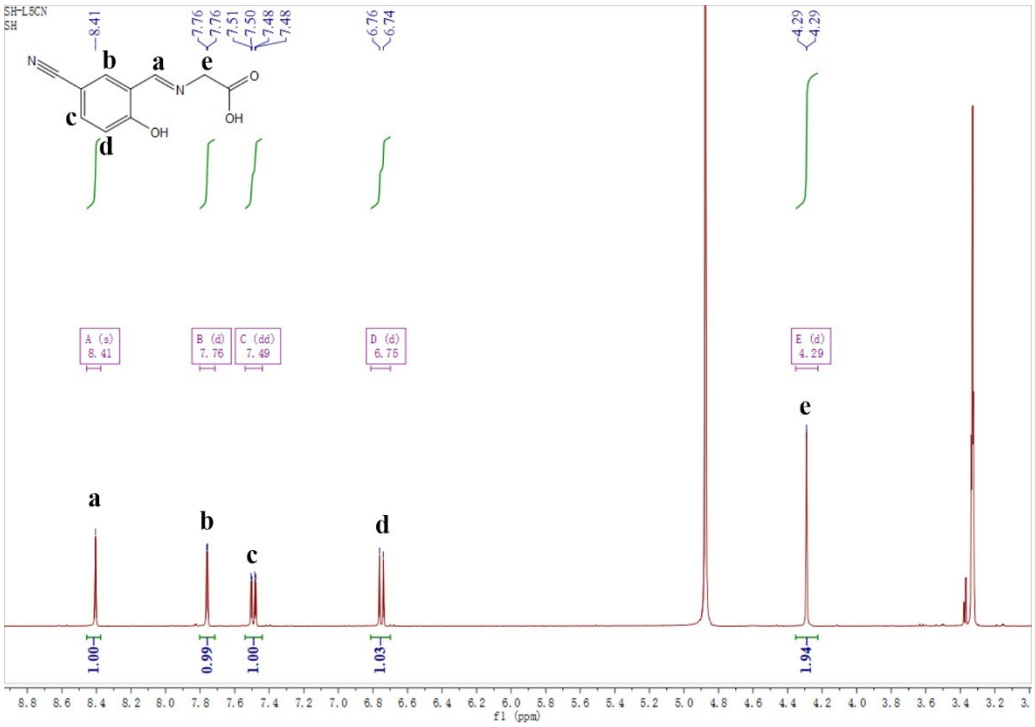

Fig. S4 NMR spectrum of L^5

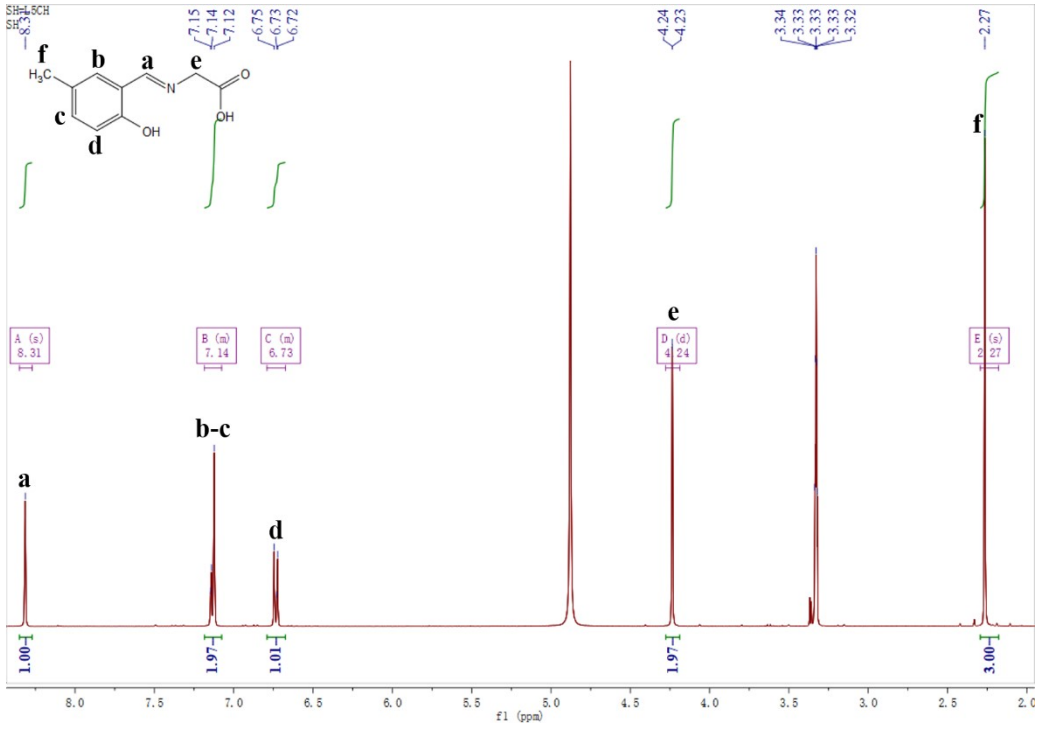

Fig. S5 NMR spectrum of L^6

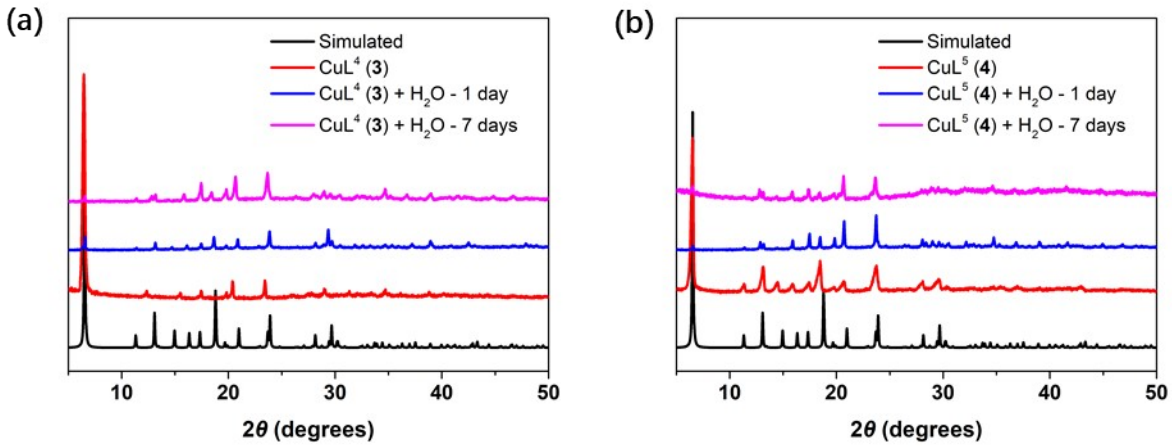

Fig. S6 The PXRD of as-synthesized samples of complexes CuL^4 (3) (a), CuL^5 (4) (b) and that soaked in water for up to 7 days

Table S1 Selected bond distances (Å) and angles (°) for complex **(1)**

Cu(1)–N(1)	1.929(3)	Cu(1)–O(2)	1.938(2)
Cu(1)–O(1)	1.944(2)	Cu(1)–O(1)#1	1.991(2)
Cu(1)–O(3)#1	2.256(2)	Cu(1)–Cu(1)	3.0097(7)
N(1)–Cu(1)–O(2)	83.99(10)	N(1)–Cu(1)–O(1)	93.02(10)
O(2)–Cu(1)–O(1)	175.22(10)	N(1)–Cu(1)–O(1)	162.42(10)
O(2)–Cu(1)–O(1)	101.59(9)	O(1)–Cu(1)–O(1)	80.21(9)
N(1)–Cu(1)–O(3)	100.70(11)	O(2)–Cu(1)–O(3)	93.52(11)
O(1)–Cu(1)–O(3)	90.70(10)	O(1)–Cu(1)–O(3)	95.62(9)

Table S2 Selected bond distances (Å) and angles (°) for complex **(2)**

Cu(1)–N(1)	1.901(4)	Cu(1)–O(2)	1.936(3)
Cu(1)–O(1)	1.937(3)	Cu(1)–O(1)#1	2.006(3)
Cu(1)–O(3)#1	2.235(3)	Cu(1)–Cu(1)	3.0363(10)
N(1)–Cu(1)–O(2)	83.94(13)	N(1)–Cu(1)–O(1)	93.22(13)
O(2)–Cu(1)–O(1)	174.80(13)	N(1)–Cu(1)–O(1)	160.17(14)
O(2)–Cu(1)–O(1)	101.98(12)	O(1)–Cu(1)–O(1)	79.30(13)
N(1)–Cu(1)–O(3)	106.45(14)	O(2)–Cu(1)–O(3)	93.16(14)
O(1)–Cu(1)–O(3)	91.83(13)	O(1)–Cu(1)–O(3)	92.23(12)

Table S3 Selected bond distances (Å) and angles (°) for complex **(3)**

Cu(1)–N(1)	1.935(4)	Cu(1)–O(2)	1.941(3)
Cu(1)–O(1)	1.926(3)	Cu(1)–O(1)#1	2.013(3)
Cu(1)–O(3)#1	2.239(3)	Cu(1)–Cu(1)	3.0578(10)
N(1)–Cu(1)–O(2)	84.08(14)	N(1)–Cu(1)–O(1)	93.01(13)
O(2)–Cu(1)–O(1)	174.27(15)	N(1)–Cu(1)–O(1)	158.52(14)
O(2)–Cu(1)–O(1)	102.85(13)	O(1)–Cu(1)–O(1)	78.71(13)
N(1)–Cu(1)–O(3)	109.77(15)	O(2)–Cu(1)–O(3)	92.36(16)
O(1)–Cu(1)–O(3)	90.44(16)	O(2)–Cu(1)–O(3)	92.36(16)

Table S4 The bond distances (Å) of complexes (1), (2), and (3)

Distance (Å)	(1)	(2)	(3)
Cu1-O1	1.944(2)	1.937(3)	1.926(3)
Cu1-O1#1	1.991(2)	2.006(3)	2.013(3)
Cu1-O2	1.938(2)	1.936(3)	1.941(3)
Cu1-N1	1.929(3)	1.901(4)	1.935(4)
Cu1-O3#1	2.256(2)	2.235(3)	2.239(3)
Cu-Cu	3.0097(7)	3.0363(10)	3.0578(10)