Fabrication of 5-R-isophthalic acid-modulated two Cu-based coordination polymers as urease inhibitors

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Table S1 Crystallographic data for **Cu-CP-COOH** and **Cu-CP-NO_2**.

Complex	**Cu-CP-COOH**	**Cu-CP-NO_2**
Empirical formula	$C_{27}H_{18}CuN_4O_9$	$C_{34}H_{24}Cu_2N_6O_{17}$
Formula weight	605.99	915.69
Temperature/K	296.0	296.0
Crystal system	Monoclinic	Monoclinic
Space group	*P*21/*n*	*Pnma*
a/Å	5.1004(7)	13.3687(6)
b/Å	20.907(3)	19.6383(9)
c/Å	21.437(3)	12.8093(5)
α/°	90	90
β/°	94.484(4)	90
γ/°	90	90
Volume/Å^3	2279.0(5)	3362.9(3)
Z	4	4
ρ_{calc}/g cm^{-3}	1.766	1.809
μ/mm^{-1}	1.031	1.360
F(000)	1236	1856.0
R_{int}	0.0927	0.0402
s	1.020	1.000
R_f/wR_f	0.0763/0.2069	0.0420/0.1094
All data R_f/wR_f	0.1570/0.2602	0.0799/0.1094

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, [b] $wR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond distances (Å) and angles (°) for **Cu-CP-COOH**.

Cu(1)–O(1)	1.938(3)	Cu(1)–N(1)	2.055(4)
Cu(1)–O(4)#1	1.953(3)	Cu(1)–N(2)#2	2.068(4)
O(1)–Cu(1)–O(4)#1	176.45(14)	O(1)–Cu(1)–N(2)#2	88.92(13)
O(1)–Cu(1)–N(1)	91.00(13)	O(4)#1–Cu(1)–N(2)#2	90.43(13)
O(4)#1–Cu(1)–N(1)	90.18(13)	N(1)–Cu(1)–N(2)#2	171.16(15)

Symmetry codes: #1 $-x + 1/2, y + 1/2, -z + 1/2$; #2 $x - 3/2, -y + 1/2, z + 1/2$.

Table S3 Selected bond distances (Å) and angles (°) for **Cu-CP-NO_2**.

Cu(1)–O(1W)	1.967(2)	Cu(1)–O(3)	1.969(2)
Cu(1)–O(1)	1.9769(19)	Cu(1)–N(1)	2.011(2)
Cu(1)–O(7)#1	2.360(2)	O(1W)–Cu(1)–O(3)	89.32(8)
O(1W)–Cu(1)–O(1)	87.77(8)	O(1W)–Cu(1)–O(7)#1	93.77(7)
O(3)–Cu(1)–O(1)	176.78(8)	O(3)–Cu(1)–O(7)#1	92.18(8)
O(1W)–Cu(1)–N(1)	176.76(9)	O(1)–Cu(1)–O(7)#1	86.64(8)
O(3)–Cu(1)–N(1)	92.13(9)	N(1)–Cu(1)–O(7)#1	89.07(9)
O(1)–Cu(1)–N(1)	90.86(9)		

Symmetry code: #1 $x - 1/2, y, -z + 3/2$.

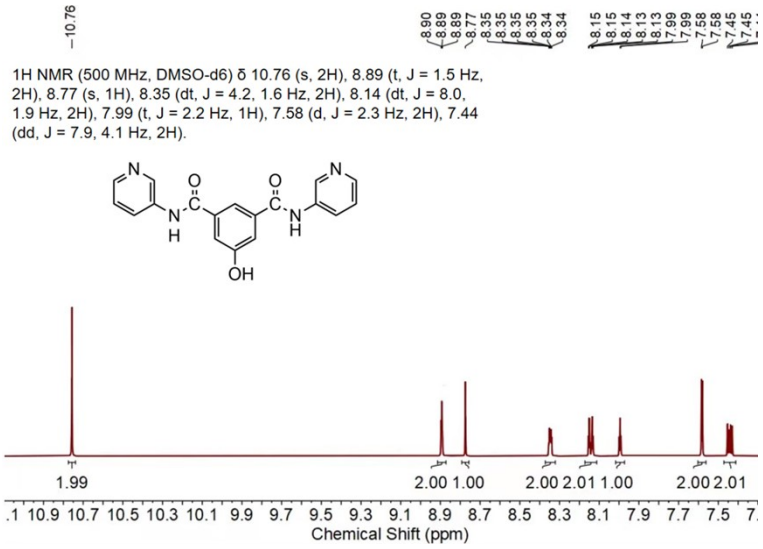

Fig. S1 NMR spectra of the 3-dpip ligand.

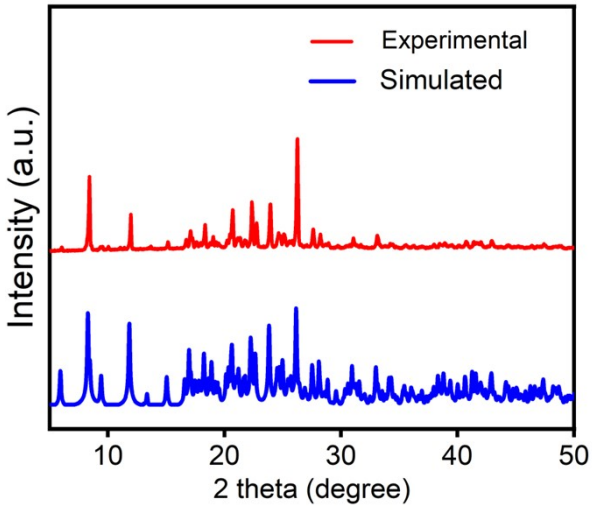

Fig. S2 The PXRD pattern of **Cu-CP-COOH**.

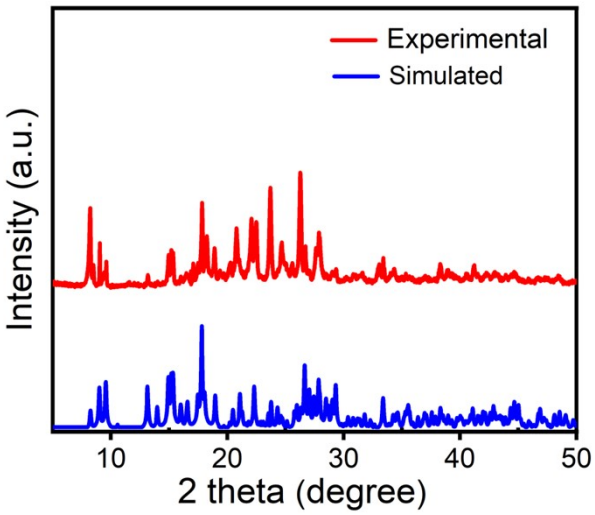

Fig. S3 The PXRD pattern of **Cu-CP-NO_2**.

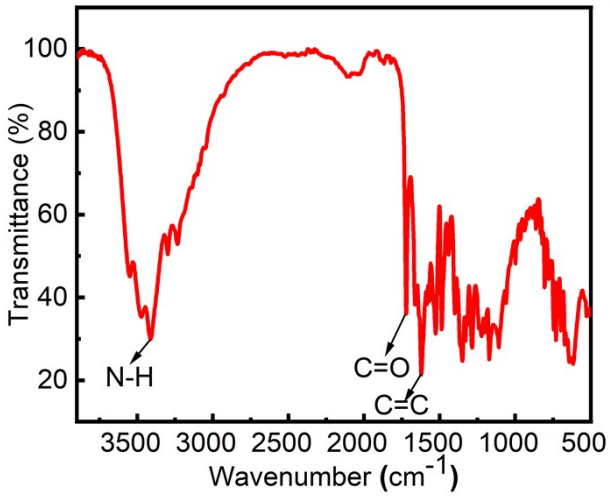

Fig. S4 The IR spectrum of **Cu-CP-COOH**.

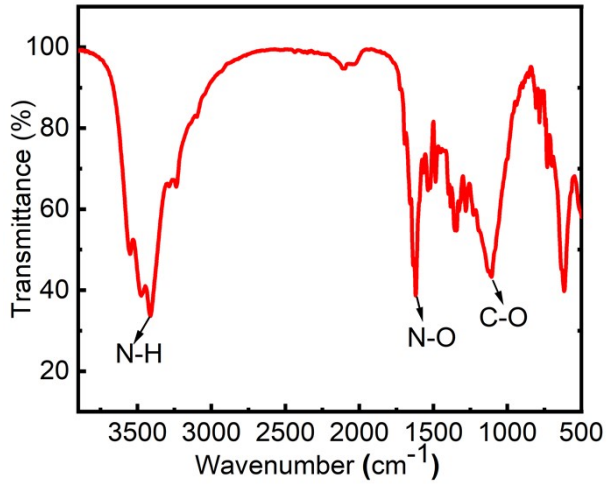

Fig. S5 The IR spectrum of **Cu-CP-NO_2**.

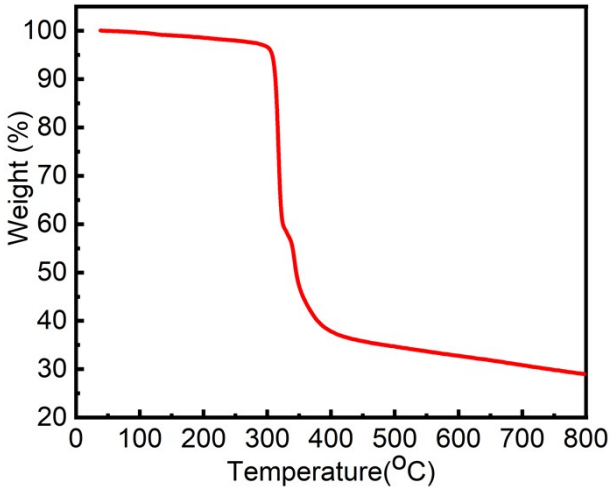

Fig. S6 TGA curve of **Cu-CP-COOH**.

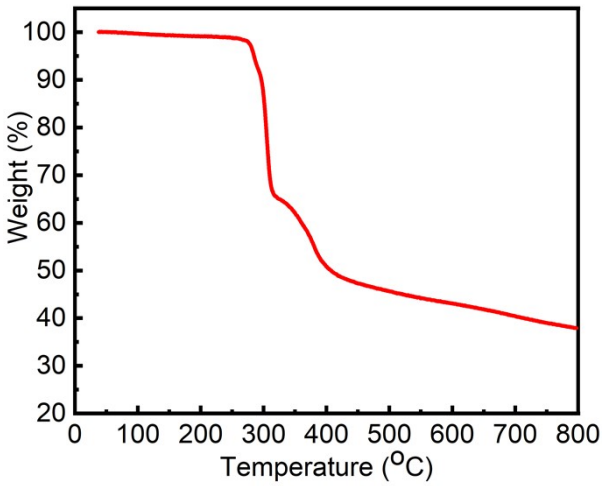

Fig. S7 TGA curve of **Cu-CP-NO_2**.

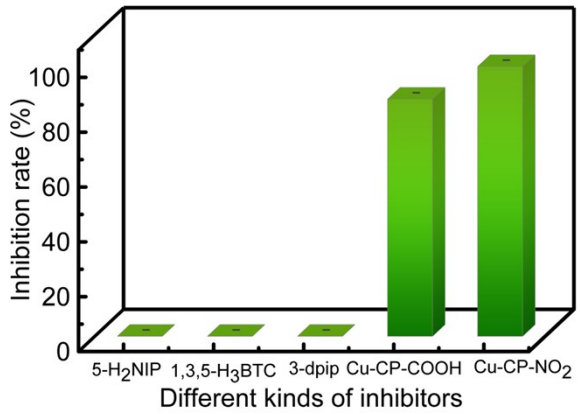

Fig. S8 Inhibition of urease by Cu-CPs and ligands at the concentration of 100 μM.

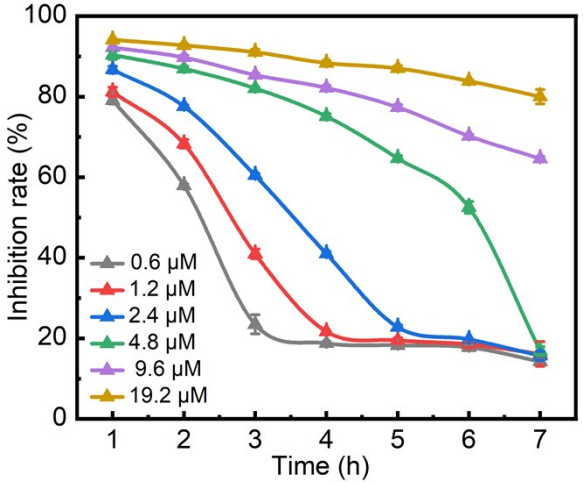

Fig. S9 Inhibitory activity curves of **Cu-CP-COOH** from the concentration of 0.6 μM to 19.2 μM.

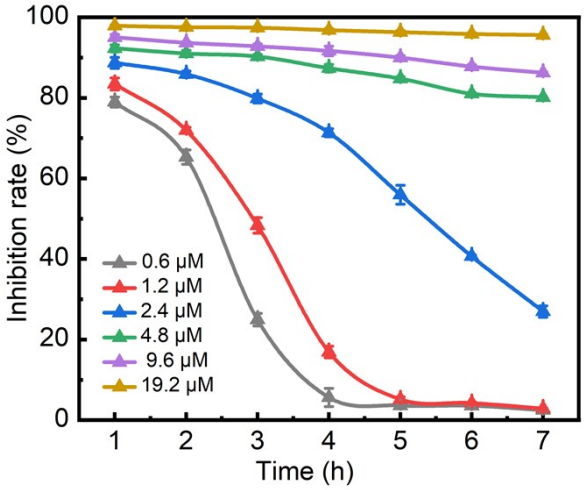

Fig. S10 Inhibitory activity curves of **Cu-CP-NO_2** from the concentration of 0.6 μM to 19.2 μM.