Fabrication of multinuclear copper cluster-based coordination polymers as urease inhibitors

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Table S1 Crystallographic data for **Cu-CP-1** and **Cu-CP-2**.

Complex	Cu-CP-1	Cu-CP-2
Empirical formula	$C_{22}H_{28}Cu_2N_4O_{15}S$	$C_{21}H_{17}CuN_2O_5$
F_w	747.62	440.91
Crystal system	Monoclinic	Triclinic
Space group	$P21/c$	$P-1$
a (Å)	10.8031(3)	9.5561(8)
b (Å)	11.9354(4)	10.8019(9)
c (Å)	23.5047(6)	11.0894(10)
α (º)	90	79.438(3)
β (º)	109.463(2)	79.785(3)
γ (º)	90	66.454(3)
V (Å^3), Z, T (K)	2857.50(14), 4, 296(2)	1024.70(15), 2, 296(2)
D_c (g cm^{-3}), F(000)	1.738, 1528	1.429, 452
Goodness-of-fit on F^2	1.049	1.021
R_{int}	0.0540	0.0716
R_1 (I > 2σ(I))[a]	0.0465	0.0555
wR_2[b] (all data)	0.0465	0.1604

[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 (º) for **Cu-CP-1**.

Cu(1)−O(1)	1.956(3)	Cu(2)−O(2)	1.941(3)
Cu(1)−O(4)#1	1.961(3)	Cu(2)−O(3)#2	1.951(3)
Cu(1)−O(8)	1.969(3)	Cu(2)−O(8)#3	1.984(3)
Cu(1)−N(1)	2.039(3)	Cu(2)−O(8)	1.997(3)
Cu(1)−O(2W)	2.227(3)	O(1W)−Cu(2)	2.321(3)
Cu(2)−Cu(2)#3	3.0082(9)	O(1)−Cu(1)−O(4)#1	152.48(14)
O(1)−Cu(1)−O(8)	92.54(11)	O(2)−Cu(2)−O(8)	92.76(11)
O(4)#1−Cu(1)−O(8)	92.07(11)	O(3)#2−Cu(2)−O(8)	161.61(13)
O(1)−Cu(1)−N(1)	88.96(13)	O(8)#3−Cu(2)−O(8)	81.85(11)
O(4)#1−Cu(1)−N(1)	86.21(13)	O(2)−Cu(2)−O(1W)	91.90(13)
O(8)−Cu(1)−N(1)	178.28(12)	O(3)#2−Cu(2)−O(1W)	93.88(13)
O(1)−Cu(1)−O(2W)	111.92(13)	O(8)#3−Cu(2)−O(1W)	89.27(11)
O(4)#1−Cu(1)−O(2W)	95.52(13)	O(8)−Cu(2)−O(1W)	104.43(11)
O(8)−Cu(1)−O(2W)	84.67(12)	O(2)−Cu(2)−Cu(2)#3	133.53(9)
N(1)−Cu(1)−O(2W)	95.55(13)	O(3)#2−Cu(2)−Cu(2)#3	138.46(9)
O(2)−Cu(2)−O(3)#2	84.82(12)	O(8)#3−Cu(2)−Cu(2)#3	41.08(7)
O(2)−Cu(2)−O(8)#3	174.60(11)	O(8)−Cu(2)−Cu(2)#3	40.77(7)
O(3)#2−Cu(2)−O(8)#3	100.36(11)	O(1W)−Cu(2)−Cu(2)#3	99.03(8)

Symmetry codes: #1 $x + 1, y, z$; #2 $–x − 1, −y − 2, −z − 1$; #3 $−x, −y − 2, −z − 1$.

Table S3 Selected bond distances (Å) and angles (º) for **Cu-CP-2**.

Cu(1)−O(4)#1	1.962(3)	Cu(1)−O(3)	1.974(3)
Cu(1)−O(2)#1	1.962(2)	Cu(1)−N(1)	2.177(3)
Cu(1)−O(1)	1.964(3)	Cu(1)−Cu(1)#1	2.6513(8)
O(4)#1−Cu(1)−O(2)#1	89.12(12)	O(1)−Cu(1)−N(1)	92.04(11)
O(4)#1−Cu(1)−O(1)	88.34(12)	O(3)−Cu(1)−N(1)	92.91(11)
O(2)#1−Cu(1)−O(1)	167.76(10)	O(4)#1−Cu(1)−Cu(1)#1	84.79(8)
O(4)#1−Cu(1)−O(3)	167.56(10)	O(2)#1−Cu(1)−Cu(1)#1	85.60(7)
O(2)#1−Cu(1)−O(3)	89.09(12)	O(1)−Cu(1)−Cu(1)#1	82.24(8)
O(1)−Cu(1)−O(3)	90.81(13)	O(3)−Cu(1)−Cu(1)#1	82.80(8)
O(4)#1−Cu(1)−N(1)	99.52(11)	N(1)−Cu(1)−Cu(1)#1	172.78(8)
O(2)#1−Cu(1)−N(1)	100.19(10)		

Symmetry code: #1 −x, −y, −z + 1.

Table S4 Hydrogen bonding geometries (Å, °) of **Cu-CP-1** and **Cu-CP-2**.

D–H···A	D–H	H···A	D···A	D–H···A
N4–H4B···O6 [i]	0.86	2.11	2.9192	156
O1W–H1WB···O9 [ii]	0.85	1.87	2.7014	164
C12–H12A···O5 [iii]	0.93	2.48	3.3079	148

Symmetry codes: [i] 2 − x, −y, −z; [ii] 1 + x, 1/2 − y, 1/2 + z; [iii] x, 1 + y, −1 + z.

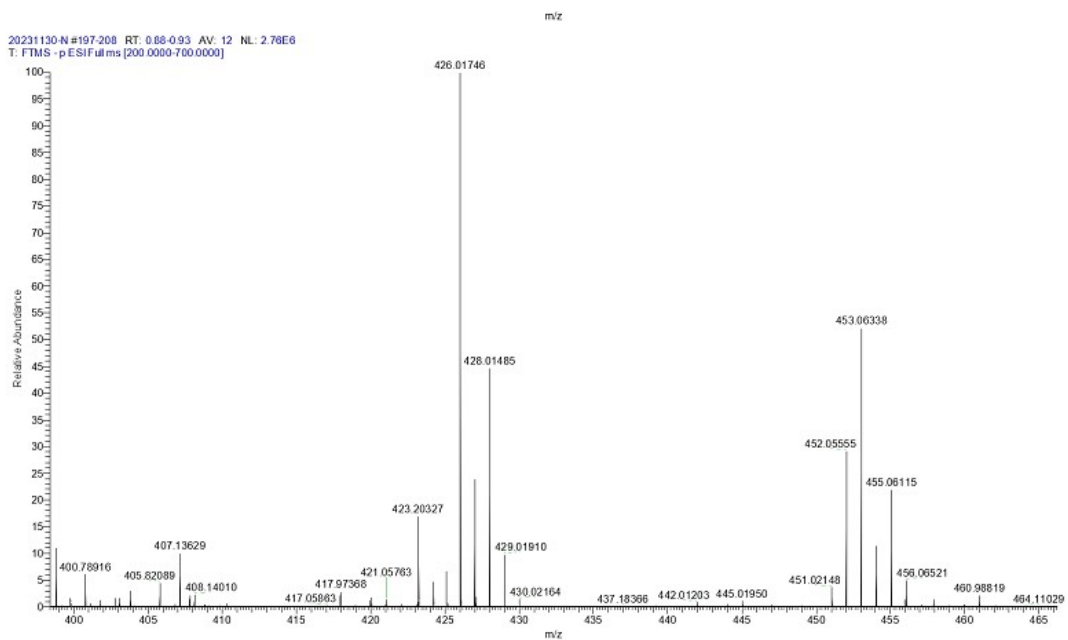**Fig. S1** The mass spectra of the **Cu-CP-1**.

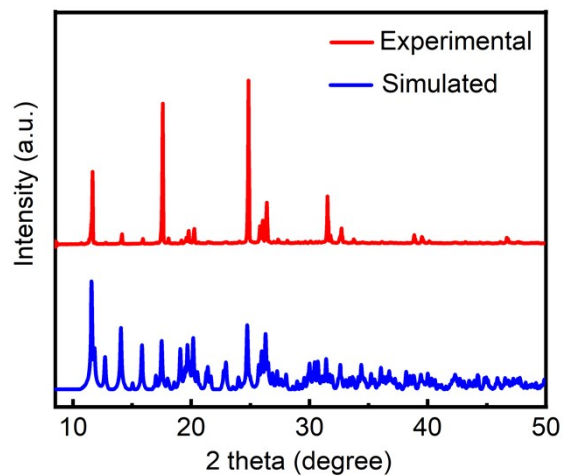**Fig. S2** The mass spectra of the **Cu-CP-2**.

Fig. S3 The PXRD patterns of **Cu-CP-1**.
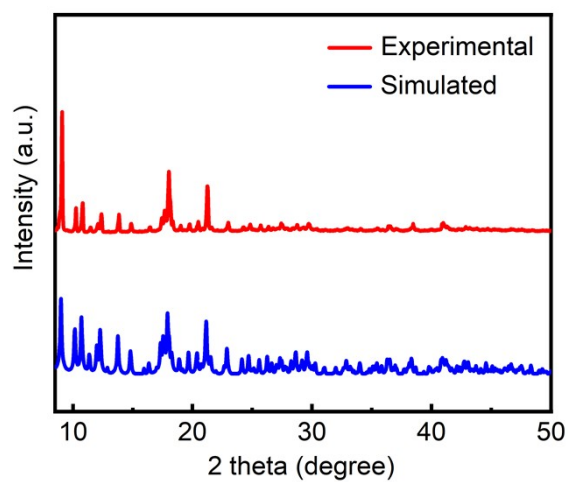

Fig. S4 The PXRD patterns of **Cu-CP-2**.
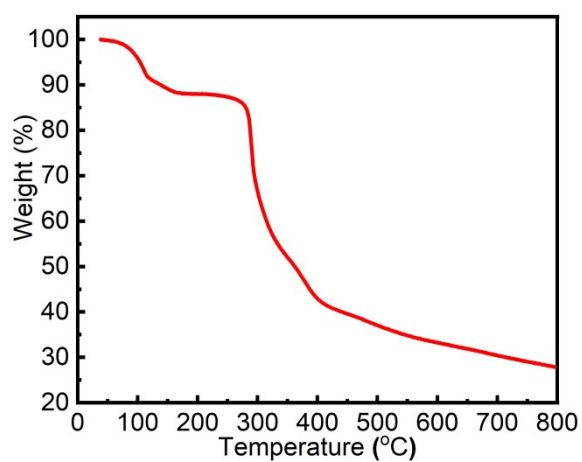

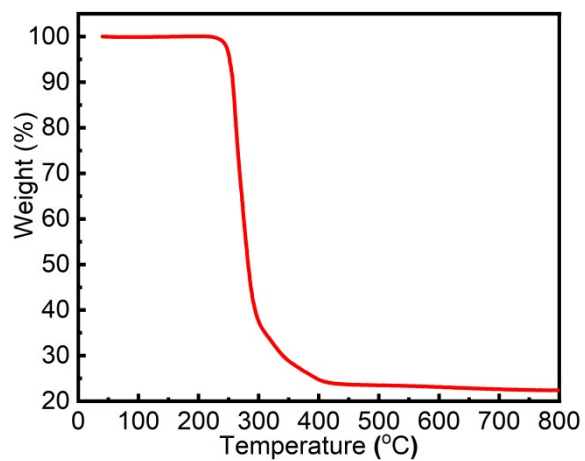**Fig. S5** TGA curve of **Cu-CP-1**.

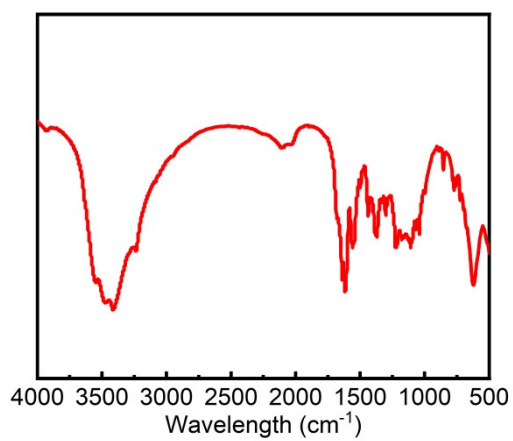**Fig. S6** TGA curve of **Cu-CP-2**.
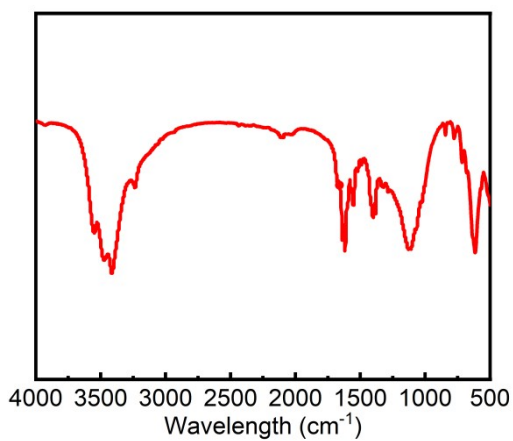

Fig. S7 The IR spectrum of **Cu-CP-1**.
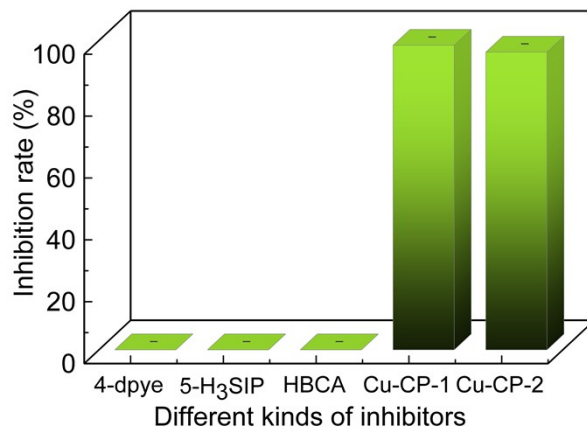

Fig. S8 The IR spectrum of **Cu-CP-2**.

Fig. S9 Inhibition of urease by Cu-CPs and ligands at 100μM concentration.
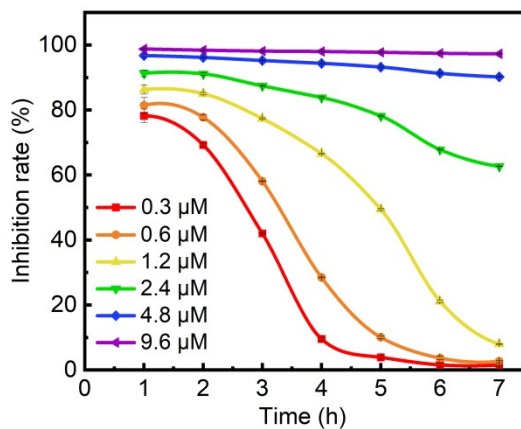

Fig. S10 Inhibitory activity curves of **Cu-CP-1** from the concentration of 0.3 μM to 9.6 μM.
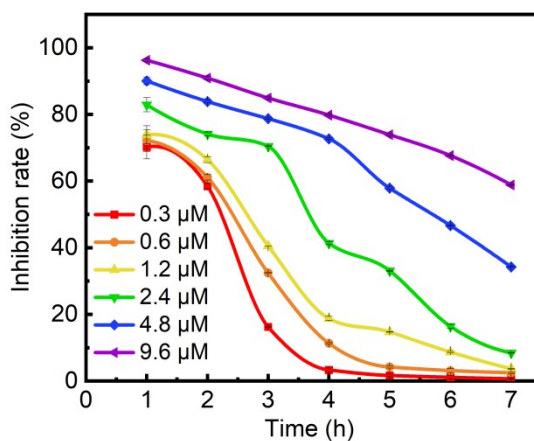

Fig. S11 Inhibitory activity curves of **Cu-CP-2** from the concentration of 0.3 μM to 9.6 μM.