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Supporting Information

A Triphenylphosphine Coordinated Cinnamaldehyde-derived Copper(I) Fenton-like agent with Mitochondrial Aggregation Damage for Chemodynamic Therapy

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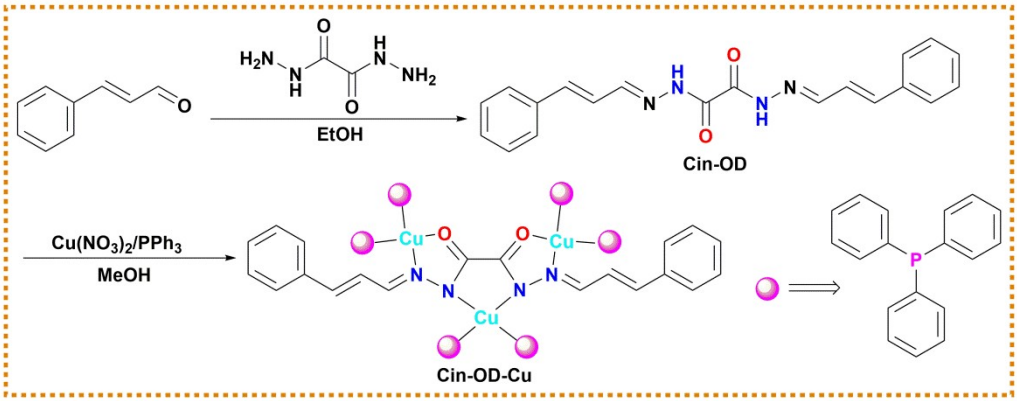

Scheme S1. Synthetic routes of **Cin-OD** and **Cin-OD-Cu**.

Table S1. Crystal data and structure refinement of **Cin-OD-Cu**.

Complex	**Cin-OD-Cu**
Empirical formula	$C_{128}H_{106}Cu_3N_4O_2P_6 \cdot NO_3$
Formula weight	2170.66
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	14.89394 (12)
b (Å)	26.78108 (18)
c (Å)	28.88607 (16)
α (°)	90
β (°)	98.0272 (7)
γ (°)	90
Volume (Å^3)	11409.06 (14)
Z	4
D_{calc} (g cm^{-3})	1.264
F (000)	4504
Reflections collected	84847
Independent reflections	20793
R_{int}	0.049
Goodness-of-fit on F^2	1.03
R_1, wR_2 [$I >= 2\sigma(I)$]	0.0448, 0.1141
R_1, wR_2[all data]	0.0579, 0.1211

Table S2. Selected bond lengths (Å) and angles (°) for **Cin-OD-Cu**.

Cin-OD-Cu			
Cu1—P1	2.2875 (7)	Cu2—O1	2.0880 (17)

Cu1—P2	2.2831 (7)	Cu2—N1	2.0760 (19)
Cu1—N2	2.0918 (18)	Cu3—P5	2.2433 (7)
Cu1—N3	2.0896 (19)	Cu3—P6	2.2591 (7)
Cu2—P3	2.2596 (7)	Cu3—O2	2.1089 (16)
Cu2—P4	2.2423 (7)	Cu3—N4	2.0550 (19)
P2—Cu1—P1	119.01 (3)	P4—Cu2—P3	121.66 (3)
N2—Cu1—P1	113.43 (6)	O1—Cu2—P3	108.78 (5)
N2—Cu1—P2	115.20 (5)	O1—Cu2—P4	112.03 (5)
N3—Cu1—P1	110.82 (6)	N1—Cu2—P3	113.62 (6)
N3—Cu1—P2	113.26 (6)	N1—Cu2—P4	114.11 (6)
N3—Cu1—N2	78.07 (7)	N1—Cu2—O1	78.21 (7)
P5—Cu3—P6	125.80 (3)	N4—Cu3—P5	117.19 (6)
O2—Cu3—P5	107.37 (5)	N4—Cu3—P6	109.35 (6)
O2—Cu3—P6	108.42 (5)	N4—Cu3—O2	77.49 (7)

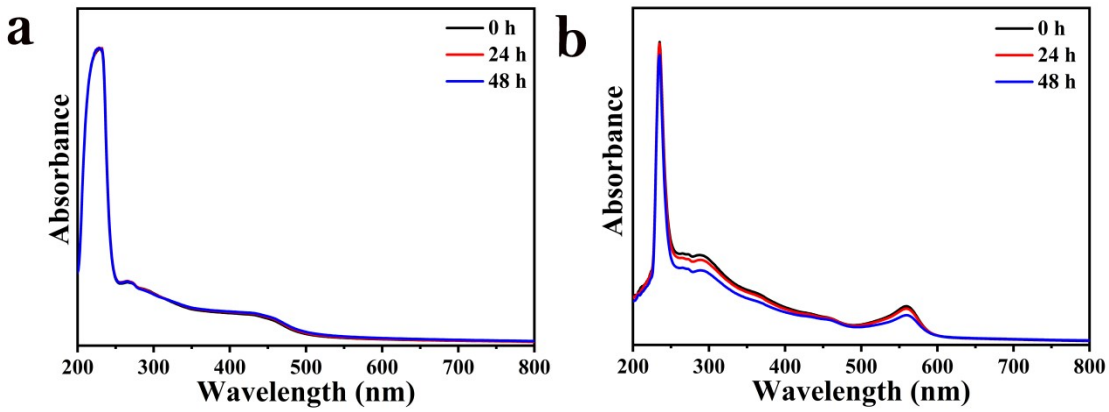

Figure S1. The absorption spectra of **Cin-OD-Cu** in Tirs-HCl buffer solution (pH=7.4) and DMEM culture medium over 48 h.

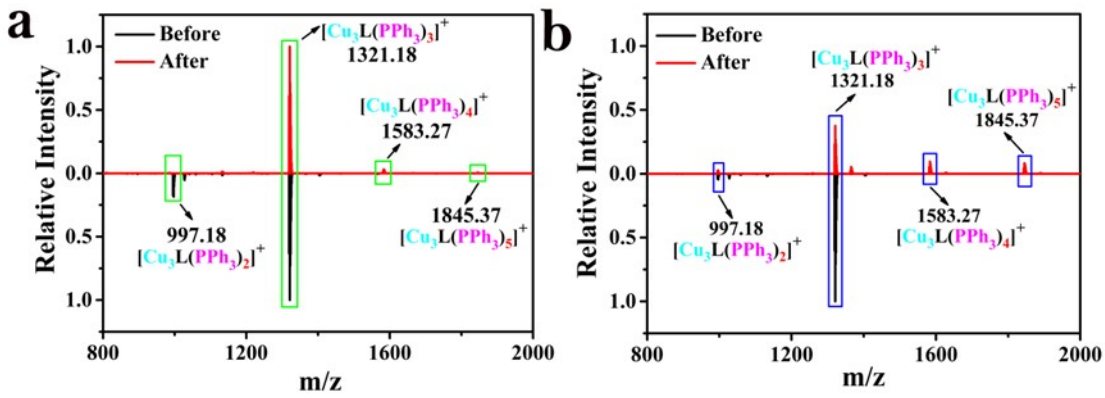

Figure S2. (a) HRMS analysis of **Cin-OD-Cu** after soaking in concentrated HCl (0.1 M) and (b) aqueous NH_3 (0.1 M) for 24 h.

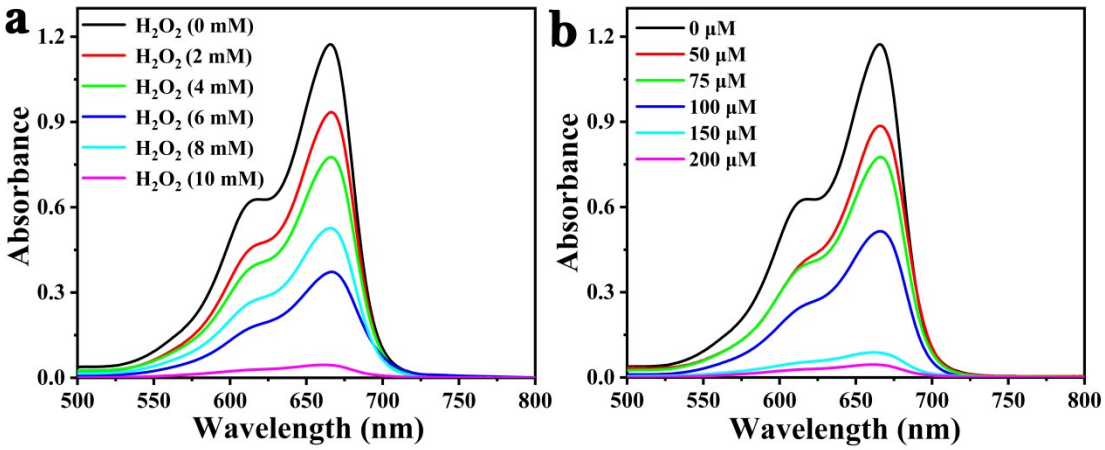

Figure S3. UV-vis absorption spectra of MB degradation after treated at different concentration of H_2O_2 (a, MB: 20 μM, **Cin-OD-Cu**: 200 μM) and **Cin-OD-Cu** (b, MB: 20 μM, H_2O_2: 10 mM) in Tris-HCl buffer (0.05 M, pH=7.4).

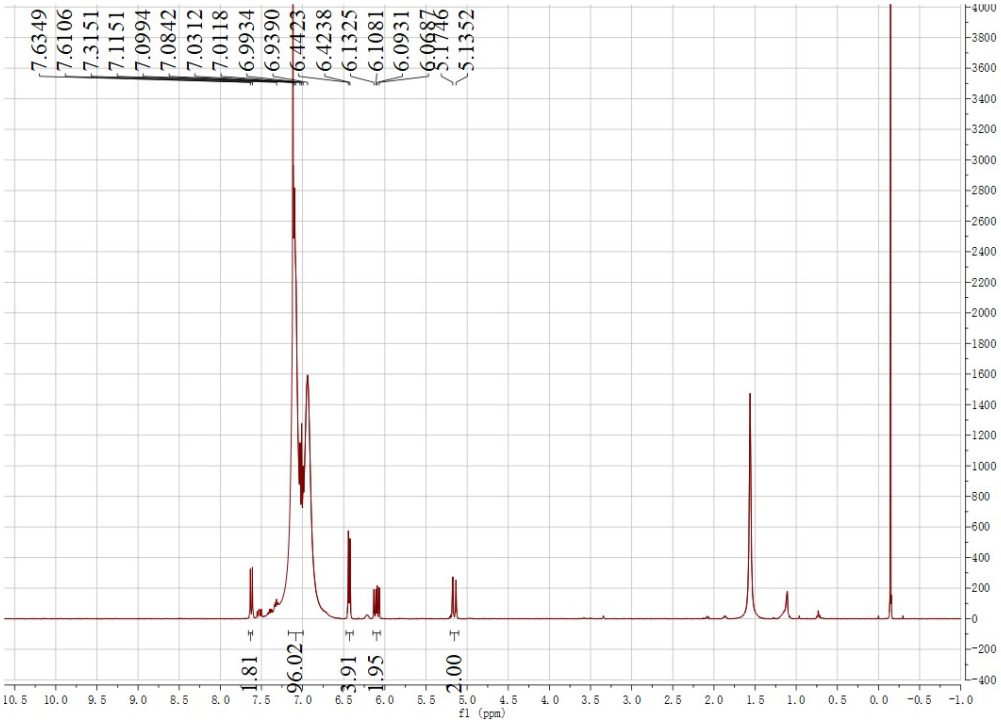

Figure S4. ^{1}H NMR spectrum of **Cin-OD-Cu**.

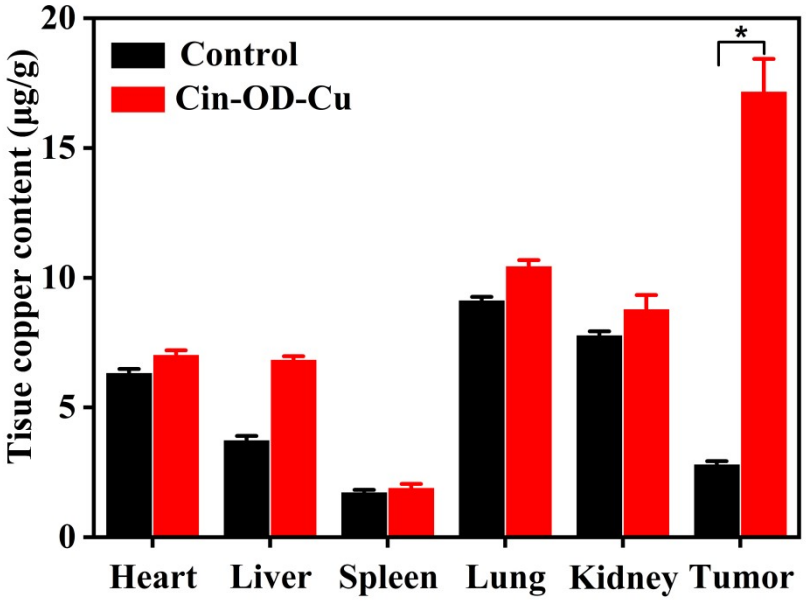

Figure S5. Tissue copper content of mice after treatment with **Cin-OD-Cu**. *P < 0.05.

Mask results for **Cin-OD-Cu** are as follows:

loop_

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  _smtbx_masks_void_nr

  _smtbx_masks_void_average_x

  _smtbx_masks_void_average_y

  _smtbx_masks_void_average_z

  _smtbx_masks_void_volume

  _smtbx_masks_void_count_electrons

  _smtbx_masks_void_content

 1 0.000 0.308 0.698 180.1 18.1 ?

 2 -0.000 0.692 0.302 180.1 18.6 ?

 3 0.500 0.808 0.802 180.1 18.0 ?

 4 0.500 0.192 0.198 180.1 18.7 ?
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That is, Mask gives 73 electrons/unit cell for the voids. If these electrons are all from MeOH ($18e^-$), each unit cell has 73/18 ≈ 4 MeOH molecules, and each formula unit has 1 MeOH molecule (since Z = 4). So the suitable formula for this compound should be $[Cu_3(Cin\text{-}OD)(PPh_3)_6]\cdot NO_3\cdot CH_3OH$.