

Supporting Information

Metal Organic Cage as Theranostic Nanoplatfrom for MRI

Guided Chemodynamic Therapy

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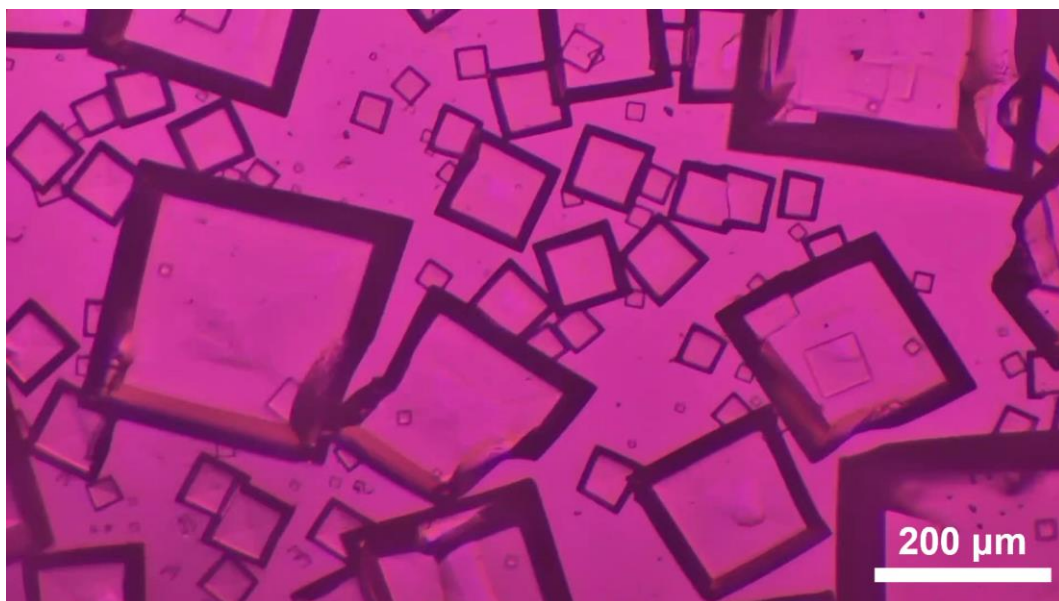


Figure S1. The morphology of crystal MOC-Mn under optical microscope.

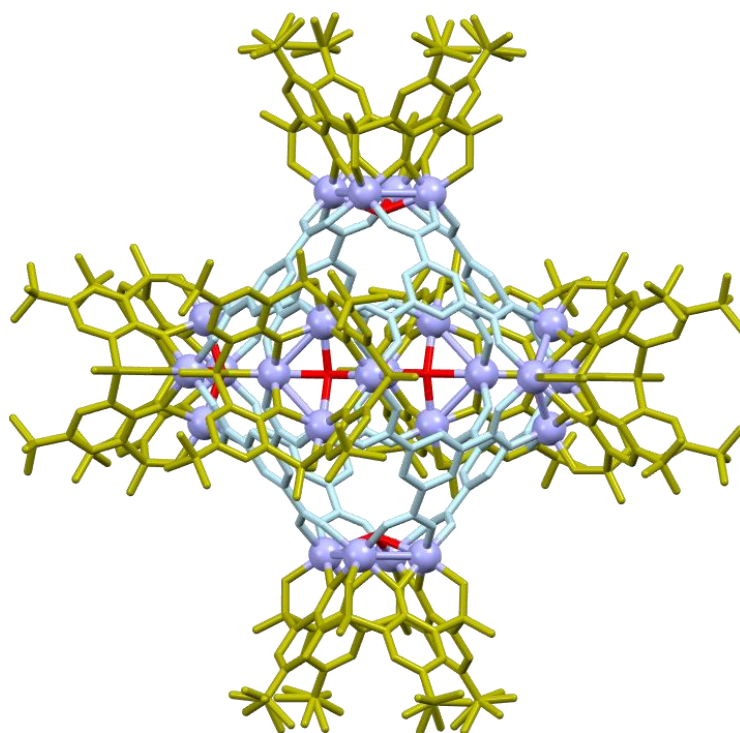


Figure S2. Structure of MOC-Mn from SC-XRD.

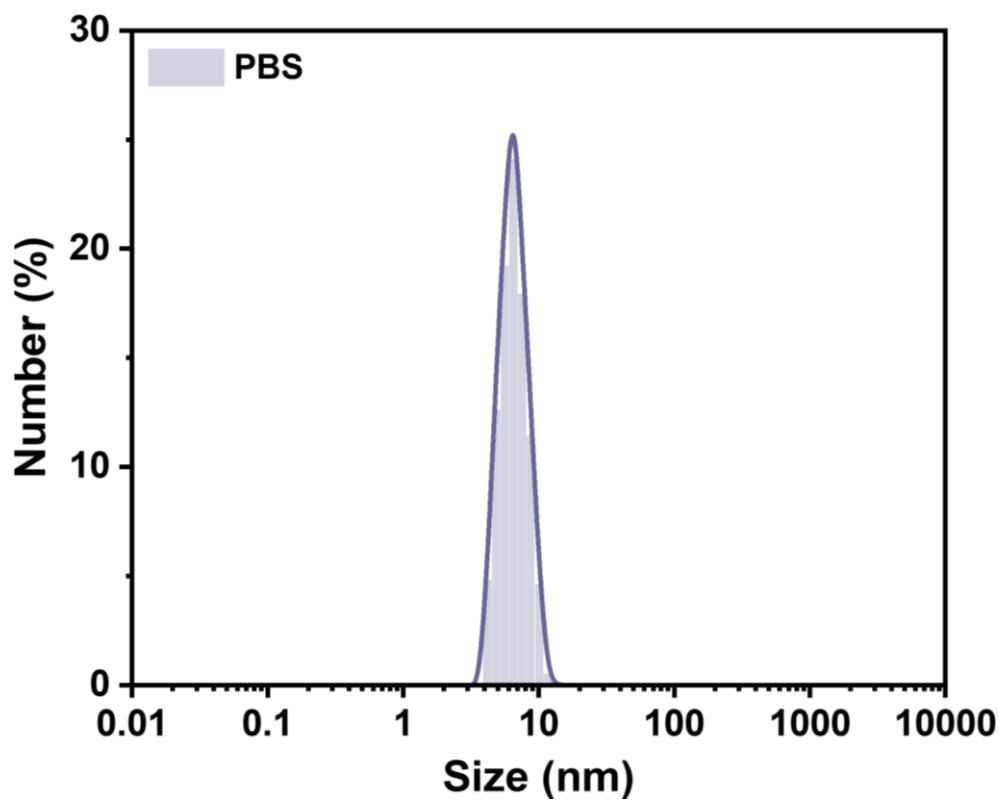


Figure S3. The DLS plots of MOC-Mn in PBS.

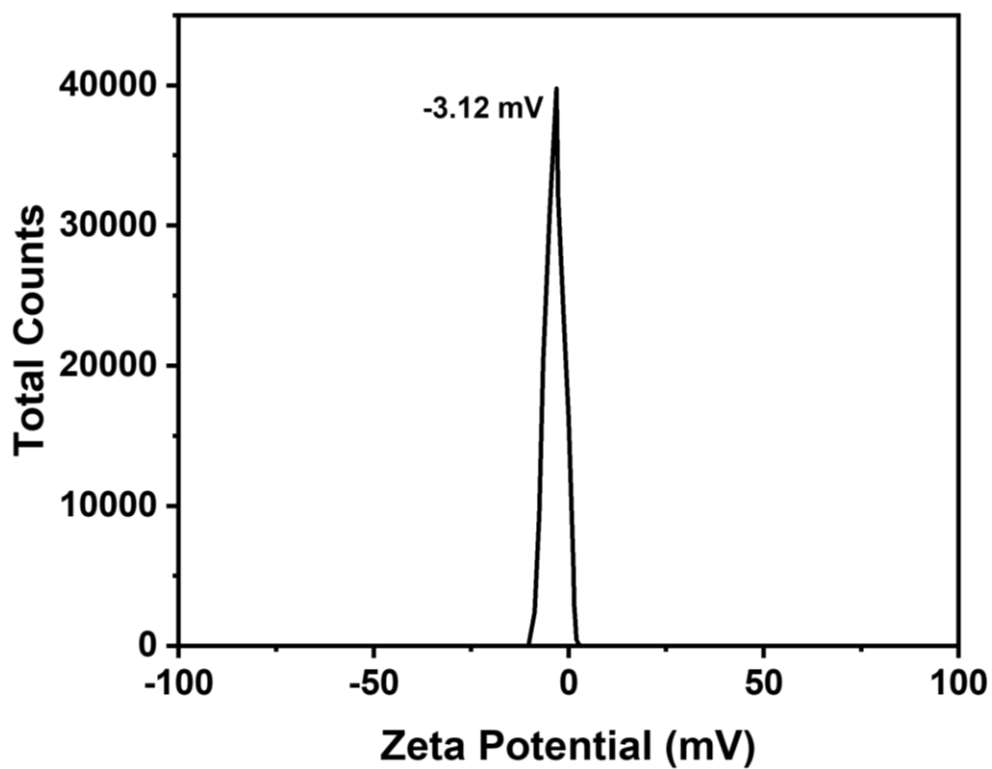


Figure S4. The zeta potential of MOC-Mn in PBS.

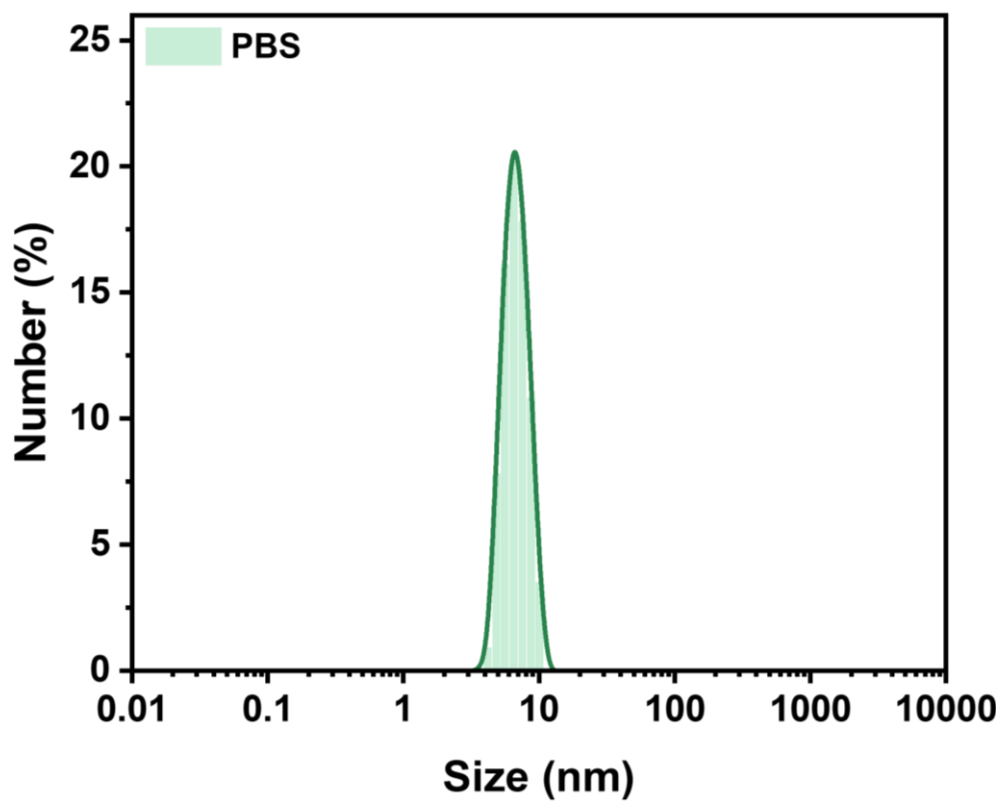


Figure S5. The DLS plots of MOC-Mn in PBS after a 5-day period.

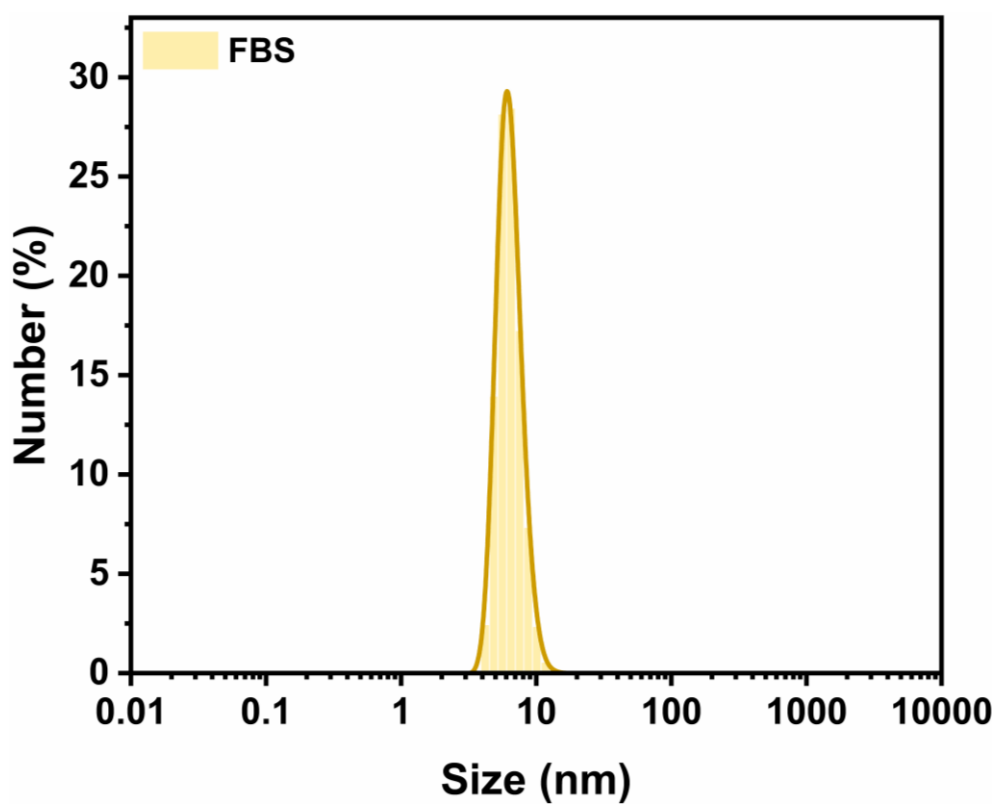


Figure S6. The DLS plots of MOC-Mn in FBS.

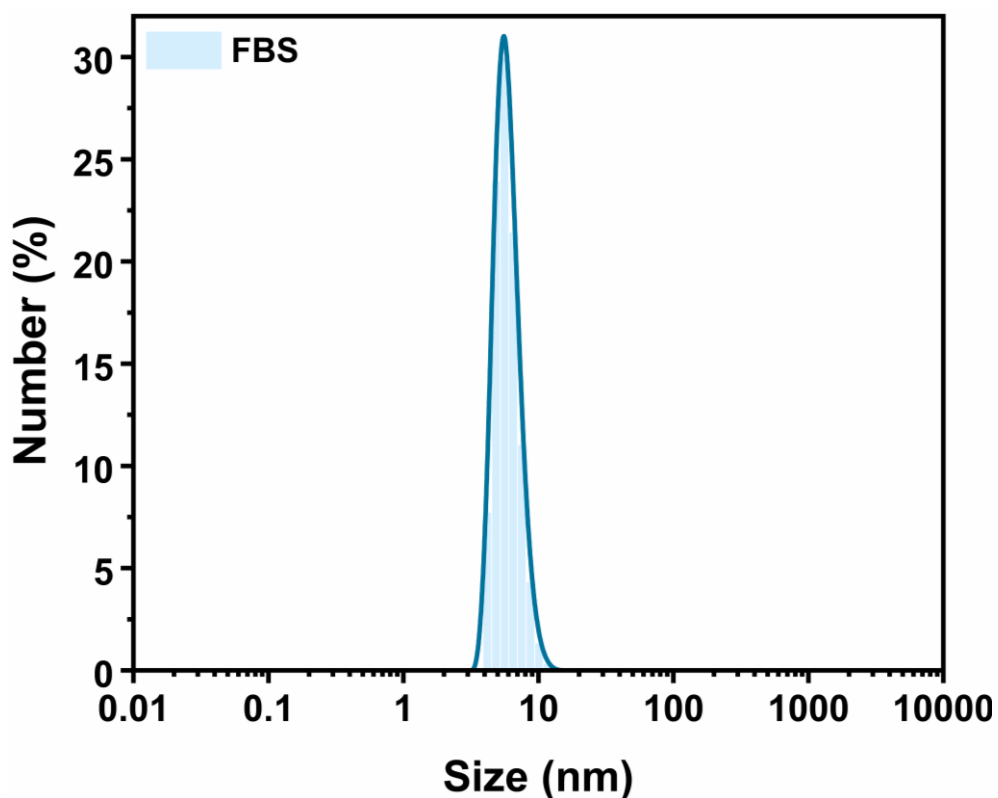


Figure S7. The DLS plots of MOC-Mn in FBS after a 5-day period.

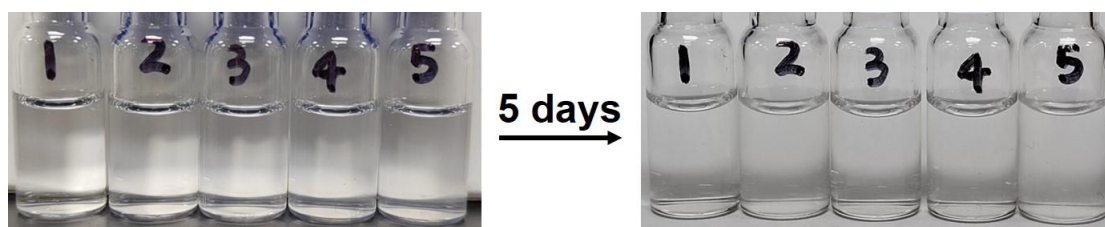


Figure S8. The photos of different concentrations of MOC-Mn (dissolved in DMSO) in PBS after a 5-day period.



Figure S9. The Tyndall effect of MOC-Mn (dissolved in DMSO) in PBS. The final concentrations are 25, 50, 75, 100, and 125 $\mu\text{g/ml}$ (designated as 1-5 in the picture).

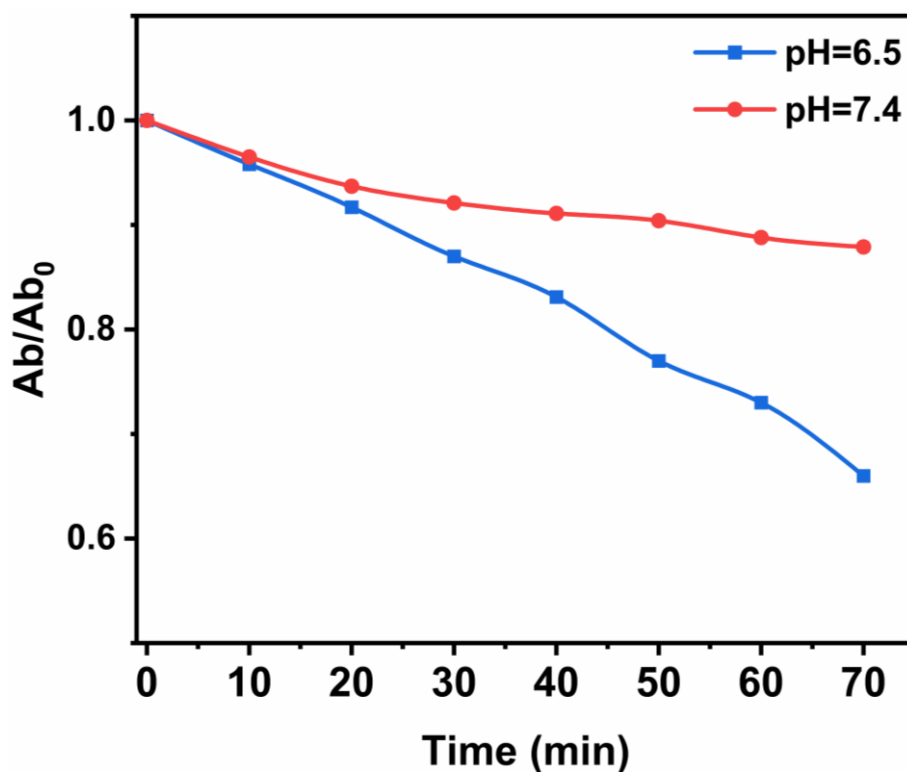


Figure S10. The UV-vis absorption spectra of MB after treatment with MOC-Mn under different conditions.

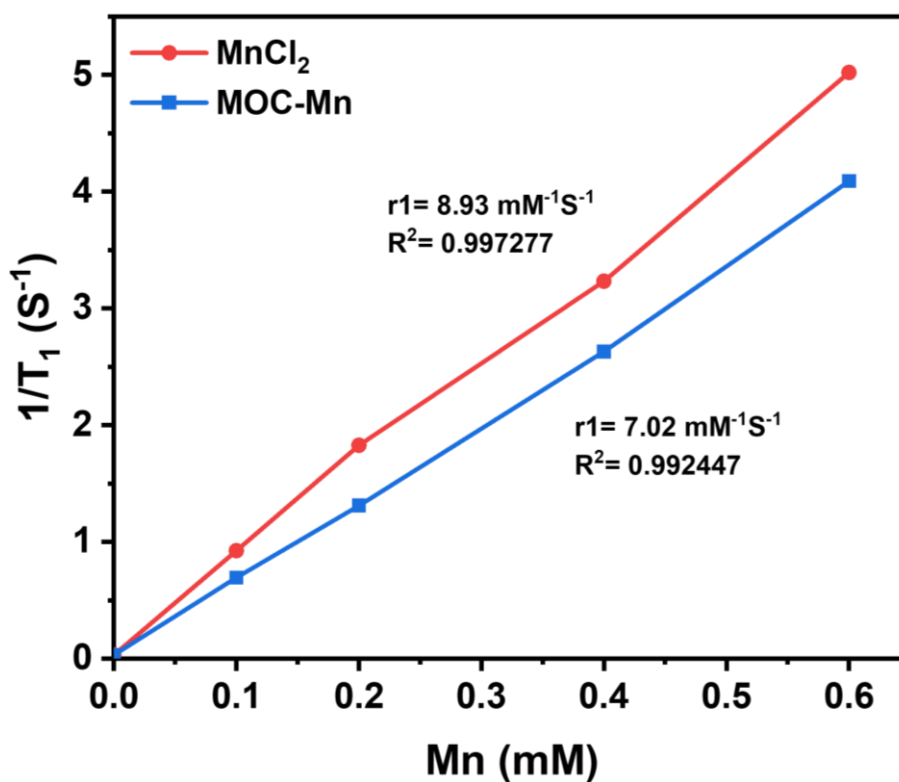


Figure S11. The relaxation rate of MnCl₂ and MOC-Mn.

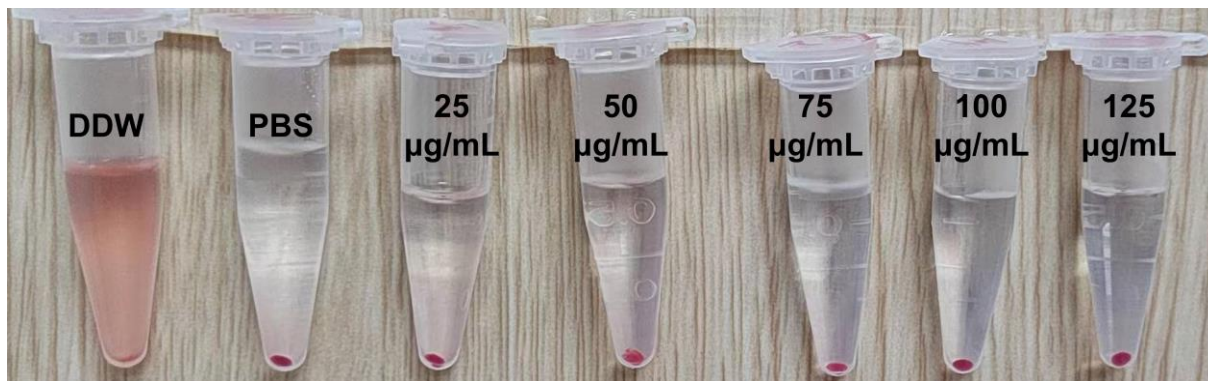


Figure S12. The hemolytic test of MOC-Mn in different concentrations.

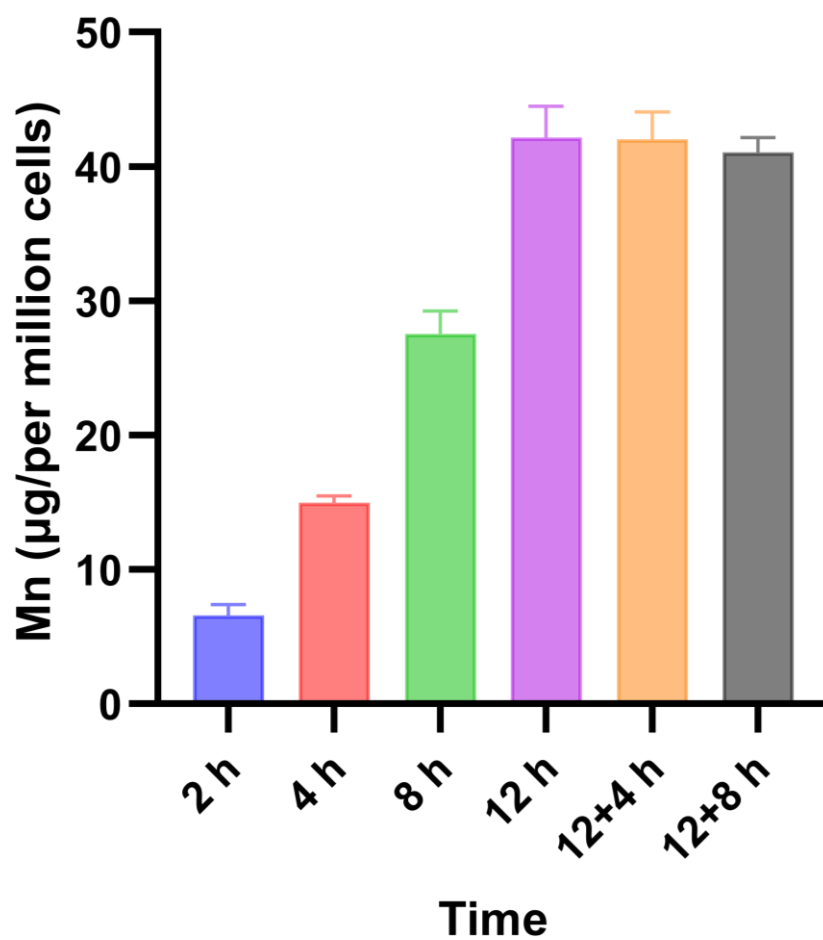


Figure S13. Cellular uptake and retention of MOC-Mn in HeLa cells.

Table S1. Crystal data and structure refinement for MOC-Mn.

Name	MOC-Mn
Empirical formula	C ₃₁₂ H ₂₈₈ Mn ₂₄ O ₁₂₆ S ₂₄
Formula weight	8141.41
Temperature/K	100
Crystal system	Tetragonal
Space group	<i>I</i> 4/m
<i>a</i> /Å	26.6066 (5)
<i>b</i> /Å	26.6066 (5)
<i>c</i> /Å	44.5181 (13)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	31514.9(15)
Z	2
ρ_{calc} /cm ³	0.883
$M\mu$ /mm ⁻¹	4.946
F(000)	8552.0
<i>h</i> , <i>k</i> , <i>l</i> _{max}	32,32,53
Nref	14737
Radiation	Cu K α (λ =1.54184)

Table. S2 The elemental distribution of MOC-Mn from EDS mapping.

Element	Atomic %	Atomic % Error	Weight %	Weight % Error	Net Counts
C	64.8	0.3	55.7	0.2	364 257
O	33.2	0.3	38.0	0.3	72 524
S	0.8	0.0	1.9	0.0	16 718
Mn	1.1	0.0	4.4	0.1	7 604