

Supporting information

Ultraviolet irradiation-mediated formation of A β ₄₂ oligomers and reactive oxygen species in Zn²⁺-bound A β ₄₂ aggregates irrespective removal of Zn²⁺

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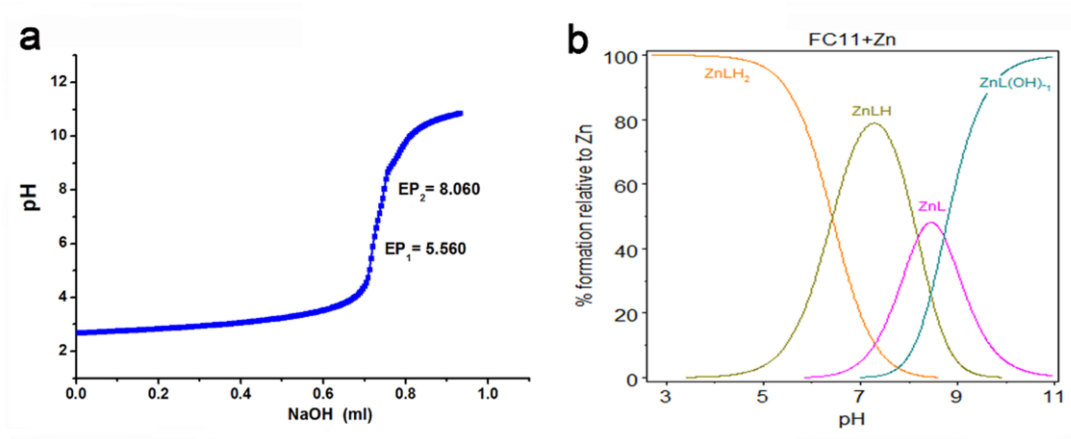
Supporting information Table S1. Crystal data and structure refinement for [Zn(FC-11)(H₂O)₂]Cl₂.

Empirical formula	C ₂₇ H ₂₇ N ₇ O ₁₀ S Zn	
Formula weight	706.99	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2c	
Unit cell dimensions	a = 35.144(7) Å	α = 90°
	b = 10.1699(17) Å	β = 148.402(8)°
	c = 33.644(6) Å	γ = 90°
Volume	6300(2) Å ³	
Z	8	
Density (calculated)	1.491 Mg/m ³	
Absorption coefficient	0.912 mm ⁻¹	
F(000)	2912	
Crystal size	0.16 x 0.12 x 0.11 mm ³	
Theta range for data collection	2.10 to 25.50°.	
Index ranges	-42 ≤ h ≤ 42, -12 ≤ k ≤ 12, -40 ≤ l ≤ 38	
Reflections collected	18165	
Independent reflections	5856 [R(int) = 0.0471]	
Completeness to theta = 25.50°	99.8 %	
Absorption correction	None	
Max. and min. transmission	0.9063 and 0.8678	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5856 / 108 / 426	
Goodness-of-fit on F²	1.118	
Final R indices [I > 2σ(I)]	R1 = 0.0838, wR2 = 0.2188	
R indices (all data)	R1 = 0.0940, wR2 = 0.2262	

Supporting information Table S2. The major data of bond lengths (Å) and angles (°) for [Zn(FC-11)(H₂O)₂]Cl₂.

Zn(1)-O(2)	2.018(4)
Zn(1)-N(2)	2.086(3)
Zn(1)-N(3)	2.096(3)
Zn(1)-O(3)	2.122(4)
Zn(1)-O(1)	2.189(4)
Zn(1)-N(1)	2.243(5)
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O(2)-Zn(1)-N(2)	101.96(18)
O(2)-Zn(1)-N(3)	101.44(17)
N(2)-Zn(1)-N(3)	156.59(14)
O(2)-Zn(1)-O(3)	100.10(19)
N(2)-Zn(1)-O(3)	86.71(17)
N(3)-Zn(1)-O(3)	89.60(18)
O(2)-Zn(1)-O(1)	85.84(16)
N(2)-Zn(1)-O(1)	83.58(16)
N(3)-Zn(1)-O(1)	97.75(16)
O(3)-Zn(1)-O(1)	169.51(17)
O(2)-Zn(1)-N(1)	162.92(17)
N(2)-Zn(1)-N(1)	79.12(17)
N(3)-Zn(1)-N(1)	78.41(17)
O(3)-Zn(1)-N(1)	96.98(18)
O(1)-Zn(1)-N(1)	77.31(15)

Supporting information Figure S1: Potentiometric titration of FC-11 with $\text{Zn}(\text{NO}_3)_2$. (a) Potentiometric titration curve of the solutions containing **FC-11** and equimolar amount $\text{Zn}(\text{NO}_3)_2$ at 25°C. (b) Species distribution plot in the Zn^{2+} -**FC-11** system.



Supporting information Figure S2: Fluorescence titration of FC-11 with a Zn²⁺ solution. (a)

Fluorescence spectra of **FC-11** at varied ratios of Zn²⁺/FC-11 in pH 7.4 buffer at room temperature.

(b) Job plotting using the data of fluorescence titration with the Zn²⁺ solution.

