Supporting Information for:

Synthesis, Crystal Structure, Photophysical Property and Ion Binding Behavior of a Cyclometalated Platinum(II) Terpyridylacetylide with Efficient π-Conjugation Degree

Dongqin Bi, Yuquan Feng, Qian Zhao, Hongwei Wang, Yongsheng Zhu, Xiaoyu Bao, Huitao Fan, Lintao Yu, Qichao Yang, Dongfang Qiu*

College of Chemistry and Pharmacy Engineering, Nanyang Normal University, Nanyang, 473061, P. R. China

Table S1. Crystal data and crystal structure parameters.

Compound	2	3
Empirical formula	$C_{50}H_{43}N_3Pt$	$C_{65}H_{52}N_6Pt$
Formula weight	880.96	1112.22
Temperature/ K	296(2)	296(2)
Wavelength/Å	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/*c*	*P*2(1)/*c*
a / Å	50.582(12)	9.7741(19)
b / Å	9.149(2)	44.237(8)
c / Å	17.832(4)	11.821(2)
α / (°)	90.00	90.00
β / (°)	104.312(7)	99.749(4)
γ / (°)	90.00	90.00
Volume / Å^3	7996(3)	5037.1(17)
Z	8	4
D_c / (g • cm^{-3})	1.464	1.467
Absorption coefficient / mm^{-1}	3.548	2.835
F(000)	3536	2248
Crystal size / mm	0.16×0.13×0.09	0.24×0.17×0.12
θ range for data collection /(°)	1.66 to 25.00	1.81 to 25.00
Limiting indices	-60≤*h*≤50, -10≤*k*≤10, -21≤*l*≤20	-11≤*h*≤8, -52≤*k*≤47, -13≤*l*≤14
Completeness to *θ* = 25.00°	99.9 %	100.0 %
Data / restraints / parameters	7017/2638/487	8864/4149/649
Goodness-of-fit on F^2	1.091	1.046
Final R indices [$I>2\sigma(I)$][a]	R_1 = 0.0337, wR_2 = 0.0957	R_1 = 0.0529, wR_2 = 0.1193
R indices (all data)	R_1 = 0.0490, wR_2 = 0.1054	R_1 = 0.0783, wR_2 = 0.1282
Largest diff. peak and hole/(e.Å^{-3})	1.058 and -1.054	1.426 and -1.218

[a] $R_1=\sum||F_0|-|F_c||/\sum|F_0|$, $wR_2=\{\sum w[(F_0)^2-(F_c)^2]^2/\sum w[(F_0)^2]^2\}^{1/2}$

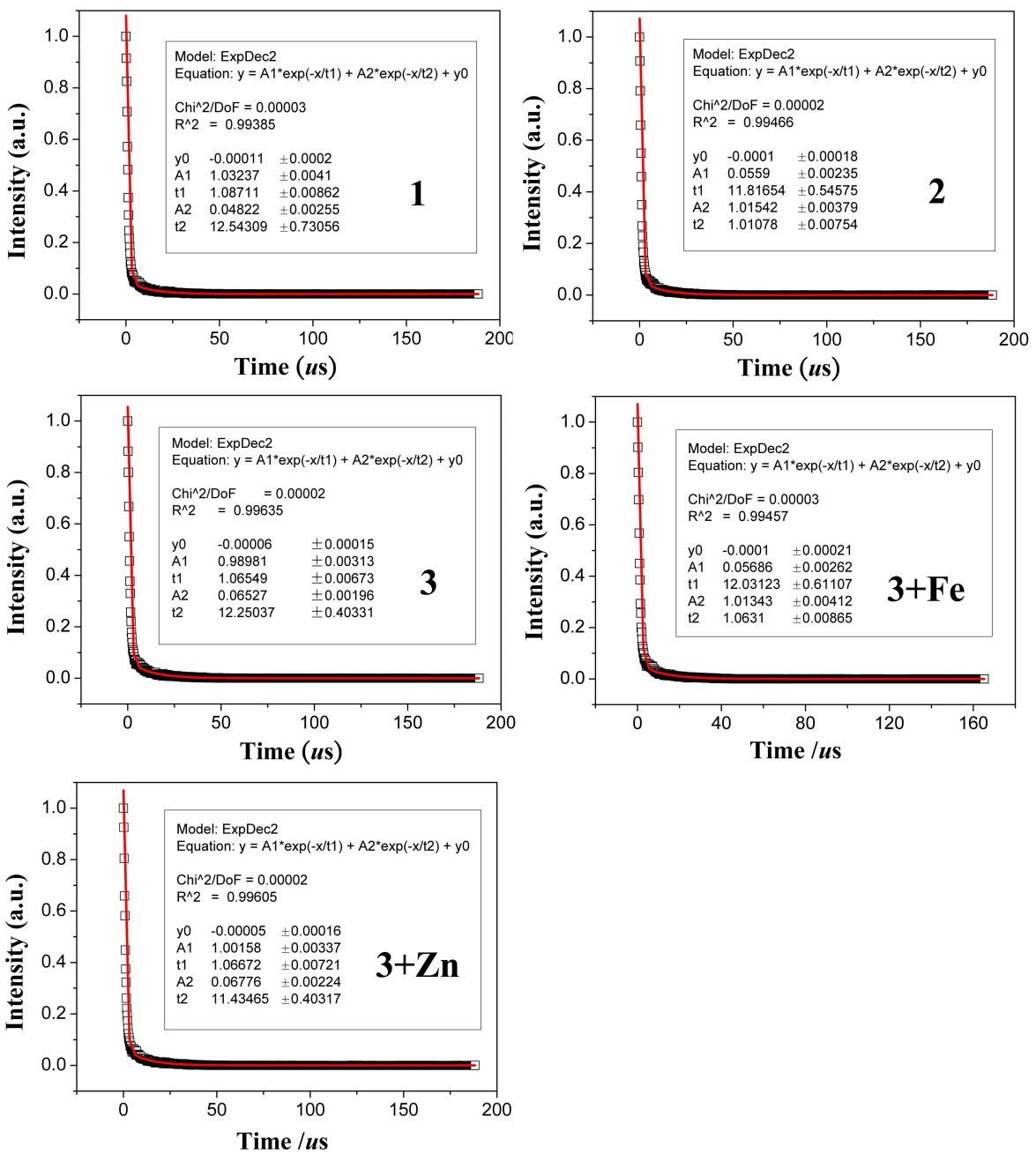

Figure S1. The luminescence intensity decay and bi-exponential fit of the complex **1**-**3** and the titration products of **3** with Fe^{2+} and Zn^{2+}, respectively.

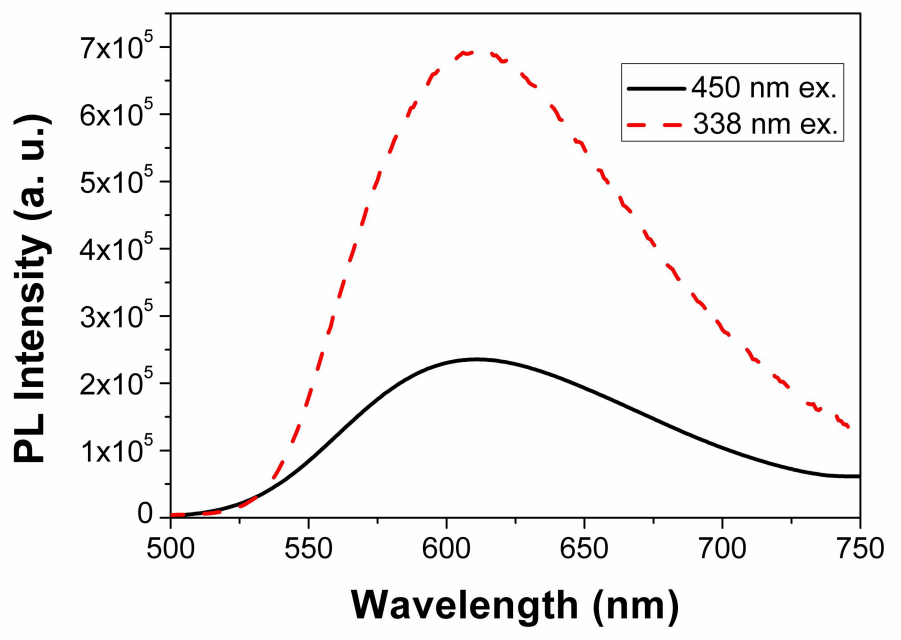

Figure S2. PL spectra of **3** under 338 and 450 nm excited wavelength.

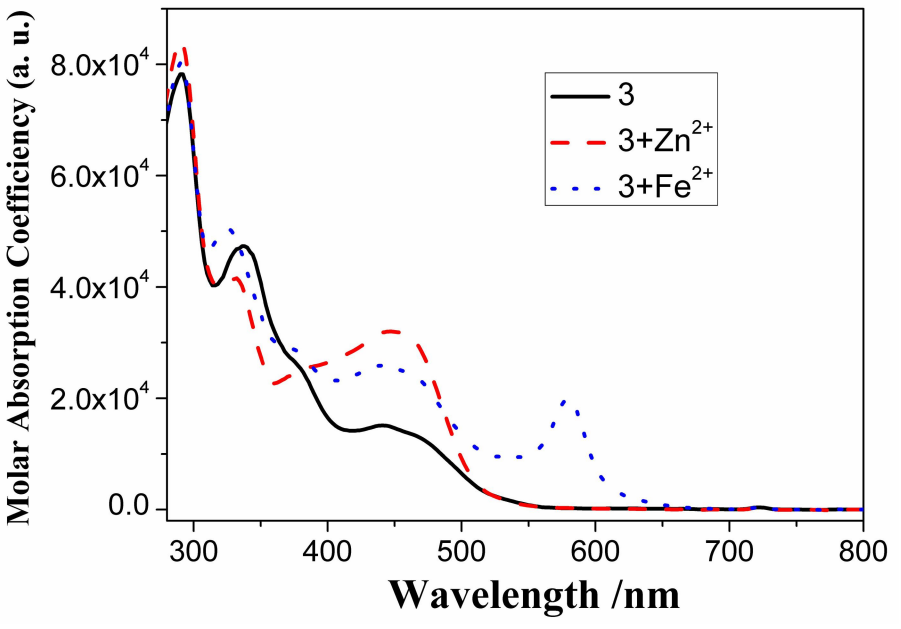

Figure S3. UV-vis absorption spectra of **3** before and after respective titration of 0.5 equiv Zn^{2+} and Fe^{2+}.

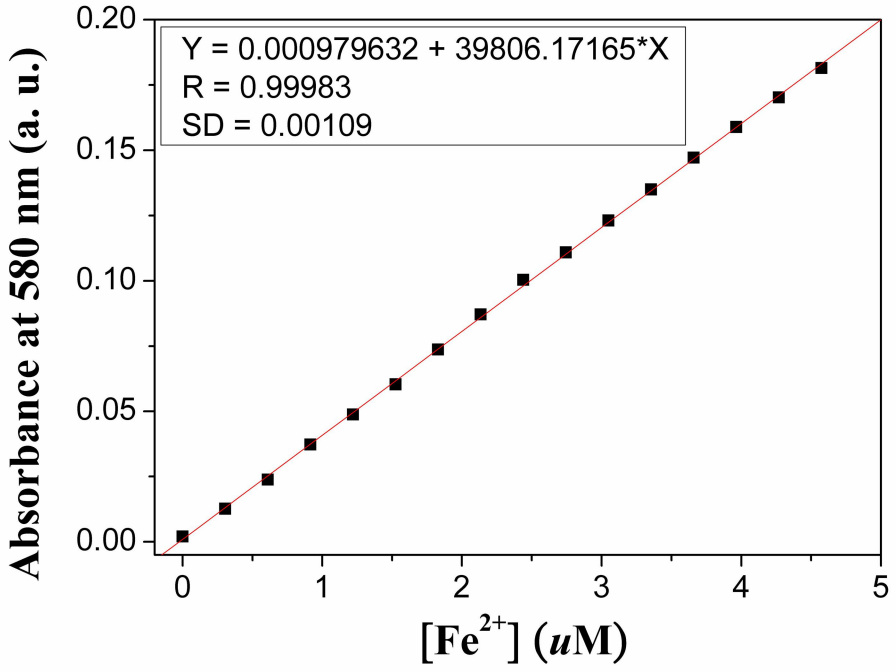

Figure S4. Linear analysis of the absorption data of **3** with consecutive titration of Fe^{2+}.

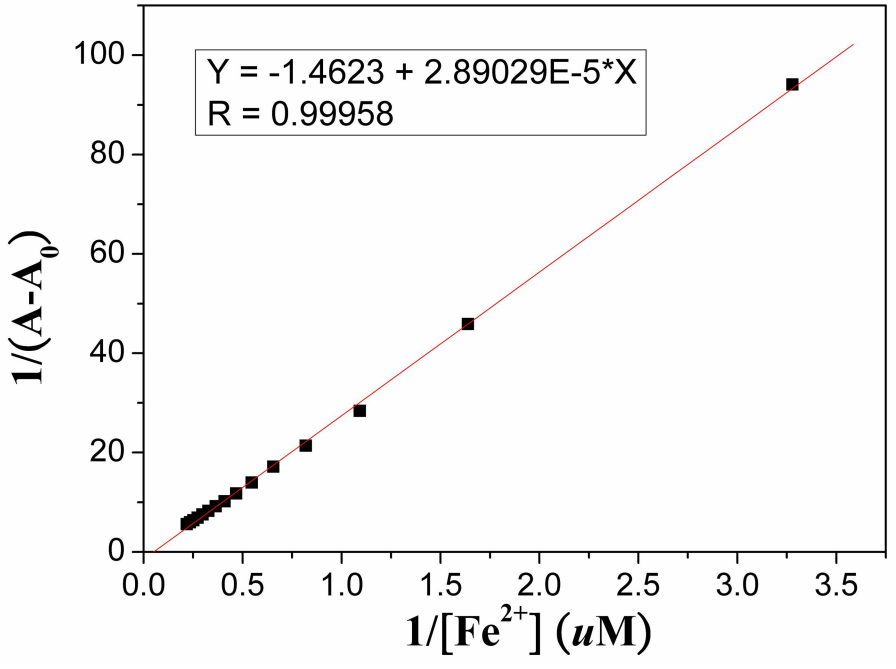

Figure S5. Benesi-Hildebrand plot of the absorption data of **3** with consecutive titration of Fe^{2+}.

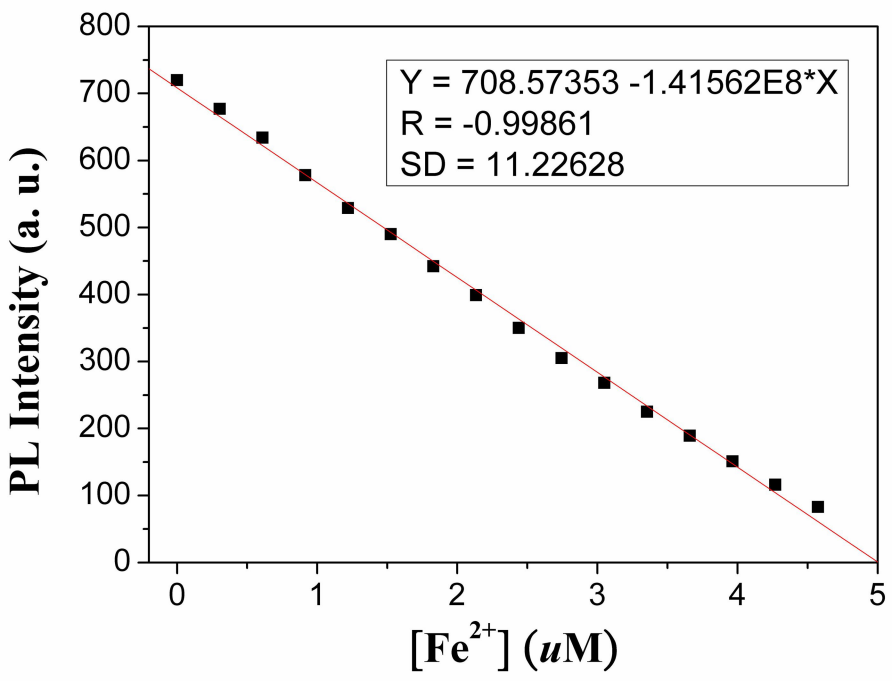

Figure S6. Linear analysis of the PL data of **3** with consecutive titration of Fe^{2+}.

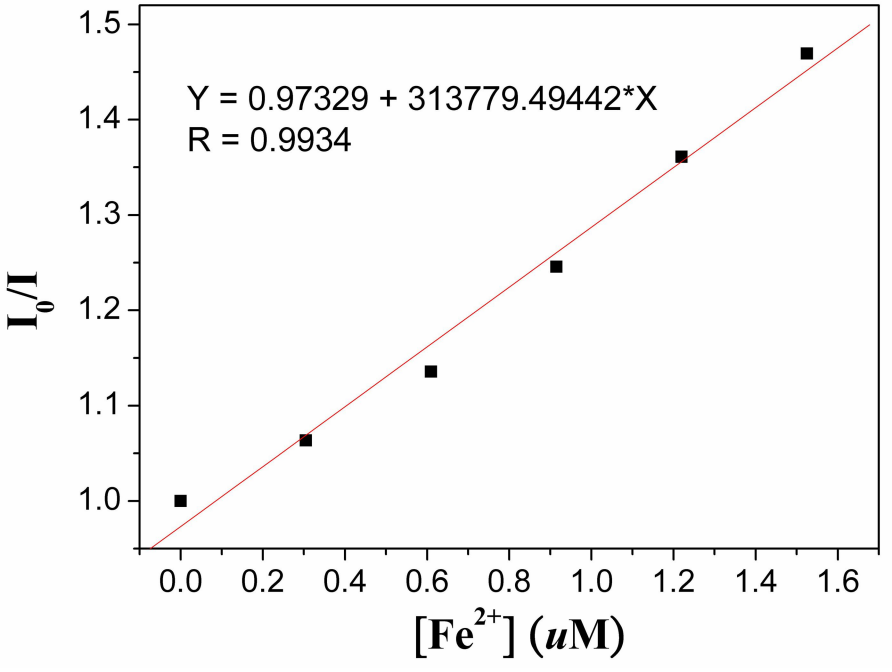

Figure S7. Stern-Volmer plot of the PL data of **3** with consecutive titration of Fe^{2+}.

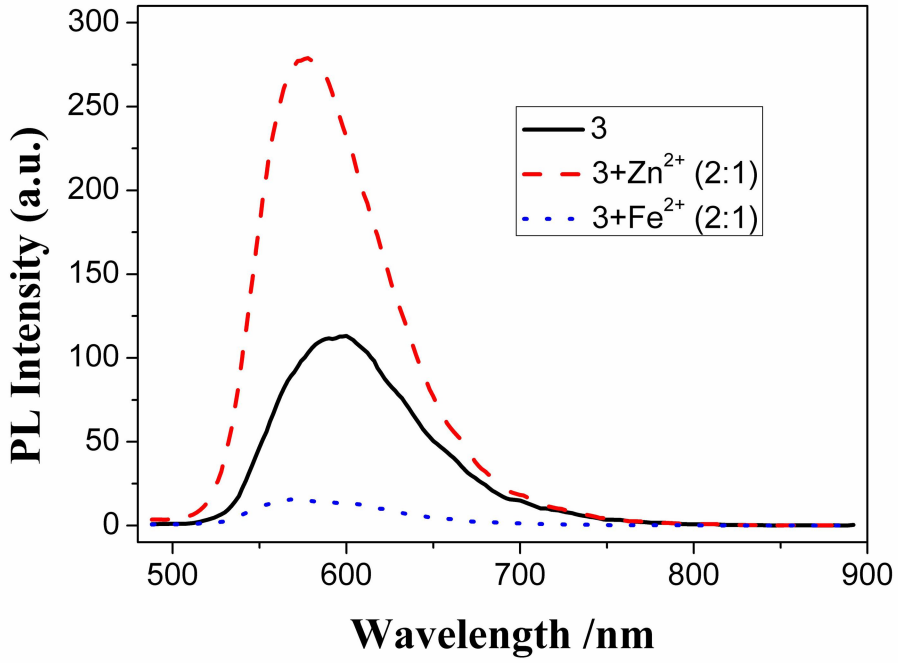

Figure S8. PL spectra of **3** before and after respective titration of 0.5 equiv Zn^{2+} and Fe^{2+}.

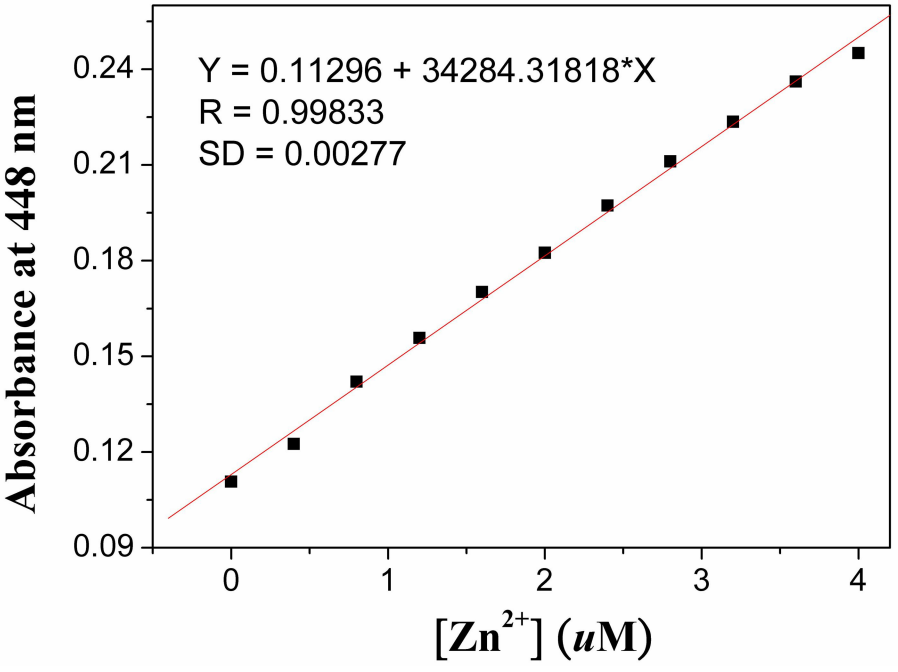

Figure S9. Linear analysis of the absorption data of **3** with consecutive titration of Zn^{2+}.

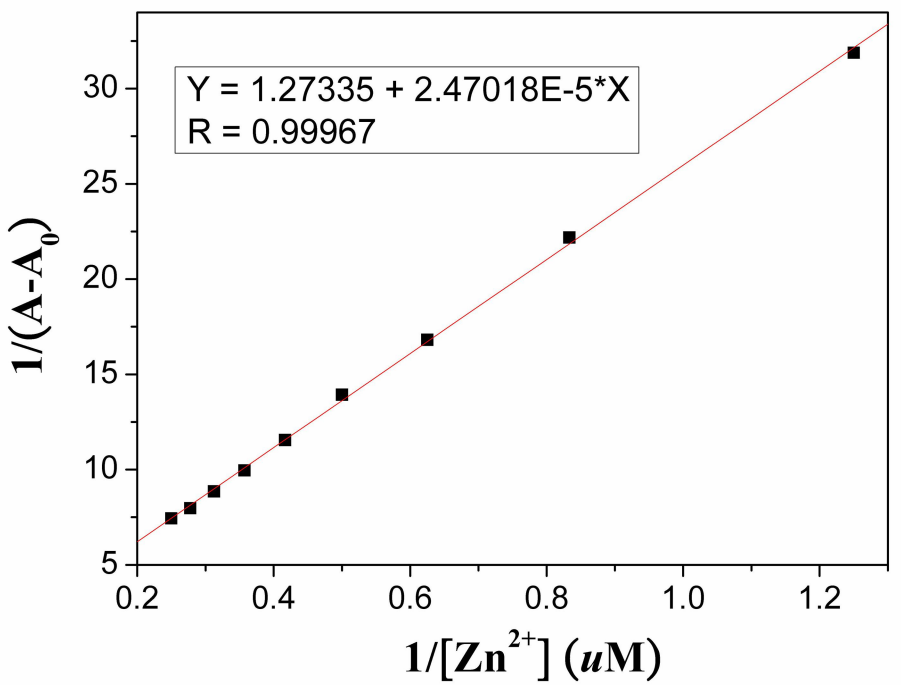

Figure S10. Benesi-Hildebrand plot of the absorption data of **3** with consecutive titration of Zn^{2+}.

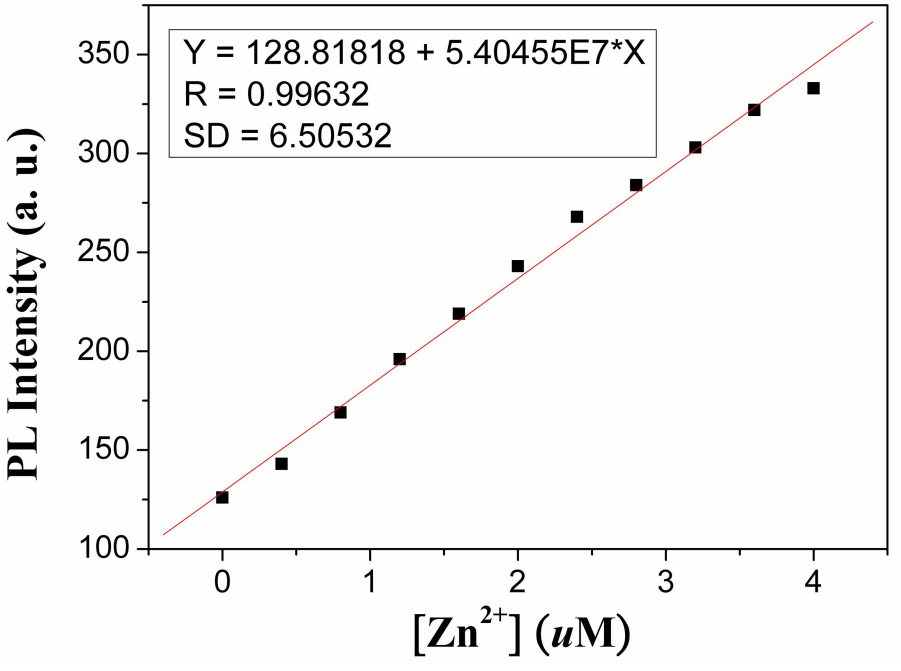

Figure S11. Linear analysis of the PL data of **3** with consecutive titration of Zn^{2+}.

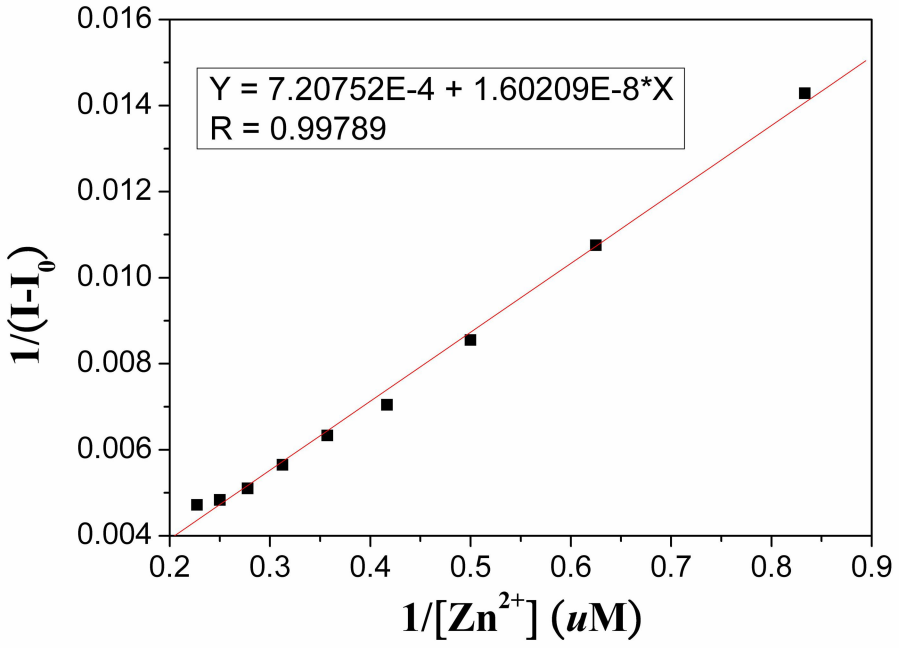

Figure S12. Benesi-Hildebrand plot of the absorption data of **3** with consecutive titration of Zn^{2+}.