

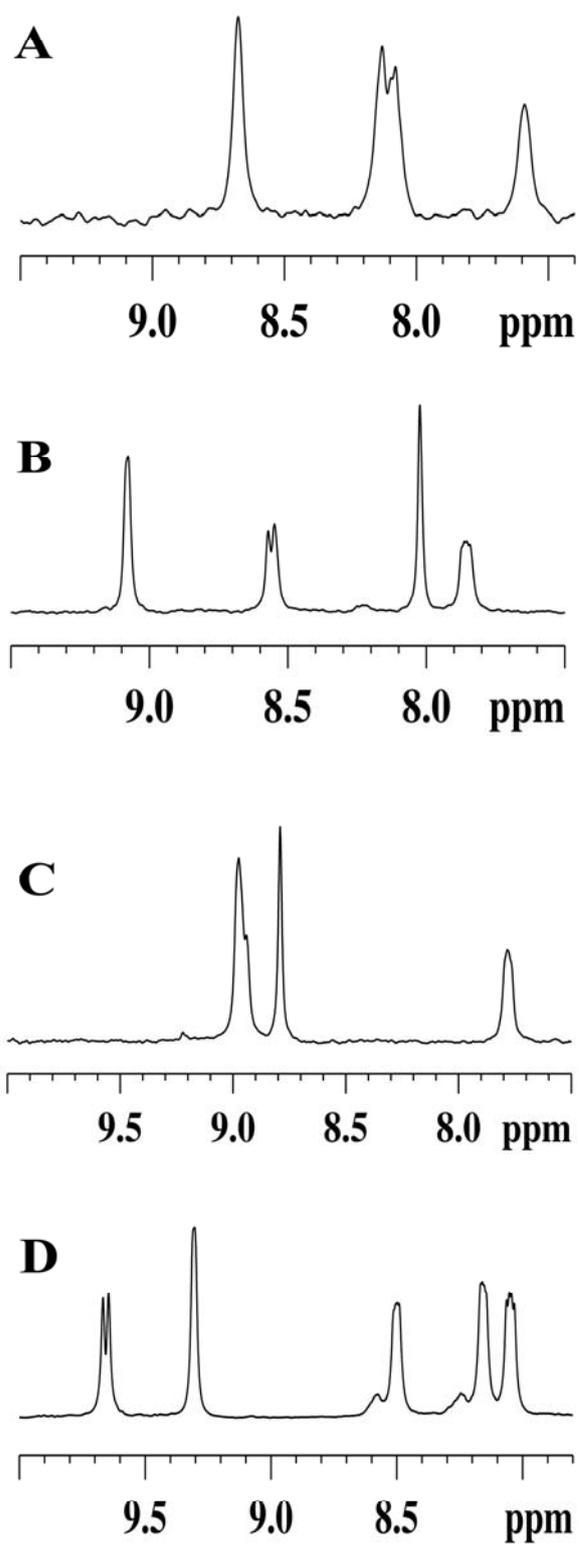
*Supporting Information for*

**Roles of DMSO-type ruthenium complexes in disaggregation  
of prion neuropeptide PrP106-126**

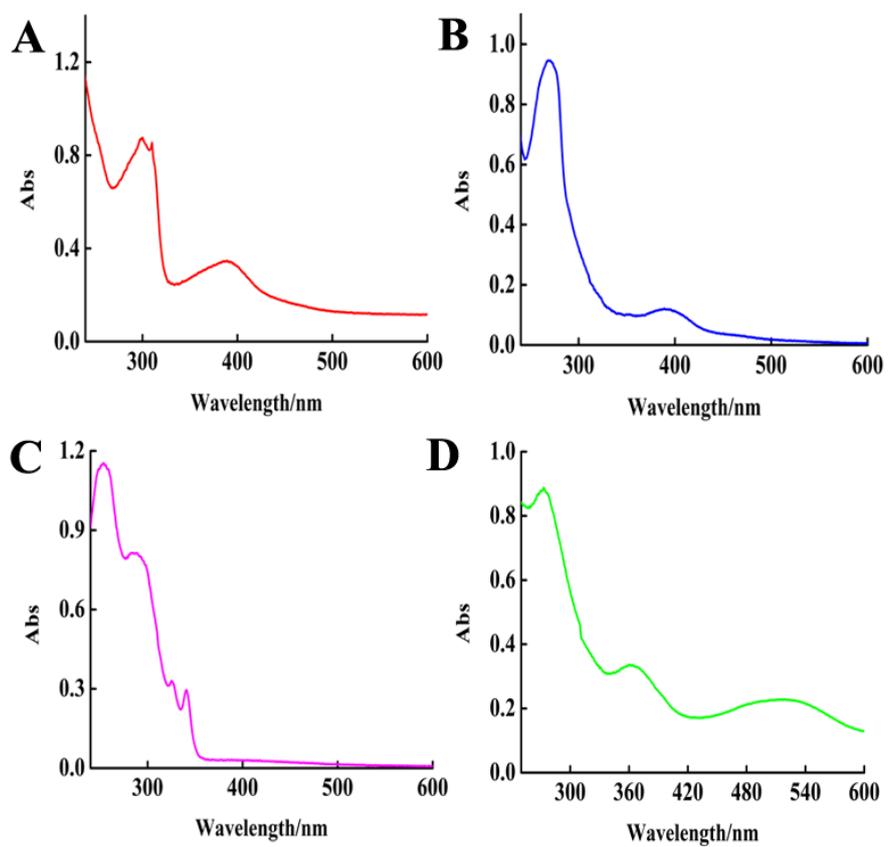
Dengsen Zhu,<sup>1</sup> Cong Zhao,<sup>1</sup> Xuesong Wang,<sup>1</sup> Wenji Wang,<sup>1</sup> Baohuai Wang,<sup>2</sup> Weihong Du<sup>1,\*</sup>

<sup>1</sup>*Department of Chemistry, Renmin University of China, Beijing, 100872, China*

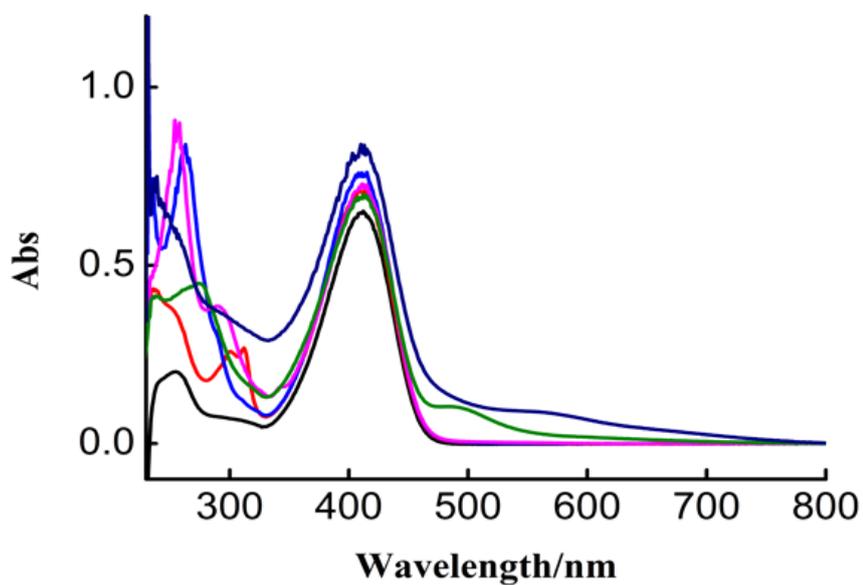
<sup>2</sup>*College of Chemistry and Molecular Engineering, Peking University, 100871, China*



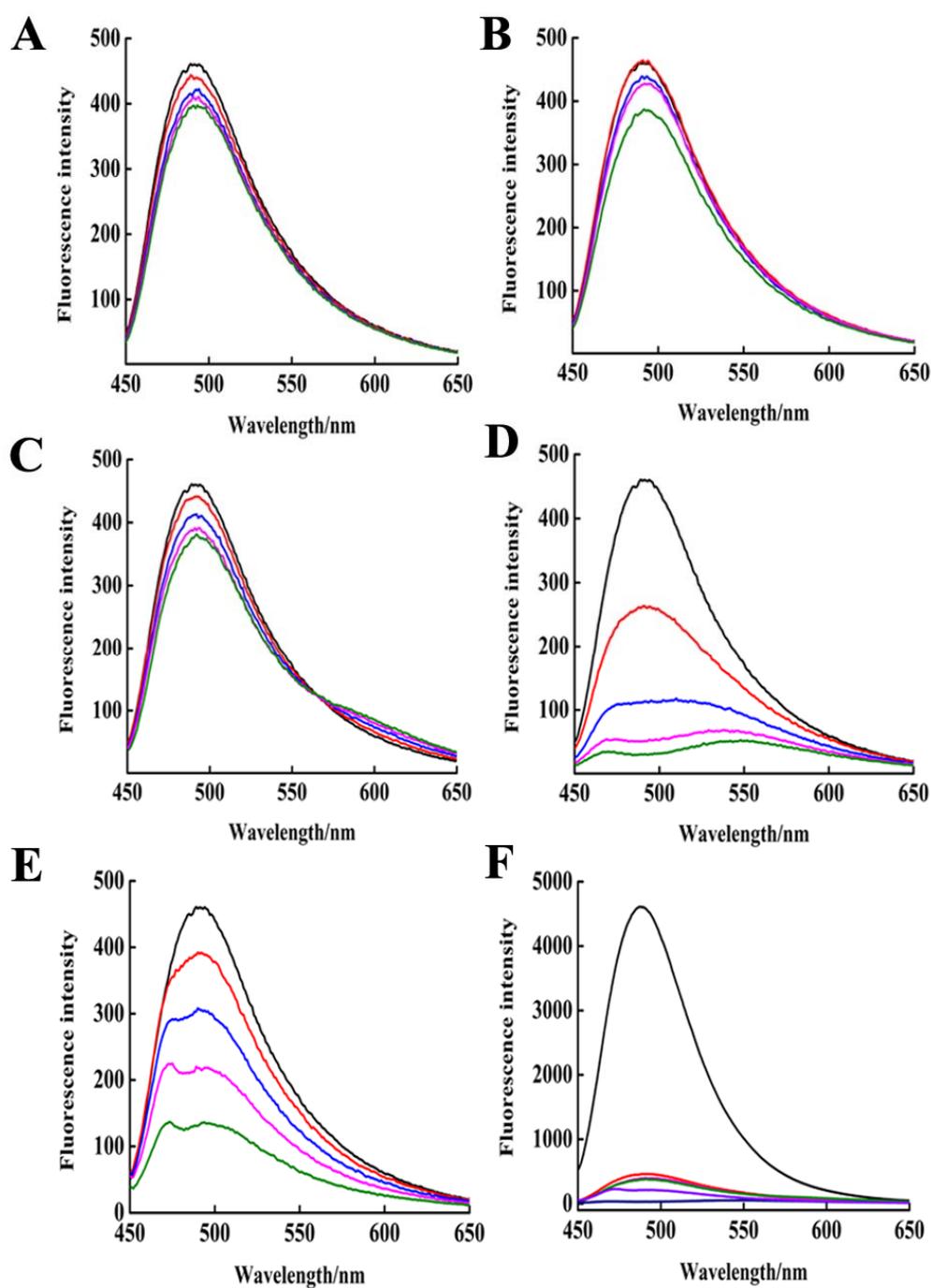
**Fig. S1**  $^1\text{H}$  NMR spectra of complexes **1**, **2**, **3**, and **4** in  $\text{H}_2\text{O}/\text{DMSO}$  at pH 5.7, 298 K, respectively.



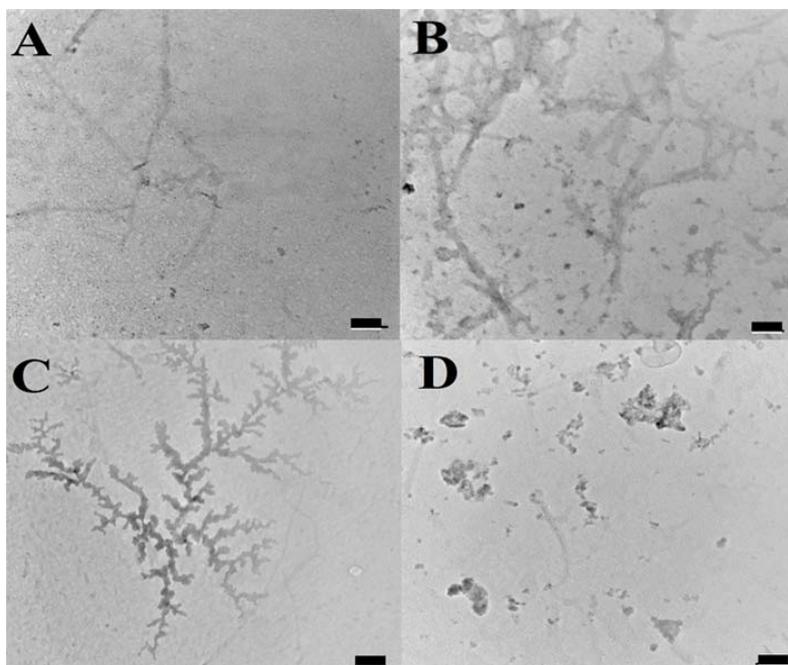
**Fig. S2** UV absorption spectra of four Ru complexes. The complexes concentration was 50  $\mu$ M. (A) 1, (B) 2, (C) 3, and (D) 4.



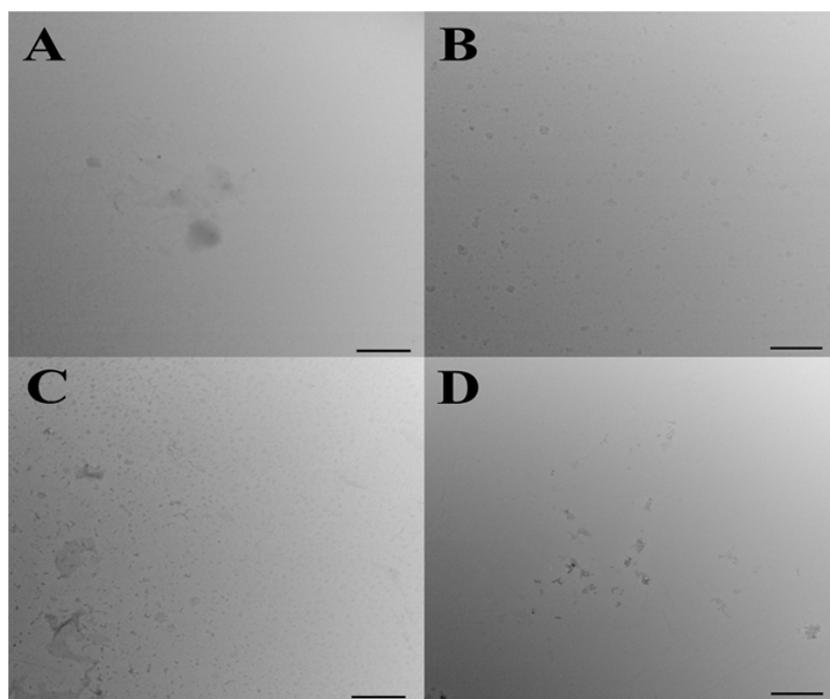
**Fig. S3** UV absorption spectra of ThT in the absence (black) and presence of complex **1** (red), **2** (blue), **3** (magenta), **4** (olive) and RuCl<sub>3</sub> (navy), after subtracting the absorption of metal complex. The concentrations of ThT and metal complex were 100  $\mu$ M both. A slight hyperchromic effect confirmed the interaction of ThT and the complex.



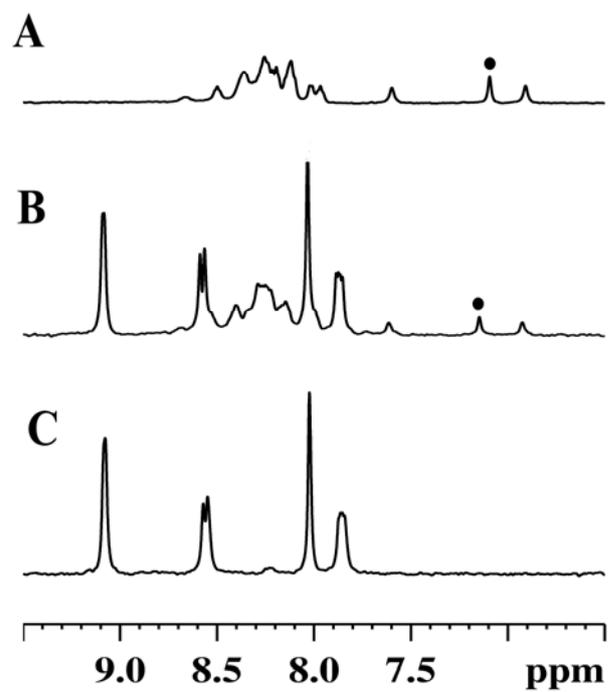
**Fig. S4** Fluorescence intensity of ThT in the absence (black) and presence of Ru complex at concentrations of 20 $\mu$ M (red), 50 $\mu$ M (blue), 80 $\mu$ M (magenta), and 100 $\mu$ M (olive) for **1**(A), **2**(B), **3**(C), **4** (D) and RuCl<sub>3</sub> (E) respectively. (F) Comparison of the fluorescence intensity of ThT with aggregated PrP106-126 (black), ThT alone (red), ThT with complex **1**(blue), **2** (magenta), **3**(olive), **4**(navy) and RuCl<sub>3</sub> (violet) respectively at 100 $\mu$ M .



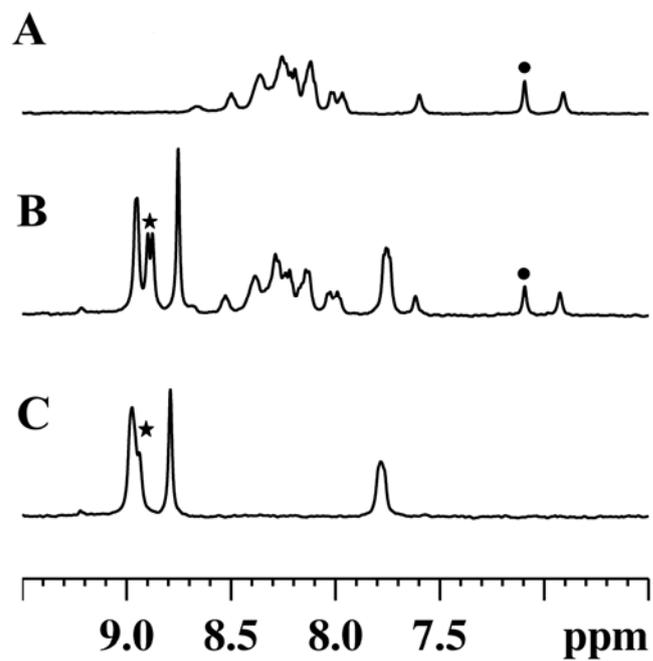
**Fig. S5** TEM images of PrP106-126 in presence of **1** (A), **2** (B), **3** (C), and **4** (D) respectively. The molar ratio of Ru complex to peptide was 0.2. The scale bar is 100 nm.



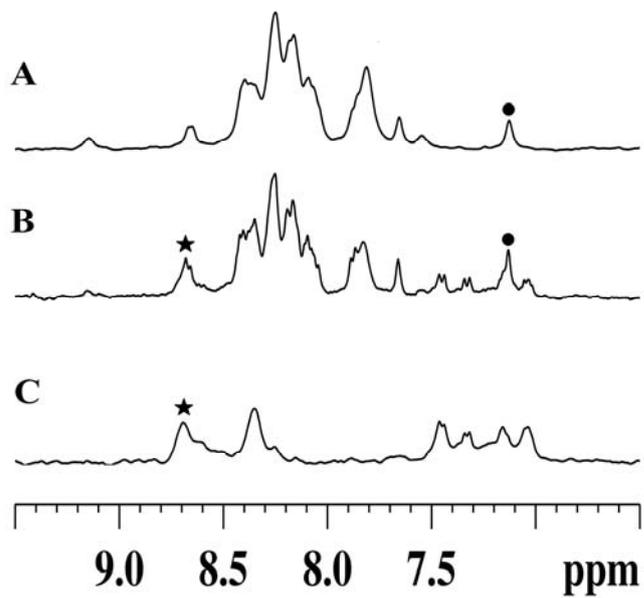
**Fig. S6** TEM images of PrP106-126 in presence of complex **1** (A), **2** (B), **3** (C) and **4** (D) respectively. The molar ratio of Ru complex to peptide was 3.0. The scale bar is 500 nm.



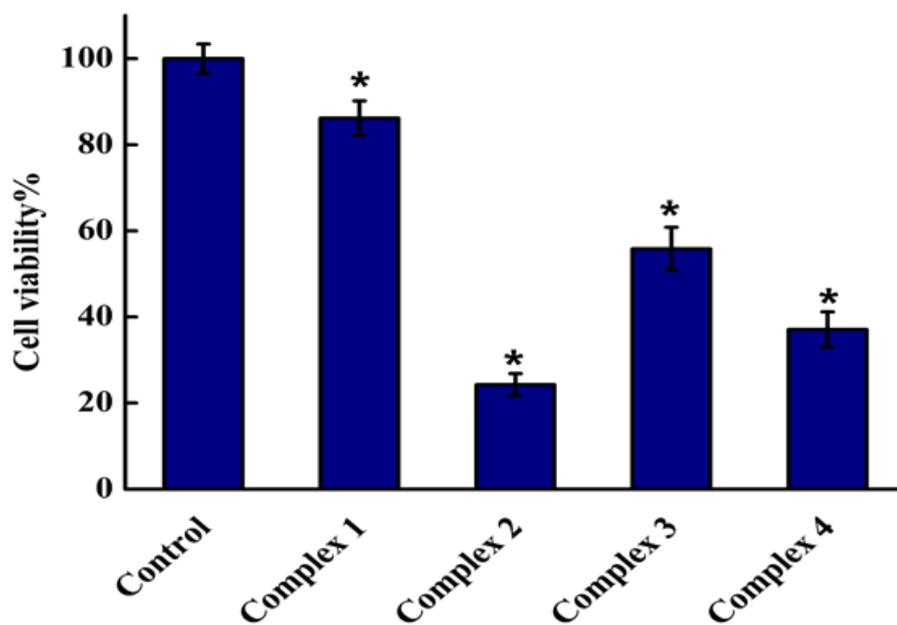
**Fig. S7** <sup>1</sup>H NMR spectra of PrP106-126 in H<sub>2</sub>O/DMSO at pH 5.7, 298 K. PrP106-126 alone (A), PrP106-126 in the presence of triple amounts of complexes **2** (B) and complex **2** alone (C).



**Fig. S8**  $^1\text{H}$  NMR spectra of PrP106-126 in  $\text{H}_2\text{O}/\text{DMSO}$  at pH 5.7, 298 K. PrP106-126 alone (A), PrP106-126 in the presence of triple amounts of complexes **3** (B) and complex **3** alone (C).



**Fig. S9**  $^1\text{H}$  NMR spectra of PrP106-126 in  $d_6$ /DMSO at pH 5.7, 298 K. PrP106-126 alone (A), PrP106-126 in the presence of triple amounts of complexes **4** (B) and complex **4** alone (C).



**Fig. S10** Effects of ruthenium complexes on the cytotoxicity of determined through an MTT assay. Human SH-SY5Y neuroblastoma cells were treated with ruthenium complexes (10  $\mu$ M). \*P<0.01 versus control group. The data were from the average of four repeated experiments.