Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Inofrmation for

Influence of Oxodiperoxovanadate Complexes on Prion Neuropeptide Fibril Formation

Table S1 Equilibration time in NMR time course experiments.

Vanadium complexes	**Equilibration time /min**	
	PrP106-126	**M109F**
$[NH_4]_3[VO(O_2)_2(OX)]\cdot 2H_2O$, **1**	92	60
$Na[VO(O_2)_2]\cdot Na_2SO_4$, **3**	142	132
$K_2[nicH\{VO(O_2)_2\}_2]\cdot H_2O$, **4**	60	50

Table S2 Equilibration time in NMR time course experiments.

Compound	**Equilibration time /min**	
	PrP106-126	**M109F**
H_2O_2	967	646

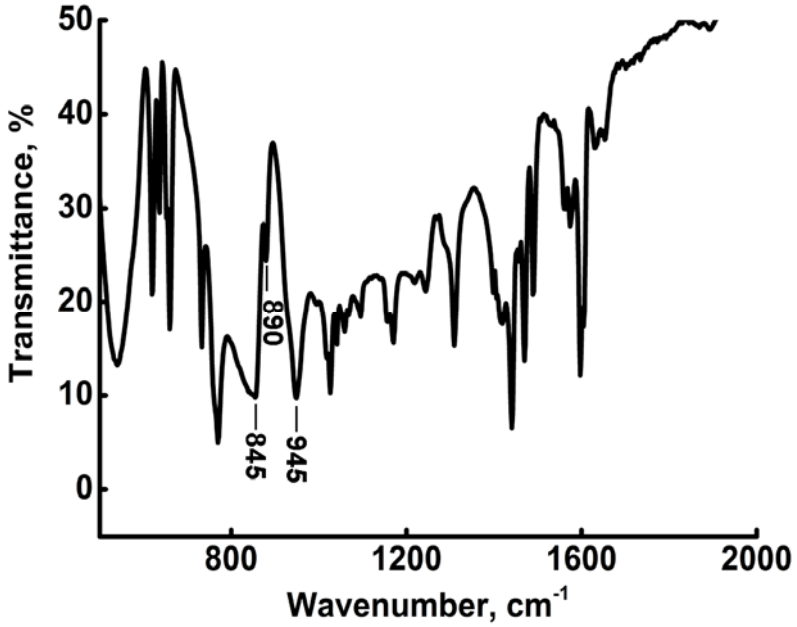

Figure S1. The IR spectrum of complex **2**, in which the peaks match those reported in ref.[44].

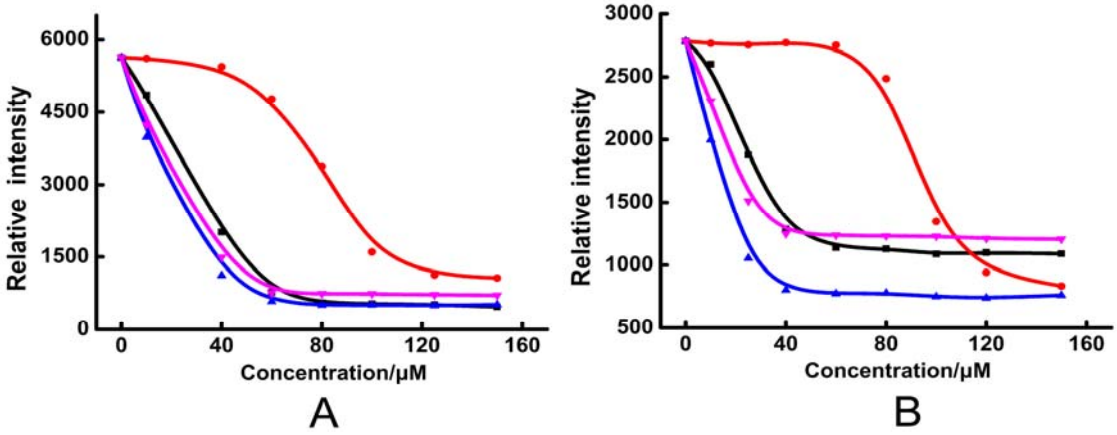

Figure S2. The IC_{50} determination for PrP106-126(A) and M109F(B) in the presence of **1** (black), **2** (red), **3** (blue) and **4** (magenta). The peptide concentration is 50 μM.

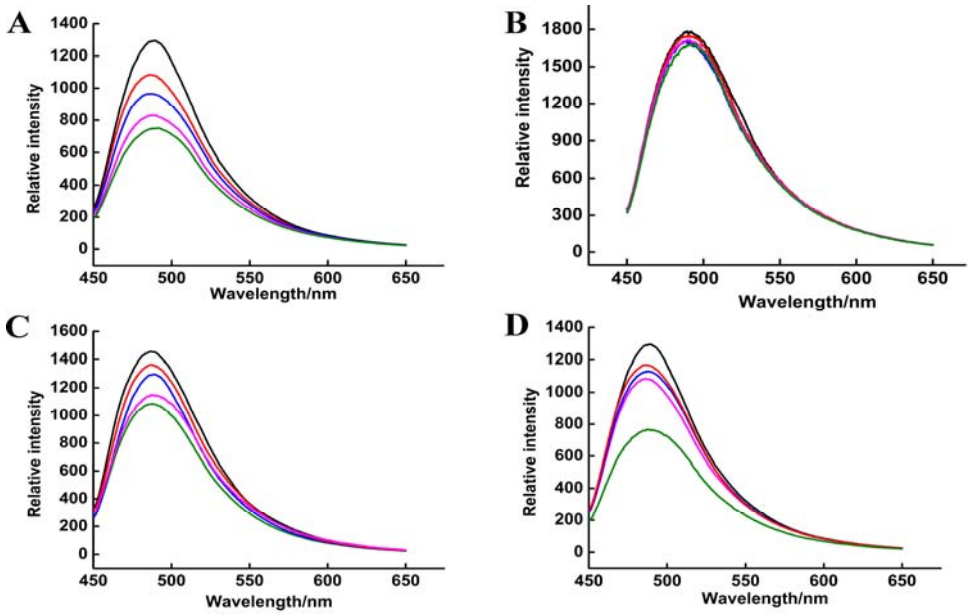

Figure S3. Competition of vanadium complex with ThT to bind PrP106-126. The sample was composed of 10 μM PrP106-126 and 40 μM ThT in the absence and presence of complex **1** (A), **2** (B), **3** (C) and **4** (D). The concentrations of vanadium complexes were 0 (black), 3 μM (red), 6 μM (blue),10 μM (megenta) and 20 μM (olive).

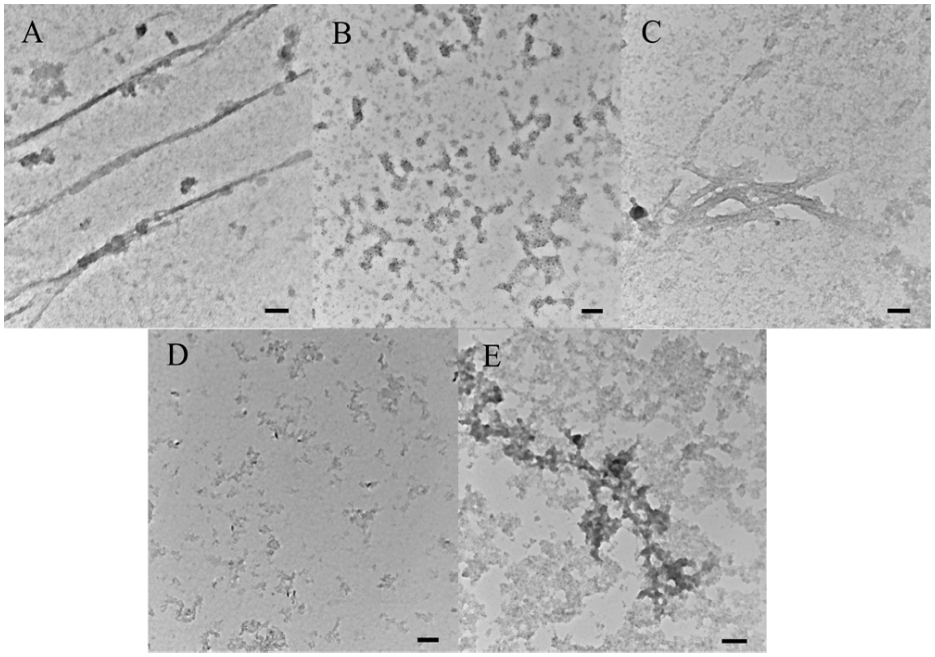

Figure S4. TEM images of peptide M109F in the absence (A) and presence of two equivalents of **1** (B), **2** (C), **3** (D) and **4** (E). The scale bar is 100 nm.

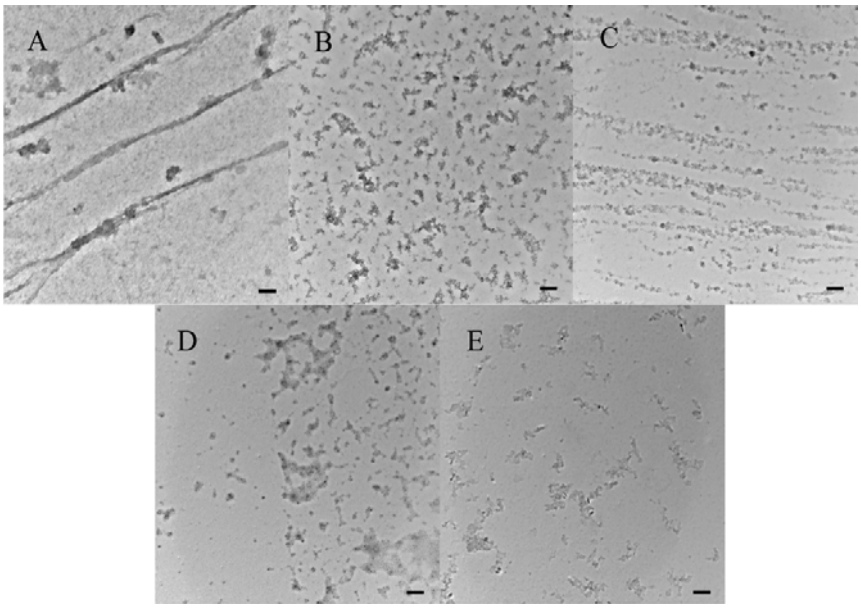

Figure S5. TEM images of peptide M109F in the absence (A) and presence of ten equivalents of **1** (B), **2** (C), **3** (D) and **4** (E). The scale bar is 100 nm.

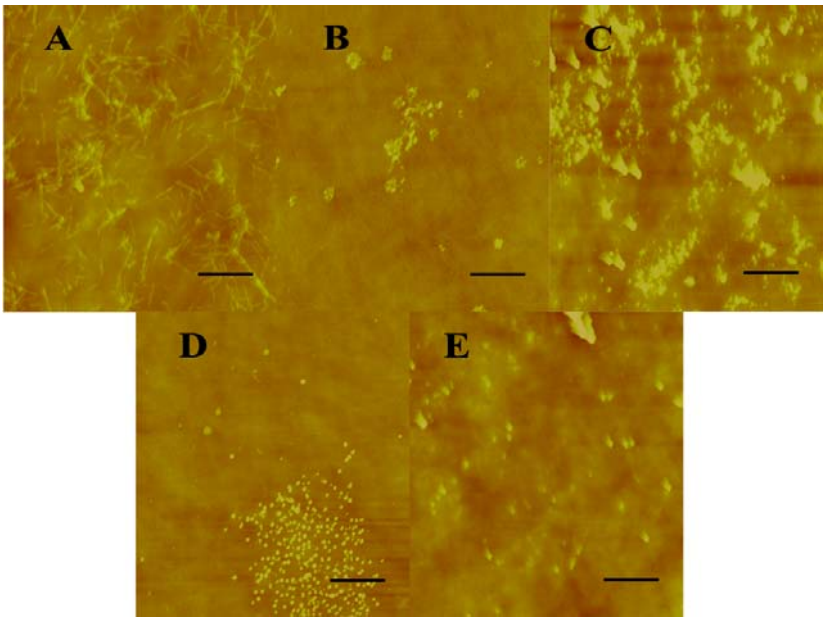

Figure S6. AFM images of peptide M109F in the absence (A) and presence of two equivalents of **1** (B), **2** (C), **3** (D) and **4** (E). The scale bar is 1μm.

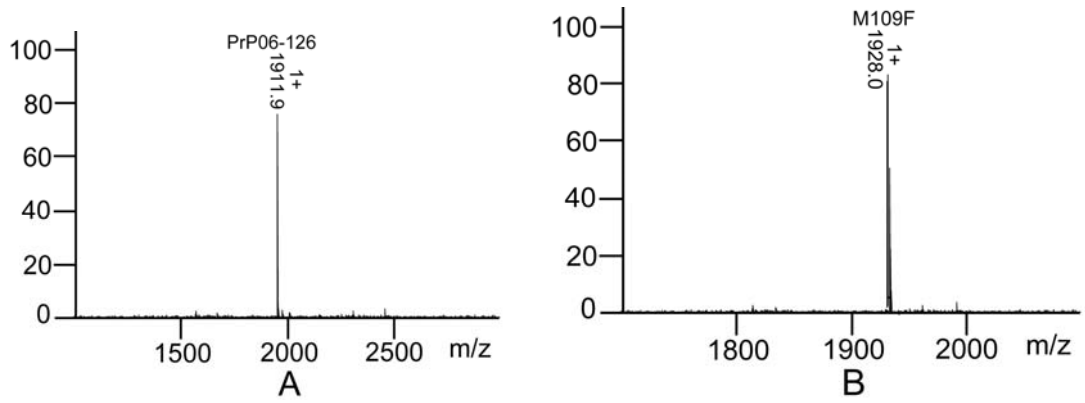

Figure S7. ESI-MS spectra of free PrP106-126 (A) and peptide M109F (B) alone.

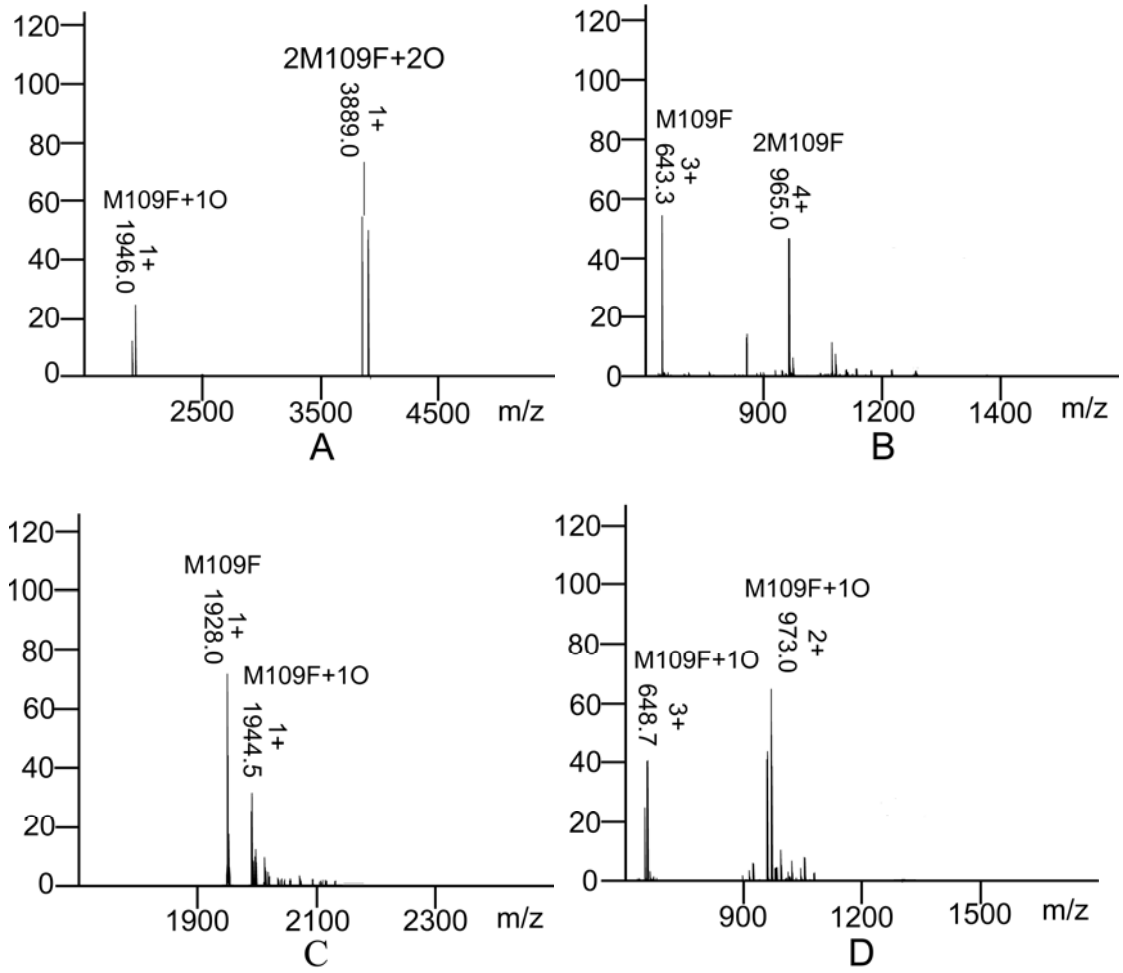

Figure S8. ESI-MS spectra for the peptide M109F in the presence of two equivalents of **1** (A), **2** (B), **3** (C) and **4** (D).

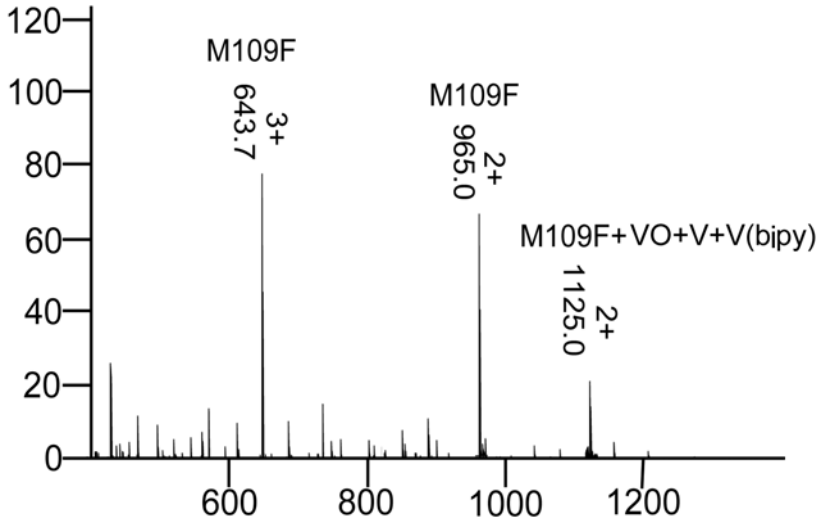

Figure S9. ESI-MS spectra for the peptide M109F in the presence of ten equivalents of **2**.

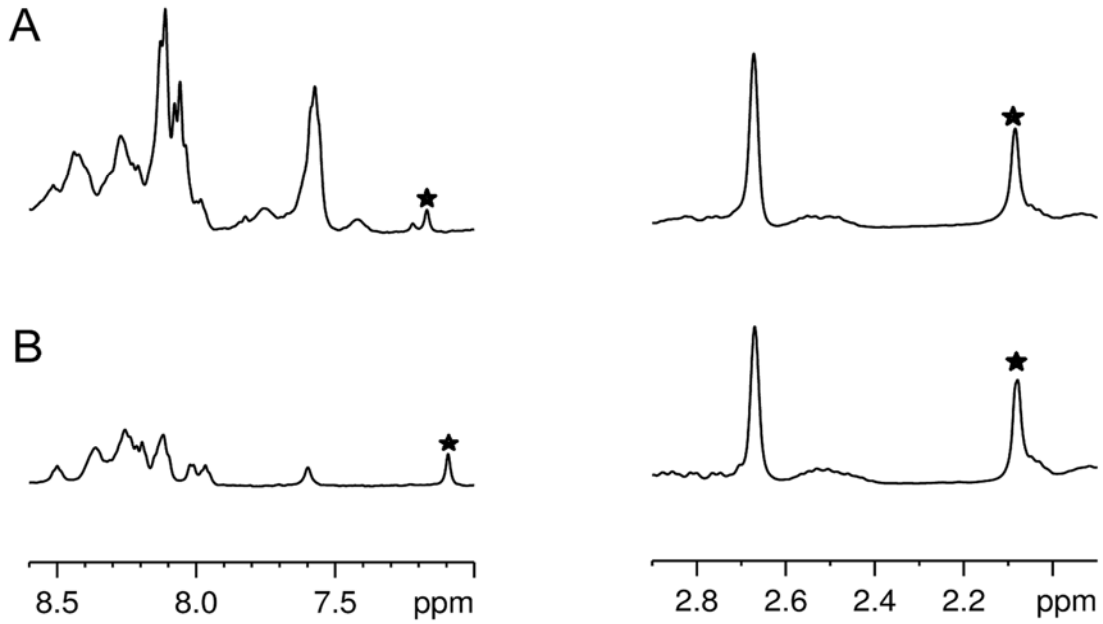

Figure S10. ^{1}H NMR spectra of PrP106-126 in the presence (A) and absence (B) of **2**. The marked peaks at 7.09 ppm and 2.08 ppm are assigned to the side chain of His111 and Met109/112. Addition of **2** made the peak at 7.09 ppm shift toward down-field. No oxidized methionine peak was observed.

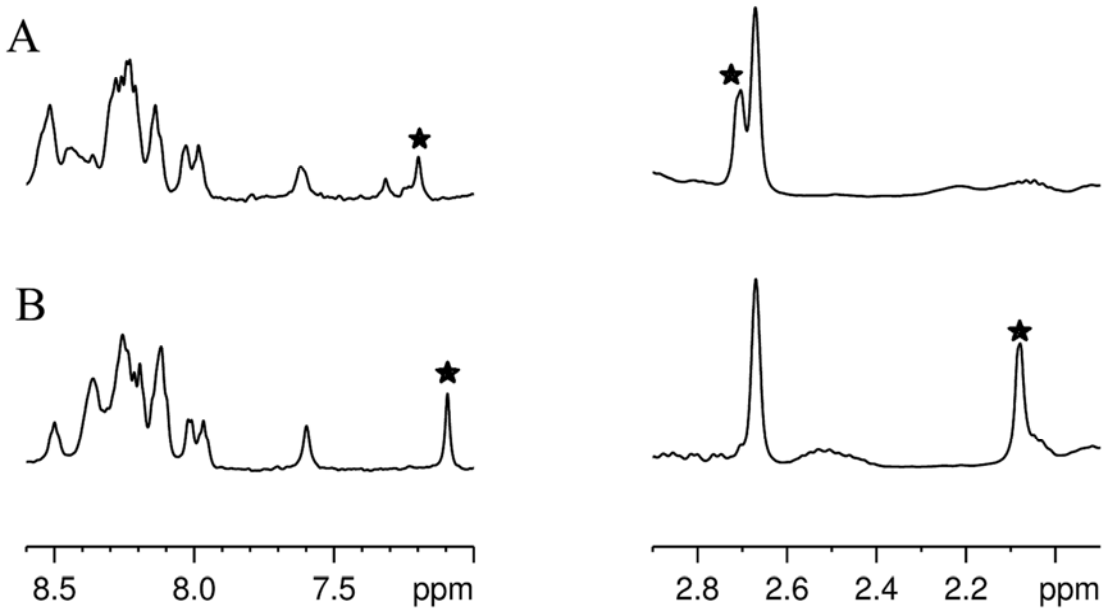

Figure S11. ^{1}H NMR spectra of PrP106-126 in the presence (A) and absence (B) of **3**. The marked peaks at 7.09 ppm and 2.08 ppm are assigned to the side chain of His111 and Met109/112. The peak at 2.71 ppm is attributed to methyl protons of oxidized methionines. Addition of **3** made the peak at 7.09 ppm shift toward down-field.

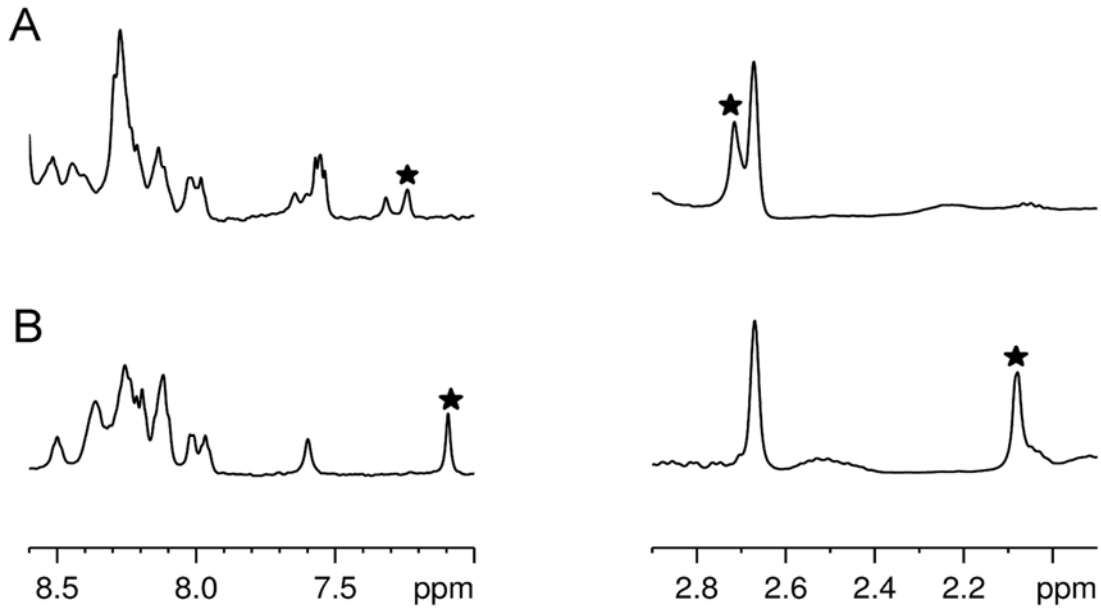

Figure S12. ^{1}H NMR spectra of PrP106-126 in the presence (A) and absence (B) of **4**. The marked peaks at 7.09 ppm and 2.08 ppm are ascribed to the side chain of His111 and Met109/112. The peak at 2.71 ppm is attributed to methyl protons of oxidized methionines. Addition of **4** made the peak at 7.09 ppm shift toward down-field.

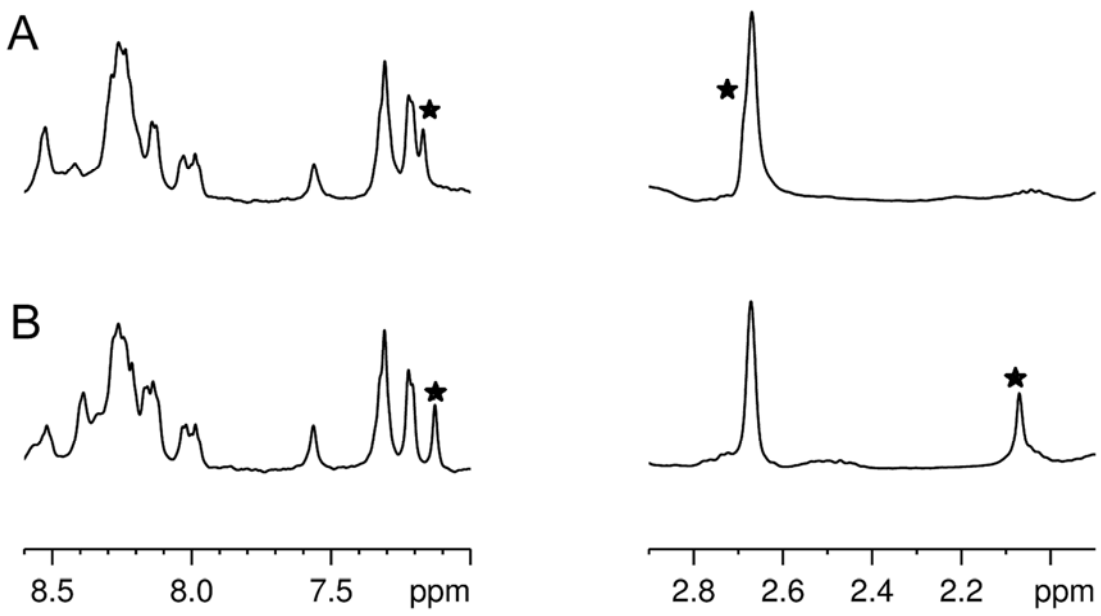

Figure S13. ^{1}H NMR spectra of peptide M109F in the presence (A) and absence (B) of **1**. The marked peaks at 7.13 ppm and 2.08 ppm are ascribed to the side chain of His111 and Met112. The new shoulder peak at 2.69 ppm is attributed to methyl protons of oxidized Met112. Addition of **1** made the peak at 7.13 ppm shift toward down-field.

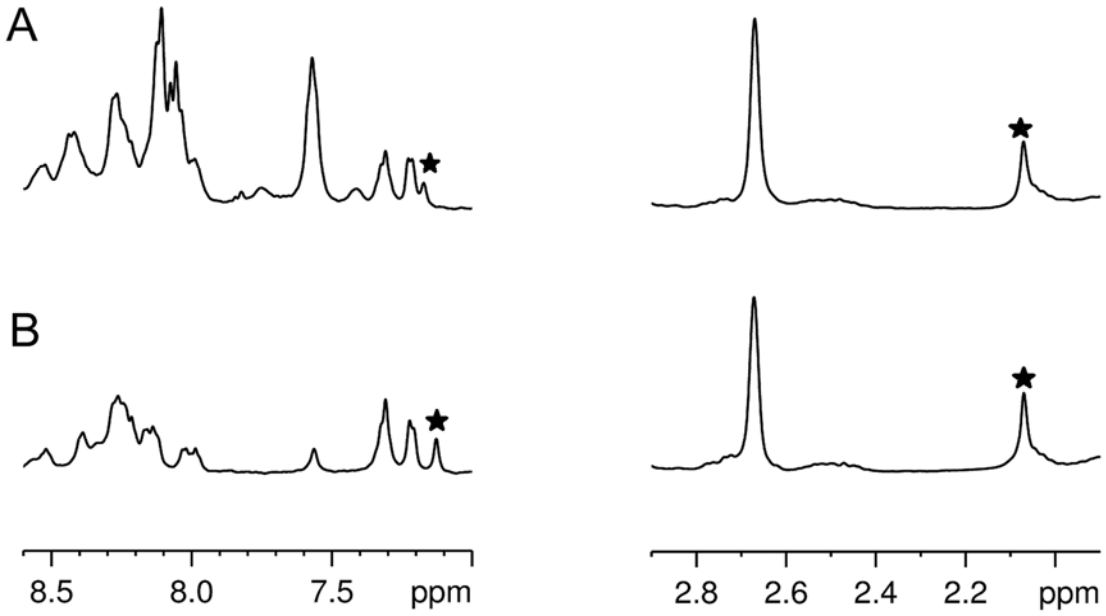

Figure S14. ^{1}H NMR spectra of peptide M109F in the presence (A) and absence (B) of **2**. The marked peaks at 7.13 ppm and 2.08 ppm are ascribed to the side chain of His111 and Met112. Addition of **2** made the peak at 7.13 ppm shift toward down-field and relaxed. No oxidized Met112 was observed.

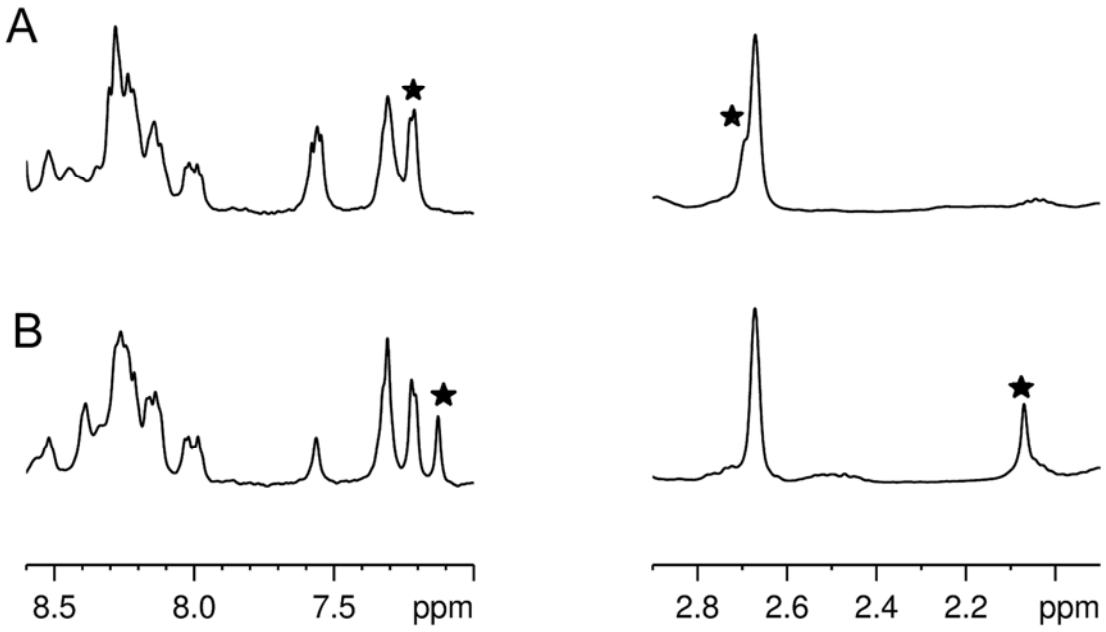

Figure S15. ^{1}H NMR spectra of peptide M109F in the presence (A) and absence (B) of **3**. The marked peaks at 7.13 ppm and 2.08 ppm are ascribed to the side chain of His111 and Met112. The new shoulder peak at 2.69 ppm is attributed to methyl protons of oxidized Met112. Addition of **3** made the peak at 7.13 ppm shift toward down-field.

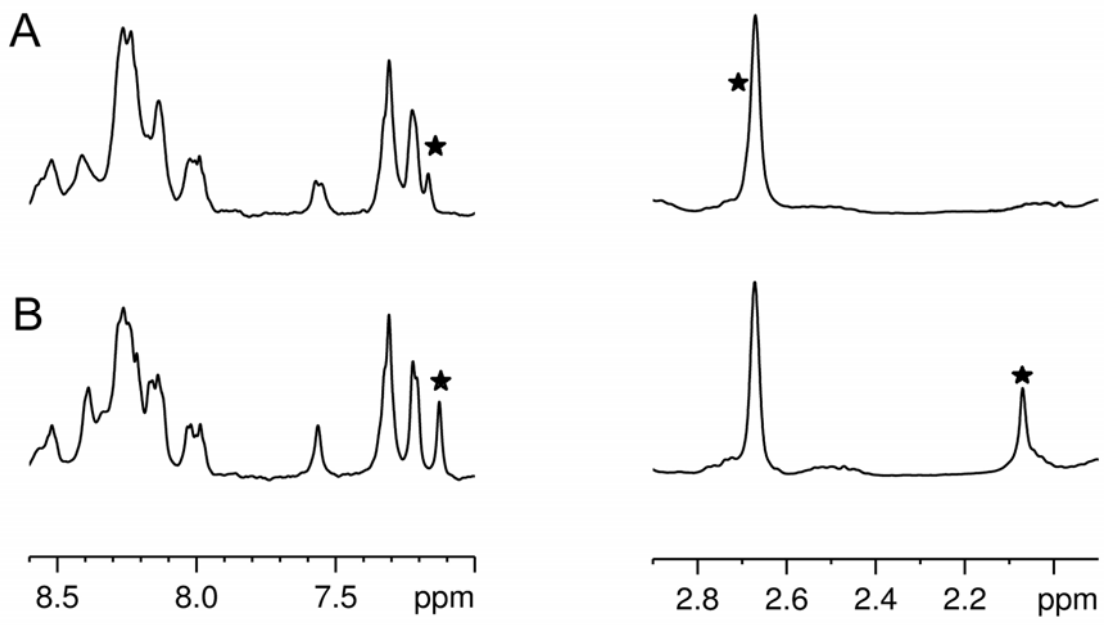

Figure S16. ^{1}H NMR spectra of peptide M109F in the presence (A) and absence (B) of **4**. The marked peaks at 7.13 ppm and 2.08 ppm are ascribed to the side chain of His111 and Met112. The peak at 2.08 ppm was decreased and the methyl protons of oxidized Met112 was overlapped with the peak of DMSO at 2.67 ppm. Addition of **4** made the peak at 7.13 ppm shift toward down-field and relaxed.

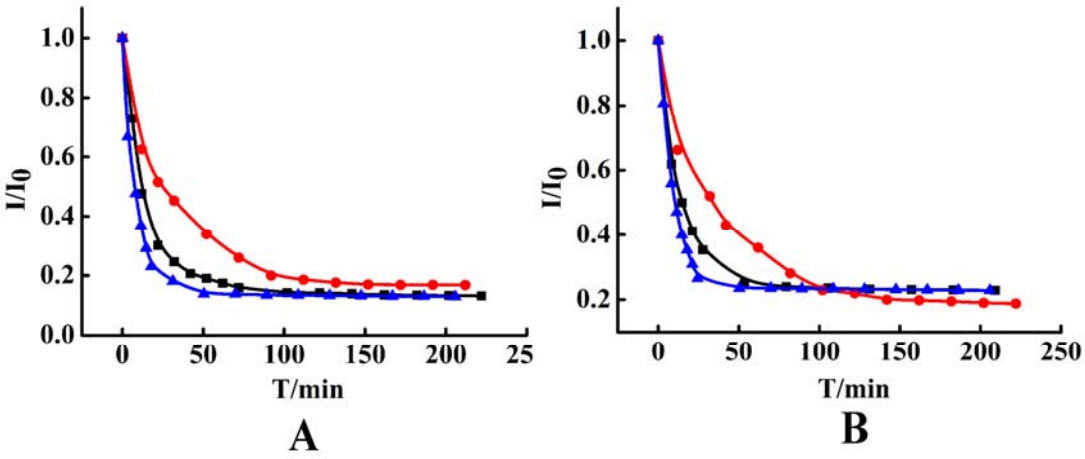

Figure S17. NMR time course experiments detected at 2.08 ppm for PrP106-126 (A) and M109F (B) in the presence of **1** (balck), **3** (red) and **4** (blue). The concentration of peptide is 500 μM and the molar ratio is 2 for each sample.

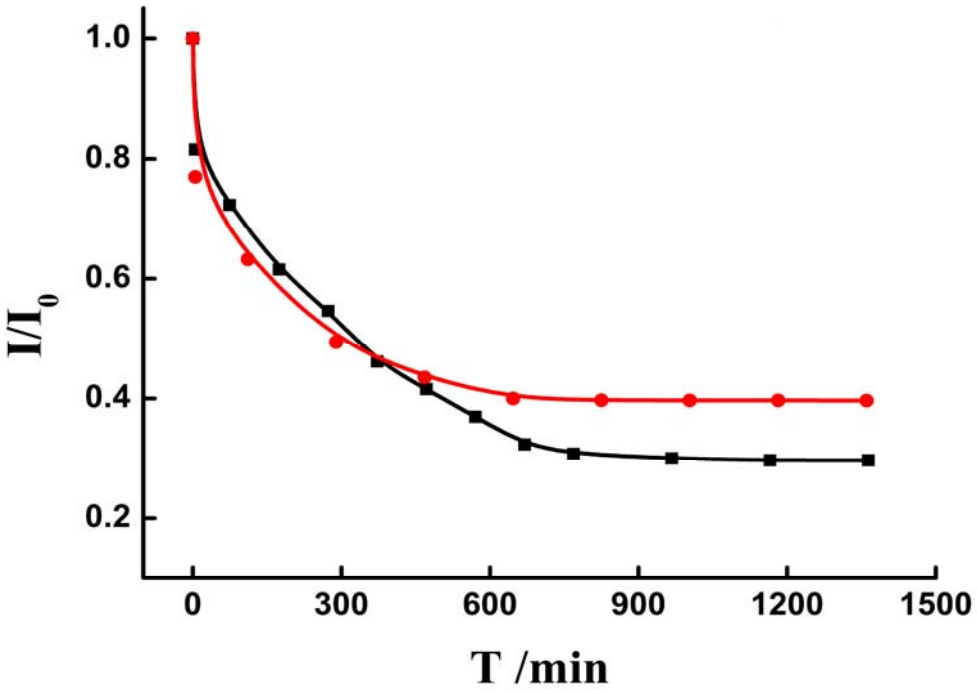

Figure S18. NMR time course experiments detected at 2.08 ppm for PrP106-126 (black) and M109F (red) in the presence of H_2O_2. The concentration of peptide is 500 μM and the molar ratio is 2 for each sample.

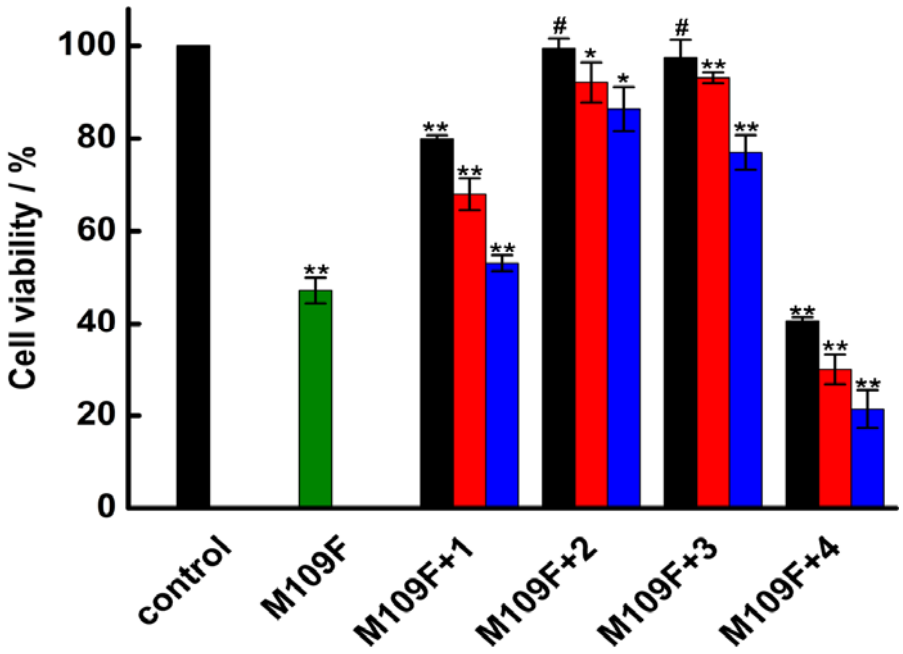

Figure S19. Cell viability was monitored using the MTT assay. SH-SY5Y cells were treated with peptide M109F and different concentrations of vanadium complexes, i.e. 1.0 μM (black), 10 μM (red) and 50 μM (blue). The cytotoxicity test of M109F alone (olive) was used for comparison. The data are shown as means ±SD, n=3.** $p<0.01$ and *$p<0.05$ compared to the control. # denotes not significant.

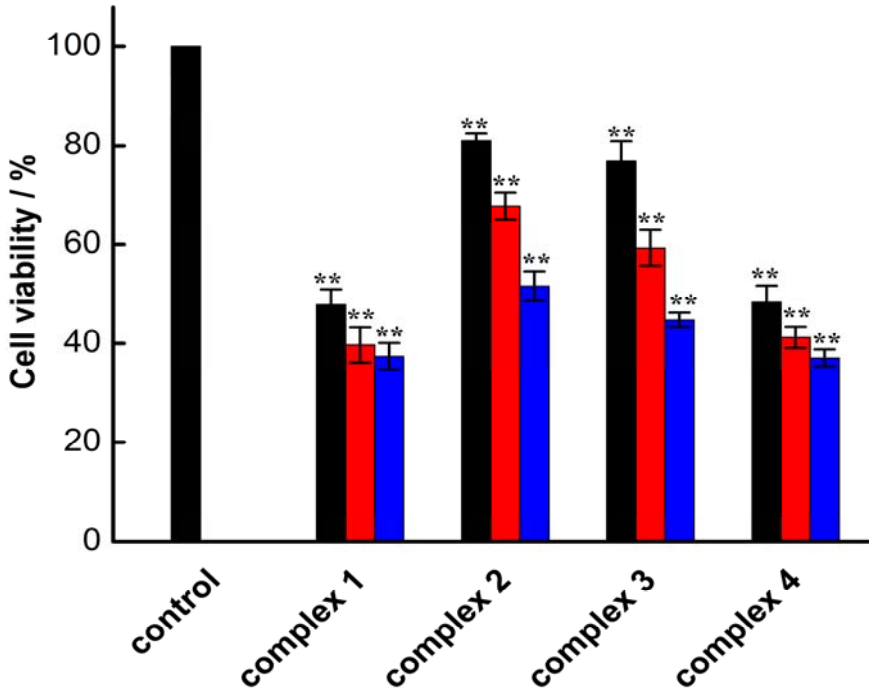

Figure S20. Cell viability was monitored using the MTT assay. SH-SY5Y cells were treated with different concentrations of vanadium complexes, i.e. 1μM (black), 10 μM (red) and 50 μM (blue) to detect the cytotoxicity of vanadium complex independently. The data are shown as means±SD, n=3.** $p<0.01$ and *$p<0.05$ compared to the control.