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硫黄素 T 对淀粉样 β -蛋白质 40 聚集成核动力学的双重影响

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Dual Effect of Thioflavin T on the Nucleation Kinetics of Amyloid β-Protein 40

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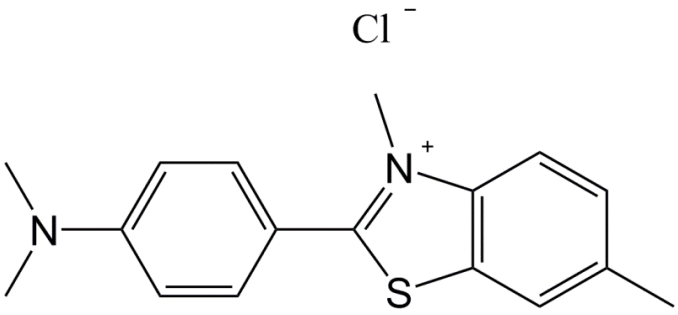

Fig.S1 Chemical structure of ThT

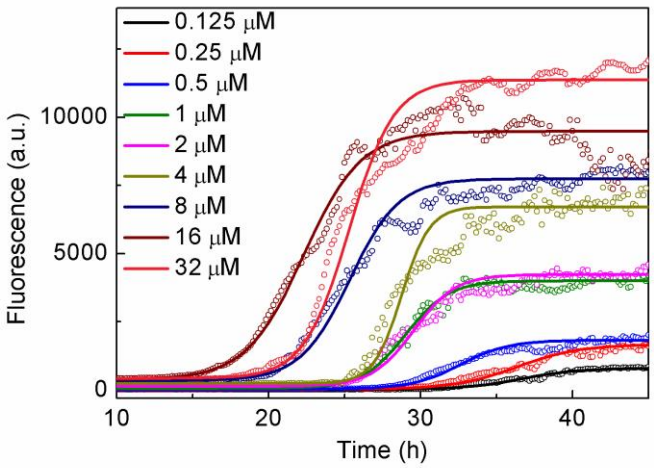

Fig.S2 Aggregation kinetics of 25 μmol·L^{-1} Aβ40 incubated with 0–32 μM ThT

The *in situ* incubations were done in PBS plus 0–32 μmol·L^{-1} ThT at 37 ℃. The solid lines are based on Eqs. (1) and (2).

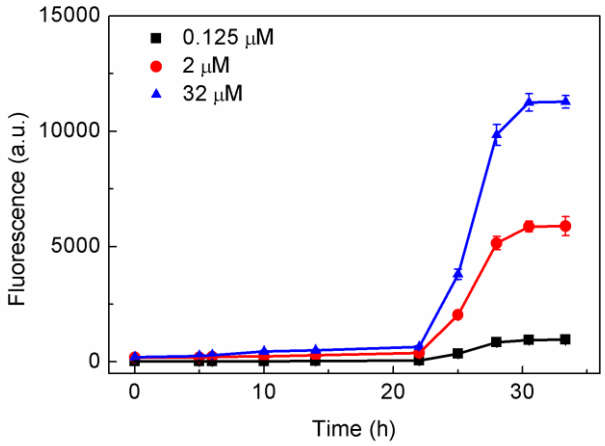

Fig.S3 Aggregation kinetics of 50 μM Aβ40 labeled with ThT of different concentrations (0.125, 2, and 32 μmol·L^{-1})

The *ex situ* incubations were done in PBS at 37 ℃. ThT for labeling was added after the incubation of the scheduled time.

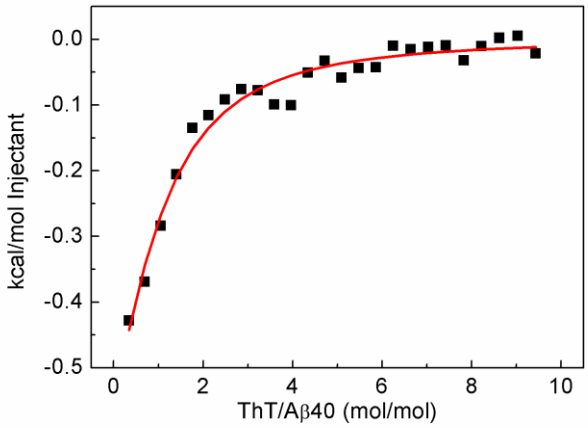

Fig.S4 ITC result of the binding of ThT to Aβ40

The initial concentrations of ThT and Aβ40 were 2.5 mmol·L^{-1} and 50 μmol·L^{-1}, and the final concentrations of them were 396.25 and 40.22 μmol·L^{-1}, respectively. Experiments were carried out in PBS at 37 ℃. The solid line was calculated by fitting the single-site binding model[1] to the experimental data.

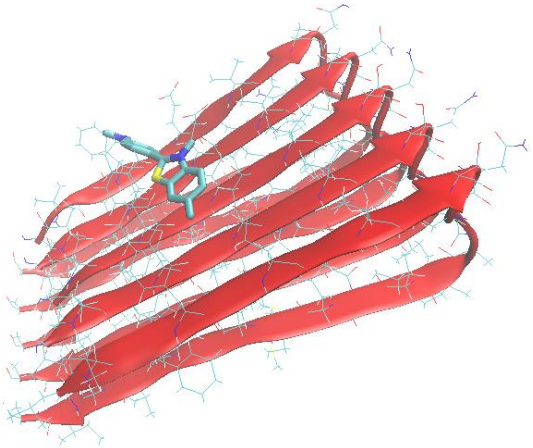

Fig.S5 Primary binding site of ThT on the Aβ17-42 fibrils

The backbone and side chains of Aβ17-42 monomer are shown by a red NewCartoon model and thin sticks, respectively. The ThT molecule is represented in licorice model. Atoms are colored red for oxygen, blue for nitrogen, white for hydrogen, green for carbon and yellow for sulphur. The snapshot is plotted with the visual molecular dynamics (VMD) software.

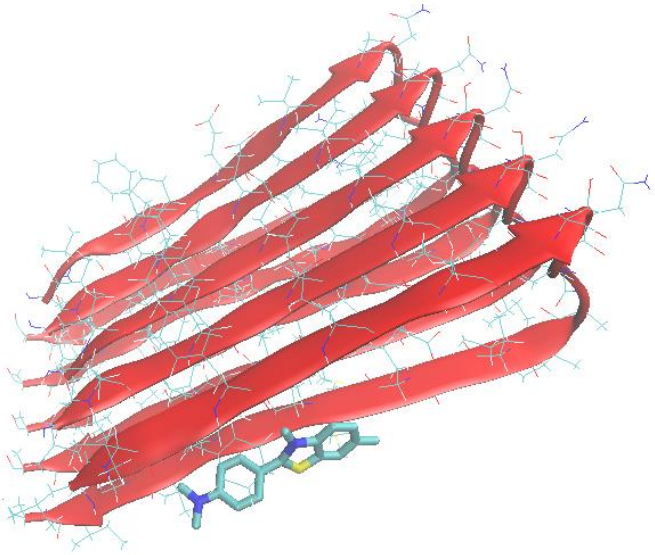

Fig.S6 Secondary binding site of ThT on the Aβ17-42 fibrils

The illustrations of the snapshot is the same as those described in the caption to Fig.S5.