Electronic Supplymentory Information

Genesis of Neuroprotective Peptoid from Aβ30-34 Inhibits Aβ Aggregation and AChE Activity

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Supplementary Figures

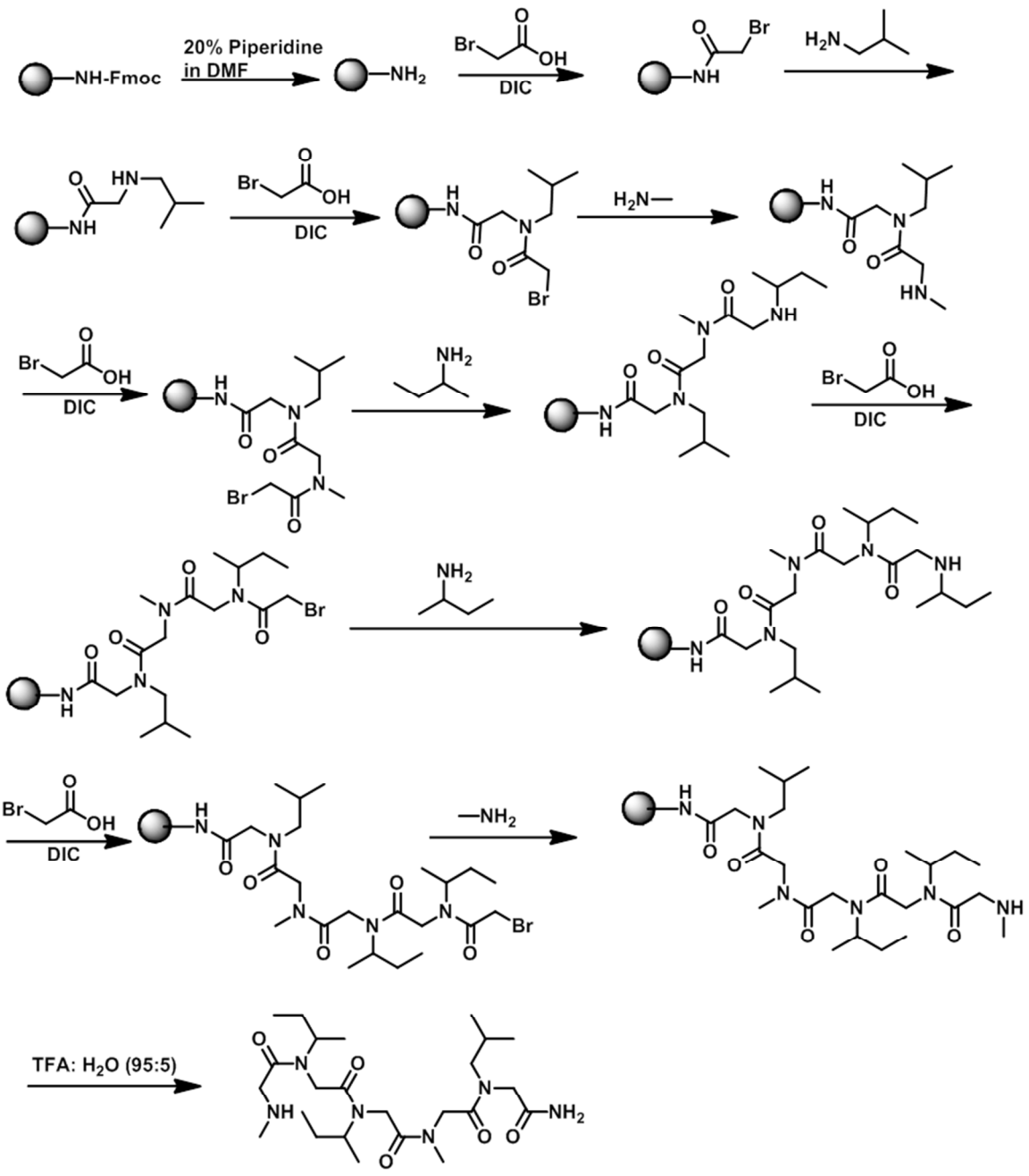
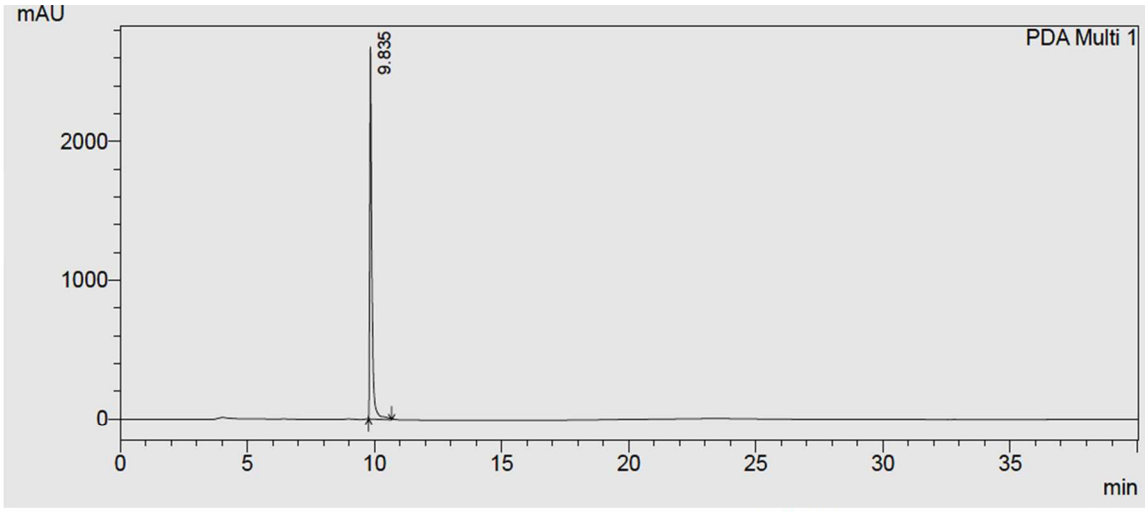


Figure S1. Synthetic scheme for preparation of AIIAL peptoid by solid phase method.



PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	9.835	15373686	2677058	100.000	100.000
Total		15373686	2677058	100.000	100.000

Figure S2. HPLC chromatogram of AI peptoid.

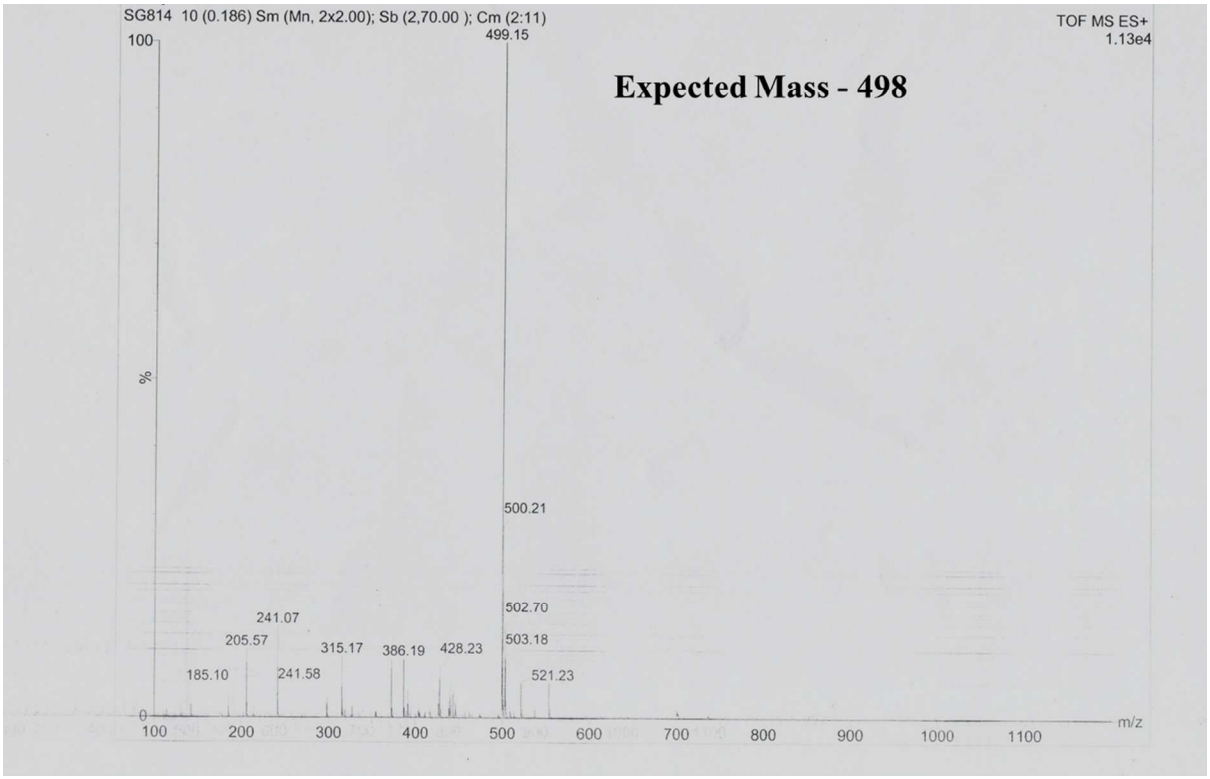
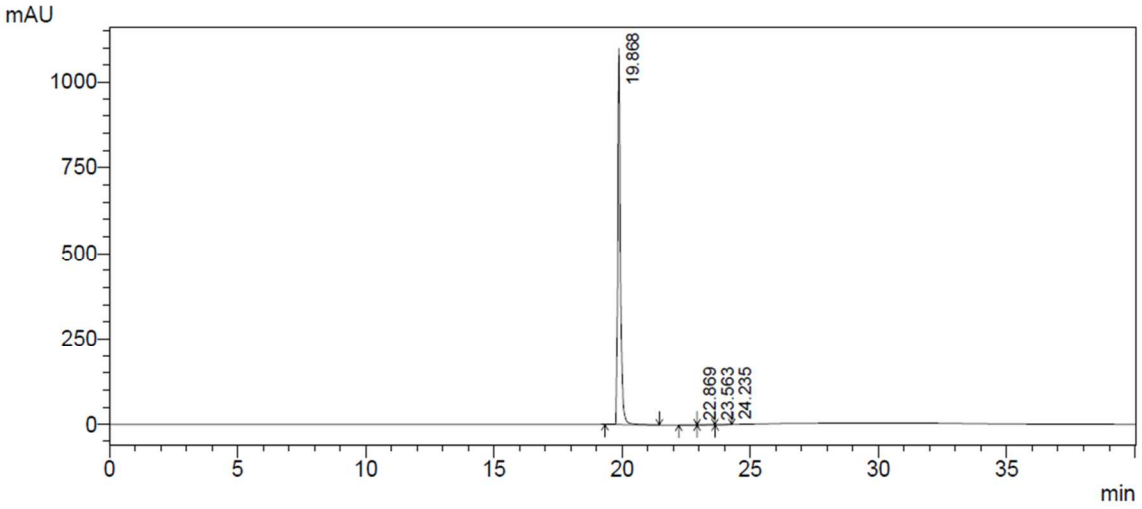


Figure S3. MASS data of AI peptoid shows 499 (498+H^+) Da.



PeakTable

PDA Ch1 210nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	19.893	33972675	4004353	100.000	100.000
Total		33972675	4004353	100.000	100.000

Figure S4. HPLC chromatogram of 5(6)-Carboxyfluorescein attached AI peptoid.

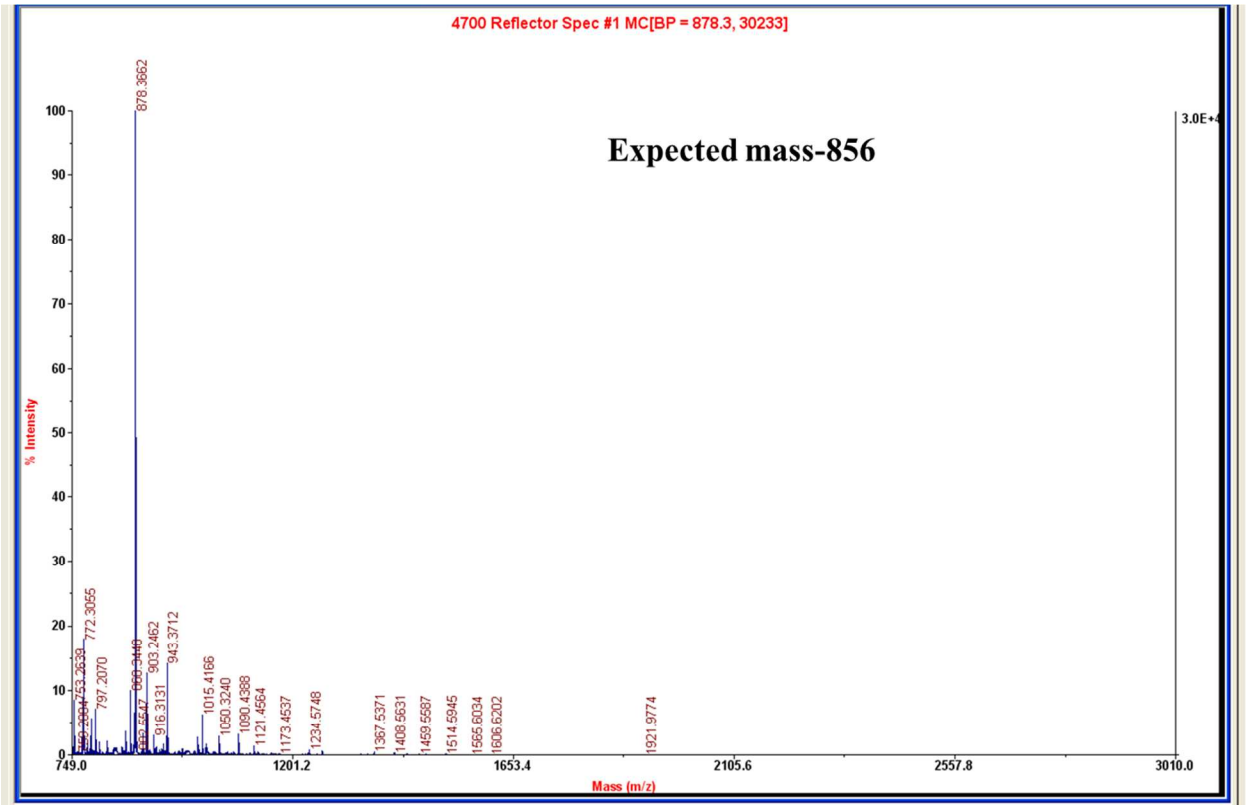
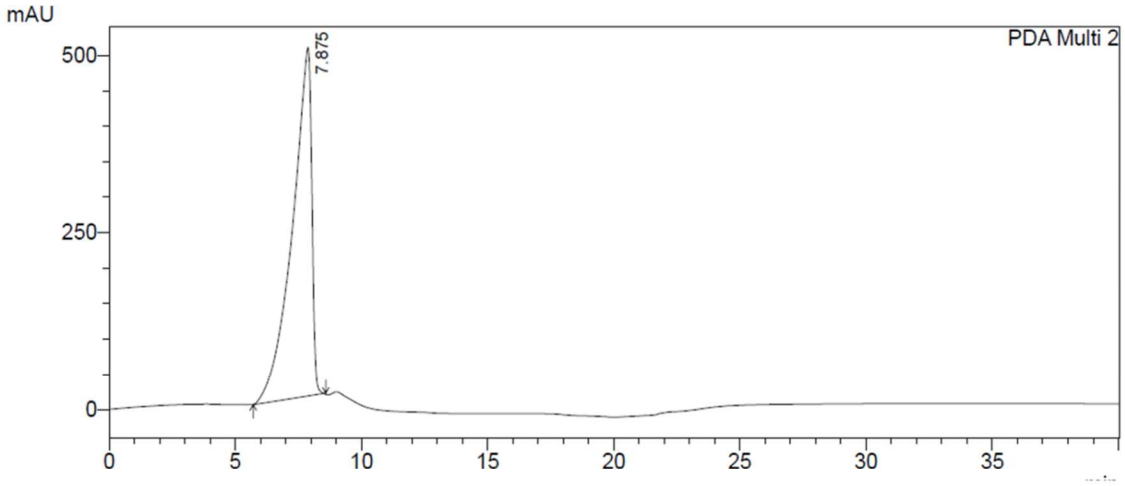


Figure S5. MASS data of 5(6)-Carboxyfluorescein attached AI peptoid.



PeakTable

PDA Ch2 260nm 4nm

Peak#	Ret. Time	Area	Height	Area %	Height %
1	7.875	26090686	492451	100.000	100.000
Total		26090686	492451	100.000	100.000

Figure S6. HPLC chromatogram of AI peptide.

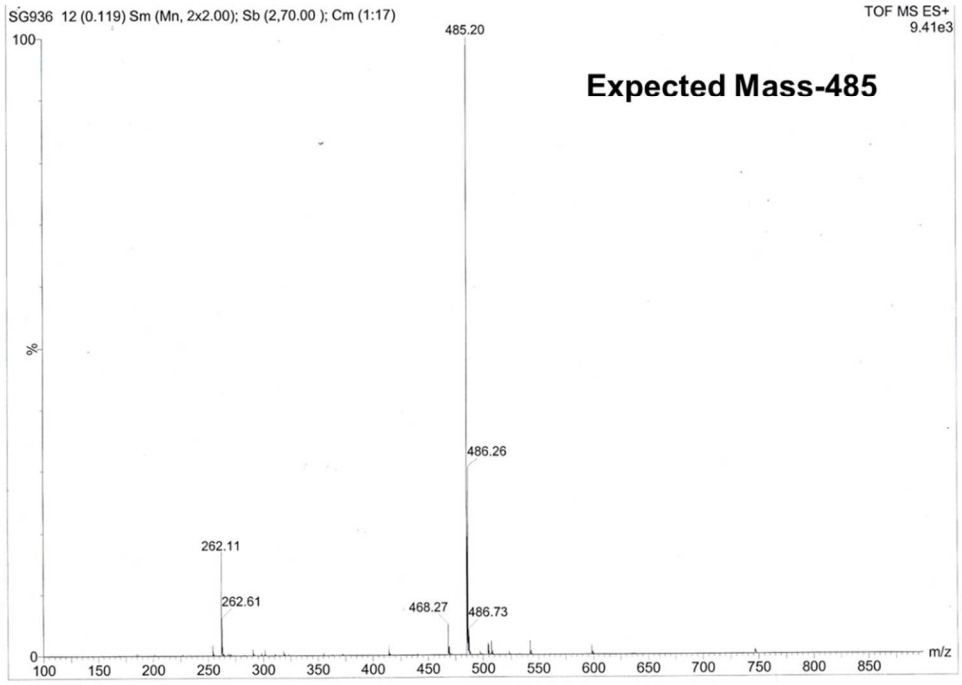


Figure S7. MASS data of AI peptide shows 485 Da.

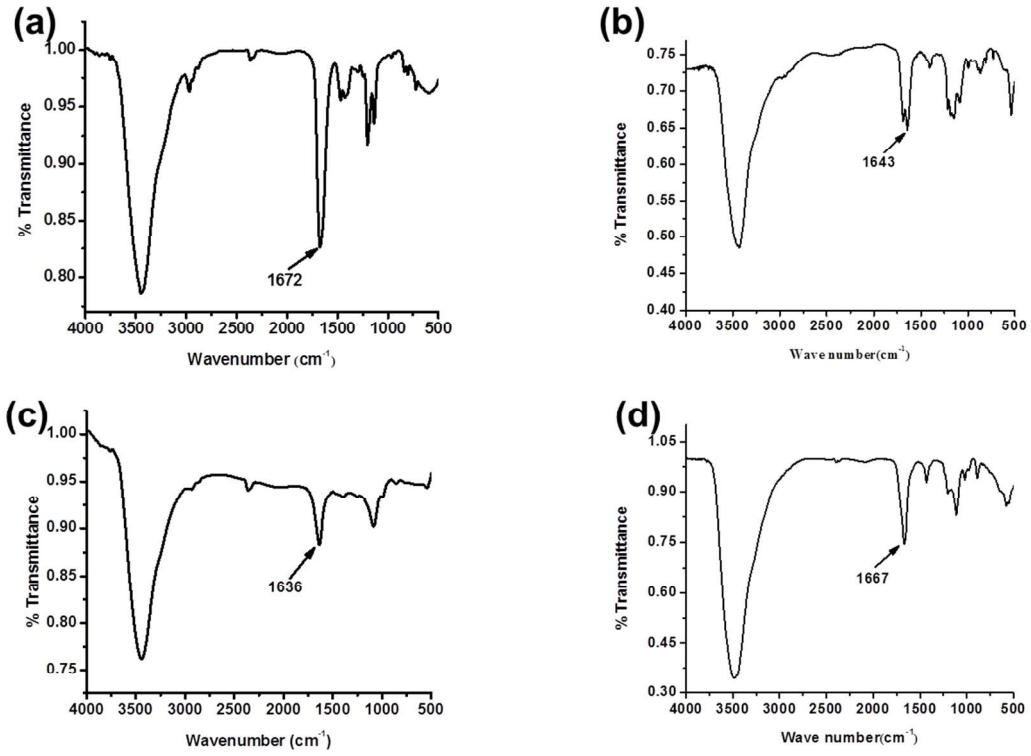


Figure S8. FT-IR spectrums reveal that AI peptoid inhibits fibril formation of Aβ42 (a) AI peptoid at 0 day incubation, (b) AI peptoid after 7 days incubation, (c) Aβ peptide after 7 days incubation and (d) Aβ peptide with AI peptoid after 7 days incubation.

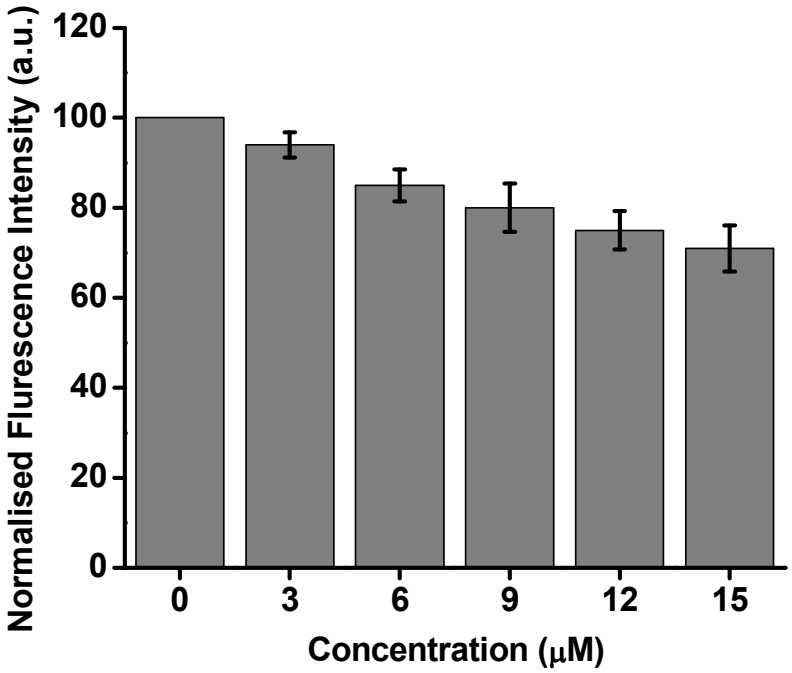


Figure S9. ThT assay with AI peptide for amyloid fibril inhibition.

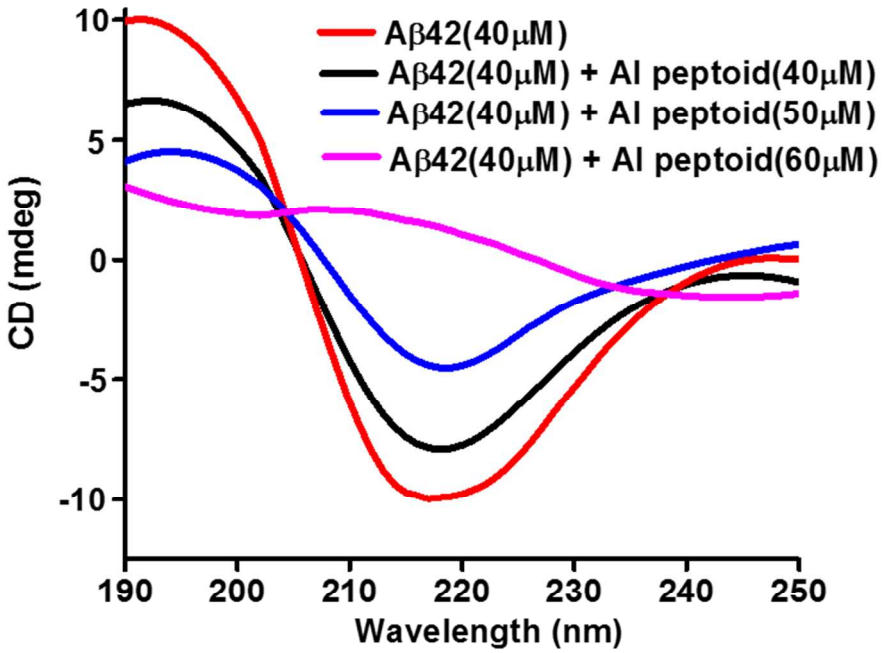


Figure S10. CD spectra of Aβ42 peptide without and with AI peptoid in different concentrations showing inhibition of β-sheet structure.

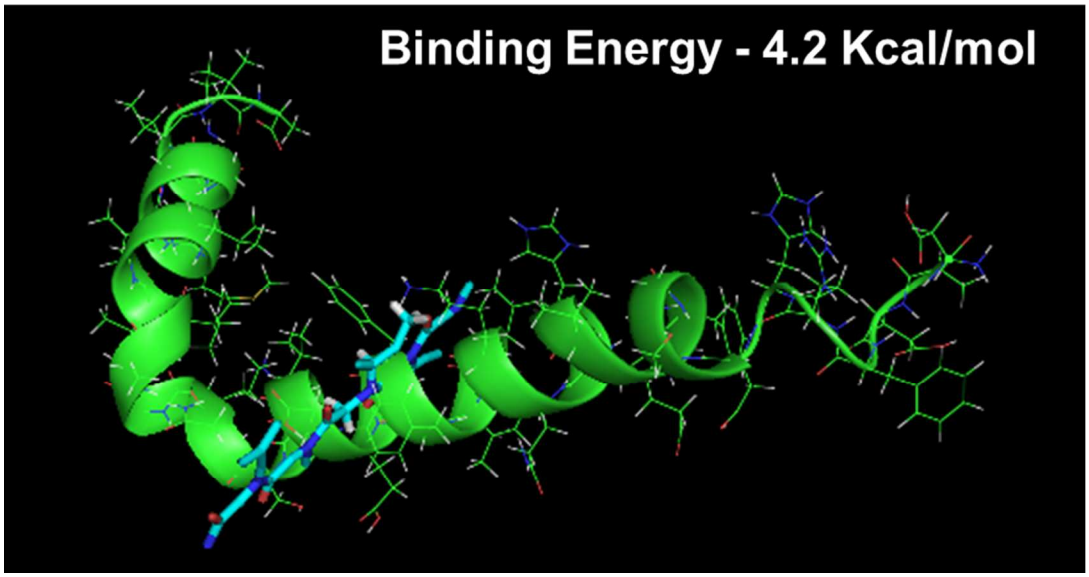


Figure S11. Docking study reveals that AI peptoid binds to the hydrophobic region (Aβ17-21) of Aβ peptide.

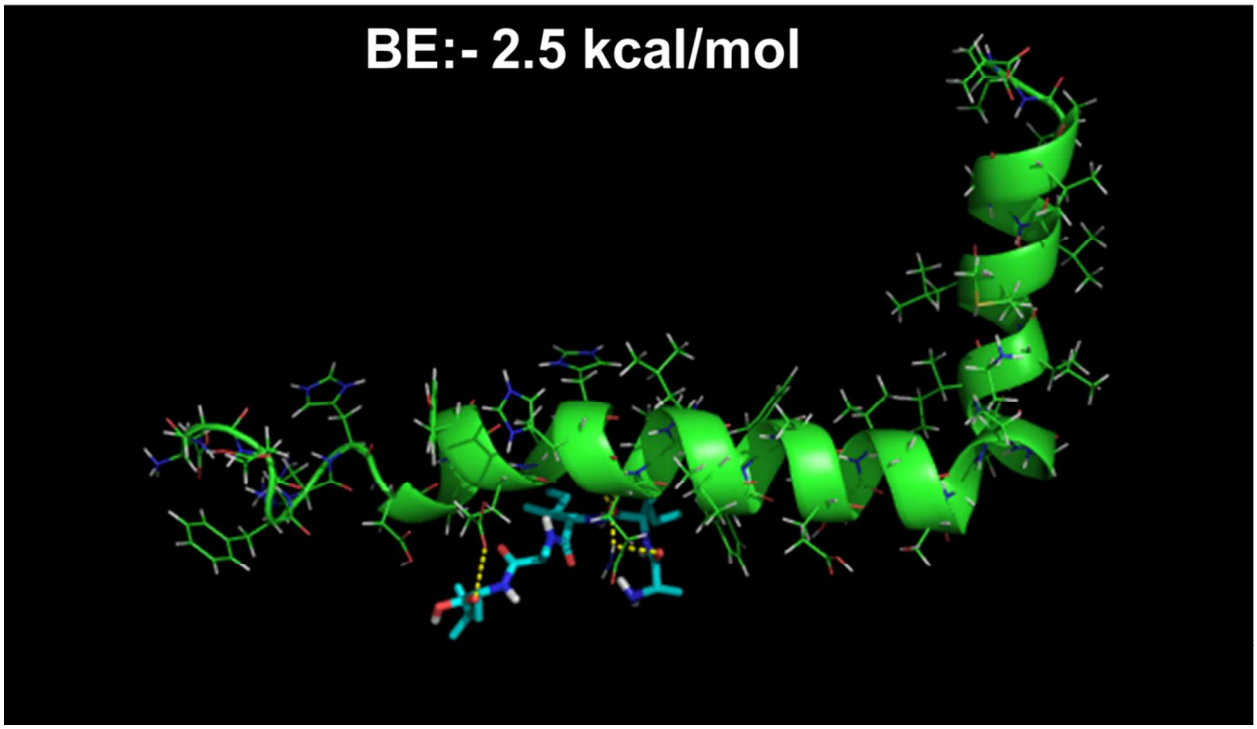


Figure S12. Docking study reveals that AI peptide binds to the Aβ11-16 of Aβ peptide.

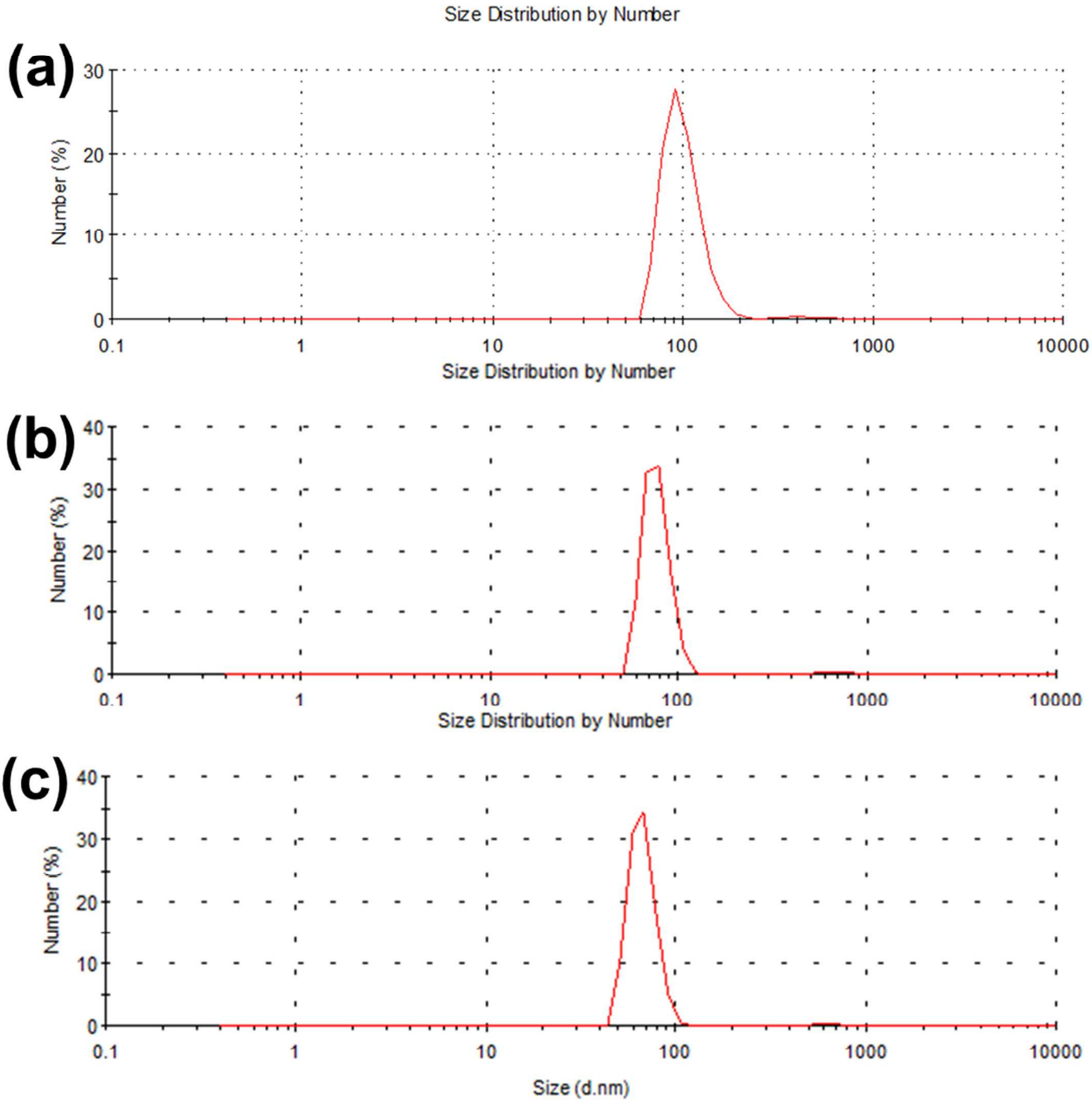


Figure S13. DLS study of AI peptoid (a) at 0 day incubation (b) at 2 days incubation and (c) at 5 days incubation.

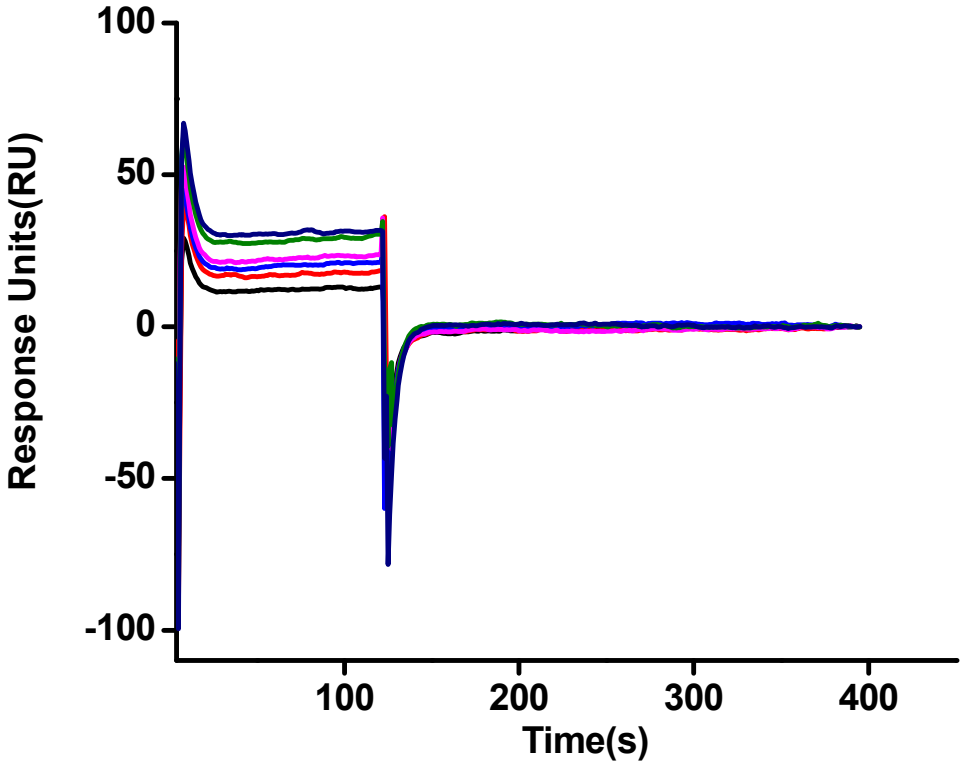


Figure S14. SPR sensogram for the kinetic analysis of the binding of AI peptide with tubulin on a NTA biosensor chip using a Biacore 3000 instrument.

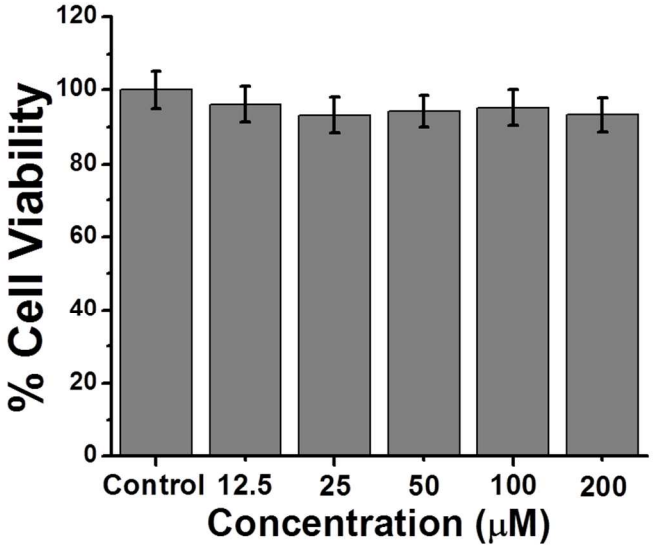


Figure S15. MTT assay of the AI peptoid treated PC12 cells showing no effect on cell viability.

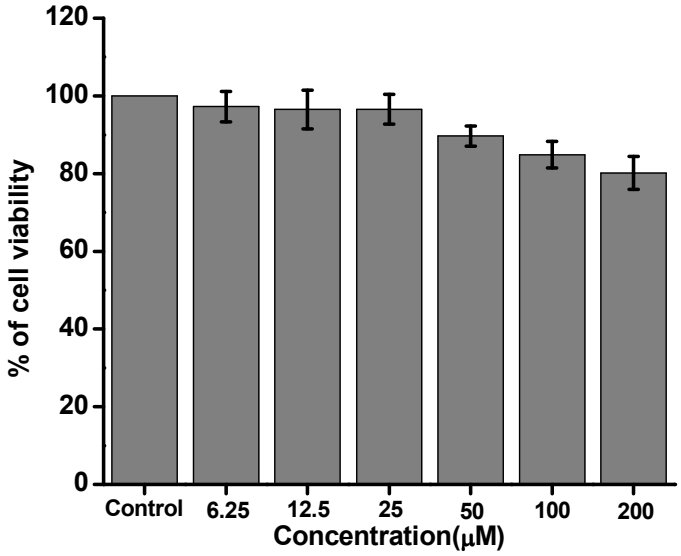


Figure S16. MTT assay of the AI peptide in the PC12 cells showing around 10% toxicity.

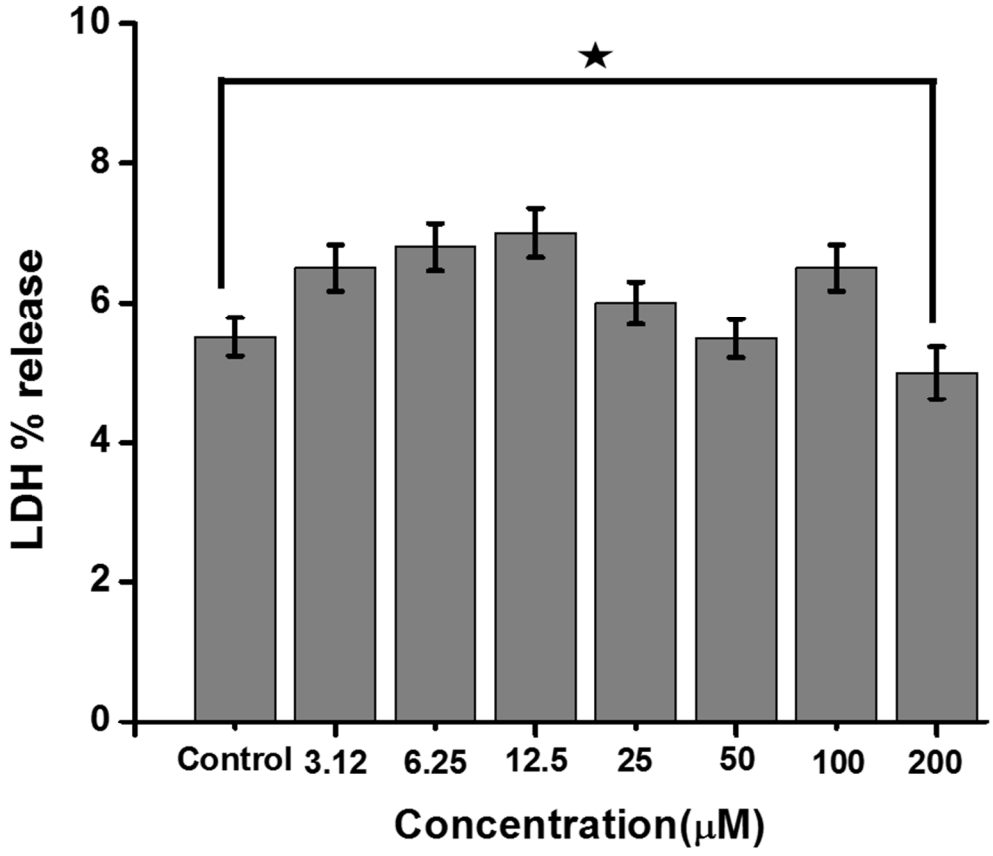


Figure S17. LDH assay reveals no cytotoxic effect of AI peptoid on treated PC12 cells.

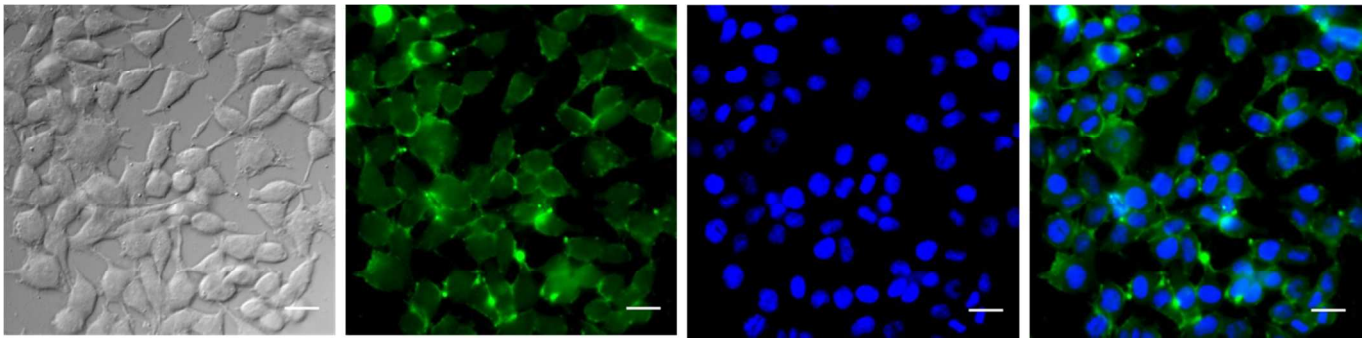


Figure S18. Cellular uptake of 5(6)-Carboxyfluorescein attached AI peptoid into the PC12 derived neurons.

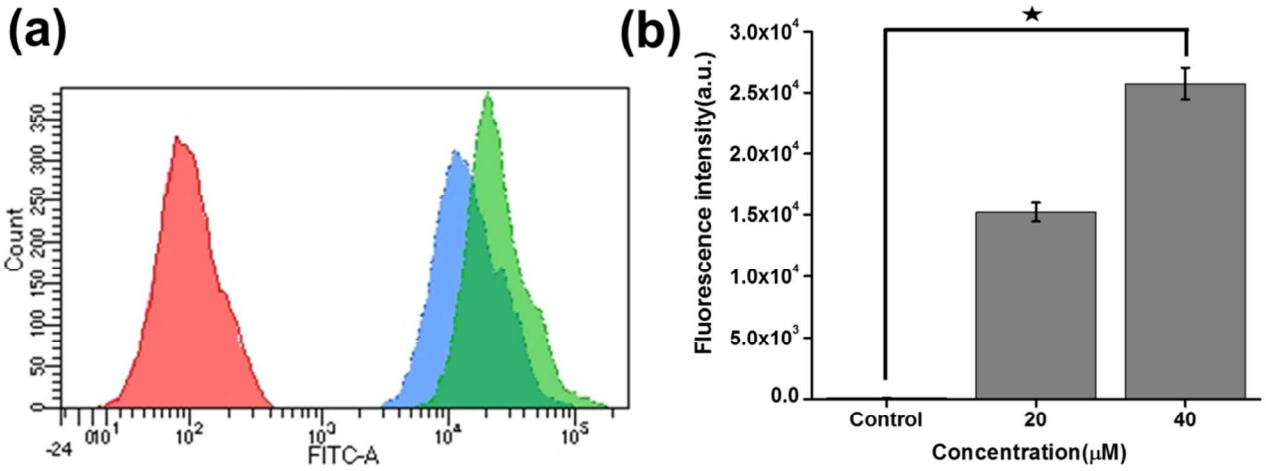


Figure S19. (a) Cellular uptake of 5(6)-Carboxyfluorescein attached AI peptoid into the PC12 cells at 20 μM and 40 μM concentrations was monitored using FACS. Graph reveals increasing trend of cellular uptake upon increasing the AI peptoid concentrations. (b) Bar diagram represents quantitative cellular uptake of 5(6)-Carboxyfluorescein attached AI peptoid.

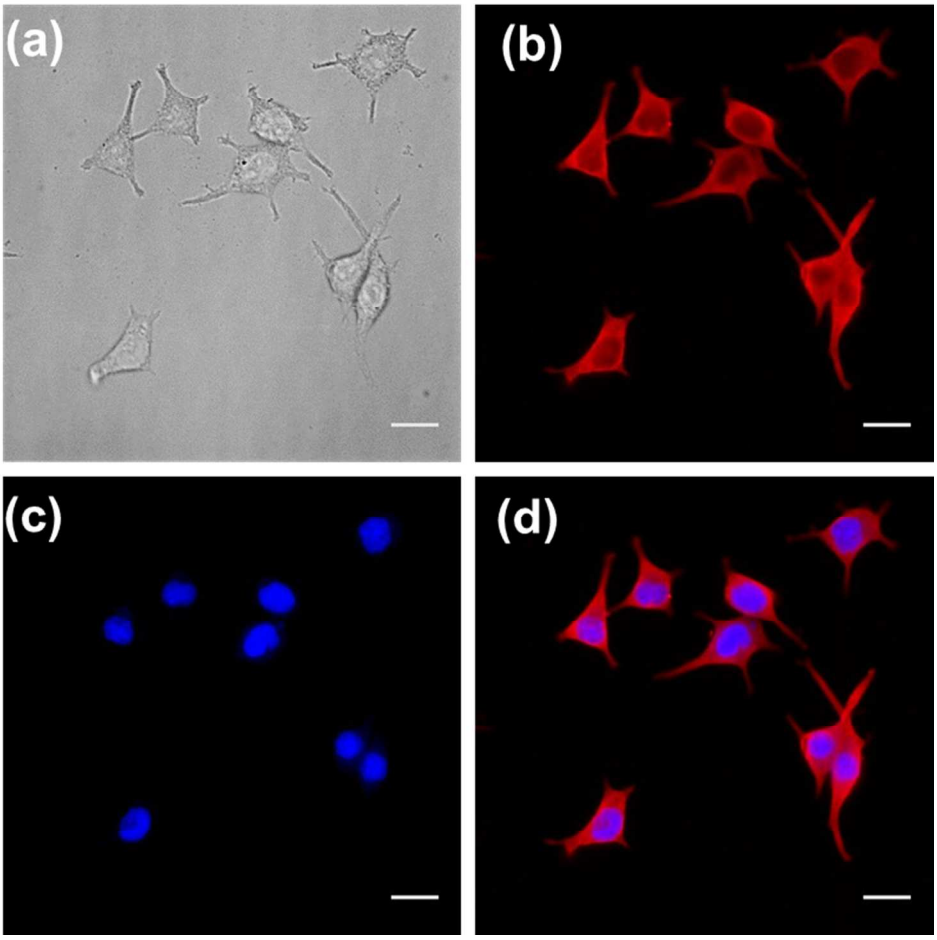


Figure S20. Microscopic images of PC12 derived neurons (control) for neurite outgrowth (a) DIC mode (b) TRITC channel (c) DAPI channel and (d) merged channel.

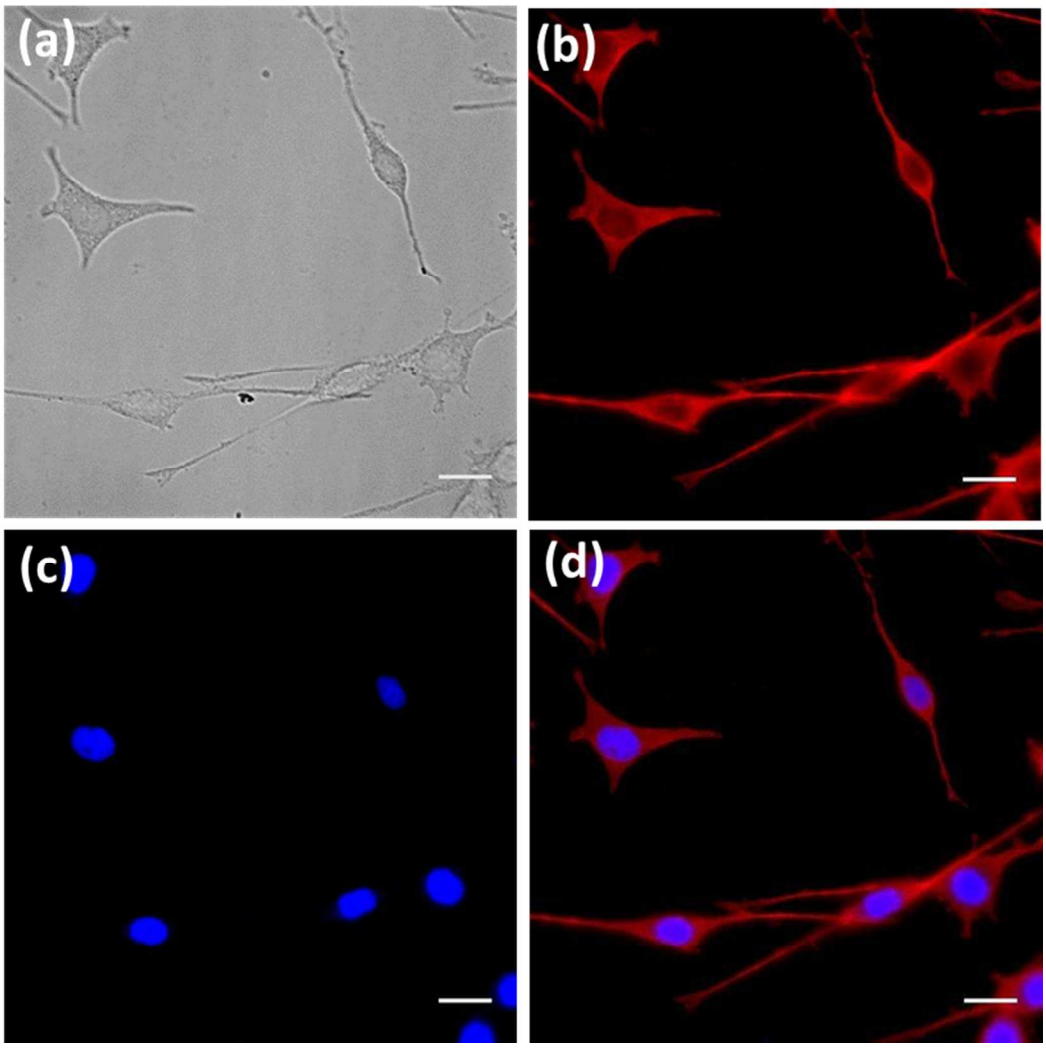


Figure S21. Microscopic images of PC12 derived neurons upon treatment with AI peptoid showing healthy microtubule netowrks and significant neurite outgrowth compared to the control (a) DIC channel (b) TRITC channel (c) DAPI channel and (d) merged channel.

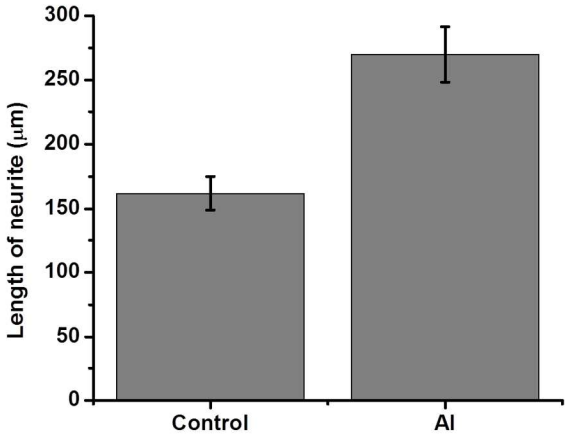


Figure S22. Quantitative analysis of neurite outgrowth of PC12 derived neurons upon treatment with AI peptoid.

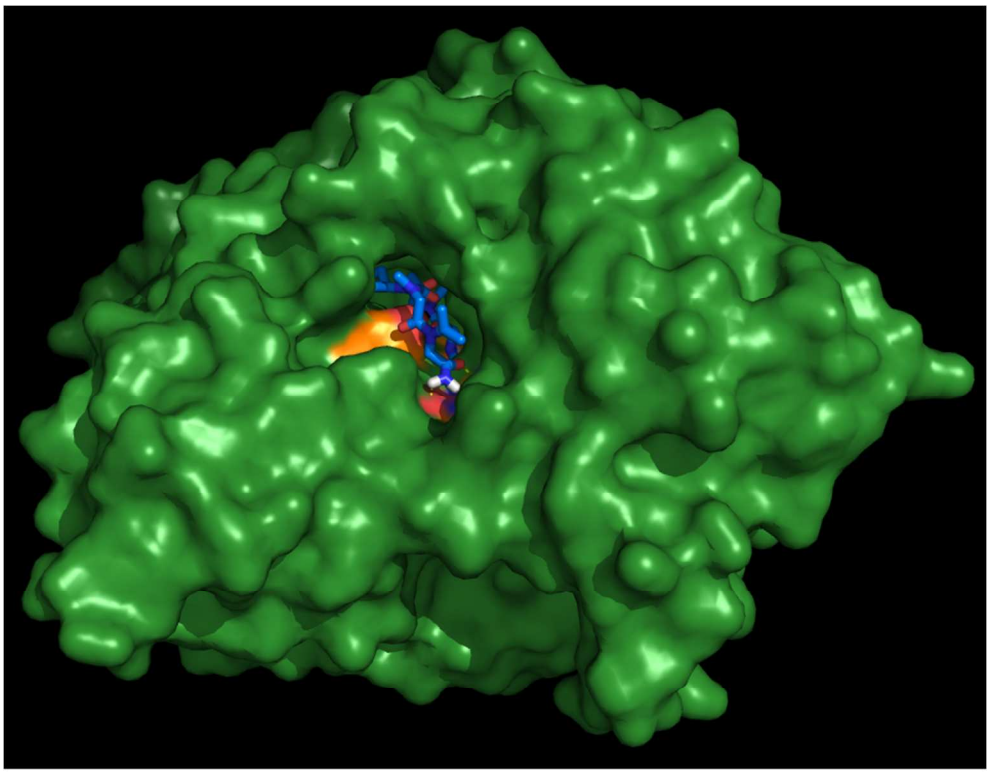


Figure S23. Docking study of AI peptoid with AChE reveals that AI peptoid binds with CAS and PAS site of AChE.

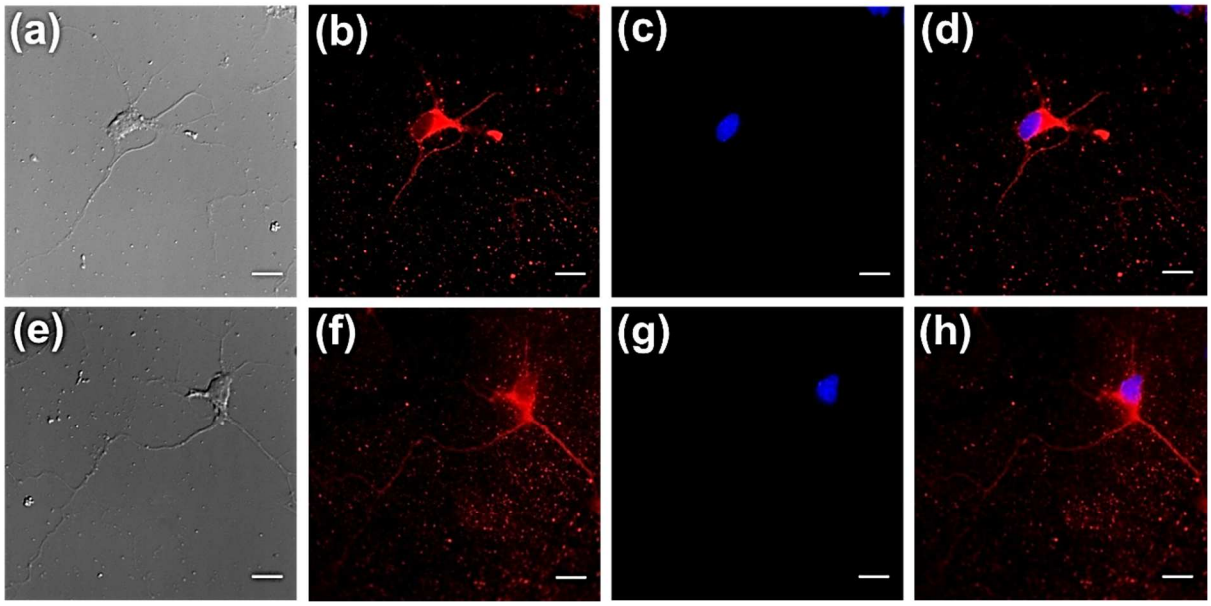


Figure S24. Microscopic images of primary cortical neurons without AI (a-d) peptoid and with AI peptoid treatment (e-h) showing healthy microtubule netowrks and significant neurite outgrowth compared to the control. (a,e) DIC channel (b,f) TRITC channel (c,g) DAPI channel and (d,h) merged channel.

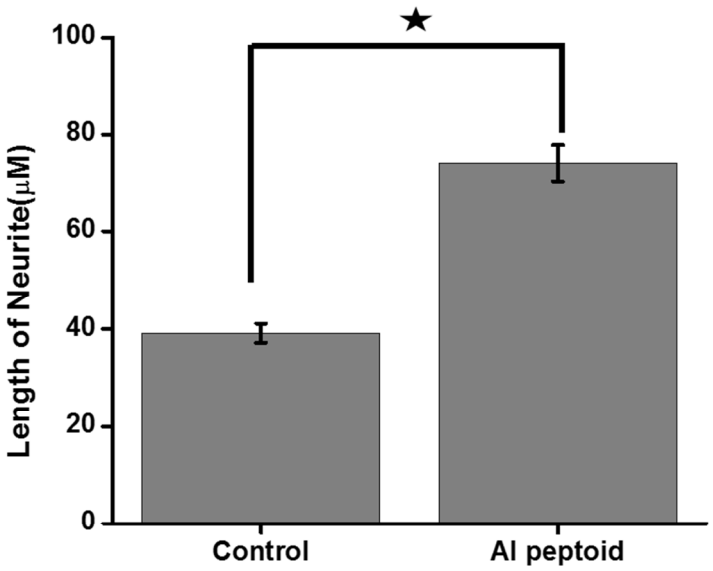


Figure S25. Quantitative analysis of neurite outgrowth of Primary cortical neurons upon treatment with AI peptoid.