

1 Cyanidin-3-O-glucoside inhibits A β 40 fibrillogenesis, disintegrates
2 preformed fibrils, and reduces amyloid cytotoxicity

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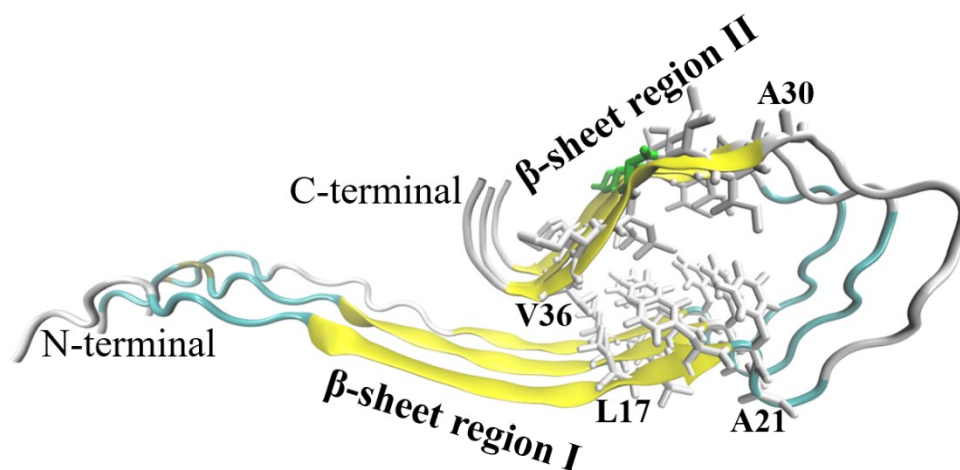
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21 **Figure S1.** The initial conformation of A β 40 trimer obtained from the A β 40 nonamer.

22 A β 40 were displayed using a New cartoon drawing method, and the residues of

23 hydrophobic core of the A β 40 trimer were displayed using Licorice drawing method.

24 The non-polar and polar residues of the A β 40 trimer are colored by white and green,

25 respectively.

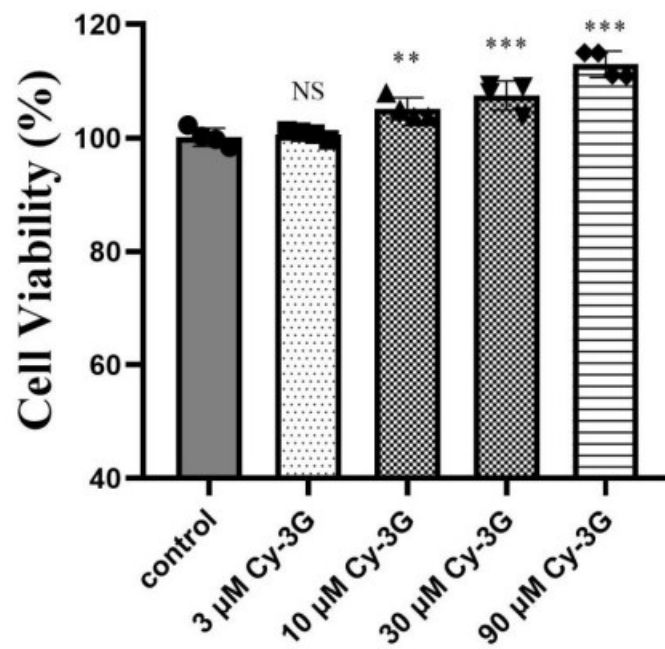
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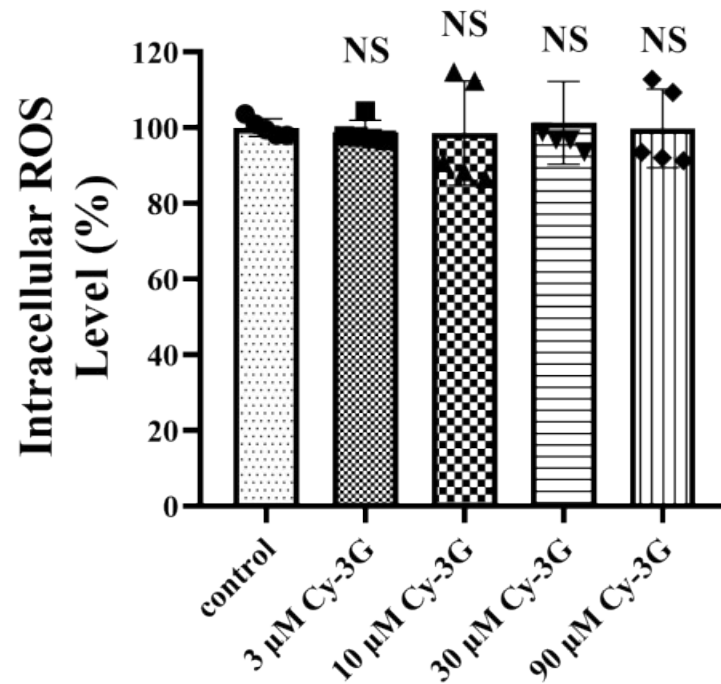
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32 **Figure S2.** Effect of Cy-3G on the cytotoxicity of PC12 cells. The cellular viability
 33 treated with PBS buffer alone (negative control) was set as 100%. All values represent
 34 means $\pm$ s.d. (n=3). NS, no significant, **, $P < 0.01$ compared to the control group, ***,
 35 $P < 0.001$ compared to the control group.

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39 **Figure S3.** The intracellular ROS production induced by cyanidin-3-O-glucoside as
 40 evidenced by the fluorescein dye 2',7'-dichlorofluorescein diacetate in the absence and
 41 presence of different concentrations of Cy-3G. The intracellular ROS level treated with
 42 PBS buffer alone was set as 100%. All values represent means $\pm$ s.d. (n=5). NS, no
 43 significant. NS, no significant.

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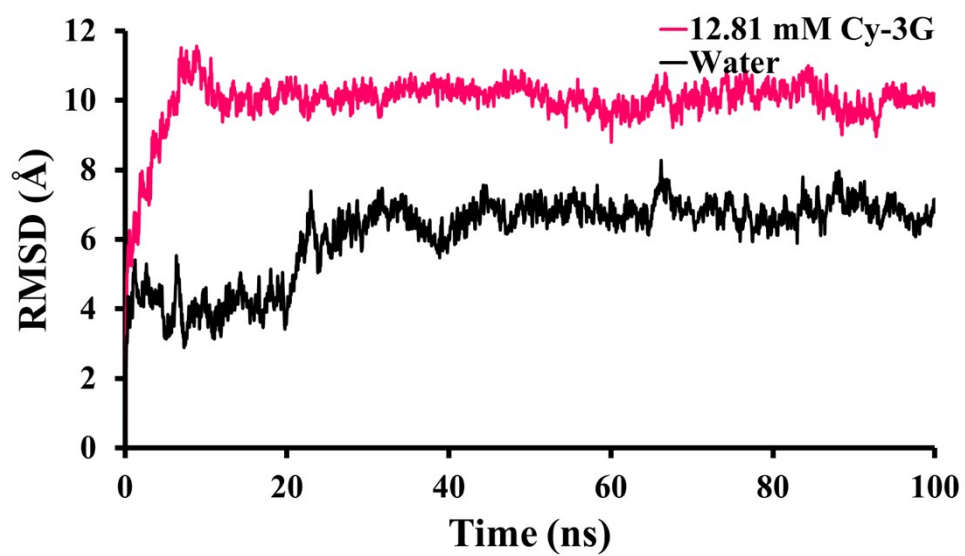
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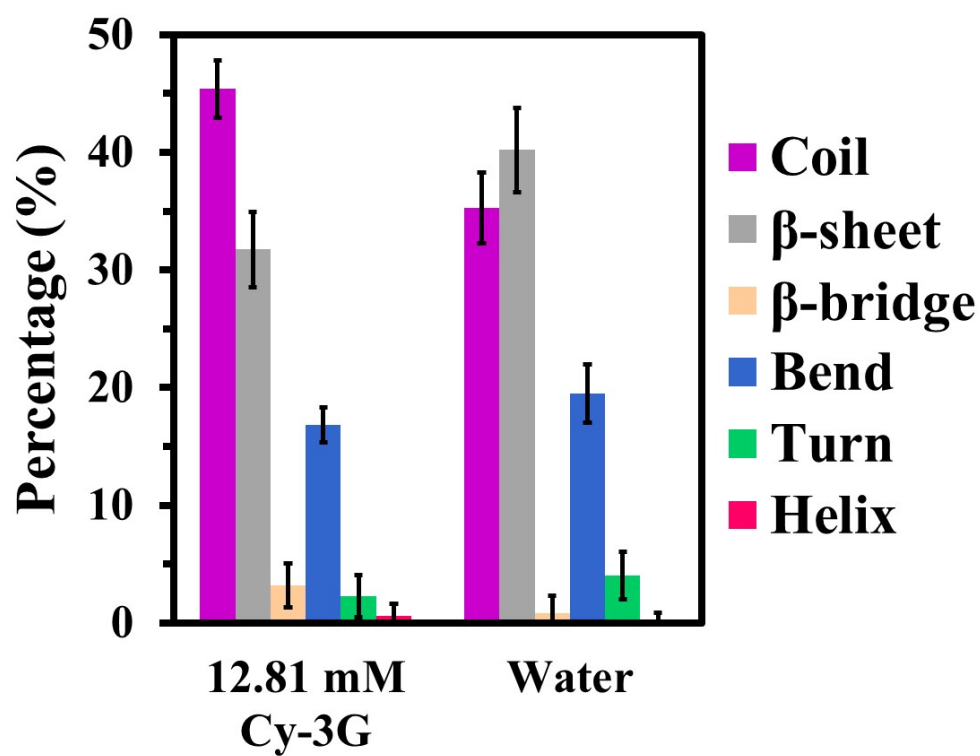
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53 **Figure S4.** Time-dependent of root mean square deviation (RMSD) of the atom C α of
 54 the A β 40 trimer.

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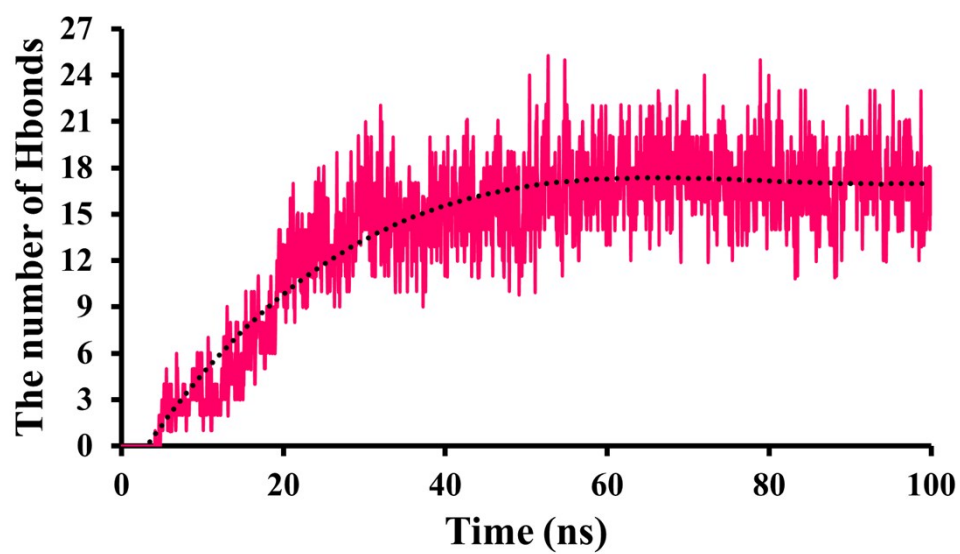


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59 **Figure S5.** Proportion of each secondary structure of the Aβ40 trimer in the total
 60 amount. The secondary structure content of the Aβ40 trimer was calculated in the last
 61 10 ns.

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65 **Figure S6.** The number of hydrogen bonds between the A β 40 trimer and Cy-3G during
 66 100 ns simulation time.

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