Inhibition of Acetylcholinesterase and Amyloid-β Aggregation by Piceatannol and Analogs: Assessing In Vitro and In Vivo Impact on a Murine Model of Scopolamine-Induced Memory Impairment

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Supplementary materials

Table S1. CDOCKER interaction energy for piceatannol, gnetol, resveratrol, rhapontigenin, and isorhapontigenin docked in AChE and Aβ peptide (1-42)

Compound	AChE	Aβ peptide (1-42)
	CDOCKER Interaction Energy (kcal/mol)	CDOCKER Interaction Energy (kcal/mol)
Piceatannol	-36.3392	-19.3083
Gnetol	-34.6363	-13.7451
Resveratrol	-31.4709	-17.0259
Rhapontigenin	-34.5302	-14.7856
Isorhapontigenin	-35.1776	-14.2737

Figure S1

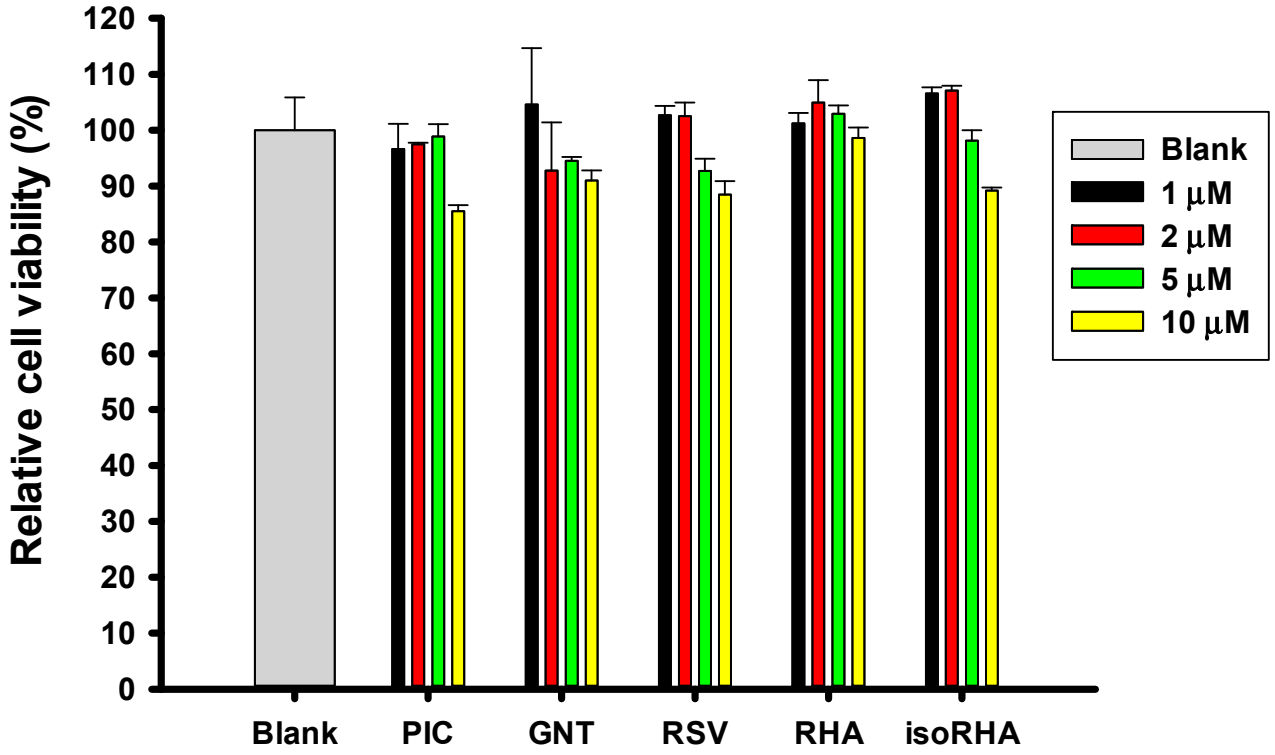

Figure S1. Effects of different concentrations (1, 2, 5, and 10 μM) of hydroxylated stilbenes (PIC, GNT, RSV, RHA, and isoRHA) on cytotoxicities of SH-SY5Y cells. The MTT was used to evaluate cell viability, and the absorbance at 570nm was determined. The DMSO used instead of sample solution was the blank (recognized as 100%), and each treatment was expressed as relative cell viability (%).

Figure S2

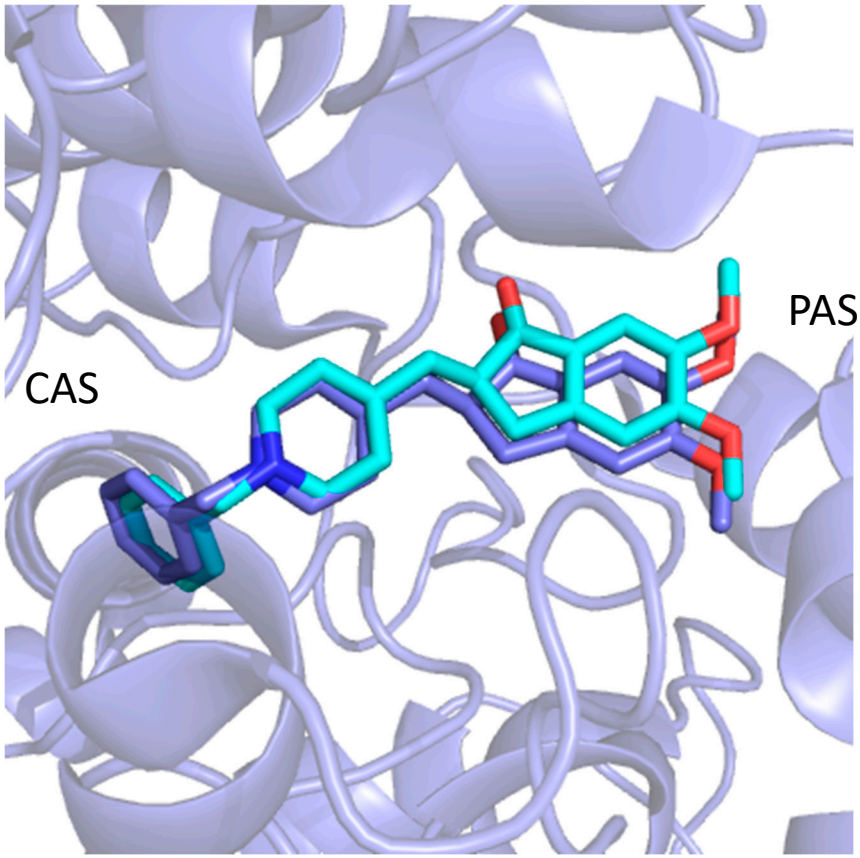

Figure S2. Validation of the docking protocol by using donepezil. The co-crystallized ligand was re-docked to confirm the docking protocol of AChE. The co-crystallized ligand (light blue) and the docked ligand (cyan) displayed similar poses. The RMSD values of the re-docking results in AChE is 1.6494 Å. The catalytic anionic site (CAS) and the peripheral anionic site (PAS) of AChE.