

1 ***Supporting Information***

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3 *Docking Study of Ginkgolide J, P and Q* From Figure S1A and Table S1, ginkgolide
4 J established H-bonding with amino acid residues Tyr70 and hydrophobic interactions
5 interactions with Ile287, Phe331, Tyr334, Phe290, Gly335, Ser286, Trp279, Gln74 and
6 Tyr121 inside AChE. The illustration of molecular docking for the interactions of
7 ginkgolide P and AChE was shown in Figure S1B and Table S1. Ginkgolide P formed
8 4 hydrophobic interactions with different residues namely Gln74, Tyr121, Tyr334 and
9 Trp279. Moreover, a hydrogen bonding interaction with residue like Tyr70 was also
10 observed. The molecular docking model of ginkgolide C is illustrated in Figure 9C and
11 Table S1. Ginkgolide Q formed 2 hydrogen bonding interactions with residues like
12 Tyr70 and Tyr121. Ginkgolide Q also formed five hydrophobic interactions with
13 Tyr334, Phe290, Gly335, Trp279 and Gln74 located in AChE.

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TABLE S1: Docking scores and interactions of compounds (Ginkgolide J, P and

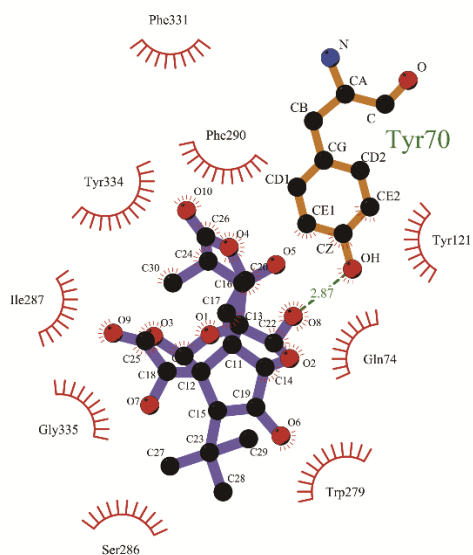
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Q) with AChE.

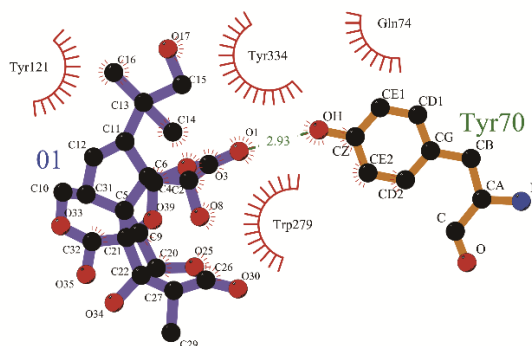
Compounds	Glide Score (kcal/mol)	No of H-bonds	H-bonds interacting residues	Van der Waals interacting residues
Ginkgolide_J	-6.1	1	Tyr70	Ile287, Phe331, Tyr334, Phe290, Gly335, Ser286, Trp279, Gln74, Tyr121
Ginkgolide_P	-6.5	1	Tyr70	Gln74, Tyr121, Tyr334, Trp279
Ginkgolide_Q	-6.2	2	Tyr70, Tyr121	Tyr334, Phe290, Gly335, Trp279, Gln74

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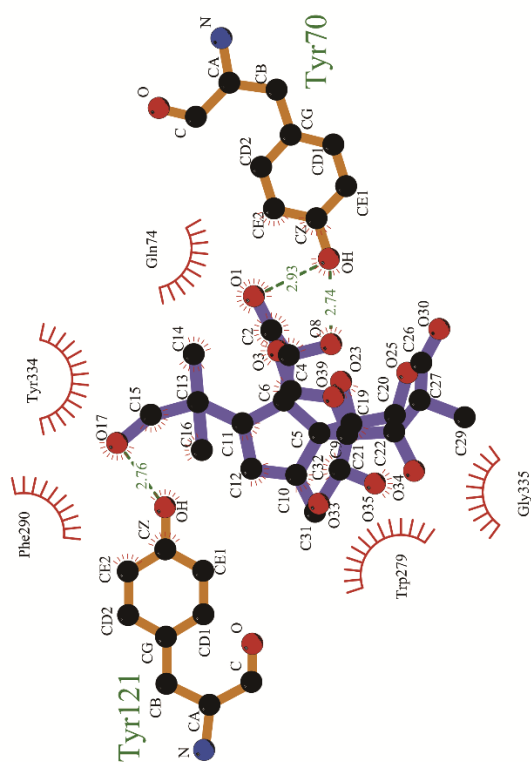
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(A)



(B)



(C)

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24 FIGURE S1: 2D ligand interaction diagram of AChE inhibition by ginkgolide J (A), ginkgolide P
25 (B) and ginkgolide Q (C). Green and red dashed lines were indicated hydrogen and hydrophobic
26 bonds, respectively. Carbons are in black, nitrogens in blue and oxygens in red.