Supplementary Information - 1 (SI1)

Table SI1 Selected plants for the study and the source of finding

	Plant Name	**Source of Information**
1.	*Coriandrum sativum*	Mani and Parle (2009), Hosseini et al. (2021), Chakraborty et al. (2022)
2.	*Ficus carica*	Chakraborty et al. (2022)
3.	*Magnolia officinalis*	Chakraborty et al. (2022)
4.	*Myristica fragrans*	Chakraborty et al. (2022)
5.	*Terminalia chebula*	Afshari et al. (2016)
6.	*Emblica officinalis*	Ahmadian-Attari et al. (2016)
7.	*Nigella sativa*	Ahmadian-Attari et al. (2016)
8.	*Bambusa bambos*	Ahmadian-Attari et al. (2016)
9.	*Elettaria cardamomum*	Ahmadian-Attari et al. (2016)
10.	*Cyperus rotundus*	Ahmadian-Attari et al. (2016)
11.	*Piper longum*	Ahmadian-Attari et al. (2016)
12.	*Piper nigrum*	Ahmadian-Attari et al. (2016)
13.	*Pimpinella anisum*	Ahmadian-Attari et al. (2016)
14.	*Zingiber officinale*	Ahmadian-Attari et al. (2016)
15.	*Argyreia speciosa*	Kashyap et al. (2020)
16.	*Boerhavia diffusa*	Personal communication
17.	*Benincasa hispida*	Rapaka et al. (2021)
18.	*Glycyrrhiza glabra*	Cui et al. (2008)
19.	*Celastrus paniculatus*	Mehla et al. (2020)
20.	*Desmodium gangeticum*	Personal communication
21.	*Tinospora cordifolia*	Sharma et al. (2020)
22.	*Allium sativum*	Personal communication
23.	*Asparagus racemosus*	Personal communication
24.	*Withania somnifera*	Chakraborty et al. (2022)
25.	*Ferula foetida*	Personal communication
26.	*Convovulus pluricaulis*	Chakraborty et al. (2022)
27.	*Ocimum tenuiflorum L.*	Personal communication
28.	*Barleria prionitis Linn*	Personal communication
29.	*Hemidesmus indicus*	Personal communication

Supplementary Information - 2 (SI2)

Table SI2 Phytochemicals reported with good binding affinity but already reported and the references of published evidence

Phytochemical	**Binding Affinity of conformations (kcal/mol)**			**Reference**
	7e3d	**1b41**	**4moe**	
27-deoxy-14-hydroxywithaferin A	-10	-10	-10.2	https://doi.org/10.1051/bioconf/20248601043
piperine	-10.3	-10.4	-9.6	doi: 10.3390/biomedicines10010154
Pipernonaline	-10.1	-10.8	-9.9	https://doi.org/10.1080/07391102.2012.10507408
Piperlonguminine	-9.5	-10.3	-9.8	https://ijobb.esaunggul.ac.id/index.php/IJOBB/arti...
Withaferin	-9.5	-10.2	-9.4	https://doi.org/10.1016/j.arabjc.2021.103529
Boeravinone B	-9.2	-10.2	10.0	Hussain BS, Raj KK, Rao P, Singh BJ, Talluri VR. Molecular docking and simulation of acetyl-cholinesterase with compounds derived from Boerhaavia diffusa. Bioinformation. 2014;10:664-71.
Withanolide A	-9.2	-11	-9.1	https://doi.org/10.1080/07391102.2012.10507408
Tetrahydropiperine	-9	-10.6	-9	DOI: 10.18311/jnr/2022/30194
Withanolide P	-9	-9.2	-10.2	https://doi.org/10.1051/bioconf/20248601043

Supplementary Information - 3 (SI3)

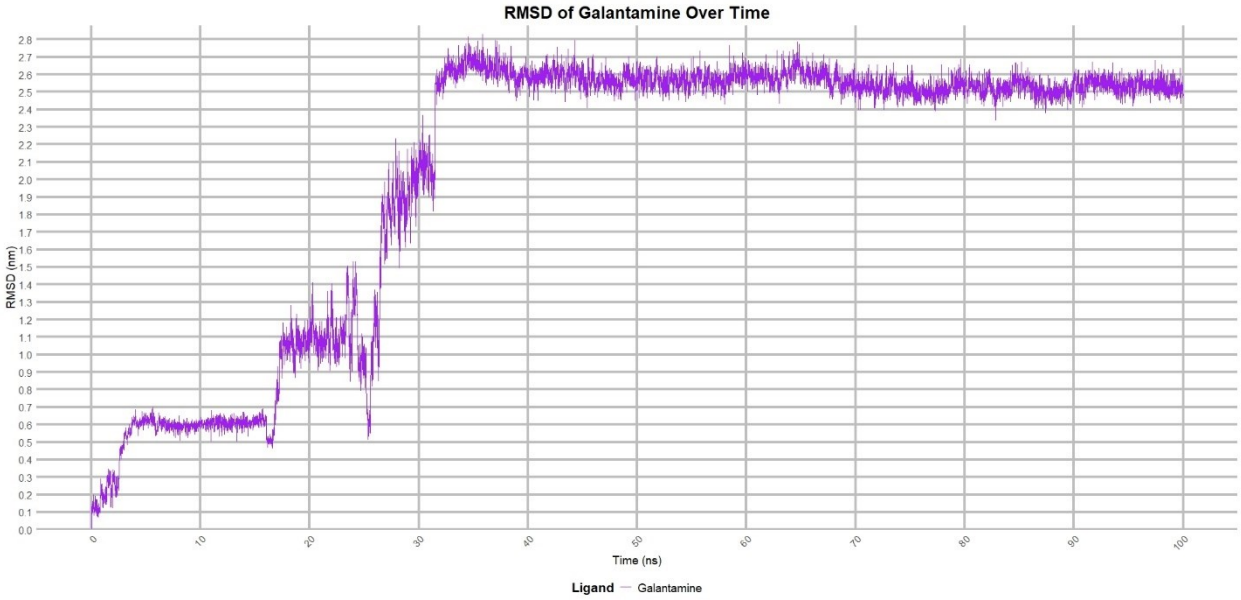

Fig. SI1 Root mean square deviation (RMSD) analysis of AChE complexes with Galantamine

Supplementary Information - 4 (SI4)

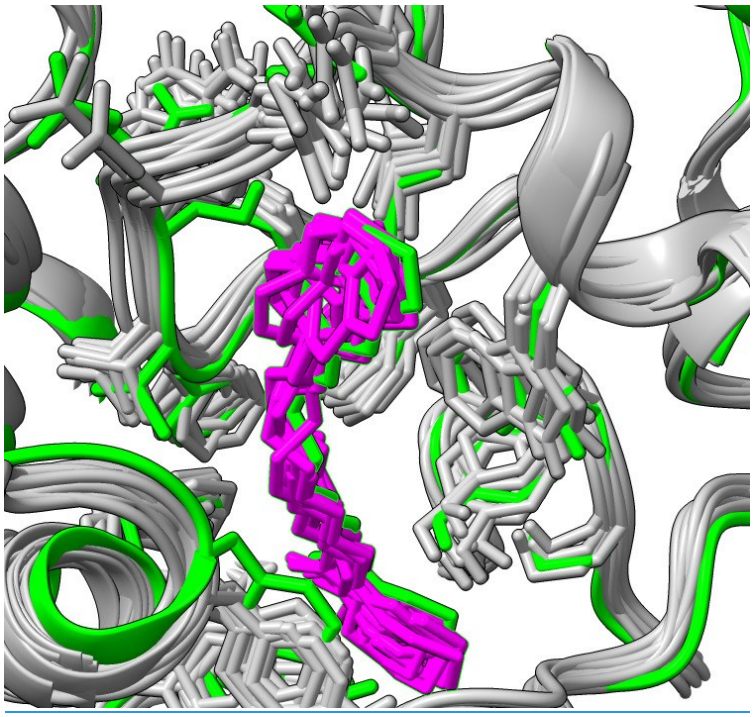

Fig. SI2 Superimposed snapshots of AChE-Dehydropipernonaline complex constructed using snapshots extracted every 10 ns of the MD trajectory