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In Silico Analysis of *Eriobotrya japonica* Leaf Extract as an Acetylcholinesterase Inhibitor in *Spodoptera litura*

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Abstract
Spodoptera litura is a destructive agricultural pest, and increasing resistance to synthetic insecticides highlights the need for alternative control strategies. This study investigates the acetylcholinesterase (AChE) inhibitory potential of *Eriobotrya japonica* methanolic leaf extract against *S. litura* using GC-MS profiling and in silico molecular docking. GC-MS analysis identified 59 phytochemicals belonging to fatty acids, terpenoids, phenolics, and chroman derivatives. A three-dimensional model of *S. litura* AChE was generated and validated for docking studies. Several phytoconstituents exhibited stronger binding affinity toward AChE than the control ligand acetylcholine (-4.1 kcal/mol), with 13-docosenamide (-13.1 kcal/mol), 1-heptacosanol (-12.0 kcal/mol), and chroman derivatives showing the highest affinities. These compounds interacted with key residues within the AChE catalytic pocket, indicating effective inhibitory potential. Overall, the findings suggest that *E. japonica* leaf extract is a promising source of natural AChE inhibitors and may serve as an eco-friendly alternative for the management of *S. litura*.

Keywords: Spodoptera litura

Introduction
Spodoptera litura (Commonly known as tobacco cutworm) a phytophagous insect pest (Brown & Dewhurst, 1975) [3] was selected for this study. The insect is known for causing huge economic injury to crop production (Dhir *et al.*, 1992) [7]. Development of resistance to existing pesticides has resulted in sporadic outbreaks stressing the need for finding alternatives (Armes *et al.*, 1997) [1].

Eriobotrya japonica (Thunb.) Lindl., commonly known as loquat, is an evergreen species in the Rosaceae family, native to subtropical and temperate regions of China, India, and Japan. Taxonomically, it is classified within the kingdom Plantae, division Tracheophyta, class Magnoliopsida, order Rosales, family Rosaceae, and genus Eriobotrya. This plant has a long-standing role in traditional medicine, where it is valued for its wide range of therapeutic benefits. Phytochemical investigations have shown that *E. japonica* leaves contain various bioactive constituents-such as flavonoids, terpenoids, and phenolic compounds-which contribute to its antibacterial, antifungal, and anti-inflammatory properties (Ibrahim, 2021) [15]

Acetylcholinesterase (AChE) plays a vital role in hydrolyzing the neurotransmitter acetylcholine at synaptic junctions, thereby terminating nerve impulses and ensuring proper neuromuscular function (Colovic *et al.*, 2013). Because insect survival depends on precise regulation of these signals, disruption of AChE activity leads to the accumulation of acetylcholine, continuous nerve stimulation, paralysis, and ultimately death. This makes AChE a critical and widely validated biochemical target for insecticides, particularly organophosphates and carbamates, which exert their toxicity by inhibiting the enzyme. Understanding the physiological importance of AChE in insects not only highlights its central role in neural regulation but also underscores its value as an effective target for developing pesticides with high specificity and potency.

In this study, we investigated the inhibitory effects of *E japonica* methanol leaf extract on the acetylcholinesterase (AChE) enzyme of *S litura* through in-silico molecular docking analyses. Targeting AChE is a well-established strategy for controlling insect pests, as its inhibition disrupts neurotransmission and leads to impaired physiological function. The in-silico studies provided insight into the binding interactions and affinity of the extract's bioactive compounds toward the AChE active site. This approache offer a comprehensive understanding of how *E. japonica* phytochemicals may contribute to AChE inhibition and support their potential use in developing environmentally friendly botanical pesticides against *S. litura*.

Materials and Methods
Preparation of raw extracts
E japonica leaves were collected from district Udhampur, Jammu and Kashmir (32°47'58.17" N-75°18'33.72" E) in the month of March and April. These leaves were shade dried and ground into fine powder form. The powder form was added methanol in the ratio of (1:10 W: V). The solution was kept under room temperature for one week on a magnetic stirrer. After that the solution was filtered twice using whatman filter paper number one. The solvent was then removed from the solution using a rotatory evaporator leaving extracted phytochemicals in the flask. Different formulations (based on solvent use and concentration) of the extract were prepared in 5%DMSO and stored at 4 degrees Celsius for further use.

GC-MS Analysis
GC-MS analysis was performed using a Shimadzu GC-MS QP2020NX equipped with an EI source operating at 70 eV. Helium (99.999%) served as the carrier gas at a constant flow rate of 1 mL/min. A 2 µL sample was injected in split mode (10:1), with injector and ion-source temperatures set at 250 °C and 200 °C, respectively. The oven program began at 110 °C (2 min), increased by 10 °C/min to 200 °C,

then by 5 °C/min to 280 °C, followed by a 9-min hold. Mass spectra were recorded from 45-450 m/z at 0.5-s intervals. The total run time was 36 min, and component percentages were calculated based on peak area normalization. The column used was SH-I-5Sil MS (30 m × 0.25 mm × 0.25 µm).

Identification of Phytocomponents

Phytochemicals were identified by matching mass spectra with the NIST library (>62,000 reference spectra). Compounds were identified based on similarity score, molecular weight, and structural data (NIST, 2020).

Protein Structure Retrieval and Modeling

Protein sequences of AChE were retrieved from NCBI in FASTA format (NCBI, 2023). AChE lacked a resolved structure and was modelled using Swiss-Model (Waterhouse *et al.,* 2018) [40]. Template selection was based on GMQE, QSQE, and sequence identity. Model quality was further validated using PROCHECK to assess Ramachandran plot statistics.

Ligand Preparation

Phytochemicals identified through GC-MS were used as ligands for docking. Control ligands included acetylcholine (for AChE). 3D structures were retrieved from PubChem (Kim *et al.,* 2025) [18] and ChemSpider (Pence *et al.,* 2010) [29], then energy-minimized and converted to PDBQT format.

Molecular Docking

Docking was performed using AutoDock Vina (Trott & Olson, 2010) [38]. Protein models were prepared by removing water molecules, adding polar hydrogens, and assigning charges in AutoDock Tools (Morris *et al.,* 2009) [24]. Grid boxes (figure 1) were defined around enzyme's active site with its center at (10.772, -18.482, -11.643) and dimensions of 22 × 22 × 28 units along the x, y, and z axes, respectively. Docking simulations generated multiple binding poses, ranked by predicted binding energy (kcal/mol). Top poses were analyzed for key molecular interactions using Discovery Studio.

Docking Analysis

A total of 59 test compounds and a control ligand were docked into each enzyme's active site using a uniform protocol. Binding affinities (ΔG values) and interaction Residues were evaluated using discovery studio 2021 (BIOVIA, 2021) [2] to identify compounds with equal or superior binding to the control ligands. Interactions such as hydrogen bonds, hydrophobic contacts, and π-π stacking were used to assess inhibitory potential, and promising phytochemicals were shortlisted for further investigation.

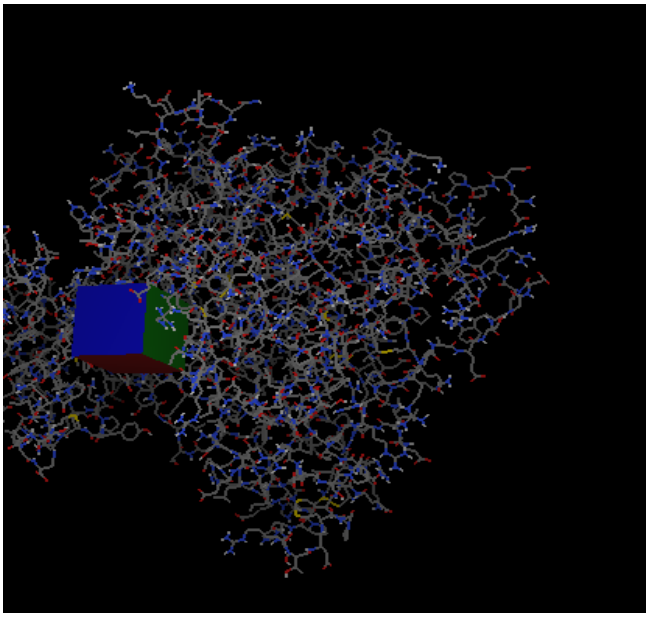

Fig 1: Grid box around the catalytic site of AChE using auto dock tools

Results

GC-MS analysis

The gas chromatography-mass spectrometry (GC-MS) analysis of the sample yielded a total of 59 distinct peaks (table), representing a diverse array of phytoconstituents. Retention times (RT) ranged from 2.78 min to 29.81 min, and identified compounds belonged to multiple chemical classes including fatty acids and their esters, hydrocarbons, aldehydes, alcohols, chromans, and terpenoids. Peak area percentages indicated the relative abundance of compounds, with 1,2,3,5-Cyclohexanetetrol (1α,2β,3α,5β) showing the highest abundance (31.64%), followed by Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester (4.33%), 13-Docosenamide (Z) (4.27%), and n-Hexadecanoic acid (4.21%).

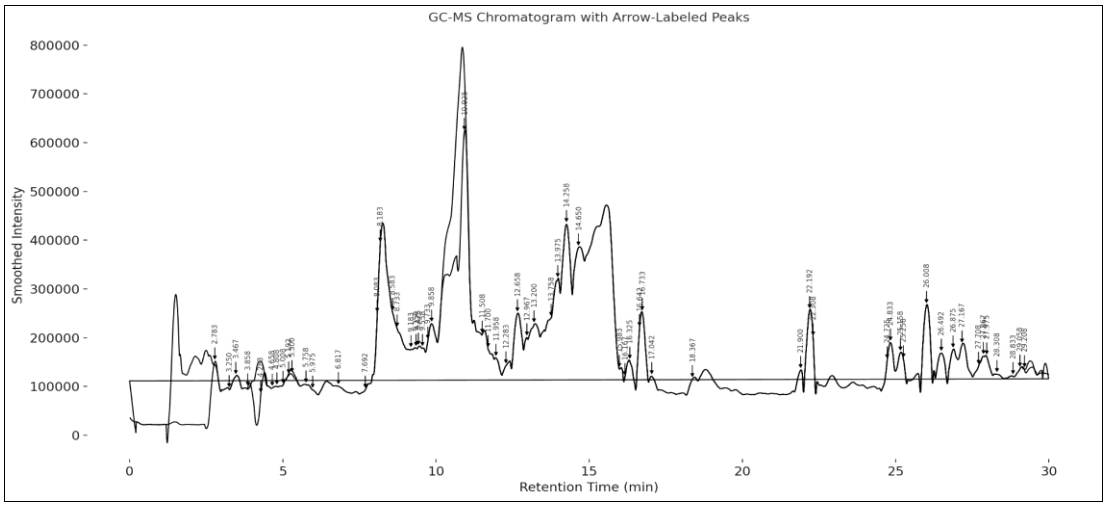

Fig 2: Chromatogram from the GC-MS analysis of the methanol extract of *E. japonica* leav

Table 1: Identified phytochemical constituents from the GC-MS analysis of *E. japonica* leaves

S.N.	Compound Name	RT (min)	Area (%)	Bioactivity	Database ID
1	2-Hexenoic acid, (E)	2.78	1.25	Antifungal, AChE inhibition (NCBI, 2025)	PubChem CID 5282707
2	3-Trifluoroacetoxypentadecane	3.247	0.13	Antifungal (Emara *et al.*, 2025) [11]	PubChem CID 534406
3	Methyl 6-oxoheptanoate	3.463	0.82	No major activity reported but present in bioactive extracts	ChemSpider ID: 254002
4	Propanoic acid, 3-(2-propynyloxy)	3.859	0.11	No major activity reported but present in bioactive extracts	PubChem C ID: 287934
5	Glucosamine, N-acetyl-N-benzoyl	4.281	1.21	No major activity reported but present in bioactive extracts	PubChem C ID: 569182
6	2,3-Diydroxy-2-methylpentanoic acid	4.662	0.08	No major activity reported but present in bioactive extracts	PubChem C ID: 317030
7	β-D-Glucopyranose, 4-O-β-D-galactopyranosyl	4.807	0.06	No major activity reported but present in bioactive extracts	ChemSpider ID: 9199494
8	4-Vinylphenol	5.009	0.06	Anticancer (Girawale *et al.*, 2023) [14], Toxic-metabolite (Vogie *et al.*, 2004) [39]	PubChem ID: 62453
9	1H-Pyrrole-2,5-dione, 3-ethyl-4-methyl-	5.196	0.17	No major activity reported but present in bioactive extracts	PubChem C ID: 29995
10	1,2,3-Propanetriol, 1-acetate	5.3	0.4	No major activity reported but present in bioactive extracts No major activity reported but present in bioactive extracts	PubChem C ID: 33510
11	2-Undecanone	5.973	0.15	Repellent and nematocidal activity (Dai *et al.*, 2025) [5], Antimicrobial (Gibka *et al.*, 2009) [13]	PubChem CID 8163
12	Benzaldehyde, 4-(octyloxy)-	6.819	0.08	No major activity reported but present in bioactive extracts	PubChem CID 90358
13	trans-Cinnamic acid	7.691	0.15	Antifungal (Li *et al.*, 2023) [20]	PubChem CID 444539
14	(E)-β-Farnesene	8.085	0.65	Insecticidal activity (Sun *et al.*, 2011) [35], alarm pheromone (Sun *et al.*, 2022) [34]	PubChem CID 5281517
15	4,8,12-Tetradecatrienenitrile, 5,9,13-trimethyl	8.184	8.63	No major activity reported but present in bioactive extracts	PubChem CID 5365871
16	2,5-Difluorobenzoic acid, 5-pentadecyl ester	8.58	0.13	No major activity reported but present in bioactive extracts	PubChem CID 76339
17	α-Farnesene	8.732	0.3	No major activity reported but present in bioactive extracts	PubChem CID 5362889
18	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	9.187	0.26	No major activity reported but present in bioactive extracts	PubChem CID 6432173
19	Dodecanoic acid	9.348	0.09	Antimicrobial activity, Antitumor activity (MA *et al.*, 2024) [21]	PubChem CID 3893
20	1,2,4-Cyclopentanetrione, 3-(2-pentenyl)	9.429	0.11	No major activity reported but present in bioactive extracts	PubChem CID 27507
21	2-Butanone, 4-[5-isopropyl-2-methyl...cyclopentenyl]	9.562	0.14	No major activity reported but present in bioactive extracts	PubChem CID 3775692
22	Megastigmatrienone	9.733	0.17	No major activity reported but present in bioactive extracts	PubChem CID 18645216
23	1,3-Benzenediol, 4-propyl-	9.859	1.56	Antibacterial (Deryabin & Tolmacheva, 2015) [6]	PubChem CID 87874
24	1,2,3,5-Cyclohexanetetrol, (1α,2β,3α,5β)	10.925	31.64	Anticancer (Jayaraj & Kanagarajan, 2025) [16]	PubChem CID 548226
25	(E)-4-(3-Hydroxyprop-1-en-1-yl)-2-methoxyphenol	11.505	1.77	No major activity reported but present in bioactive extracts	PubChem CID 1549095
26	Tetradecanoic acid	11.7	0.84	Larvicidal and repellent activity (Sivakumar *et al.*, 2011) [32]	PubChem CID 11005
27	6-Hydroxy-4,4,7a-trimethylbenzofuran-2(4H)-one	11.957	0.7	Anti-inflammatory (Jayawardena *et al.*, 2019) [17]	PubChem CID 14334
28	2-Hydroxy-5-methylisophthalaldehyde	12.284	0.41	No major activity reported but present in bioactive extracts	PubChem CID 81744
29	3,7,11,15-Tetramethyl-2-hexadecen-1-ol (Phytol)	12.963	0.49	Phytol derivatives as drug resistance reversal agents	PubChem CID 145386
30	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, acetate	13.201	0.94	Phytol derivatives as drug resistance reversal agents	ChemSpider ID:4933940
31	Hexadecanoic acid, methyl ester	13.762	0.47	Anti-inflammatory (El-Demerdash, 2011) [9]	PubChem CID 8181
32	Palmitoleic Acid	13.973	2.41	Antibacterial (Wille & Kydonieus, 2003) [41]	PubChem CID 445638
33	n-Hexadecanoic acid	14.255	4.21	Antimicrobial (Pu *et al.*, 2010) [30]	PubChem CID

					985
34	trans-Sinapyl alcohol	14.653	1.05	Antimicrobial (Tiz *et al.*, 2024) [37]	PubChem CID 5280507
35	Sorbitol	15.984	0.37	No major activity reported but present in bioactive extracts	PubChem CID 5780
36	9,12,15-Octadecatrienoic acid, methyl ester (Z,Z,Z)-	16.163	0.29	No major activity reported but present in bioactive extracts	PubChem CID 9316
37	Phytol	16.323	1.73	Phytol derivatives as drug resistance reversal agents	PubChem CID 5280435
38	9,12-Octadecadienoic acid (Z,Z)-	16.643	0.16	Antimicrobial, (Kusumah *et al.*, 2020) [19] Anticancer (Manosalva *et al.*, 2024) [22]	PubChem CID 3931
39	7-Tetradecenal, (Z)-	16.735	2.15	Key component of female sex pheromone blends in several Lepidoptera species (Steck *et al.*, 1982) [33]	PubChem CID 5364468
40	Octadecanoic acid	17.046	0.33	Antimicrobial (Pu *et al.*, 2010) [30]	PubChem CID 5281
41	Benzyl β-d-glucoside	18.368	0.53	No major activity reported but present in bioactive extracts	PubChem CID 188977
42	Oleoyl chloride	21.897	0.93	Enhances Antimicrobial activity (Evran *et al.*, 2010) [12]	PubChem CID 5364783
43	Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	22.194	4.33	No major activity reported but present in bioactive extracts	PubChem CID 129853056
44	Linolenic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	24.837	1.45	No major activity reported but present in bioactive extracts	PubChem CID 5367459
45	Octadecanoic acid, 2,3-dihydroxypropyl ester	25.161	1.45	No major activity reported but present in bioactive extracts	PubChem CID 256388
46	13-Docosenamide, (Z)	26.009	4.27	Antimicrobial and cytotoxic (El-Gazzar *et al.*, 2025) [10]	PubChem CID 87172336
47	Squalene	26.496	1.51	Precursor to sterols (Du *et al.*, 2023) [8], Antioxidant (Micera *et al.*, 2020) [23].	PubChem CID 638072
48	α-Tocospiro B	26.877	1.45	No major activity reported but present in bioactive extracts	ChemSpider ID:10286571
49	1-Heptacosanol	27.708	0.44	No major activity reported but present in bioactive extracts	PubChem CID 74822
50	Dotriacontanal	27.864	0.29	No major activity reported but present in bioactive extracts	ChemSpider ID:10542
51	Tetracosahexaen-3-ol, hexamethyl-, (all-E)-	27.974	0.34	No major activity reported but present in bioactive extracts	PubChem CID 5366014
52	δ-Tocopherol	28.308	0.2	Antioxidant, Anticancer, Enhances phase II detoxifying enzymes (Szewczyk *et al.*, 2021) [36].	PubChem CID 92094
53	Oxirane, 2,2-dimethyl-3-(pentamethyl)	29.058	0.32	No major activity reported but present in bioactive extracts	PubChem CID 693
54	Octadecatetraenoic acid, 5,9,13,17-tetramethyl	29.212	0.06	No major activity reported but present in bioactive extracts	PubChem CID 54190803
55	(R)-6-Methoxy-2,8-dimethylchroman derivative	29.811	0.22	No major activity reported but present in bioactive extracts	PubChem CID 77299178
56	5,9,13,17-Tetramethyl 4,8,12,16-octadecatetraenoic acid	29.212	0.06	No major activity reported but present in bioactive extracts	PubChem CID 54190803
57	Neophytadiene			Anti-inflammatory, antioxidant, anticancer, and hepatoprotective effects (Rajeswaran & Rajan, 2025) [31]	PubChem CID 10446

A representative chromatogram is shown in figure 2, with peak labels corresponding to the identified compounds. The early-eluting peaks (< 10 min) primarily consisted of low-molecular-weight organic acids and esters, while mid-range peaks (10-18 min) were dominated by fatty acids, phenolics, and sugar derivatives. The late-eluting peaks (> 20 min) contained long-chain hydrocarbons, sterol precursors, tocopherols, and chroman derivatives, reflecting the non-polar nature of these constituents.

Among the detected metabolites, δ-tocopherol (RT = 28.31 min) showed well-documented antioxidant and anticancer properties, enhancing phase II detoxifying enzymes, while 13-docosenamide (Z) (RT = 26.01 min) exhibited antimicrobial and cytotoxic activity. Additionally, squalene (RT = 26.50 min) was identified as a biosynthetic precursor of sterols with antioxidant significance. Several compounds with unreported or limited activity—such as α-tocospiro B, tetracosahexaen-3-ol, hexamethyl (all-E), and octadecatetraenoic acid, 5,9,13,17-tetramethyl were present in minor quantities (< 1%), suggesting potential for further pharmacological investigation.

Overall, the GC-MS profiling demonstrates a complex phytochemical composition comprising both primary metabolites (sugars, fatty acids) and secondary metabolites (phenolics, terpenoids, and chromans). This biochemical diversity underlies the observed biological potential of the extract, particularly in antioxidant, antimicrobial, anti-inflammatory, and cytotoxic contexts.

Validation of 3D model

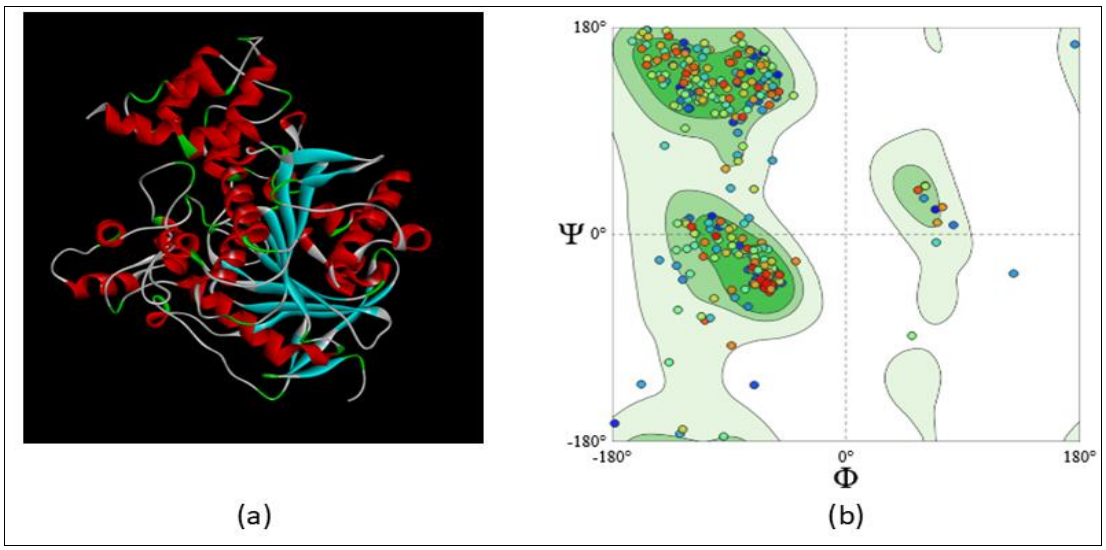

Fig 3: (a) 3D modeled structure of AChE1 (b) Ramachandran plot for 3D modeled structure of AChE1

The structural quality of the modeled proteins, Acetylcholinesterase 1 (AChE1) and Phenoloxidase 1, was evaluated using MolProbity analysis and Ramachandran plot assessment. The Ramachandran plot for AChE1 (Fig. 1) revealed that 95.16% of the residues are located within the favored regions, indicating excellent stereochemical quality. Only 0.56% of residues (A152 PRO, A478 ASP, and A606 ILE) were identified as outliers. The model exhibited a MolProbity score of 1.54 and a clash score of 2.13, with minor steric clashes observed between residue pairs A532 PHE-A608 TRP and A535 TYR-A632 LEU. The percentage of rotamer outliers was 1.95%, further confirming that the model geometry is well within acceptable limits. Overall, the AChE1 homology model demonstrates high structural integrity and is suitable for downstream molecular studies.

Molecular docking results

Molecular docking analysis of 60 phytocompounds against acetylcholinesterase (AChE) revealed that many constituents of *E japonica* exhibited stronger binding Affinities than the control ligand acetylcholine (-4.1 kcal/mol). Several compounds demonstrated notably higher inhibitory potential, including 13-docosenamide (-13.1 kcal/mol), 1-heptacosanol (-12.0 kcal/mol), tetracosahexaen-3-ol (-9.2 kcal/mol), and the (R)-6-methoxy-2,8-dimethylchroman derivative (-10.1 kcal/mol). Additional compounds such as octadecatetraenoic acid tetramethyl (-7.7 kcal/mol), 5,9,13,17-tetramethyl octadecatetraenoic acid (-7.9 kcal/mol), α-farnesene and benzyl β-D-glucoside (both -7.4 kcal/mol), megastigmatrienone (-7.3 kcal/mol), and neophytadiene (-7.3 kcal/mol) also displayed strong binding, clearly outperforming the control. Overall, the majority of the phytochemicals showed moderate to high affinity (-5.0 to -7.0 kcal/mol), indicating their potential to interact effectively with the AChE active site. These findings suggest that *E japonica* leaf extract contains multiple compounds with superior predicted inhibitory activity compared to acetylcholine, highlighting its promise as a natural AChE inhibitor (table).

Table 2: Comparison of acetylcholinesterase binding affinities and interaction profiles of the top five phytochemicals and acetylcholine (control)

S. No.	Compound	Binding affinity (kcal/mol)	Interacting residues	Interactions type
1.	Acetylcholine	-4.1	TYR235, SER313, PHE443, GLY233	Hydrogen bonds
			TRP198, TYR442,	Cation-anion attractive charge
			GLU312	π-cation attractive charge
			GLY232, PHE402, PHE513, HIS553	Van der waals interactions
2.	13-docosenamide	-13.1	TRP198, TYR235, TRP394, LEU397, PHE402, TYR442, PHE443, TYR446, TYR447	Non-covalent hydrophobic interactions
			TYR244	Hydrogen bonds
3.	1-heptacosanol	-12.0	PRO345, TYR475, TYR511, TRP640, LEU644, PRO 645	Non-covalent hydrophobic interactions
			GLN641	Hydrogen bonds
4.	tetracosahexaen-3-ol	-9.2	TRP198, TRP394, LEU397, PHE402, TYR442, PHE443, TYR446, TYR447, ALA554	Non-covalent hydrophobic interactions
5.	R)-6-methoxy-2,8-dimethylchroman derivative	-10.1	GLU 398, TRP394, CYS400, PHE402, TYR235, LEU397, GLU401, GLY231, GLY232, ALA554, GLU312	Van der waals interactions
			TYR447, ILE399, TYR446, HIS553, TRP198, TYR442, PHE443	Non-covalent hydrophobic interactions
6.	Octadecatetraenoic	-7.7	GLY232, GLY231, CYS400, ILE399, PHE402, GLU312,	Van der waals interactions

	acid tetramethyl		SER236	
			TYR 235	Hydrogen bonds
			ALA554, HIS553, TRP198, TYR442, PHE443, TYR446, TYR447	Non-covalent hydrophobic interactions

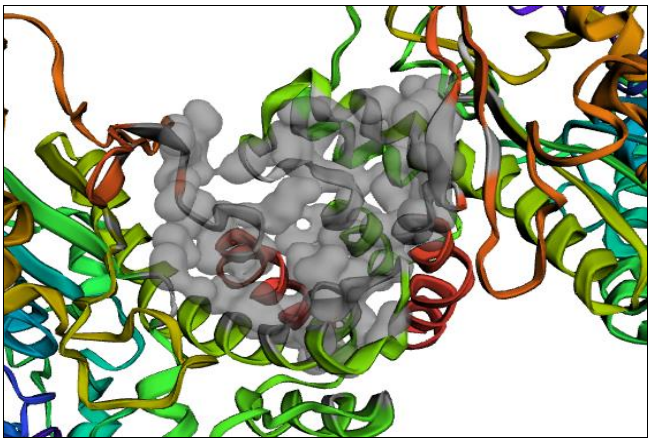

Fig 4: Catalytic pocket of AChE as predicted by CASTp

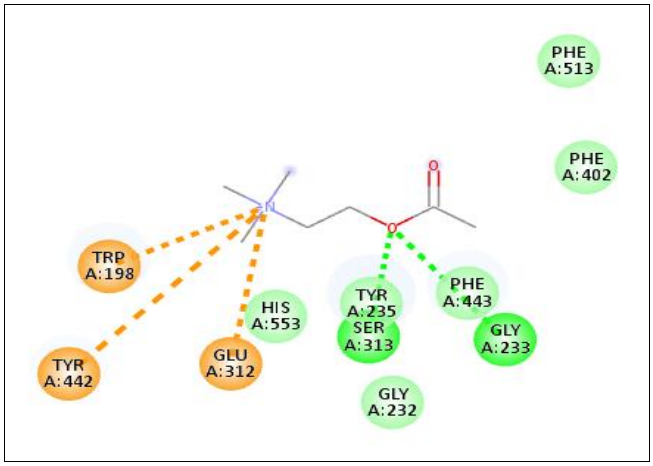

Fig 5: Binding-site residues involved in the interaction between acetylcholinesterase and acetylcholine.

Discussion

E japonica methanolic leaf extract possesses strong potential as a natural inhibitor of acetylcholinesterase (AChE) in *S litura*. GC-MS analysis confirmed the presence of a wide range of phytochemicals, indicating that the leaf extract is a rich source of biologically active compounds. Homology modeling and validation of *S. litura* AChE demonstrated that the predicted protein structure was of high stereochemical quality and suitable for molecular interaction studies.

Molecular docking results clearly showed that several phytoconstituents exhibited higher binding affinity toward AChE than the natural substrate acetylcholine, with key compounds such as 13-docosenamide, 1-heptacosanol, and chroman derivatives showing particularly strong interactions within the enzyme's catalytic pocket. These interactions suggest effective inhibition of AChE, which could disrupt normal neurotransmission and ultimately impair insect survival.

Conclusion

Overall, the findings confirm that *E. japonica* leaf extract contains multiple compounds capable of targeting AChE, supporting its potential use as an eco-friendly botanical insecticide against *S. litura*. The study establishes a scientific basis for further experimental validation and development of plant-derived pest management strategies, offering a sustainable alternative to conventional synthetic pesticides.

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