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Original Article

Computational Pharmacokinetics and Docking Insights into Conjugated Schiff Base Scaffold for Acetylcholinesterase Inhibition

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ABSTRACT

Aim: To evaluate the pharmacokinetic profiles and docking interactions of Schiff base scaffolds as potential Acetylcholinesterase (AChE) inhibitors using computational models. **Background:** Schiff bases exhibit diverse biological activities, including AChE inhibition relevant for neurodegenerative disorders. Computational evaluation of their pharmacokinetics and drug-likeness aids in prioritising ligands for further experimental validation. **Objectives:** To assess pharmacokinetics, drug-likeness, and molecular docking interactions of Schiff base ligands in comparison with Donepezil, an established AChE inhibitor. **Materials and Methods:** A series of Schiff ligands (L1-L11) was analysed for physicochemical properties, using SwissADME. Docking of the molecule and their studies were carried out with AutoDock Vina to investigate the binding interactions of the compounds with acetylcholinesterase (AChE), using its crystal structure (PDB ID: 1EVE) as the target. Medicinal chemistry filters were applied to assess synthetic feasibility and potential assay interference. **Results:** The Schiff base ligands (L1-L11) showed drug-like properties, good solubility, high GI absorption, and predicted BBB penetration in select cases. All passed drug-likeness rules with a bioavailability score of 0.55 and low medicinal chemistry alerts. Docking revealed stable AChE binding, supporting their potential as effective AChE inhibitors. **Conclusion:** Schiff base scaffolds demonstrate favourable pharmacokinetic properties, drug-likeness, and stable docking interactions with AChE.

Keywords: Schiff Base, Acetylcholinesterase Inhibition, *in silico* Pharmacokinetics, Molecular Docking, Drug-likeness, ADME Profiling.

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INTRODUCTION

The development of effective therapies to help manage conditions like Alzheimer's and other neurodegenerative diseases remains a key focus in medicinal chemistry and pharmaceutical research.[1] One prominent therapeutic strategy for managing Alzheimer's disease involves the inhibition of Acetylcholinesterase (AChE), the enzyme that breaks down acetylcholine in the spaces between nerve cells.[2] By blocking AChE activity, these compounds enhance cholinergic neurotransmission, thereby helping to alleviate cognitive impairments associated with neurodegeneration.[3]

To assess the pharmacokinetic properties, efficacy, and safety of potential AChE inhibitors, extensive *in vivo* studies using animal models are traditionally conducted. However, due to ethical concerns, high costs, and the time-intensive nature of animal testing, the scientific community has increasingly turned to *in silico* methods to accelerate early-stage drug development while reducing reliance on animal models.[4,5]

In silico methods, including "Quantitative Structure-Activity Relationship (QSAR) analysis, molecular docking, and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) evaluation," play a crucial role in predicting and assessing the biological activities and pharmacokinetic properties of drug candidates.[6,7] These computational approaches enable the rapid screening of extensive compound libraries, allowing researchers to prioritise the most promising molecules for further experimental validation while significantly reducing costs and development time. "Lipinski's Rule of Five," which evaluates oral bioavailability based on specific physicochemical parameters, serves as a fundamental guideline for assessing the drug-likeness of small molecules intended for oral use.[8] Additionally, evaluating parameters like skin permeability, Blood-Brain Barrier (BBB) penetration, interactions with Cytochrome P450 (CYP) enzymes, clearance rates, half-life, and acute toxicity (LD_{50}) is crucial for understanding the pharmacokinetic properties and safety profiles of potential AChE inhibitors.[9-11]

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Schiff bases, especially those with conjugated structures, have gained attention as a promising class of compounds in the search for novel AChE inhibitors.[12] Their ease of synthesis, structural adaptability, and capacity to form stable complexes with metal ions contribute to a wide range of biological activities, including antimicrobial, antiviral, anticancer, and neuroprotective effects.[13,14] The imine linkage (-C=N-) present in Schiff bases enhances their ability to interact with the active sites of enzymes like AChE, positioning them as strong candidates for further investigation as potential anti-Alzheimer's agents.[13]

Despite their promising biological activities, many Schiff base derivatives do not progress in development because of unfavourable pharmacokinetic characteristics or toxicity issues. Therefore, it is crucial to thoroughly assess their ADMET profiles using *in silico* methods to pinpoint derivatives that exhibit optimal drug-likeness and low toxicity risks before proceeding to *in vitro* and *in vivo* testing. In this study, a detailed investigation of *in silico* assessment of conjugated Schiff base scaffolds with potential AChE inhibitory activity was conducted using QSAR modelling, molecular docking, and SwissADME analysis.[14] The "drug-likeness" and pharmacokinetic properties of these compounds were assessed, focusing on key parameters such as BBB permeability-critical for CNS-active drugs-along with GI absorption, P-glycoprotein interactions, CYP metabolism, bioavailability scores, and toxicity indicators, to predict their potential as drug candidates for Alzheimer's disease treatment. By utilising computational models, this research aims to identify and prioritise conjugated Schiff base derivatives that exhibit strong predicted AChE inhibitory activity and favorable ADMET profiles, thereby facilitating their advancement in the drug development pipeline with increased efficiency and reduced reliance on animal testing.

Ultimately, this study seeks to provide meaningful insights into the potential of conjugated Schiff base scaffolds as AChE inhibitors, supporting their further development for clinical use in managing neurodegenerative diseases. This approach also aligns with the principles of ethical, cost-effective, and time-efficient drug discovery.

MATERIALS AND METHODS

Preparation of Acetylcholinesterase Structure and Optimisation of Ligands

The 3D crystal form of human "*Acetylcholinesterase Structure*" (PDB ID: 1B41), was downloaded in PDB format from the Protein Data Bank (www.rcsb.org). The reference "*Acetylcholinesterase*" inhibitor, "*Donepezil*" (PubChem CID: 3152) was retrieved from PubChem (https://pubchem.ncbi.nlm.nih.gov/). Ligands L1-L11 (as listed in Table 1) were designed using ChemDraw Ultra (CambridgeSoft Corporation, USA), with SMILES strings generated for each compound, and the structures were saved in mol format for use in subsequent docking studies. The selection of ligands L1-L11 was guided by precedent and strategic design: Schiff bases incorporating aromatic and heterocyclic cores are well-recognised for their donor versatility and coordination behaviour, as well as for their biological relevance.[15]

For theoretical validation, the ligand structures underwent geometry optimisation using OpenBabel to obtain their lowest energy conformations, ensuring their suitability for subsequent ADME and *in silico* analyses.[17] The resulting SMILES codes were then employed to assess ADME characteristics and predict other biological activities based on the structural data.[16-18]

Assessment of ADME Profiles and Molecular Docking

The distribution, metabolism, and excretion (DME) properties of the compounds were evaluated using the SwissADME tool (http://www.swissadme.ch).[19] This analysis covered various parameters, including physicochemical properties, lipophilicity, water solubility, pharmacokinetics, drug-likeness, and medicinal chemistry features. The assessment was conducted in line with Lipinski's Rule of Five, which suggests that drug candidates should have no more than five hydrogen bond donors, no more than ten hydrogen bond acceptors, a molecular weight below 500 Da, and a Log P value under 5.

For docking studies, the "CB-Dock online" platform (http://cao.labshare.cn/cb-dock/) was utilised to automatically predict binding energies. This free, user-friendly blind docking server offers interactive 3D visualisation of docking results, facilitating efficient evaluation of ligand-protein interactions.[20]

Additionally, toxicity predictions, including LD_{50} values, hepatotoxicity, and skin sensitisation, were evaluated to ensure the safety profile of the ligands by using a web-based tool for predicting the toxicity of chemical compounds (ProTox-3.0).[21]

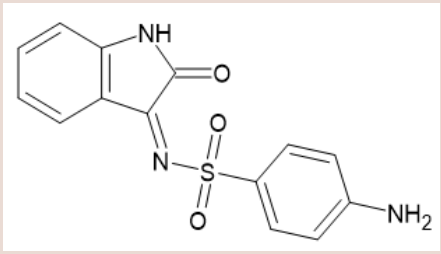
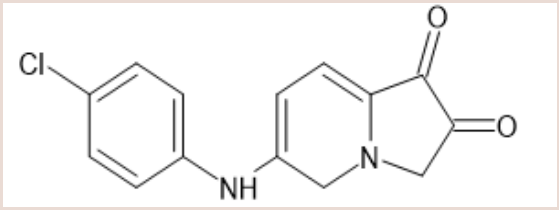
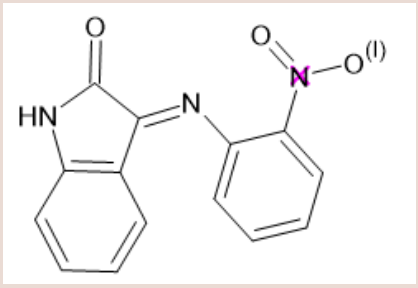
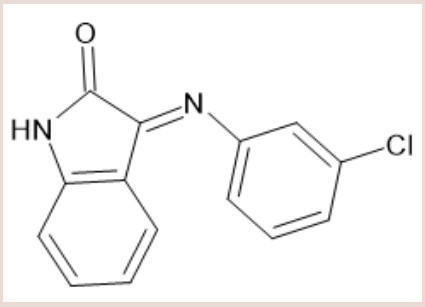
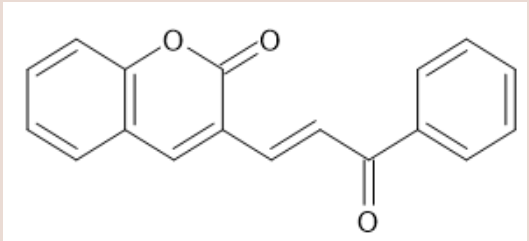
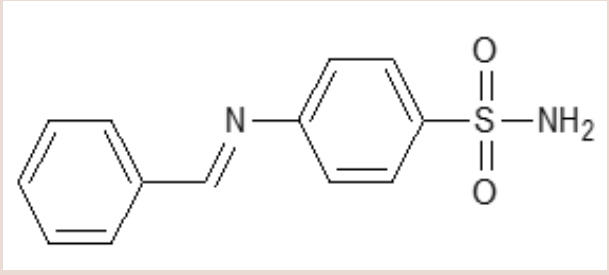
CB-Dock identifies active sites and calculates cavity sizes using an innovative curvature-based void detection method, integrating AutoDock Vina, a commonly used docking software, to carry out the molecular docking studies. Potential targets for the ligands were identified using the Swiss Target Prediction web platform (http://www.swisstargetprediction.ch/).

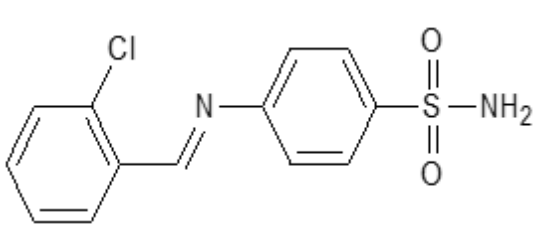
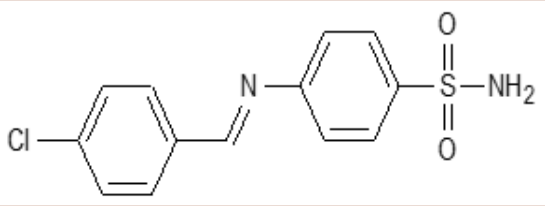
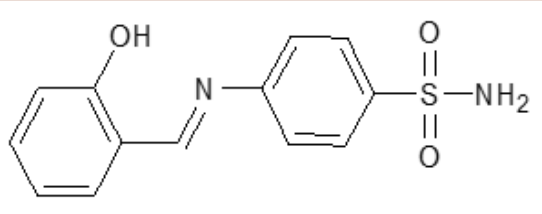
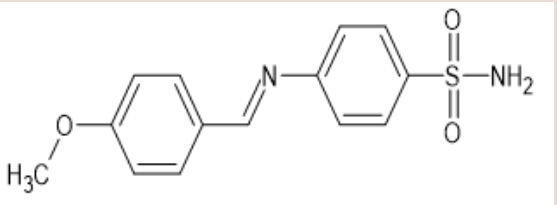
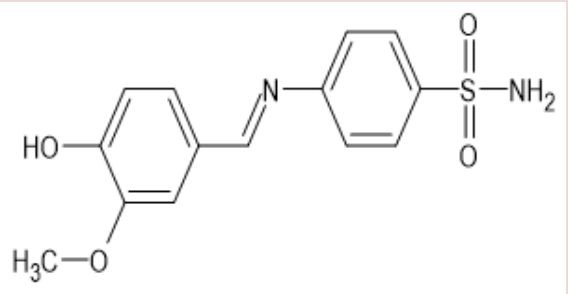
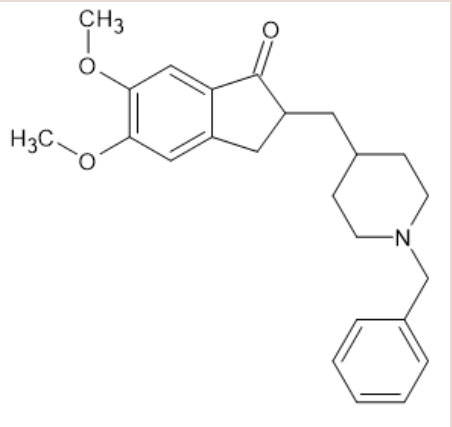
RESULTS

Molecular Properties

The ligands have molecular weights ranging from 257.69 Da (L3) to 317.34 Da (L1), all within the acceptable range for drug-likeness. Donepezil (379.49 Da) is heavier than the synthesised ligands but remains within the Lipinski threshold. TPSA values vary significantly, with L1 showing the highest TPSA (136.35 $Å^2$) and Donepezil having the lowest TPSA (38.77 $Å^2$), indicating higher polarity in L1 and better CNS permeability for Donepezil.

Table 1: Chemical name and structures of the ligands utilized in this study.

Ligand	Chemical Structure
L1 4-amino-N-[(3Z)-2-oxo-1,2-dihydro-3H-indol-3-ylidene]benzene-1-sulfonamide SMILES O=S(=O)(\N=C\1/C(=O)Nc2ccccc/12)c1ccc(N)cc1	
L2 6-(4-chloroanilino)indolizine-1,2(3H,5H)-dione SMILES O=C1C(=O)CN2CC(=CC=C21)Nc1ccc(Cl)cc1	
L3 (3E)-3-[(2-nitrophenyl)imino]-1,3-dihydro-2H-indol-2-one SMILES O=[N+]([O-])c1ccccc1\N=C1/c2ccccc2NC1=O	
L4 (3E)-3-[(3-chlorophenyl)imino]-1,3-dihydro-2H-indol-2-one SMILES O=C/1Nc2ccccc2\C\1=N/c1cc(Cl)ccc1	
L5 3-[(1E)-3-oxo-3-phenylprop-1-en-1-yl]-2H-1-benzopyran-2-one SMILES O=C1Oc2ccccc2C=C1/C=C/C(=O)c1ccccc1	
L6 N-(4-((phenylmethylene)amino)phenyl)sulfonamide SMILES O=S(=O)(N)N(Cc1ccccc1)c1ccccc1	

Ligand	Chemical Structure
L7 N-(4-((2-chlorobenzylidene)amino)phenyl)sulfonamide SMILES O=S(=O)(N)N(Cc1ccccc1Cl)c1ccccc1	
L8 4-[(4-chlorobenzylidene)amino]benzenesulfonamide SMILES O=S(=O)(N)c1ccc(cc1)/N=C/c1ccc(Cl)cc1	
L9 4-[(2-hydroxybenzylidene)amino]benzenesulfonamide SMILESO=S(=O)(N)c1ccc(cc1)/N=C/c1ccccc1O	
L10 4-{(E)-[(4-methoxyphenyl)methylidene]amino} benzene-1-sulfonamide SMILES O=S(=O)(N)c1ccc(cc1)\N=C\c1ccc(cc1)OC	
L11 4-[(4-hydroxy-3-methoxybenzylidene) amino]benzenesulfonamide SMILES O=S(=O)(N)c1ccc(cc1)/N=C/c1cc(OC)c(O)cc1	
Donepezil (Standard/ Reference drug) 2-[(1-benzylpiperidin-4-yl) methyl]-5,6-dimethoxy-2,3-dihydroinden-1-one SMILES O=C1c2cc(OC)c(OC)cc2CC1CC1CCN(Cc2ccccc2)CC1	

"Note: SMILES strings and IUPAC names are standard representations of molecular structures and may appear similar to database entries."

Lipophilicity

Most ligands exhibit moderate lipophilicity, with XLOGP3 values between 1.05 and 3.8. Donepezil shows the highest lipophilicity (XLOGP3=4.28), correlating with its good BBB penetration, while L1 has the lowest iLOGP (-3.04), indicating high hydrophilicity.

Water Solubility

Most ligands are classified as soluble, with ESOL Log S values indicating adequate aqueous solubility for oral administration. L3 and Donepezil exhibit moderate solubility, with Donepezil having the lowest solubility (ESOL Log S=-4.81) among the compounds, consistent with its high lipophilicity.

Pharmacokinetics

All ligands and Donepezil show high gastrointestinal absorption, supporting oral bioavailability potential. BBB permeability is predicted for L2, L3, L5, and Donepezil, aligning with higher lipophilicity and lower TPSA in these molecules. Several ligands (e.g., L8, L10, L11) inhibit CYP3A4, indicating possible drug-drug interaction risks, while Donepezil inhibits CYP2D6 and CYP3A4.

Druglikeness

All ligands comply with Lipinski, Ghose, Veber, Egan, and Muegge rules, confirming their drug-like nature. All have a bioavailability score of 0.55, indicating good oral bioavailability potential.

Medicinal Chemistry Alerts

Certain ligands, including L1, L3, and L4, triggered PAINS alerts, suggesting a possible risk of false-positive responses in biological assays and highlighting the need for additional validation. Although docking results indicate promising binding potential, the presence of PAINS-associated motifs raises the possibility that any observed activity could arise from assay artefacts rather than genuine target inhibition. Brenk alerts are minimal, typically 0-1 per ligand, indicating low structural complexity and fewer toxicophores. All ligands have acceptable synthetic accessibility values (2.32-3.34), suggesting practical feasibility for synthesis.

L3 and L7, which exhibited the strongest AchE binding affinities (-8.8 kcal/mol), also show moderate lipophilicity, high GI absorption, BBB permeability, and good drug-likeness. This suggests they are promising candidates for further *in vitro*/*in vivo* validation. L3 and L7 show the strongest binding affinity (-8.8 kcal/mol), surpassing Donepezil (-7.2 kcal/mol), indicating promising potential as AchE inhibitors. L10 has the weakest binding affinity (-6.2 kcal/mol) among the ligands. Overall, L3, L4, L6, L7, and L9 exhibit stronger binding than Donepezil. Ligands with high TPSA values (e.g., L1, L9, L11) may have limited BBB penetration, which may be advantageous if peripheral AchE inhibition is targeted while minimising CNS side effects.[22]

The combined analysis (Tables 2 and 3) indicates that L3, L4, L6, L7, and L9 exhibit a favourable balance between binding affinity, solubility, lipophilicity, drug-likeness, and pharmacokinetic properties, positioning them as potential AchE inhibitors for further pharmacological studies.Top of Form

DISCUSSION

The molecular profiling confirmed that all ligands met standard drug-likeness criteria and exhibited good oral bioavailability potential. Compared to Donepezil, ligands with higher TPSA (e.g., L1, L9, L11) may show limited BBB penetration, suggesting possible utility for peripheral AchE inhibition. In contrast, L3 and L7 combined moderate lipophilicity, good solubility, high GI absorption, and BBB permeability with the strongest binding affinities (-8.8 kcal/mol), surpassing Donepezil. Although some ligands showed PAINS alerts, low Brenk alerts and acceptable synthetic accessibility support their feasibility. Overall, L3, L4, L6, L7, and L9 emerged as promising AchE inhibitor candidates, with L3 and L7 being the most suitable for further experimental validation.

CONCLUSION

The computational analysis of Schiff base scaffolds highlights their promising potential as Acetylcholinesterase (AChE) inhibitors for treating neurodegenerative diseases. The ligands showed drug-like properties, with suitable molecular weights, moderate lipophilicity, and high gastrointestinal absorption, while some demonstrated the ability to cross the blood-brain barrier. Most compounds met drug-likeness criteria and showed good potential for oral bioavailability. Medicinal chemistry evaluations revealed minimal structural concerns and indicated that these ligands can be practically synthesised for further studies. Docking results showed stable interactions within the AChE active site,

Table 2: Cavity-detection guided Blind Docking-predicted biological characteristics of ligand, L1-L11 and Standard Donepezil drug with Acetylcholinesterase enzyme.

Sl. No.	Ligand	AchE Binding affinity
1	L1	-7.3
2	L2	-7.1
3	L3	-8.8
4	L4	-8.3
5	L5	-7.9
6	L6	-8.3
7	L7	-8.8
8	L8	-6.7
9	L9	-8.5
10	L10	-6.2
11	11	-6.6
12	Donepezil	-7.2

Table 3: Analysis of Physicochemical, Pharmacokinetic, and Drug-Likeness Properties of Ligands and Standard.

Property	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10	L11	Donepezil (Std)
MF	$C_{14}H_{13}N_4O_3S$	$C_{15}H_{11}ClN_2O$	$C_{14}H_{10}ClN_2O$	$C_{14}H_{10}N_3O_3$	$C_{18}H_{12}O_3$	$C_{13}H_{13}N_2O_2S$	$C_{13}H_{12}ClN_2O_2S$	$C_{13}H_{11}ClN_2O_2S$	$C_{13}H_{12}N_2O_3S$	$C_{14}H_{14}N_2O_3S$	$C_{14}H_{14}N_2O_4S$	$C_{24}H_{29}NO_3$
MW (Da)	317.34	270.71	257.69	268.25	276.29	261.32	295.76	294.76	276.31	290.34	306.34	379.49
TPSA (Å²)	136.35	41.46	41.79	87.61	47.28	80.9	80.9	80.9	101.13	90.13	110.36	38.77
iLOGP	-3.04	2.53	-1.41	-1.78	2.62	-2.61	-2.8	2.02	1.41	1.62	1.9	3.92
XLOGP3	1.05	3.24	3.8	3.0	3.32	2.13	2.76	2.41	1.65	1.77	1.61	4.28
ESOL Log S	2.74	3.96	-4.26	-3.71	4.01	3.1	3.68	-3.46	-2.86	-2.94	-2.91	-4.81
Solubility Class	Soluble	Soluble	Mod. soluble	Soluble	Mod. soluble	Soluble	Soluble	Soluble	Soluble	Soluble	Soluble	Mod. soluble
GI Absorption	High	High	High	High	High	High	High	High	High	High	High	High
BBB Permeant	No	Yes	Yes	No	Yes	No	No	No	No	No	No	Yes
Pgp Substrate	Yes	No	Yes	Yes	No	Yes	Yes	No	No	No	No	Yes
CYP Inhibition	No	1A2, 2C19	1A2	1A2	1A2, 2C19, 2C9	No	No	1A2, 2C19, 2C9, 3A4	No	3A4	2C9, 3A4	2D6, 3A4
Lipinski	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.	0 viol.
Bioavail. Score	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55
PAINS Alerts	1	0	1	1	0	0	0	0	0	0	0	0
Brenk Alerts	1	1	0	2	1	1	1	1	1	1	1	0
Leadlikeness Viol	0	0	1	0	0	0	0	0	0	0	0	2
Synth. Accessibility	2.75	2.59	2.32	2.61	3.34	2.82	2.9	2.47	2.51	2.45	2.58	2.32

suggesting these compounds may effectively inhibit AChE activity, comparable to the standard drug Donepezil. Overall, the findings support Schiff base scaffolds as promising candidates for further *in vitro* and *in vivo* investigations, moving toward the development of effective, orally available AChE inhibitors that could contribute to the management of neurodegenerative disorders.

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ABBREVIATIONS

AChE: acetylcholinesterase; **ADME:** Absorption, Distribution, Metabolism, Excretion; **GI:** Gastrointestinal; **BBB:** Blood-Brain Barrier; **QSAR:** Quantitative Structure-Activity Relationship; **ADMET:** Absorption, Distribution, Metabolism, Excretion, and Toxicity; **CYP:** Cytochrome P450enzymes; **LD_{50}:** Lethal Dose, 50%; **DME:** Distribution, metabolism, and excretion; **Da:** Dalton; **Log P:** Logarithm of the Partition Coefficient; **MF**: Molecular Formula; **MW:** Molecular Weight; **TPSA:** Topological Polar Surface Area; ***iLOGP:*** In silico *Log Partition Coefficient;* ***XLOGP:*** *Atom Additive Log Partition Coefficient;* ***Log S:*** *Estimated Solubility;* **Pgp:** *P glycoprotein*.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

SUMMARY

The Schiff base ligands we designed showed encouraging drug-like features, with suitable molecular weights, balanced lipophilicity, good solubility, and strong potential for oral absorption. Some compounds were predicted to cross the blood-brain barrier, while those with higher polarity may be better suited for peripheral AChE inhibition, reducing possible CNS side effects. Docking studies revealed that several ligands (L3, L4, L6, L7, and L9) bound more strongly than Donepezil, with L3 and L7 standing out as the most promising. Importantly, medicinal chemistry checks showed minimal structural concerns and practical ease of synthesis. Taken together, these results suggest that Schiff base scaffolds, especially L3 and L7, could serve as valuable leads for developing new AChE inhibitors and deserve further exploration through *in vitro* and *in vivo* studies for potential use in neurodegenerative disease therapy.

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