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Original Article

In silico Assessment of Bioactive Compounds from *Thaalisaathi Chooranam* Targeting Alcohol Dehydrogenase in Alcoholic Liver Disease

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ABSTRACT

Background: Alcoholic Liver Disease (ALD) is a major cause of cirrhosis-related morbidity and mortality, with limited therapies. Alcohol Dehydrogenase (ADH) plays a key role in ethanol metabolism and contributes to hepatic injury. Siddha formulations are rich in bioactive phytoconstituents with potential hepatoprotective effects. **Objectives:** To evaluate the drug-likeness and inhibitory potential of bioactive phytoconstituents from *Thaalisaathi Chooranam* against Human Alcohol Dehydrogenase using *in silico* ADME analysis and molecular docking studies. **Materials and Methods:** A total of 43 bioactive compounds were identified from previously published data of *Thaalisaathi Chooranam*. After excluding certain fatty acids, five small molecules were selected based on peak area percentage. Drug-likeness and lead-likeness were assessed using the Swiss-ADME web tool following Lipinski's Rule of Five. Three compounds that met ADME criteria were docked against human alpha-type alcohol dehydrogenase (PDB ID: 1HSO) using iGEMDOCK v2.0. Binding energies and protein-ligand interactions were analyzed. **Results:** Swiss-ADME analysis confirmed that the three selected compounds had favourable physicochemical and pharmacokinetic properties. Molecular docking demonstrated their activity against Alcohol Dehydrogenase, with Dihydroqinghaosu showing the strongest binding, stabilised by hydrogen bonds with active site residues, complemented by van der Waals interactions. The other two compounds, 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone and Apiole, also exhibited strong binding, indicating potential inhibitory activity. **Conclusion:** This study showed that bioactive compounds from *Thaalisaathi Chooranam*, particularly Dihydroqinghaosu, demonstrated strong inhibitory potential against human alcohol dehydrogenase and favourable ADME properties, endorsing their promise as therapeutic leads for ALD and supporting further *in vivo* and experimental validation.

Keywords: Alcohol dehydrogenase, Alcoholic liver disease, *In silico* study, *Thaalisaathi Chooranam*.

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INTRODUCTION

Alcoholic Liver Disease (ALD) is a sequence of hepatic diseases, ranging from alcoholic fatty liver to alcoholic hepatitis, ultimately leading to alcoholic cirrhosis, the most advanced and largely irreversible stage of alcohol-induced liver injury (Patel *et al.*, 2024). Alcohol consumption causes about 3.3 million deaths each year worldwide, representing 5.9% of global mortality, and also leads to both acute and chronic liver damage that can result in ALD. (Nagarjuna *et al.*, 2025). The leading cause of cirrhosis (43.2%) in India is alcohol consumption, followed by NAFLD/ Cryptogenic liver disease (14.4%), Hepatitis B Virus (11.5%), and Hepatitis C Virus (6.2%), with a significant rise in alcohol-related cirrhosis over recent decades and a concurrent decline in viral etiologies (Elhence *et al.*, 2024).

ALD is considered completely irreversible there are currently no FDA-approved anti-fibrotic therapies for cirrhosis, and therapeutic options remain limited (Nagarjuna *et al.*, 2025; Ohashi *et al.*, 2018). Conventional treatments suggest corticosteroids as the standard treatment for severe alcoholic hepatitis; however, they provide only short-term survival benefit without significant improvement in long-term outcomes, with six-month mortality remaining high (Nagarjuna *et al.*, 2025; Ohashi *et al.*, 2018). There is no treatment for patients with advanced liver disease, liver transplantation is the only option, yet reduced feasibility,

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rendering the need for alternative and adjunctive therapeutic strategies (Ohashi *et al*., 2018).

Alcohol Dehydrogenases (ADHs) play an important function in ethanol metabolism. Pharmacological inhibition of ADH using agents such as fomepizole (4-methylpyrazole), a non-specific ADH inhibitor currently used for methanol and ethylene glycol poisoning, has been proposed as a potential strategy to prevent the formation of toxic metabolites in substance intoxication (Di *et al*., 2021). Traditional Siddha medicine offers various formulations to promote liver health and manage liver diseases, representing the therapeutic strength of this system of medicine (Subramani *et al*., 2017).

Beyond conventional treatment strategies, there is growing scientific interest in traditional herbal remedies, especially polyherbal formulations, due to their potential to serve as sources of effective therapeutic remedies (Kotmire *et al*., 2024). This study aimed to evaluate the drug-likeness and inhibitory potential of bioactive compounds from *Thaalisaathi Chooranam* against human alcohol dehydrogenase using *in silico* ADME analysis and molecular docking studies.

MATERIALS AND METHODS

In this study, previously published GC-MS data of *Thaalisaathi Chooranam* (Mudhaliyar, 1992) were analyzed, which identified 43 compounds (Kumarasamy *et al*., 2016). From these, five small molecules were shortlisted based on peak area percentage after excluding fatty acids, due to their high structural flexibility and nonspecific Hydrophobic Interactions, which may produce unreliable binding scores. The selected compounds were evaluated for pharmacokinetic properties, drug-likeness, and lead-likeness using the SwissADME web tool (http://www.swissadme.ch/) in accordance with Lipinski's Rule of Five. Compounds that met ADME criteria were subsequently subjected to molecular docking against human alpha-type alcohol dehydrogenase (PDB ID: 1HSO) using iGEMDOCK v2.0 (Yang *et al*., 2004), and their binding affinities and protein-ligand interactions were analyzed. The method is represented diagrammatically in Figure 1.

Selection of Molecules and Ligand Preparation

The following Five Phyto-compounds (Table 1) were selected as ligands based on peak area percentage for drug-likeness analysis and ADME studies (Figure 2). The 5 selected ligand canonical SMILES were obtained from the PubChem website (https://pubchem.ncbi.nlm.nih.gov/). The canonical SMILES were converted to PDB format using Cactus software (https://cactus.nci.nih.gov/translate/).

Ethical statement

Not applicable as this is an *in silico* computational study not involving live human or animal subjects.

RESULTS

Selection of Target protein

The human liver alpha-type alcohol dehydrogenase enzyme (PDB ID: 1HSO) protein structure was acquired from the protein data bank (www.rcsb.org). The PDB format extraction was used to study the protein's crystal structure. The structure is represented in Figure 2d. Preliminary virtual screening of the extracted compounds was carried out using the iGEMDOCK v2.0 molecular docking program (Yang *et al*., 2004). Based on the binding energy scores obtained, the compounds of TSC demonstrating the highest binding affinity were shortlisted and subsequently subjected to detailed molecular docking analysis for further evaluation of their interaction with the target protein.

DISCUSSION

The selection of ADH1A (Hadi *et al*., 2023) as the molecular target is scientifically coherent, given that its inhibition could reduce the generation of acetaldehyde, a toxic ethanol metabolite central to ALD pathogenesis. The formulation's constituent *Triphala Chooranam* has documented ADH-inhibitory potential (Banjan *et al*., 2025), and *Coriandrum sativum* (Dhanalakshmi *et al*., 2019) (present in relatively high proportions) has demonstrated beneficial effects in Alcohol Use Disorder clinically. Classical Siddha literature (*Siddha Vaithiya Thirattu*) (Mudhaliyar *et al*., 1992) further indicates *Thaalisaathi Chooranam* in liver cirrhosis (*Eeral Ularal*). The present *in silico* investigation evaluated five phytochemical constituents (Compounds A-E) from GC-MS profile of *Thaalisaathi Chooranam*, a classical Siddha polyherbal formulation, as the inhibitors of human alpha-type alcohol dehydrogenase (ADH1A; PDB ID: 1HSO) (Figure 2).

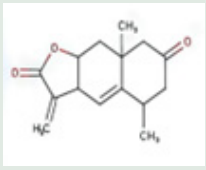
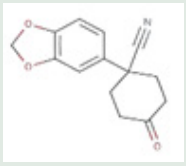
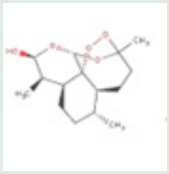
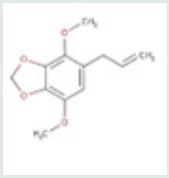
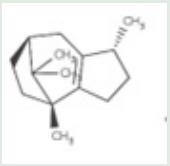
The physicochemical parameters of Compounds A-E (from Table 1) demonstrated full compliance with Lipinski's Rule of Five (MW ≤ 500 g/mol; Log p≤ 5; HBD ≤ 5; HBA ≤ 10), with molecular weights (204.35-284.35 g/mol) and consensus Log p values (2.04-3.76) falling within the oral bioavailability range of 1-3, associated with successful oral drug candidates in approved pharmaceutical inventories (Lipinski *et al*., 1997). All compounds additionally satisfied the Ghose, Veber, and Egan filters, reinforcing their pharmacokinetic acceptability. Compounds A-D exhibited moderate lipophilicity (consensus Log P ≈ 2.0-2.4), considered optimal for balancing oral absorption with solubility. These observations agree with the established pharmacokinetic principle that excessive lipophilicity can impair aqueous dissolution and limit bioavailability (Table 3). Predicted aqueous solubility across ESOL, Ali, and Silicos-IT models consistently classified all compounds as "Soluble" (log S>-4), with Compound A demonstrating the highest solubility (ESOL log S =-2.27) and Compound E the lowest (-3.81), still within acceptable drug-like limits (Tables 1 and 2).

Topological polar surface area values (0.00-59.32 Å²), established intestinal absorption threshold of 140 Å² and the BBB permeability reference limit of 90 Å², alongside rotatable bond counts (0-4) substantially below Veber's ≤10 threshold, collectively predict high gastrointestinal absorption and favourable membrane permeability for all compounds. Compound E's TPSA of 0.00 Å² reflects complete non-polarity and strong hydrophobic character, consistent with its higher consensus Log P (3.76) and lower predicted aqueous solubility (Table 2).

The absence of PAINS alerts and the uniform Abbott bioavailability score of 0.55 compare favourably against established benchmarks, given that approximately 6-10% of screening library compounds carry PAINS liabilities and a score of ≥0.55 is considered acceptable for early-stage oral candidates (Baell *et al.*, 2010) (Table). Molar refractivity values (59.59-71.34) fell within the Ghose filter range (40-130), and rotatable bond counts (0-4) were well below Veber's threshold of ≤10, indicating optimal molecular flexibility conducive to receptor binding. The Bioavailability Radar profiles (Figure 1) for all compounds predominantly occupied the optimal physicochemical space, and a uniform Abbott bioavailability score of 0.55 was predicted, suggesting a moderate but acceptable probability of oral bioavailability Table 2 (Martin *et al.*, 2005).

All compounds except Compound E show high GI absorption and BBB permeability, indicating favorable oral bioavailability and potential CNS activity; however, Compound B and D exhibit CYP inhibition, suggesting possible drug-drug interactions. Compound E demonstrates poor GI absorption, no BBB

Table 1: Molecular Structures and Physicochemical Properties of the Selected Compounds.

Compounds	2-Oxo-5,11(13)-eudesmadien-12,8-olide	4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone	Dihydroqinghaosu	Apiole	Patchoulene
	A	B	C	D	E
IUPAC Name	5,8*a*-dimethyl-3-methylidene-3*a*,5,6,8,9,9*a* hexahydrobenzo[f][1] benzofuran-2,7-dione	1-(benzo[d][1,3] dioxol-5-yl)-4-oxocyclohexane-1-carbo nitrile	(4S,5R,8S,9R,10S,12R,13R)-1,5,9-trimethyl-11,14,15,16 tetraoxatetracyclo [10.3.1.04,13.08,13] hexadecan-10-ol	4,7-dimethoxy-5-prop-2-enyl-1,3-benzodioxole	1,5,11,11-tetramethyltricyclo [6.2.1.02,6] undec-2(6)-ene
Canonical SMILES	CC1CC(=O) CC2(C1=CC3C(C2) OC(=O)C3=C)C	N#CC1(C2=C/C3=C(\C=C/2) OCO3) CCC(=O)CC1	C[C@@H]1CC[C@H]2[C@H] ([C@H] (O[C@H]3[C@@]24[C@H]1 CCC(O3)(OO4)C)O)C	COC1=C2C(=C(C(=C1) CC=C) OC) OCO2	C[C@@H]1CCC2=C1C[C@ @H]3CC[C@@]2(C3(C)C)C
Chemical Structure					
Molecular Formula	$C_{15}H_{18}O_3$	$C_{14}H_{13}NO_3$	$C_{15}H_{24}O_5$	$C_{12}H_{14}O_4$	$C_{15}H_{24}$
Molecular Weight	246.30	243.26	284.35	222.24	204.35
H bond donor	0	0	1	0	0
H bond acceptor	3	4	5	4	0
Log p	2.27	2.04	2.17	2.44	3.76
Molar refractivity	68.15	64.03	71.34	59.59	66.88
No.heavy atoms	18	18	20	16	15
No.Aromatic heavy atoms	0	6	0	6	0
Fraction Csp3	0.60	0.43	1.00	0.33	0.87
No rotatable bonds	0	1	0	4	0

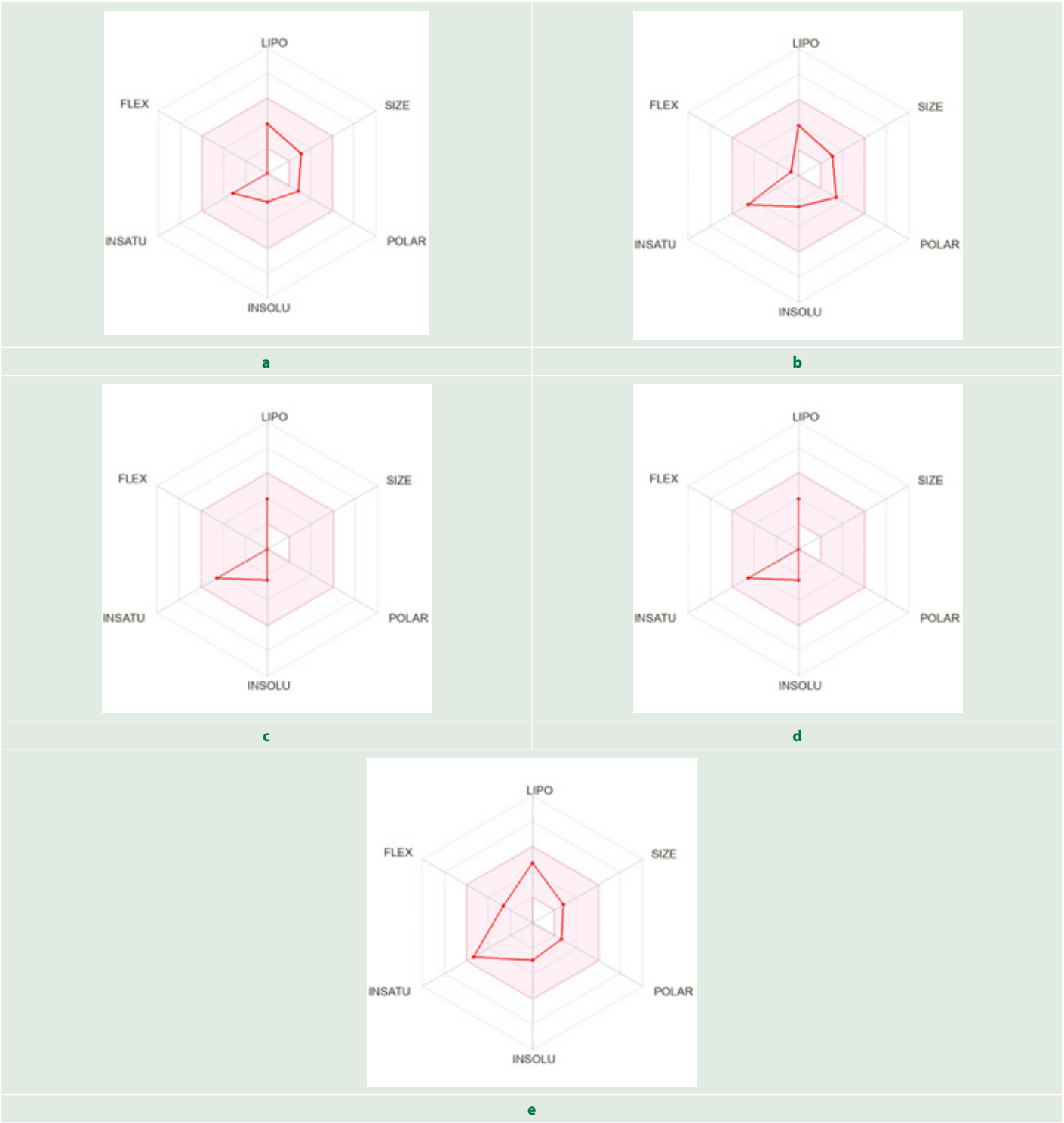


Figure 1: Evaluating Drug Likeness and Oral Availability of the Ligands by Radar Graph. a: Radar of 2-Oxo-5,11(13)-eudesmadien-12,8-olide. b: Radar of 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone. c: Radar of Dihydroqinghaosu. d: Radar of Apiole. e: Radar of Patchoulene.

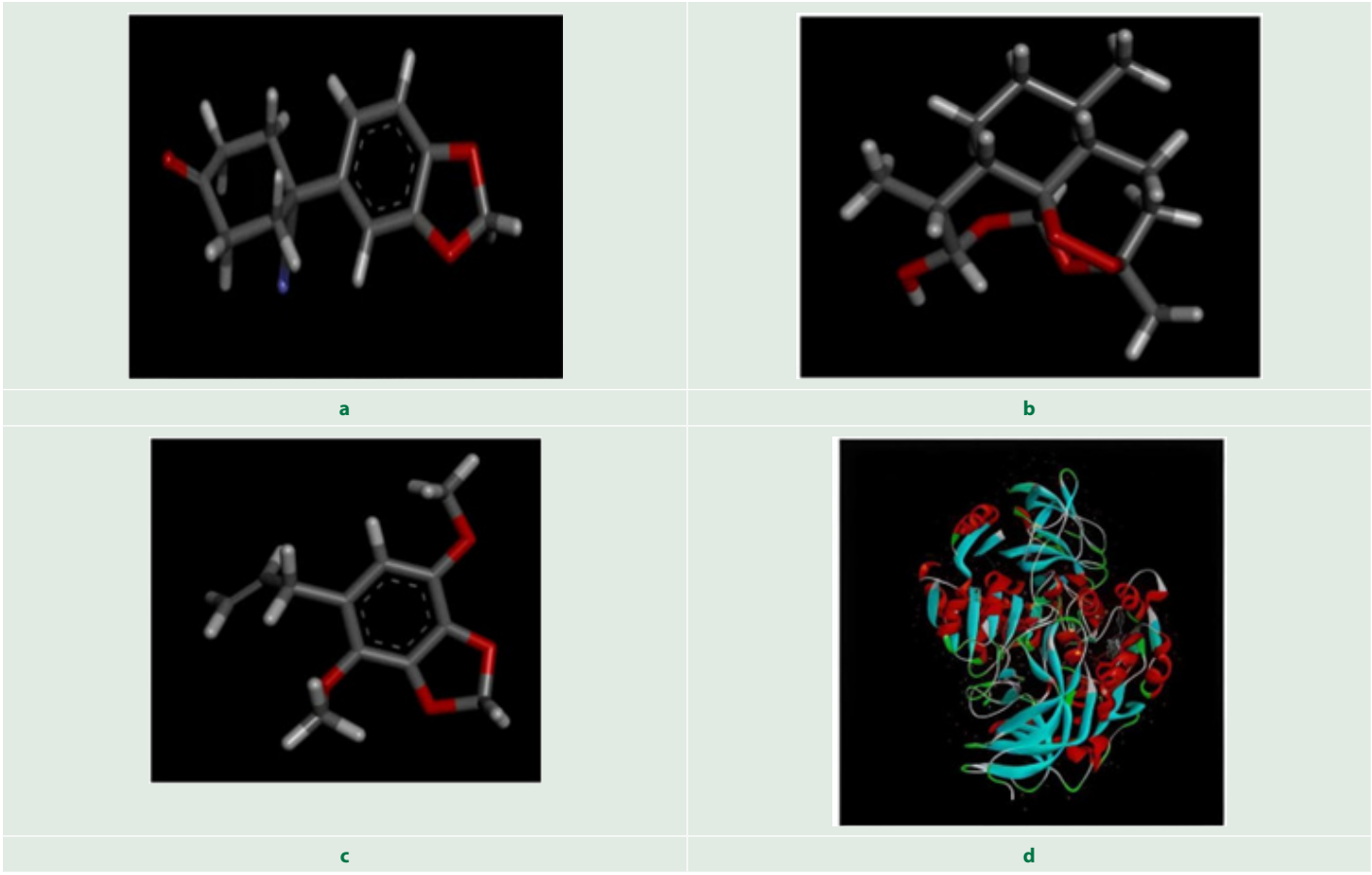


Figure 2: Selected Ligand and Target for in silico Analysis. a: Ligand 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone. b: Ligand Dihydroqinghaosu. c: Ligand Apiole. d: Target alcohol Dehydrogenase (PDB ID: 1HSO).

penetration, and P-gp efflux, indicating limited systemic and CNS availability despite relatively higher skin permeability (Log Kp) Table 3 (Bosco *et al.*, 2024).

Molecular docking analysis

Following ADME-guided exclusion of Compounds A and E, three lead compounds -Dihydroqinghaosu, 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone, and Apiole -were subjected to molecular docking against the ADH1A active site using iGEMDOCK (Kiran, 2022) (population size 200; 70 generations; very slow/accurate mode). Dihydroqinghaosu exhibited the highest binding affinity (-83.54 kcal/mol), with a strong hydrogen bonding contribution of -29.32 kcal/mol involving active site residues CYS46, THR48, HIS51, and the catalytic zinc ion ZN1376 (Figure 3 and Table 4). The prominent involvement of the zinc centre is mechanistically significant, as zinc coordinates the substrate hydroxyl group during catalysis in ADH enzymes; competitive occupancy of this site could directly attenuate enzymatic activity. These interactions suggest that Dihydroqinghaosu may act through a zinc-chelation-mediated inhibitory mechanism, meriting further investigation (Asahi *et al.*, 2023).

4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone ranked second (-82.22 kcal/mol), with dominant van der Waals interactions (-71.92 kcal/mol) through hydrophobic contacts with GLY47, THR178, VAL292, and VAL294, though its hydrogen bonding energy (-10.31 kcal/mol) was comparatively lower, implying reduced binding specificity. Apiole demonstrated moderate overall affinity (-80.25 kcal/mol) with balanced van der Waals (-61.21 kcal/mol) and hydrogen bonding (-19.05 kcal/mol) contributions, engaging CYS46, CYS174, LEU319, ZN1376, and PYZ1378 -a broader residue interaction profile suggestive of stable but less specific active-site accommodation.

Toxicity Prediction

Toxicity profiling via the ProTox-II web tool classified all five compounds (Table 3) under GHS Toxicity Classes 4 and 5 (LD_{50}: 567-5000 mg/kg), indicating low to practically non-toxic acute oral toxicity profiles, with no compound demonstrating predicted hepatotoxicity -a critically favourable finding given the hepatic disease context of the study (Venkatachalam *et al.*, 2025; Cheng *et al.*, 2012). Aqueous solubility ranged from Very Soluble to Moderately Soluble, with high GI absorption predicted for Compounds 1-4, while Patchoulene exhibited low GI absorption, moderate solubility, and a single Lipinski violation

Table 2: Predicted Solubility of the screened compounds.

Compounds	2-Oxo-5,11(13)-eudesmadien-12,8-olide	4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone	Dihydroqinghaosu	Apiole	Patchoulene
TPSA	43.37 $Å^2$	59.32 $Å^2$	57.15 $Å^2$	36.92 $Å^2$	0.00 $Å^2$
iLOGP	2.18	1.95	2.49	2.85	0.00
XLOGP3	1.44	1.42	2.99	2.75	4.29
WLOGP	2.42	2.32	2.19	2.16	4.56
MLOGP	2.38	1.31	1.95	1.40	5.65
Silicos-IT Log P	2.93	3.17	1.23	3.02	4.30
Consensus Log P	2.27	2.04	2.17	2.44	3.76
ESOL log S	-2.27	-2.42	-3.49	-2.96	-3.81
ESOL solubility [mg/mL]	1.31e+00 mg/mL	9.17e-01 mg/mL	9.27e-02 mg/mL	2.42e-01 mg/mL	3.17e-02 mg/mL
ESOL solubility [mol/l]	5.32e-03 mol/l	3.77e-03 mol/l	3.26e-04 mol/l	1.09e-03 mol/l	1.55e-04 mol/l
ESOL class	Soluble	Soluble	Soluble	Soluble	Soluble
Ali log S	-1.96	-2.27	-3.85	-3.18	-4.00
Ali solubility [mg/mL]	2.72e+00 mg/mL	1.31+00 mg/mL	3.98e-02 mg/mL	1.47e-01 mg/mL	2.03e-02 mg/mL
Ali solubility [mol/l]	1.11e-02 mol/l	5.36e-03 mol/l	1.40e-04 mol/l	6.60e-04 mol/l	9.93e-05 mol/l
Ali class	Very soluble	Soluble	Soluble	Soluble	Moderately Soluble
Silicos-IT log S	-2.94	-3.79	-1.34	-3.26	-3.97
Silicos-IT solubility [mg/mL]	2.83e-01 mg/mL	3.97e-02 mg/mL	1.30+01 mg/mL	1.21e-01 mg/mL	2.19e-02 mg/mL
Silicos-IT solubility [mol/mL]	1.15e-03 mol/l	1.63e-04 mol/l	4.58e-02 mol/l	5.45e-04 mol/l	1.07e-04 mol/l
Silicos-IT class	Soluble	Soluble	Soluble	Soluble	Soluble
Lipinski # violations	Yes; 0 Violation	Yes; 0 violation	Yes; 0 violation	Yes;0 violation	Yes; 1 violation: MLOGP>4.15
Ghose # violations	Yes	Yes	Yes	Yes	Yes
Veber # violations	Yes	Yes	Yes	Yes	Yes
Egan # violations	Yes	Yes	Yes	Yes	Yes
Muegge # violations	Yes	Yes	Yes	Yes	No;1 violation: Heteroatoms<2
Bioavailability score	0.55	0.55	0.55	0.55	0.55
PAINS # alerts	0 alert	0 alert	0 alert	0 alert	0 alert
Brenk # alerts	2 alerts: isolated_alkene, Michael_acceptor_1	0 alert	1 alert: Peroxide	1 Alert: isolated_alkene	1 alert: isolated_alkene
Leadlikeness # violations	No;1 violation: MW < 250	No; 1 violation: MW<250	Yes	No;1 violation: MW<250	No;2 violations: MW<250, XLOGP3>3.5
Synthetic accessibility	4.17	2.24	6.59	2.57	5.22

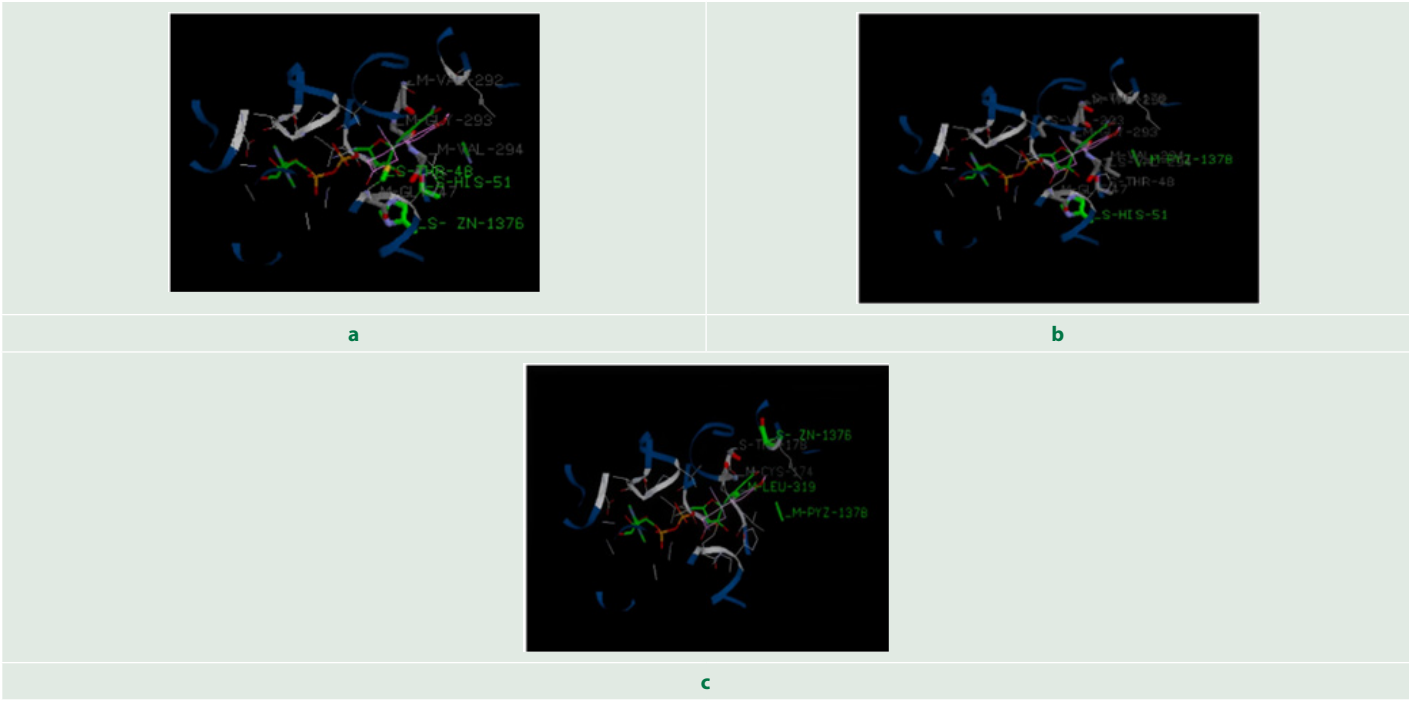


Figure 2: Docking Pose of Selected Compounds through iGemDock. Note: Green and gray colors represent the amino acids involved in Hydrogen Bonding and van der Waals interaction, respectively. a: Predicted Docking pose of Dihydroqinghaosu. b: Predicted Docking pose of 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone. c: Predicted Docking pose of Apiole.

Table 3: Predicted Pharmacokinetics (ADME-T) parameters of the screened compounds.

Compound Name	2-Oxo-5,11(13)-eudesmadien-12,8-olide	4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone	Dihydroqinghaosu	Apiole	Patchoulene
LD_{50}	5000 mg/kg	4000 mg/kg	567 mg/kg	1000 mg/kg	5000 mg/kg
Toxicity Class	5	5	4	4	5
Hepatotoxic	No	No	No	No	No
Water Solubility (SILICOS-IT)	Very Soluble	Soluble	Soluble	Soluble	Moderately Soluble
BBB Permeant	Yes	Yes	Yes	Yes	No
GI Absorption	High	High	High	High	Low
P-gp Substrate	No	Yes	No	No	Yes
Lipinski Rule	Yes; 0 Violation	Yes; 0 Violation	Yes; 0 Violation	Yes; 0 Violation	Yes; 1 Violation: MLOGP > 4.15
CYP1A2 inhibitor	No	Yes	No	Yes	No
CYP2C19 inhibitor	No	Yes	No	No	No
CYP2C9 inhibitor	No	No	No	No	No
CYP2D6 inhibitor	No	No	No	No	No
CYP3A4 inhibitor	No	No	No	No	No
Log Kp [cm/s]	-6.78 cm/s	-6.78 cm/s	-5.91 cm/s	-5.70 cm/s	-4.50 cm/s

Table 4: Total Binding energy of docked ligands obtained by igemdock.

Sl. No.	Compound	Energy	VDW	HBOND	AA-HBONDS
1.	4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone	-82.22	-71.92	-10.31	HIS51, PYZ1378
2.	Dihydroqinghaosu	-83.54	-57.22	-29.32	CYS46, THR48, HIS51, ZN1376
3.	Apiole	-80.25	-61.21	-19.05	CYS46, CYS174, LEU319, ZN1376, PYZ1378

(MLOGP>4.15), collectively reflecting a lipophilicity-driven bioavailability limitation requiring formulation-level intervention (Lipinski *et al.*, 1997). P-glycoprotein efflux substrate activity predicted for Compounds 2 and 5 suggests potential reduction in intestinal uptake and tissue distribution, Since Compounds 1, 3, and 4 are not P-gp substrates, they are less likely to be actively effluxed, allowing better systemic availability (International Transporter Consortium *et al.*, 2010).

LIMITATIONS

The present work represents a preliminary *in silico* initiative aimed at identifying potential lead compounds targeting human alcohol dehydrogenase. As the findings are based solely on computational docking predictions, further detailed *in vitro* and *in vivo* studies are required to validate the biological efficacy and therapeutic potential of the identified compounds.

CONCLUSION

The present *in silico* study demonstrated that among the screened compounds, Dihydroqinghaosu exhibited the highest binding affinity toward human alpha-type alcohol dehydrogenase (PDB ID: 1HSO), with the lowest total binding energy (-83.54 kcal/mol). The interaction analysis revealed significant hydrogen bonding with key active site residues, including CYS46, THR48, HIS51, and the catalytic Zinc Ion (ZN1376), indicating strong and specific binding within the enzyme's active pocket. Compared to 4-Cyano-4-(3,4-methylenedioxyphenyl) cyclohexanone and Apiole, Dihydroqinghaosu showed superior interaction stability due to a higher hydrogen bond contribution along with favorable van der Waals interactions. These findings suggest that Dihydroqinghaosu may act as a potential modulator of alcohol dehydrogenase activity and could be considered a promising lead candidate for further pharmacological investigation in alcohol-induced liver damage.

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ABBREVIATIONS

AA: Amino Acids; **ADH:** Alcohol Dehydrogenase; **ADH1A:** Alcohol Dehydrogenase 1A; **ADME:** Absorption, Distribution, Metabolism, and Excretion; **ALD:** Alcoholic Liver Disease; **BBB:** Blood-Brain Barrier; **CNS:** Central Nervous System; **CYP:** Cytochrome P450; **ESOL:** Estimated Solubility; **FDA:** Food and Drug Administration; **GC-MS:** Gas Chromatography Mass Spectrometry; **GI:** Gastrointestinal; **GHS:** Globally Harmonized System; **HBOND:** Hydrogen Bond; **HBA:** Hydrogen Bond Acceptor; **HBD:** Hydrogen Bond Donor; **HCV:** Hepatitis C Virus; **HBV:** Hepatitis B Virus; **iLOGP:** Internal Log Partition Coefficient; **LD_{50}:** Lethal Dose 50; **MLOGP:** Moriguchi Log Partition Coefficient; **NAFLD:** Non-Alcoholic Fatty Liver Disease; **PAINS:** Pan Assay Interference Compounds, **PDB:** Protein Data Bank; **P-gp:** P-glycoprotein, **SMILES:** Simplified Molecular Input Line Entry System, **TPSA:** Topological Polar Surface Area, **TSC:** *Thaalisaathi Chooranam*; **VDW:** Van der Waals; **WLOGP:** Wildman-Crippen Log Partition Coefficient; **XLOGP3:** Predicted Log Partition Coefficient (version 3).

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

AUTHORS CONTRIBUTION

Conceptualization, Resources, Data curation, Methodology, Investigation, Funding acquisition: Jinavani Jeevagan. Investigation, Writing original draft: Jinavani Jeevagan, Abarna Balasubramani. Writing - Review & Editing: Shaira Banu I, Priyadharshini M, Visualization: Prof. Murugesan Sannasi, Formal Analysis: Sathish Adithya Rajathinakaran, Project administration, Supervision: Prof. Madhavan Ramachandhran.

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