Molecular Docking Analysis of Bioactive Compounds from Wurfbainia compacta Against *Candida albicans* Virulence Proteins

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Abstract. *Candida albicans* is an opportunistic pathogen that causes oral and systemic candidiasis, especially in immunocompromised individuals. Natural medicines obtained from medicinal plants offer compelling alternatives for addressing virulence factors in *C. albicans*, including adhesins and enzymes secreted for biofilm development. This study examined molecular docking (using AutoDock Vina software) to test and evaluate the binding affinities of four natural compounds—2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene, dodecanoic acid 2,3-bis(acetyloxy)propyl ester, hexadecanoic acid ethyl ester, and ethyl iso-allocholate—against the virulence proteins *ALS1*, *ALS3*, *SAP4*, *SAP5*, and *SAP6* of C. albicans. Docking and physicochemical, pharmacokinetic, and toxicity assessments were conducted to ascertain their potential as antifungal drugs. Ethyl iso-allocholate exhibited the highest binding affinity, especially towards SAP6 (-8.4 kcal/mol), suggesting that is a promising antifungal agent. Among the tested compounds, ethyl iso-allocholate demonstrated the strongest and most consistent binding interactions with key virulence proteins of *C. albicans,* particularly SAP6, indicating its potential as a promising lead molecule for the development of novel antifungal therapeutics targeting pathogenic mechanisms.

1 Introduction

Multiple studies have confirmed that *Candida albicans* is the most common cause of serious fungal infections, with a particularly high impact on immunocompromised populations. These infections range from superficial mucosal diseases to life-threatening systemic candidiasis, with mortality rates for invasive disease reaching up to 50% in vulnerable groups [1–4]. Immunocompromised individuals, including those with HIV/AIDS, cancer patients undergoing chemotherapy, organ transplant recipients, and those receiving immunosuppressive therapies, are at a markedly increased risk of both mucosal and systemic *C. albicans* infections [1,2,4,5]. Oral and systemic candidiasis are common in HIV/AIDS patients and often serve as early indicators of immune deficiency [4]. Similarly, patients undergoing chemotherapy or other immunosuppressive treatments are highly susceptible to invasive candidiasis, which is associated with high morbidity and mortality [1–5].

Recent reviews and studies have consistently shown that the effectiveness of existing antifungal drugs is limited by their significant toxicity and increased drug resistance. The main antifungal groups, polyenes, azoles, echinocandins, and flucytosine, are associated with side effects, drug interactions, and fewer treatment options due to resistance, especially in immunocompromised patients [6–9]. Toxicities, such as amphotericin B-induced nephrotoxicity and azole-related hepatotoxicity often limit their use or require careful monitoring [7,8]. Simultaneously, resistance among Candida and Aspergillus species is increasing, with more multidrug-resistant strains emerging, further weakening current therapies [6–8]. These challenges underscore the urgent need for new antifungal agents with improved safety profiles and novel mechanisms for overcoming resistance. This study aimed to identify potential antifungal lead compounds by evaluating the binding affinity, pharmacokinetic properties, and toxicity profiles of selected natural bioactive molecules against the key virulence proteins of *C. albicans* through molecular docking analysis.

The software uses applications such as PyRx and Discovery Studio 2024, Protein Data Bank (https://www.rcsb.org/), PubChem (https://pubchem.ncbi.nlm.nih.gov/), SwissADME (http://www.swissadme.ch), pkCSM (http://biosig.unimelb.edu.au/pkcsm/),SwissModel(https://swissmodel.expasy.org/interactive/ZhjW6V/models/), and Lipinski filter (http://www.scfbio-iitd.res.in/software/drugdesign/lipinski.jsp). The materials used in this study included the target protein structures of agglutinin-like sequence proteins (*ALS1* and *ALS2*) and secreted aspartic protease (*SAP4*, *SAP5*, and *SAP6*), which were obtained from the Protein Data Bank (PDB). The natural ligands used include 2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene, dodecanoic

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acid, 2,3-bis(acetyloxy)propyl ester, hexadecanoic acid, ethyl ester, and ethyl iso-allocholate as anti-candidiasis ligands obtained through: 1) GC-MS testing results, 2) preparation of receptor and ligand using the PyRX application, 3) modelling and validation the quality of the receptor for use in in silico research, 4) molecular docking procedure and results vaisualization using Biovia Discovery Studio Visualizer 2024 displaying a 2D image of interactions between bonds and residues, and 5) pharmacokinetic and toxicological analyses included LD50, bioavailability, potential hepatotoxicity, skin sensitization, and adherence to Lipinski's "rule of five".

2 Results and Discussion

2.1 Molecular Docking and Visualization

GC-MS analysis of the cardamom extract (*W. compacta*) revealed several bioactive compounds, including: 2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene, dodecanoic acid, 2,3-bis(acetyloxy)propyl ester, hexadecanoic acid, ethyl ester, and ethyl iso-allocholate. The presence of 2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene ($C_8H_8O_2$) indicated the presence of a relatively stable oxygenated cyclic compound. In addition, dodecanoic acid, 2,3-bis(acetyloxy)propyl ester is a fatty ester that may be derived from the lipid modification of lauric acid (dodecanoic acid). It may contribute to emollient properties, thermal stability, and potential biological activities, such as antibacterial activity. This ester structure also confers lipophilic properties, allowing for cell membrane penetration and potential bioactivity.

Another bioactive compound, hexadecanoic acid, ethyl ester (ethyl ester of palmitic acid), was also detected in W. compacta tap water. This compound is known to be a moisturising component and may contribute to its antimicrobial or antioxidant properties. In addition, ethyl iso-allocholate, a steroid/triterpenoid ethyl derivative compound related to cholic glycosides, was also identified. This compound also exhibits anti-inflammatory activity and pharmacological activities. This composition shows that cardamom oil contains not only major monoterpenes such as eucalyptol and α-terpinyl acetate [10], but also non-volatile compounds, including amino acids, fatty esters, and steroids. The molecular docking results (Table 1-5) indicate that among the five tested compounds against each target protein, ethyl iso-allocholate exhibited the lowest binding energy of –8.4 kcal/mol (with ALS3 protein), suggesting that it has the strongest binding affinity to the active site compared to the other ligands. These long-chain lipid compounds can also act as membrane stabilizers and antibacterial agents by disrupting the cell membranes [6].

The hexadecanoic acid ethyl ester showed stable binding conformations with low RMSD values (0.0–4.5 Å) to ALS1, indicating good flexibility and strong hydrophobic interactions mediated by van der Waals forces between the steroidal and ethoxy groups [11]. A lower binding energy corresponds to a more stable ligand-protein complex [12]. Overall, ethyl iso-allocholate is the most stable and promising active ligand for further in vitro testing, with diverse functional groups such as carbonyl, hydroxy, and ethoxy enhancing hydrophobic and hydrogen bonding, which is crucial for complex stability [13]. Analysis of the relationship between structure and activity showed that the presence of polar and aromatic groups in ligands plays a vital role in increasing the binding affinity to the active site of the protein.

Table 1. Docking results of test compounds on the target protein ALS1

No.	Ligand	Conformation	Binding Afinity	RSMD LB	RSMD UB
1.	2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	0	-4.8	0.0	0.0
		1	-4.8	0.089	2.259
		2	-4.8	0.136	2.259
		3	-4.3	25.617	26.762
		4	-4.2	10.342	11.576
		5	-4.0	9.804	11.015
		6	-3.9	19.265	20.269
		7	-3.9	19.324	20.461
		8	-3.5	81.375	82.324
2.	Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	0	-4.2	0.0	0.0
		1	-3.9	16.99	21.085
		2	-3.9	2.038	5.144
		3	-3.8	2.44	4.087
		4	-3.8	1.955	5.256
		5	-3.7	52.29	62.469
		6	-3.6	16.979	20.875
		7	-3.6	59.425	61.661
		8	-3.5	5.533	9.24
3.	Hexadecanoic acid, ethyl ester	0	-2.4	0.0	0.0
		1	-2.2	1.819	2.434
		2	-1.6	2.02	3.148
		3	-1.6	3.06	4.152
		4	-1.4	2.277	3.364
		5	-0.9	1.656	2.956
		6	-0.0	3.605	8.5
		7	-0.2	2.862	5.55
4.	Ethyl iso-allocholate	0	-5.6	0.0	0.0
		1	-5.6	2.398	4.574
		2	-5.6	11.434	13.228
		3	-5.6	10.903	14.913
		4	-5.5	1.055	1.95
		5	-5.5	3.886	6.079
		6	-5.3	1.548	2.178
		7	-5.2	10.181	14.28
		8	-5.0	3.186	9.07

Table 2. Docking results of test compounds on the target protein ALS3

No	Ligand	Conformation	Binding Afinity	RSMD LB	RSMD UB
1.	2,7-Dioxa-	0	-4.7	0.0	0.0
		1	-4.7	1.505	2.58

	tricyclo[4.4.0.0(3,8)]deca-4,9-diene	2	-4.4	1.407	2.53
		3	-3.9	33.605	34.552
		4	-3.9	20.07	21.481
		5	-3.9	20.066	21.564
		6	-3.9	19.963	21.36
		7	-3.8	19.803	21.394
		8	-3.7	19.509	20.63
2.	Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	0	-5.0	0.0	0.0
		1	-5.0	2.177	3.961
		2	-4.7	1.849	4.979
		3	-4.7	16.851	20.698
		4	-4.5	1.95	5.72
		5	-4.0	48.281	51.645
		6	-3.9	17.576	21.295
		7	-3.9	2.561	5.164
		8	-3.7	3.458	7.279
3.	Hexadecanoic acid, ethyl ester	0	-4.6	0.0	0.0
		1	-3.8	32.901	35.206
		2	-3.7	2.432	4.825
		3	-3.6	1.801	3.56
		4	-3.6	29.137	30.625
		5	-3.5	30.25	33.945
		6	-3.5	28.961	31.18
		7	-3.4	21.79	24.51
		8	-3.3	33.48	35.533
4.	Ethyl iso-allocholate	0	-6.7	0.0	0.0
		1	-6.5	1.934	8.862
		2	-6.3	2.215	3.406
		3	-6.0	3.33	8.897
		4	-5.9	3.137	8.12
		5	-5.9	24.222	26.099
		6	-5.8	23.735	26.421
		7	-5.8	3.646	9.764
		8	-5.7	23.886	26.605

Table 3. Docking results of test compounds on the target protein SAP4

No	Ligand	Conformation	Binding Afinity	RSMD LB	RSMD UB
1.	2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	0	-4.7	0.0	0.0
		1	-4.7	0.139	2.864
		2	-4.6	1.388	2.159
		3	-4.6	1.382	3.012
		4	-4.6	1.073	2.405
		5	-4.4	30.273	31.588
		6	-4.4	30.288	31.599
		7	-4.4	30.478	31.615
		8	-4.2	1.359	2.345
2.	Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	0	-5.7	0.0	0.0
		1	-5.6	18.533	20.782
		2	-5.5	28.201	29.752
		3	-5.3	20.546	22.84
		4	-5.3	2.469	5.183
		5	-5.2	27.351	29.02
		6	-5.2	13.771	16.517
		7	-5.1	27.051	30.595
		8	-5.1	10.762	13.21
3.	Hexadecanoic acid, ethyl ester	0	-5.0	0.0	0.0
		1	-4.9	6.282	9.751
		2	-4.7	5.98	8.888
		3	-4.5	6.92	10.312
		4	-4.4	39.653	41.875
		5	-4.4	33.901	36.966
		6	-4.3	6.185	9.081
		7	-4.3	10.973	13.394
		8	-4.3	4.326	10.504
4.	Ethyl iso-allocholate	0	-7.3	0.0	0.0
		1	-7.1	3.081	7.187
		2	-7.0	4.032	6.933
		3	-6.9	31.083	34.685
		4	-6.7	7.776	10.742
		5	-6.6	4.35	7.275
		6	-6.5	31.345	34.373
		7	-6.4	9.03	11.456
		8	-6.4	16.402	18.701

Table 4. Docking results of test compounds on the target protein SAP5

No	Ligand	Conformation	Binding Afinity	RSMD LB	RSMD UB
1.	2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	0	-5.2	0.0	0.0
		1	-5.2	0.009	2.864
		2	-5.2	0.04	2.91
		3	-4.8	2.753	4.329
		4	-4.8	2.752	4.069
		5	-4.3	27.107	28.299
		6	-4.2	26.969	28.286
		7	-4.2	27.132	28.39
		8	-4.2	27.173	28.473
2.	Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	0	-6.4	0.0	0.0
		1	-6.1	1.635	3.968
		2	-5.7	1.889	3.697
		3	-5.7	3.186	8.349
		4	-5.2	2.165	7.831
		5	-4.9	16.294	18.887
		6	-4.8	3.367	8.644
		7	-4.7	18.363	21.3

		8	-4.7	15.608	18.642
3.	Hexadecanoic acid, ethyl ester	0	-4.0	0.0	0.0
		1	-4.0	34.414	36.622
		2	-4.0	2.339	5.756
		3	-3.9	35.043	37.342
		4	-3.8	35.201	37.417
		5	-3.7	1.374	2.049
		6	-3.7	35.051	37.252
		7	-3.6	35.212	37.636
		8	-3.6	25.459	27.224
4.	Ethyl iso-allocholate	0	-7.3	0.0	0.0
		1	-7.2	3.332	5.844
		2	-6.9	2.317	3.317
		3	-6.8	20.844	25.99
		4	-6.8	1.8	2.351
		5	-6.7	10.331	12.86
		6	-6.6	22.685	26.637
		7	-6.5	2.446	4.108
		8	-6.5	23.347	26.648

Table 5. Docking results of test compounds on the target protein SAP6

No	Ligand	Conformation	Binding Afinity	RSMD LB	RSMD UB
1.	2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	0	-5.6	0.0	0.0
		1	-5.6	3.243	5.711
		2	-5.6	18.035	19.698
		3	-5.5	8.531	10.598
		4	-5.5	1.742	2.448
		5	-5.5	2.86	4.23
		6	-5.5	18.489	19.475
		7	-5.5	19.145	20.241
		8	-5.4	19.268	20.915
2.	Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	0	-5.1	0.0	0.0
		1	-5.0	7.754	10.088
		2	-4.9	11.312	13.165
		3	-4.7	11.857	14.588
		4	-4.7	2.423	5.696
		5	-4.6	8.598	11.157
		6	-4.6	11.537	14.804
		7	-4.5	8.113	10.764
		8	-4.5	11.659	13.054
3.		0	-4.7	0.0	0.0
	Hexadecanoic acid, ethyl ester	1	-4.5	10.23	12.936
		2	-4.5	10.306	12.892
		3	-4.5	12.981	15.181
		4	-4.5	10.675	12.77
		5	-4.4	12.215	15.017
		6	-4.3	2.698	5.688
		7	-4.3	9.867	12.003
		8	-4.3	9.789	10.964
4.	Ethyl iso-allocholate	0	-8.4	0.0	0.0
		1	-7.8	2.452	4.142
		2	-7.1	13.124	16.729
		3	-7.1	2.445	3.914
		4	-7.0	29.626	31.641
		5	-7.0	17.926	20.133
		6	-6.9	13.258	14.957
		7	-6.9	12.519	16.115
		8	-6.9	11.617	15.336

2.2 Physiochemical Analysis Based on Lipinski's Rule of Five

Analysis of the physicochemical properties of the test compounds was conducted to assess their pharmacokinetic feasibility in silico, particularly in the context of potential oral biological activity based on Lipinski's Rule of Five. The evaluated parameters included molecular weight (MW), number of hydrogen bond donors and acceptors (HBD and HBA), and lipophilicity (LogP) (Table 6). All ligands complied with Lipinski's Rule of Five, showing zero to one violation, suggesting good potential for membrane permeability and oral bioavailability.

Table 6. Physicochemical Analysis Based on Lipinski's Rules of Five

Ligand	Mol Weight (g/mol)	HB Acceptor	HB Donor	Liphopolicity	Lipinski Rule of Five
2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	136.15	2	0	0.65	Yes, 0 error
2-Amino-3-(4-hydroxyphenyl)-	181.19	4	3	-1.70	Yes, 0 error

propanoic acid					
Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	358.5	6	0	2.95	Yes, 0 error
Hexadecanoic acid, ethyl ester	284.5	2	0	4.15	Yes, 1 error
Ethyl iso-allocholate	436.62	5	3	3.46	Yes, 0 error

According to [14], compounds with one or fewer violations are considered to be suitable for drug development. Overall, all five compounds demonstrated acceptable pharmacokinetic properties and did not violate Lipinski's Rule, supporting their potential as bioactive candidates with adequate membrane permeability.

2.3 Pharmacokinetic and Toxicity Analysis (ADMET Profiling)

In silico pharmacokinetic assessment evaluated the absorption, distribution, metabolism, excretion, and possible toxicity of the docked compounds by analyzing water solubility, gastrointestinal absorption, blood-brain barrier permeability, P-glycoprotein substrate status, and cytochrome P450 enzyme inhibition (Table 7).

Table 7. Pharmacokinetic Analyses

Compound Name	WS	GI Abs	BBB	P-gp Sub	Log Kp (cm/s)
2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	0.32	*High*	*No*	*No*	-6.92
2-Amino-3-(4-hydroxyphenyl)-propanoic acid	-1.29	*High*	*No*	*No*	-9.01
Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	-4.97	*High*	*No*	*Yes*	-4.65
Hexadecanoic acid, ethyl ester	-6.41	*High*	*No*	*No*	-2.44

All compounds showed high gastrointestinal (GI) absorption, indicating good potential for oral absorption. None of the ligands showed permeability to the blood–brain barrier (BBB), thus they were safe from neurotoxic effects. These results indicate that the five ligands likely act on the peripheral system, rather than the central nervous system, which is relevant for the development of antimicrobial or antifungal agents [15].

2.4 Toxicity Analysis of Test Compounds

In silico toxicity analysis predicted the biological safety of docked compounds by assessing toxicity level, LD_{50} value (mg/kg), and potential hepatotoxicity, mutagenicity, carcinogenicity, immunotoxicity, and cytotoxicity (Table 8).

Table 8. Toxicity Analysis of Test Compounds

Compound Name	Level	LD50 mg/kg	Hepatotoxicity	Mutagenicity	Carcinotoxicity	Immunotoxicity	Cytotoxicity
2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene	5	5000	*Inactive*	*Inactive*	*Inactive*	*Inactive*	*Inactive*
Dodecanoic acid, 2,3-bis(acetyloxy)propyl ester	5	5000	*Inactive*	*Active*	*Active*	*Inactive*	*Inactive*
Hexadecanoic acid, ethyl ester	5	5000	*Inactive*	*Inactive*	*Active*	*Inactive*	*Inactive*
Ethyl iso-allocholate	5	5000	*Inactive*	*Inactive*	*Inactive*	*Active*	*Inactive*

All compounds demonstrated low to very low toxicity, with LD_{50} values of ≥ 1460 mg/kg, placing them in a mild toxicity category based on the OECD classification. Values in levels 4–5 suggest that most compounds are non-toxic or minimally toxic, which is suitable for biopharmaceutical candidate development [8,11]. None of the compounds showed hepatotoxic activity, indicating their safety for liver function. This aligns with earlier ADMET findings that revealed no significant inhibition of major CYP enzymes, indicating a minimal hepatic metabolic risk.

3 Conclusion

This study revealed that bioactive compounds from *W. compacta* have promising antifungal effects against *C. albicans* virulence proteins. Among the compounds tested, ethyl iso-allocholate showed the highest binding affinity, especially for the SAP6 protein (–8.4 kcal/mol), indicating a stable and strong interaction through

hydrogen bonds and hydrophobic contacts within the active site. All compounds met Lipinski's Rule of Five with minimal exceptions, suggesting good pharmacokinetics and oral bioavailability. ADMET and toxicity assessments confirmed its safety, showing no toxicity, hepatotoxicity, mutagenicity, or carcinogenicity risks. These results highlight ethyl iso-allocholate, along with 2,7-Dioxa-tricyclo[4.4.0.0(3,8)]deca-4,9-diene as promising natural antifungal candidates for further laboratory and clinical studies. Molecular docking findings provide a solid basis for developing plant-based antifungal agents to tackle *Candida* infections and combat antifungal resistance

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