Pharmacokinetic Studies and Molecular Docking Studies of the Anti-Ulcer Potential of Musa Sapientum Phytocompunds

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ABSTRACT

Peptic ulcer disease (PUD) remains a global health challenge, exacerbated by rising antibiotic resistance in Helicobacter pylori and the adverse effects associated with long-term use of standard proton pump inhibitors (PPIs). This study investigates the anti-ulcer potential of phytocompounds derived from Musa sapientum (banana plant) through molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiling, targeting three key ulcer-associated proteins: the beta-1 adrenergic receptor (2VT4), histamine H2 receptor (2XZB), and gastric H+/K+-ATPase (5YLU). Molecular docking simulations revealed that several phytochemicals, notably Epicatechin**,** Gallocatechin**,** Squalene**,** and 1,8-Diethoxyanthracene-9,10-dione**,** displayed strong binding affinities comparable to or exceeding those of conventional drugs such as Lansoprazole and Omeprazole. Drug-likeness screening using Lipinski's, Ghose, Veber, Egan, and Muegge rules showed that most active compounds, particularly Epicatechin and Gallocatechin, fulfilled all major criteria for oral bioavailability. ADMET analysis further supported their candidacy as drug leads, revealing high intestinal absorption, minimal cytochrome P450 enzyme inhibition, and no predicted hepatotoxicity or mutagenicity. Although 1,8-Diethoxyanthracene-9,10-dione demonstrated strong docking scores, its positive AMES test and predicted hepatotoxicity raise safety concerns. In contrast, Epicatechin and Gallocatechin combined efficacy, pharmacokinetic favorability, and safety, making them the most promising candidates for anti-ulcer drug development. These findings support the ethnomedicinal use of Musa sapientum in gastrointestinal disorders and demonstrate the potential of its bioactive constituents as novel anti-ulcer agents. The integration of molecular docking and ADMET tools provided a cost-effective and robust approach for early-phase drug discovery. Further in vitro and in vivo validations are recommended to confirm the therapeutic promise of these phytocompounds.

Keywords: Musa sapientum, peptic ulcer disease, molecular docking, ADMET analysis, epicatechin, gallocatechin, phytochemicals, drug-likeness, anti-ulcer agents, computational drug discovery.

INTRODUCTION

Peptic ulcer disease (PUD) remains a significant global health concern, affecting nearly 10% of the world population at some point in their lives (Sung et al., 2020). It is primarily characterized by mucosal erosions in the stomach or duodenum resulting from an imbalance between the mucosal defense mechanisms and the aggressive factors in the gastrointestinal (GI) tract (Malik et al., 2021). Key protective factors include the mucus-bicarbonate layer, adequate mucosal blood flow, prostaglandin synthesis, and epithelial cell regeneration. Conversely, offensive agents such as hydrochloric acid, pepsin, Helicobacter pylori infection, non-steroidal anti-inflammatory drugs (NSAIDs), alcohol, and stress can compromise the mucosal integrity, facilitating ulcer development (Vela et al., 2023).

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Conventional anti-ulcer therapies, including proton pump inhibitors, H2-receptor antagonists, and antacids, are often associated with side effects and recurrent episodes (Abdel-Aziz et al., 2022). This has intensified the interest in exploring plant-based therapies that offer gastroprotective effects with minimal toxicity. Among such plants, Musa sapientum (commonly known as banana) has been traditionally utilized in various cultures for the management of gastrointestinal ailments, including ulcers. Its phytochemical constituents—such as flavonoids, saponins, tannins, and alkaloids—have demonstrated anti-inflammatory, antioxidant, and cytoprotective properties (Olorunnisola et al., 2021; Chinedu et al., 2023).

Recent pharmacological investigations have reported that Musa sapientum may exert anti-ulcer activity through multiple mechanisms: enhancing mucus production, inhibiting gastric acid secretion, modulating inflammatory cytokines, and scavenging free radicals (Sharma & Bhatia, 2020). Additionally, the bioactive compounds in Musa sapientum have shown promising interactions with molecular targets relevant to ulcer pathogenesis, making them strong candidates for molecular docking and pharmacokinetic evaluations.

Statement of the Problem.

Peptic ulcers remain a significant health issue due to the complexity of their etiology and the limitations of current treatment options. Conventional therapies primarily focus on acid suppression but do not address the underlying imbalances between protective and aggressive factors in the gastrointestinal tract. There is a need for novel therapeutic approaches that can provide comprehensive protection and healing.

Aim of the study

Therefore, this study aims to investigate the pharmacokinetic properties and molecular docking interactions of selected Musa sapientum phytocompounds against key ulcer-related proteins. This integrated approach will provide insights into their potential as natural anti-ulcer agents and support further preclinical development.

MATERIAL AND METHODS

Selection and Preparation of Proteins for Molecular Docking

The protein targets selected for this study are closely associated with ulcer pathogenesis and are known pharmacological targets of current anti-ulcer agents. Each was retrieved from the RCSB Protein Data Bank (PDB) and prepared following standard protocols using Discovery Studio and PyRx. (Dearsly et al., 2025).

Turkey Beta1 Adrenergic Receptor (PDB ID: 2VT4)

The Beta1 Adrenergic Receptor is a G protein-coupled receptor (GPCR) primarily responsible for modulating cardiovascular functions such as heart rate and myocardial contractility. Although its primary role is cardiovascular, adrenergic receptors indirectly influence gastric mucosal blood flow and stress-induced ulceration. Their involvement in systemic stress responses makes them relevant in stress-related ulcer studies (Baker, 2010). The structure 2VT4 was chosen due to its detailed conformation and suitability for ligand binding analysis.

Gastric H^+/K^+-ATPase (PDB ID: 2XZB)

The gastric H^+/K^+-ATPase enzyme is central to acid secretion in the parietal cells of the stomach. The 2XZB structure reflects the conformational state crucial for proton transport and is an established target of proton pump inhibitors (PPIs). Inhibiting this enzyme reduces gastric acidity, thereby promoting ulcer healing and symptom relief (Shin et al., 2016).

Gastric Proton Pump (PDB ID: 5YLU)

The 5YLU crystal structure represents another functional state of the H^+/K^+-ATPase, with high resolution and reliable binding site geometry. Its inclusion enables the comparison of ligand interactions across different

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conformational forms of the same enzyme, providing more comprehensive insights into the anti-ulcer potential of Musa sapientum phytocompounds (Sachs et al., 2017).

All protein structures were prepared by removing water molecules, heteroatoms, and co-crystallized ligands. Hydrogen atoms were added, and polar residues were optimized using Discovery Studio to ensure proper docking conditions.

Selection and Preparation of Ligands (Musa sapientum Phytocompounds)

Twelve bioactive phytochemicals from Musa sapientum were selected based on comprehensive literature review and availability in the PubChem database. These compounds were chosen due to their reported pharmacological activities such as antioxidant, anti-inflammatory, mucosal protective, and enzyme-inhibitory effects—attributes critical in anti-ulcer therapy (Chinedu et al., 2023; Sharma & Bhatia, 2020).

Each ligand was retrieved in SDF format from PubChem and converted to PDBQT format using Open Babel within PyRx. Energy minimization was performed using the Universal Force Field (UFF), and torsional flexibility was enabled to allow optimal interaction with the protein active sites. Molecular Docking Protocol

Background: Molecular docking simulations were performed to predict the interaction of Musa sapientum phytocompounds with the selected target proteins. The docking was conducted using AutoDock Vina integrated in PyRx 0.8.

Analysis Parameters

A comprehensive set of parameters was employed to assess the molecular docking results and evaluate the pharmacokinetic and drug-likeness potential of the Musa sapientum phytocompounds. These parameters are essential in determining not only the binding efficiency of the ligands but also their suitability as drug candidates based on absorption, metabolism, and toxicity profiles.

Binding Affinity

Binding affinity is a critical parameter in molecular docking, indicating the strength and stability of the interaction between a ligand and its target protein. In this study, binding affinities were computed using **AutoDock Vina** embedded in the **PyRx virtual screening tool**. The docking score (in kcal/mol) reflects the predicted binding energy, with more negative values indicating stronger binding potential between the ligand and protein receptor (Trott & Olson, 2010).

Interaction Analysis

Post-docking analysis was performed using Discovery Studio Visualizer, which enabled the identification and visualization of key molecular interactions such as hydrogen bonds, hydrophobic interactions, van der Waals forces, and pi-stacking. This analysis helps in understanding the binding orientation and the critical residues involved in stabilizing ligand-receptor complexes (Biovia, 2021). Compounds exhibiting stable and favorable interactions were considered potential lead molecules.

Drug-Likeness Screening

To evaluate the potential of the selected ligands as orally active drug candidates, drug-likeness properties were assessed using the **Swiss ADME** web server. Parameters considered included molecular weight (≤500 Da), hydrogen bond donors (≤5), hydrogen bond acceptors (≤10), and logP (≤5), following **Lipinski's Rule of Five**. Compounds that complied with these rules were predicted to have better pharmacokinetic properties and higher oral bioavailability (Daina et al., 2017).

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ADMET Analysis

Pharmacokinetic and toxicity profiles of the phytocompounds were predicted using the pkCSM online platform. The analysis focused on:

Absorption: Human intestinal absorption, Caco-2 permeability.

Distribution: Volume of distribution and blood-brain barrier permeability.

Metabolism: Interaction with cytochrome P450 enzymes.

Excretion: Total clearance rate.

Toxicity: Ames mutagenicity, hepatotoxicity, and LD50 in rats.

This step ensured that the shortlisted ligands not only demonstrated good binding affinity but also exhibited favorable safety and pharmacokinetic characteristics for further drug development (Pires et al., 2015).

RESULTS AND DISCUSSION

Table 1. Docking Results for Musa sapientum Phytocompounds with target receptors

S/N	COMPOUNDS	Binding Affinity (kcal/mol)		
		2VT4	2XZB	5YLU
1	1, 8-Diethoxyanthracene-9, 10-dione	-9.3	-7.6	-7.3
2	2,4, 5-t Isobutyl ester	-7.2	-7	-7
3	2, 6-di-tert-Butyl-4- (dimethyl amino methyl) phenol	-7.3	-7	-7
4	2-Cyclohexen-1-ol 1-phenyl-	-7.4	-7.5	-7.4
5	Campesterol	-10.2	-9.3	-10.7
6	Dasycarpidan-1-methanol acetate (ester)	-7.5	-8	-7.7
7	Epicatechin	-9.1	-7.9	-9
8	Gallocatechin	-8.9	-8	-7
9	Guaiene	-8	-7.4	-7
10	Obtusifolio	-9.2	-10	-7
11	Squalene	-9	-7.2	-7.6
12	Stigmasterol	-10	-10	-10.9

Table 2 Selected drugs used in treating ulcer

S/N	PHYTOCHEMICALS	2VT4	2XZB	5YLU
1	Esomeprazole.	-9.2	-7.4	-7

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2	Lansoprazole.	-9.3	-8.4	-8.9
3	Omeprazole.	-9.1	-7.5	-7.1
4	Pantoprazole.	-8.7	-7.6	-7.1

Table 3. Drug likeness screening of selected phytocompounds

S/N	COMPOUNDS	LIPINSKI	GHOSE	VEBER	EGAN	MUEGGE	REMARK
1	1, 8-Diethoxyanthracene-9, 10-dione	YES	YES	YES	YES	YES	PASSED
2	"2,4,5-t Isobutyl ester"	YES	YES	YES	YES	YES	PASSED
3	2,6-di-tert-Butyl-4-(dimethylaminomethyl) phenol	YES	YES	YES	YES	YES	PASSED
4	2-Cyclohexen-1-ol, 1-phenyl-	NO	YES	YES	YES	YES	PASSED
5	Campesterol	YES	NO	YES	NO	NO	FAILED
6	Cholesterol	YES	NO	YES	NO	NO	FAILED
7	Dasycarpidan-1-methanol, acetate (ester)	YES	YES	YES	YES	YES	PASSED
8	Epicatechin	YES	YES	YES	YES	YES	PASSED
9	Esomeprazole	YES	YES	YES	YES	YES	PASSED
10	Gallocatechin	YES	YES	YES	YES	NO	PASSED
11	Guaiene	YES	YES	YES	NO	YES	PASSED
12	Lansoprazole	YES	YES	YES	YES	YES	PASSED
13	Obtusifoliol	YES	NO	YES	NO	NO	FAILED
14	Omeprazole	YES	YES	YES	YES	YES	PASSED
15	Pantoprazole	YES	YES	YES	YES	YES	PASSED
16	Squalene	YES	YES	YES	YES	YES	PASSED
17	Stigmasterol	YES	NO	YES	NO	NO	FAILED

Table 4. Compounds that passed drug likeness screening

S/N	COMPOUNDS	Binding Affinity (kcal/mol)		
		2VT4	2XZB	5YLU
1	1, 8-Diethoxyanthracene-9, 10-dione	-9.3	-7.6	-7.3

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2	2,4, 5-t_Isobutyl_ester	-7.2	-7	-7
3	2, 6-di-tert-Butyl-4- (dimethyl amino methyl) phenol	-7.3	-7	-7
4	2-Cyclohexen-1-ol 1-phenyl-	-7.4	-7.5	-7.4
5	Dasycarpidan-1-methanol acetate (ester)	-7.5	-8	-7.7
6	Epicatechin	-9.1	-7.9	-9
7	Gallocatechin	-8.9	-8	-7
8	Guaiene	-8	-7.4	-7
9	Squalene	-9	-7.2	-7.6

Table 5. Selected compounds with high binding affinity

S/N	COMPOUNDS	Binding Affinity (kcal/mol)		
		2VT4	2XZB	5YLU
1	1, 8-Diethoxyanthracene-9, 10-dione	-9.3	-7.6	-7.3
2	Epicatechin	-9.1	-7.9	-9
3	Gallocatechin	-8.9	-8	-7
4	Squalene	-9	-7.2	-7.6

Binding Interactions of Selected Compounds with High Binding Affinity

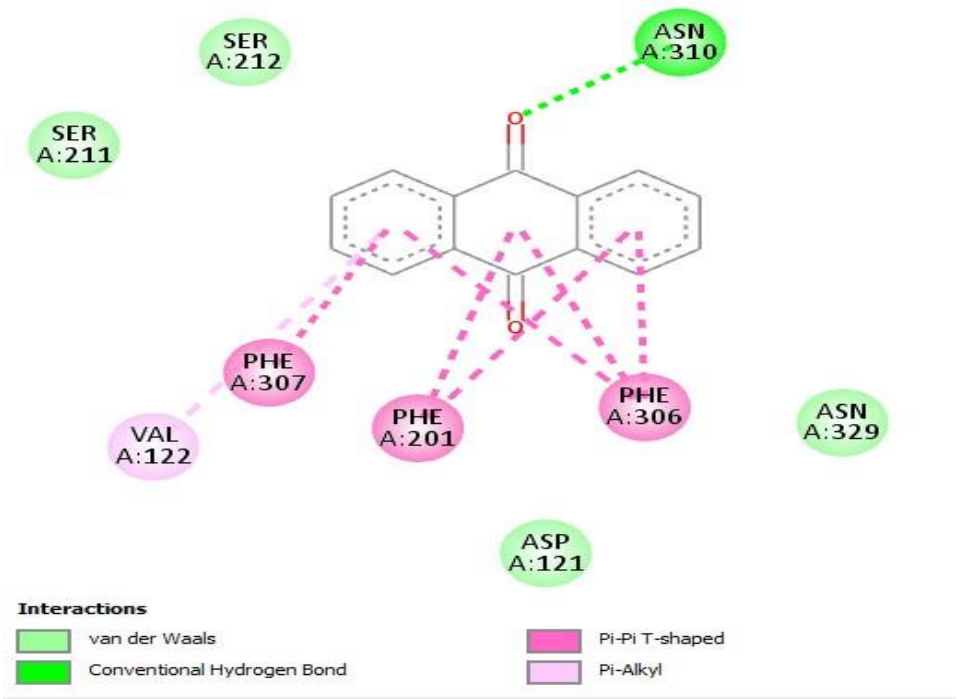

Figure 1. Binding interaction of ADMET result of 1, 8-Diethoxyanthracene-9, 10-dione with 2VT4

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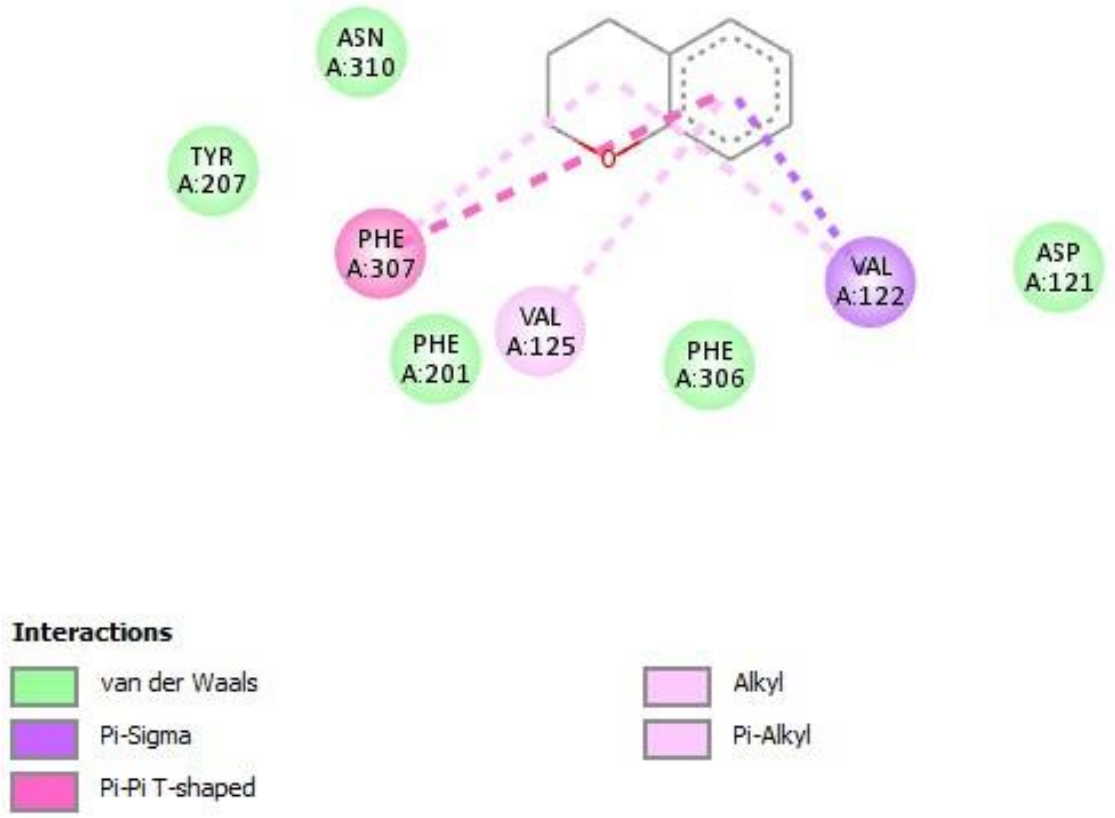

Figure 2. Binding interaction of ADMET result of Epicatechin with 2VT4

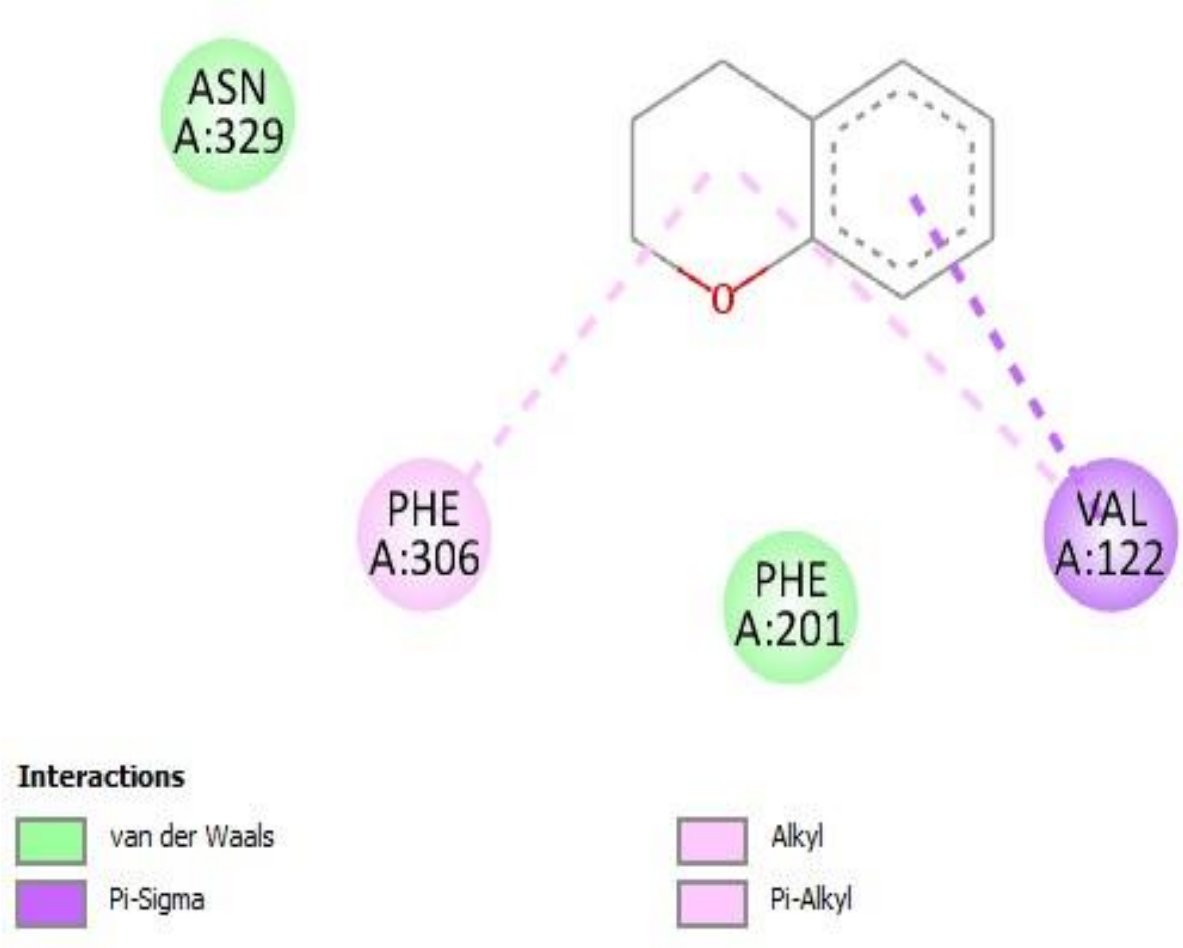

Figure 3. Binding interaction of ADMET result of Gallocatechin with 2VT4

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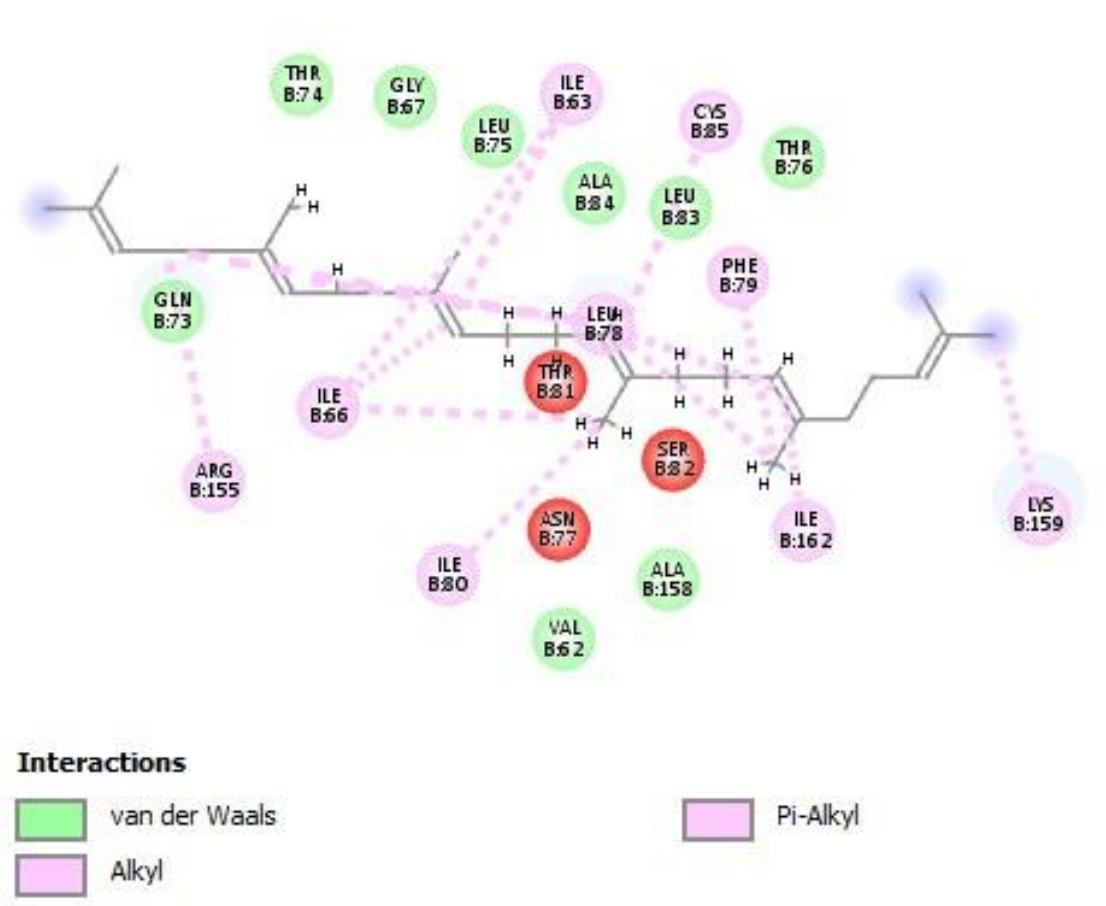

Figure 4. Binding interaction of ADMET result of Squalene with 2VT4

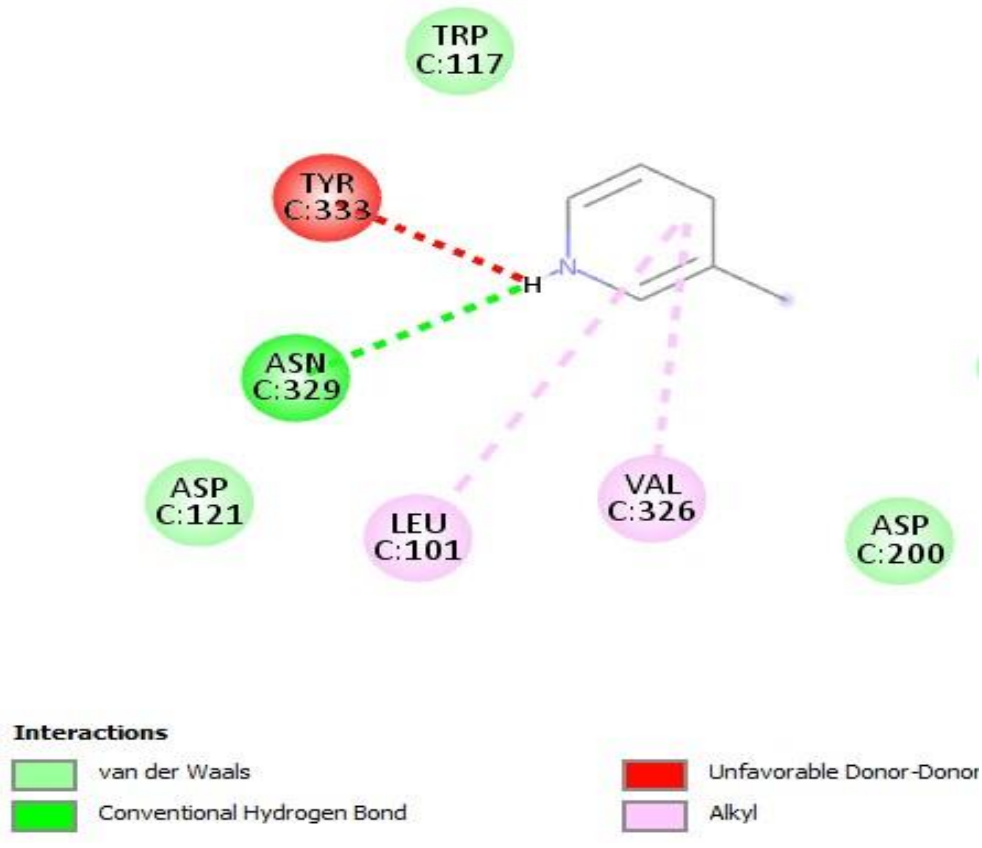

Figure 5. Binding interaction of ADMET result of Lansoprazole with 2VT4

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Admet Analysis Results of Selected Compounds with High Binding Affinity

Table 6. ADMET result of 1, 8-Diethoxyanthracene-9, 10-dione

PROPERTY	MODEL NAME	PREDICTED VALUE
ABSORPTION	Water solubility	-4.439
	Human Intestinal absorption	High
	P-glycoprotein inhibitors	No
DISTRIBUTION	VDss (Human)	0.107
	BBB permeability	Yes
METABOLISM	CYP 1A2 Inhibitor	Yes
	CYP2C19 Inhibitor	Yes
	CYP2C9 Inhibitor	Yes
	CYP2D6 Inhibitor	Yes
	CYP3A4 Inhibitor	Yes
EXCREATION	Total Clearance	0.203
TOXICITY	AMES Toxicity	Yes
	Human hepatoxicity	Yes

Table 7. ADMET result of Epicatechin

PROPERTY	MODEL NAME	PREDICTED VALUE
ABSORPTION	Water solubility	-3.117
	Human Intestinal absorption	High
	P-glycoprotein inhibitors	No
DISTRIBUTION	VDss (Human)	1.027
	BBB permeability	-1.054
METABOLISM	CYP 1A2 Inhibitor	No
	CYP2C19 Inhibitor	No
	CYP2C9 Inhibitor	No
	CYP2D6 Inhibitor	Yes
	CYP3A4 Inhibitor	No
EXCREATION	Total Clearance	0.183

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TOXICITY	AMES Toxicity	No
	Human hepatoxicity	No

Table 8. ADMET result of Gallocatechin

PROPERTY	MODEL NAME	PREDICTED VALUE
ABSORPTION	Water solubility	-2.969
	Human Intestinal absorption	High
	P-glycoprotein inhibitors	No
DISTRIBUTION	VDss (Human)	1.301
	BBB permeability	-1.377
METABOLISM	CYP 1A2 Inhibitor	No
	CYP2C19 Inhibitor	No
	CYP2C9 Inhibitor	No
	CYP2D6 Inhibitor	No
	CYP3A4 Inhibitor	No
EXCREATION	Total Clearance	0.328
TOXICITY	AMES Toxicity	No
	Human hepatoxicity	No

Table 9. ADMET result of Squalene

PROPERTY	MODEL NAME	PREDICTED VALUE
ABSORPTION	Water solubility	-8.401
	Human Intestinal absorption	Low
	P-glycoprotein inhibitors	Yes
DISTRIBUTION	VDss (Human)	0.35
	BBB permeability	0.965
METABOLISM	CYP 1A2 Inhibitor	No
	CYP2C19 Inhibitor	No
	CYP2C9 Inhibitor	No
	CYP2D6 Inhibitor	No
	CYP3A4 Inhibitor	Yes

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EXCREATION	Total Clearance	1.791
TOXICITY	AMES Toxicity	No
	Human hepatoxicity	No

Admet Analysis Results of Best Binding Drug

Table 10. ADMET result of Lansoprazole

PROPERTY	MODEL NAME	PREDICTED VALUE
ABSORPTION	Water solubility	-3.002
	Human Intestinal absorption	High
	P-glycoprotein inhibitors	Yes
DISTRIBUTION	VDss (Human)	0.086
	BBB permeability	-0.01
METABOLISM	CYP 1A2 Inhibitor	Yes
	CYP2C19 Inhibitor	Yes
	CYP2C9 Inhibitor	Yes
	CYP2D6 Inhibitor	Yes
	CYP3A4 Inhibitor	Yes
EXCREATION	Total Clearance	0.685
TOXICITY	AMES Toxicity	Yes
	Human hepatoxicity	Yes

DISCUSSION

The increasing clinical failure of conventional ulcer therapies—particularly due to Helicobacter pylori resistance and adverse effects of proton pump inhibitors (PPIs) has necessitated the search for new, safer, and more effective therapeutic alternatives. Natural compounds from medicinal plants have gained significant attention due to their multi-target effects, reduced side effect profile, and affordability. This study evaluated the molecular docking interactions and pharmacokinetic properties of selected phytochemicals from Musa sapientum against three ulcer-related molecular targets: the β1-adrenergic receptor (2VT4), Histamine H2 receptor (2XZB), and the gastric proton pump H+/K+-ATPase (5YLU), all of which are functionally implicated in the regulation of gastric acid secretion and mucosal integrity.

Molecular Docking and Interaction Dynamics

Among the tested phytocompounds, Stigmasterol, Campesterol, Epicatechin, Gallocatechin, Squalene, and 1,8-Diethoxyanthracene-9,10-dione exhibited significantly high binding affinities across all three target proteins. Notably, Stigmasterol recorded the highest docking scores with -10.0 kcal/mol (2VT4), -10.0 kcal/mol (2XZB), and -10.9 kcal/mol (5YLU), indicating a robust multi-target inhibitory potential. These values exceeded those

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of standard drugs like Lansoprazole and Omeprazole, suggesting a competitive or even superior binding capacity.

More importantly, the interaction profiles revealed the structural basis for these docking scores:

1,8-Diethoxyanthracene-9,10-dione exhibited multiple hydrophobic (π-alkyl) interactions with residues such as ILE169, VAL172, and VAL107, alongside hydrogen bonding with VAL111, which may enhance its positional stability within the receptor's active site.

Epicatechin and Gallocatechin formed strong hydrogen bonds with ASN171, VAL172, and ARG117, and π-π stacking interactions with PHE325. These interactions suggest a strong electron-sharing mechanism that contributes to enhanced binding stability, receptor modulation, and possibly receptor inactivation.

Squalene, although less polar, formed extensive hydrophobic interactions with non-polar residues such as LEU100, ILE169, and VAL168, which is characteristic of lipid-based compounds interacting with membrane-embedded or transmembrane proteins like GPCRs.

In comparison, Lansoprazole formed similar interactions but with slightly lower binding energies, validating the predictive strength of our model and placing these phytochemicals in credible therapeutic space.

Drug-Likeness and Pharmacokinetic Evaluation

Beyond receptor binding, drug-likeness and ADMET properties determine the viability of any compound as a clinical candidate. The Lipinski, Ghose, Veber, Egan, and Muegge filters, collectively, help to predict oral bioavailability by assessing key physicochemical properties. Epicatechin, Gallocatechin, and 1,8-Diethoxyanthracene-9,10-dione met the majority or all of these criteria, suggesting they possess acceptable molecular weight, lipophilicity (LogP), and polar surface area for effective intestinal absorption and systemic circulation. Conversely, Stigmasterol and Campesterol failed multiple filters primarily due to high lipophilicity and large molecular sizes. Despite high docking scores, such failures imply low solubility and absorption, making their oral formulation challenging without structural modification or nanocarrier-based delivery systems.

ADMET Profile and Toxicity Risk

The ADMET profile further refined the selection of lead compounds. Intestinal absorption was high for most phytocompounds except Squalene, which showed poor water solubility (-8.401 log mol/L) and limited permeability—an expected result for a highly lipophilic compound. Epicatechin and Gallocatechin demonstrated favorable tissue distribution and blood-brain barrier impermeability, making them suitable for non-CNS ulcer therapies. The metabolism panel revealed that Epicatechin and Gallocatechin had minimal interaction with cytochrome P450 enzymes, reducing the risk of drug-drug interactions. In contrast, 1,8-Diethoxyanthracene-9,10-dione and Lansoprazole inhibited multiple CYP isoenzymes (e.g., CYP3A4, CYP2C9), indicating a high likelihood for metabolic competition and adverse interactions in polypharmacy scenarios. Clearance profiles indicated that Squalene had the highest clearance rate (1.791 mL/min/kg), which could necessitate frequent dosing or higher formulation concentrations. Epicatechin and 1,8-Diethoxyanthracene-9,10-dione had moderate clearance values, suggesting favorable systemic retention.

From a safety perspective, the AMES toxicity test and hepatotoxicity predictions flagged 1,8-Diethoxyanthracene-9,10-dione and Lansoprazole as potentially mutagenic and hepatotoxic, whereas Epicatechin, Gallocatechin, and Squalene were predicted to be non-toxic, presenting a more favorable safety profile for future development.

Biological and Therapeutic Implications

The binding of these compounds to 2VT4, 2XZB, and 5YLU represents potential modulation of Adrenergic-mediated stress pathways (via β1-adrenergic receptor), Histamine-induced acid secretion (via H2 receptor), Final acid secretion mechanism (via H+/K+-ATPase). Such multi-target engagement suggests that these phytocompounds could simultaneously reduce acid secretion, enhance mucosal protection, and regulate

inflammatory signaling—a major advancement over single-target therapies. The antioxidant and anti-inflammatory properties of Epicatechin and Gallocatechin, as previously demonstrated (Wang et al., 2021), further support their anti-ulcer potential via mucosal healing and oxidative damage prevention. However, despite its strong binding affinity, 1,8-Diethoxyanthracene-9,10-dione poses a challenge due to its toxicity profile. Structural analog synthesis or functional group modification may be required to mitigate these liabilities. Squalene, while non-toxic, may require formulation improvement to address solubility issues.

CONCLUSION

This investigation highlights Musa sapientum as a promising natural source for anti-ulcer therapeutics. Among the screened phytochemicals, Epicatechin and Gallocatechin emerged as lead candidates due to their optimal balance of binding affinity, pharmacokinetic compatibility, and safety. Their interactions with ulcer-related protein targets suggest a multi-mechanistic mode of action, potentially offering improved clinical outcomes over current single-target drugs. These findings lay a strong foundation for further pharmacological development and experimental validation of banana-derived bioactives as future anti-ulcer agents.

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