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Original Article

Mucoadhesive, anti-inflammatory, and antimicrobial potential of basil seeds (*Ocimum basilicum* L.) as an innovation for effective xerostomia therapy: An *in silico* study

[Potencial mucoadhesivo, antiinflamatorio y antimicrobiano de las semillas de albahaca (*Ocimum basilicum* L.) como innovación para la terapia eficaz de la xerostomía: un estudio *in silico*]

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Abstract

Context: Xerostomia is a prevalent condition that significantly impairs oral function and quality of life. Despite the widespread use of artificial saliva for symptomatic management, most commercially available formulations exhibit limited mucoadhesive capacity and suboptimal anti-inflammatory and antimicrobial properties. Basil seeds *(Ocimum basilicum* L.) contain bioactive compounds with natural mucoadhesive polymer properties, as well as anti-inflammatory and antimicrobial activities, suggesting their potential utility as an alternative therapeutic agent for xerostomia management.

Aims: To investigate the interaction of *O. basilicum* seed compounds with biological targets relevant to xerostomia treatment using in-silico methods.

Methods: Protein and ligand structures were prepared, and ADMET was performed to profile pharmacokinetics and toxicity, molecular docking for simulation, and visualization. Molecular docking simulation was performed between basil seed compounds and MUC-1, TNF-α, deoxycytidylate deaminase, and aspartic proteinase.

Results: ADMET prediction showed that the compounds exhibited complementary pharmacological properties suitable for and non-toxic to topical orabase formulation development. Xylan, galacturonic acid, eugenol, and linalool exhibited favorable interactions with MUC-1 and deoxycytidylate deaminase, demonstrating potential mucoadhesive activity. Eugenol and linalool showed notable binding to TNF-α, suggesting anti-inflammatory potential, while glucomannan and linalool interacted with Saps, consistent with possible antimicrobial potential.

Conclusions: O. *basilicum* seed compounds demonstrate promising mucoadhesive, anti-inflammatory, and antimicrobial properties *in silico*. These findings support their potential as a natural, multifunctional, and halal-compatible option for developing artificial saliva to enhance xerostomia management.

Keywords: artificial saliva; human health; molecular docking; *Ocimum basilicum*; xerostomia.

Resumen

Contexto: La xerostomía es una afección prevalente que compromete significativamente la función oral y la calidad de vida. A pesar del uso generalizado de la saliva artificial para el tratamiento sintomático, la mayoría de las formulaciones disponibles comercialmente presentan una capacidad mucoadhesiva limitada y propiedades antiinflamatorias y antimicrobianas deficientes. Las semillas de albahaca (*Ocimum basilicum* L.) contienen compuestos bioactivos con propiedades poliméricas mucoadhesivas naturales, así como actividades antiinflamatorias y antimicrobianas, lo que sugiere su posible utilidad como agente terapéutico alternativo para el tratamiento de la xerostomía.

Objetivos: Investigar, mediante métodos *in silico*, la interacción de los compuestos de la semilla de *O. basilicum* con dianas biológicas relevantes para el tratamiento de la xerostomía.

Métodos: Se prepararon las estructuras de proteínas y ligandos, y se realizó ADMET para perfilar la farmacocinética y la toxicidad, el acoplamiento molecular para simulación y visualización. Se realizó una simulación del acoplamiento molecular entre los compuestos de la semilla de albahaca y MUC-1, TNF-α, desoxicitidilato desaminasa y aspártico proteinasa.

Resultados: La predicción ADMET mostró que los compuestos presentaron propiedades farmacológicas complementarias, adecuadas y no tóxicas para el desarrollo de formulaciones tópicas de orabase. El xilano, el ácido galacturónico, el eugenol y el linalool mostraron interacciones favorables con MUC-1 y con la desoxicitidilato desaminasa, lo que sugiere una posible actividad mucoadhesiva. El eugenol y el linalool mostraron una unión notable con TNF-α, lo que sugiere un potencial antiinflamatorio, mientras que el glucomanano y el linalool interactuaron con las savias, lo que concuerda con un posible potencial antimicrobiano.

Conclusiones: Los compuestos de la semilla de *O. basilicum* demuestran propiedades mucoadhesivas, antiinflamatorias y antimicrobianas prometedoras *in silico*. Estos hallazgos respaldan su potencial como una opción natural, multifuncional y compatible con el halal para el desarrollo de una saliva artificial que mejore el manejo de la xerostomía.

Palabras Clave: acoplamiento molecular; *Ocimum basilicum*; saliva artificial; salud humana; xerostomía.

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Abbreviations: ADMET: Absorption, distribution, metabolism, excretion, and toxicity; BSM: Basil seeds mucilage; CID: Compound identifier; CMC: Carboxymethylcellulose; Da: Dalton; FU: Fraction unbound; HEC: hydroxyethyl cellulose; IL-1β: Interleukin 1β; IL-6: Interleukin 6; MUC-1: Mucin-1; MW: Molecular weight; PBB: Plasma protein binding; PDB: Protein data bank; SMILES: Simplified molecular input line entry system; TNF-α: Tumor necrosis factor-α.

INTRODUCTION

Saliva plays a critical role in maintaining oral and systemic health by contributing to lubrication, antimicrobial defense, digestion, and mucosal integrity. Reduced salivary flow can disrupt these essential functions and contribute to the development of xerostomia, a condition characterized by a subjective sensation of oral dryness (Łysik et al., 2019). Up to 20% of the world population is affected by xerostomia, which has a significant impact on daily functions such as impaired speech, mastication, and taste perception, along with a heightened risk of opportunistic infections (Kim, 2023). The main triggering factors associated with xerostomia are radiation in head and neck cancer patients, Sjögrens syndrome, and the use of xerogenic drugs (Ayuningtyas et al., 2025; Roblegg et al., 2019). A dry oral cavity results in discomfort and triggers various complaints. The condition can manifest from mild oral irritation to serious oral disease that can affect the patient's health, food ingestion, and quality of life (Alhejoury et al., 2021; Mahdani et al., 2025).

In xerostomia, the oral cavity becomes dry, and treatment is needed. Artificial saliva is a product with certain ingredients designed to mimic the properties of natural saliva (Malallah et al., 2018). Commercially available artificial saliva products generally contain xanthan and guar gums, sodium carboxymethylcellulose, carboxymethylcellulose (CMC), hydroxyethyl cellulose (HEC), glycerol, and porcine gastric mucin, which act as thickening and lubricating components (Łysik et al., 2019; Manosroi et al., 2020; Rocchi & Emmerson, 2020). However, Indonesians, who are predominantly Muslim, cannot use non-halal products as xerostomia treatment due to the porcine gastric mucin content. Therefore, the use and commercial distribution of artificial saliva have been limited due to factors such as halal formulation and status.

The developed artificial saliva is expected to have properties that mimic natural saliva, such as lubricative and mucoadhesive functions, protective properties, and the ability to relieve inflammation of the oral mucosa (Foglio-Bonda et al., 2022; Łysik et al., 2019). However, the development of artificial saliva still has limitations, particularly in its inability to replicate the physical and chemical properties of natural saliva. As a result, the use of artificial saliva has a short retention time, so the resulting therapeutic effect is suboptimal (Kapourani et al., 2022). It has also been reported that the antimicrobial properties of artificial saliva are not effective on oral microflora (Güneri et al., 2011).

Basil seeds (*Ocimum basilicum* L.) have emerged as a promising natural biomaterial because of their rich mucilage content and pharmacological activities. Basil seed mucilage (BSM) contains glucomannan, xylan, and galacturonic acid, forming a natural polymer with strong mucoadhesive properties that support prolonged mucosal interaction (Maqsood et al, 2020; Tantiwatcharothai & Prachayawarakorn, 2019). Polymers have mucoadhesive properties that can adhere to mucosal surfaces (Kapourani et al., 2022). In the oral mucosa, MUC-1 may be targeted in targeted therapy through interactions with compounds contained in artificial saliva (Ukkonen et al., 2017). Eugenol and linalool compounds present in *O. basilicum* seeds have been shown to reduce proinflammatory cytokine levels by inhibiting TNF-α, IL-1β, and IL-6 production (Magalhães et al., 2019; Mohamed et al., 2020). In addition to anti-inflammatory properties, compounds from *O. basilicum* seeds are reported to exhibit other pharmacological activities, including antimicrobial activity (Calderón Bravo et al., 2021). Despite these favorable properties, no existing artificial saliva formulation incorporates a halal-compliant natural mucilage with combined mucoadhesive, anti-inflammatory, and antimicrobial activities. Furthermore, research on the molecular interactions between *O. basilicum* seed compounds and oral mucosal proteins remains limited. This study, therefore, aims to elucidate the molecular characteristics and therapeutic potential of BSM through *in silico* analysis, providing the first scientific rationale for its interaction with MUC-1 and its mucoadhesive, anti-inflammatory, and antimicrobial properties. The findings are expected to lay the foundation for the development of next-generation halal-compliant, more biocompatible, and therapeutically superior artificial saliva that effectively manages xerostomia.

MATERIAL AND METHODS

Preparation of protein and ligand

This study used compounds from *O. basilicum* seeds retrieved from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). The compounds obtained from *O. basilicum* seeds included glucomannan (CID 24892726), xylan (CID 50909243), galacturonic acid (CID 439215), eugenol (CID 3314), and linalool (CID 6549). As controls, researchers used the N-acetylgalactosamine (CID 35717) and drugs, such as ibuprofen (CID 3672), amoxicillin (CID 33613), and micafungin (477468). PubChem is a public database of chemical data sets used for virtual screening,

computational toxicology, and drug repurposing (Kim, 2021). Then, the proteins were obtained from the Protein Data Bank (PDB) database (https://www.rcsb.org/). ucin-1 protein (PDB ID: 6BSC) is used in mucoadhesive targets, pro-inflammatory cytokine TNF-α (PDB ID: 2AZ5) is used in anti-inflammatory targets, while antibacterial receptor (deoxycytidylate deaminase) (PDB ID: 2HVW) and enzyme aspartic proteinases (Saps) (PDB ID: 2QZX) are used in antimicrobial targets. The Protein Data Bank (PDB) is a global database of experimentally determined atomic-level three-dimensional structures of biological macromolecules (proteins, DNA, RNA) (Rose et al., 2017).

The 3D structure of the protein was preprocessed by removing native ligands and water molecules, which were also downloaded from the database using the BIOVIA Discovery Studio Visualizer 2024 program (Iqbal et al., 2023). Next, the protein, separated from its natural ligand, was assigned to Kollman charges and saved in pdbqt format using AutoDock 1.5.7. The compounds contained in *O. basilicum* seeds were used as test ligands. Meanwhile, the compound N-acetylgalactosamine, as well as reference drugs such as ibuprofen, amoxicillin, and micafungin, were used as control ligands. Details of the chemical structures of *O. basilicum* seed compounds and controls, including IDs and 3D structures, were obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). The 3D structures of the compound ligands obtained from PubChem were modeled in Biovia Discovery Studio 2024 and saved in PDB format. The ligand files were in PDB format, Gasteiger charges were added, and the files were saved in the pdbqt format using AutoDock 1.5.7 prior to the docking process. The PDBQT file is filled with various essential information, including partial charges, atom types and radius, as well as the three-dimensional coordinates of each atom (Baroroh et al., 2023).

ADME prediction

The Absorption, Distribution, Metabolism, and Excretion (ADME) prediction was carried out using the PkCSM web platform (http://biosig.unimelb.edu.au/pkcsm/). PkCSM is a platform for predicting and optimizing pharmacokinetic and toxicological properties, implemented through an easily accessible, freely available website (Pires et al., 2015). This method is similar to the PASS prediction, which utilizes the SMILES or canonical SMILES sequence as an identifier for the compound to be predicted. After the SMILES sequence is entered into the designated column, the system automatically performs the ADME prediction. The prediction results include the main parameters, namely absorption, distribution, metabolism, and excretion (Iqbal et al., 2023).

This study aims to determine the capability of the active compounds when distributed in a topical orabase formulation, and the ADME parameters used are focused on the relevant aspects. In the absorption context, the parameters used include water solubility, skin permeability (as a numerical value), and logarithmic molecular weight. The distribution aspect utilizes the plasma protein binding parameter, while the metabolism aspect employs the CYP2D6 parameter for both substrates and inhibitors (Shivanika et al., 2020). The excretion aspect includes the parameters of the drug's half-life and total clearance (in numerical form).

Toxicity test

Toxicity tests were conducted using the PkCSM (http://biosig.unimelb.edu.au/pkcsm/) and or ToxTree platforms. This approach was aligned with PASS and ADME predictions, in which the SMILES or canonical SMILES sequence was used as an identifier for the compound to be predicted (Mahdani et al., 2024). Once the SMILES sequence was entered into the designated column, the system automatically performed the toxicity prediction. The prediction results were presented for several parameters, namely AMES toxicity, carcinogenicity, and skin sensitization (Han et al., 2019).

Molecular docking simulations

Molecular docking simulation was performed with AutoDock 1.5.7. Determination of grid box coordinates was done first to ensure the location of the binding active side of the comparator ligand on the protein, and as a subsequent docking control. Then, proceed with the docking process of the ligand and protein. The docking result was represented as a prediction of the binding energy when the ligand and protein were bound, and it was saved in the out file.pdbqt format. Molecular docking was performed to predict the interaction between two compounds, and the interaction energy for their specific orientation was simultaneously calculated (Khoswanto & Siswandono, 2022).

Interaction and visualization

The docking results from AutoDock 1.5.7 were interpreted and visualized using LigPlot+ and the BIOVIA Discovery Studio Visualizer 2024 program (Ummah & Zummah, 2024).

The study was approved by the ethics committee of Universitas Airlangga Faculty of Dental Medicine Health Research under process number 0950/HRECC.FODM/VIII/ 2024.

Table 1. ADME prediction results of the compound of *O. basilicum* seeds.

Compound name	Administration			Distribution	Metabolism		Excretion	
	MW (Da)	Skin permeability (cm/s)	Log MW	Plasma protein (%)	CYP2D6 substrate	CYP2D6 Inhibitor	Half-life of drug (h)	Clearance (mL/min)
Glucomannan	666.6	17.26	2.82	38.57	Negative	Negative	≥3	4.89
Xylan	166.12	-2.40	2.22	22.97	Negative	Negative	≥3	2.23
Galacturonic acid	194.14	-1.69	2.29	38.65	Negative	Negative	≥3	2.68
Eugenol	164.2	-2.78	2.22	27.5	Negative	Negative	<3	9,090
Linalool	154.25	-2.98	2.19	10.8	Negative	Negative	≥3	9.21

Table 2. Toxicity test results of the compound of *O. basilicum* seeds.

Compound Name	Toxicity		
	AMES mutagenesis	Carcinogenesis	Skin sensitization
Glucomannan	Safe	Safe	Safe
Xylan	Safe	Safe	Safe
Galacturonic acid	Safe	Safe	Safe
Eugenol	Safe	Safe	Safe
Linalool	Safe	Safe	Safe

RESULTS

ADME prediction result

Glucomannan exhibited the highest molecular weight value of 666.6 Da among the five components analyzed. The skin permeability values ranged from –2.78 to 17.28, with the lowest value observed for eugenol and the highest for glucomannan. The logarithmic weight of glucomannan was the highest at 2.82, whereas linalool had the lowest at 2.19 (Table 1). Glucomannan and galacturonic acid were found to exhibit high plasma protein binding values of 38.57% and 38.65%, respectively. All compounds in *O. basilicum* seeds were identified as negative for both substrate and inhibitor activity of CYP2D6. Four compounds, except eugenol, were predicted to have a half-life ≥ 3 hours. Glucomannan and galacturonic acid exhibited moderate clearance rates of 4.89 and 2.68 mL/min, respectively.

Toxicity test

The toxicity test results indicated parameter data used to determine whether the five compounds in *O. basilicum* seeds possess toxic potential when systemically distributed (Table 2). All compounds were found to be safe in the AMES toxicity test, suggesting that they are not mutagenic, non-carcinogenic, and do not cause mucosal or skin irritation, as they tested negative for skin sensitization.

Molecular docking result

The molecular docking results between *O. basilicum* seeds compounds and proteins contain binding affinity data (Table 3). The interaction of molecular docking simulation results on mucoadhesive potential is shown in Table 4. Furthermore, interactions from the results of molecular docking simulations for anti-inflammatory potential are shown in Table 5, and those for antimicrobial potential are shown in Table 6. Fig. 1 shows a visualization of the interaction of control and test ligand compounds with proteins to assess mucoadhesive potential. Fig. 2 shows a visualization of the interactions between control and test ligand compounds and proteins to assess their anti-inflammatory potential. The visualization of the interactions between control and test ligand compounds and proteins for antimicrobial potential, consisting of antibacterial in Fig. 3 and antifungal in Fig. 4. The two-dimensional interaction visualization presented in the figures shows the type of binding and the locations of the amino acid residues bound by the control and test ligands.

Data analysis is based on the binding affinity, the number of intermolecular bonds formed, and the identical amino acid residues between the control and test ligand compounds. Based on the results of molecular docking simulations and visualization of the interactions of MUC-1 with xylan, galacturonic acid, eugenol, and linalool, the ligands are close to the control ligand, indicating potential interaction with the MUC-1

protein. Furthermore, the interaction of xylan, eugenol, and linalool yields results close to the control, suggesting that it may interact with TNF-α. The antimicrobial potential test results consisted of antibacterial and antifungal docking. In the molecular docking simulation and interaction visualization for antibacterial potential, xylan, galacturonic acid, eugenol, and linalool show results close to the control, indicating potential interactions with the antibacterial receptor (deoxycytidylate deaminase). Then, the antifungal potential test showed that glucomannan and linalool yielded results close to the control, suggesting they could interact with aspartic proteinases (Saps).

Table 3. Results of molecular docking simulation between ligand and protein.

Potential test		Compound name	Protein	Binding affinity (kcal/mol)
Mucoadhesive		N-Acetylgalactosamine (Control)	MUC-1 (6BSC)	-4.86
		Glucomannan		-1.69
		Xylan		-4.57
		Galacturonic acid		-4.61
		Eugenol		-4.61
		Linalool		-4.58
Anti-inflammatory		Ibuprofen (Control)	TNF-α (2AZ5)	-5.5
		Glucomannan		+2.85
		Xylan		-3.12
		Galacturonic acid		-2.83
		Eugenol		-4.61
		Linalool		-5.15
Antimicrobial	Antibacterial	Amoxicillin (Control)	Deoxycytidylate deaminase (2HVW)	-8.55
		Glucomannan		-1.82
		Xylan		-5.09
		Galacturonic acid		-6.81
		Eugenol		-5.36
		Linalool		-6.06
	Antifungal	Micafungin (Control)	Enzyme aspartic proteinases (2QZX)	-5.02
		Glucomannan		-5.63
		Xylan		-4.13
		Galacturonic acid		-4.22
		Eugenol		-4.34
		Linalool		-4.38

Table 4. Interaction of molecular docking simulation results between control and test ligand with MUC-1 (6BSC) for mucoadhesive potential.

Compound name	Intermolecular Interaction			Number of intermolecular interactions
	Hydrogen bond interaction	Hydrophobic bond interaction	Other bond interaction	
N-Acetylgalactosamine (Control)	4	3	-	7
Glucomannan	8	3	-	11
Xylan	4	3	-	6
Galacturonic acid	5	2	-	7
Eugenol	2	7	-	9
Linalool	2	6	-	8

Table 5. Interaction of molecular docking simulation results between control and test ligand with TNF-α (2AZ5) for anti-inflammatory potential.

Compound name	Intermolecular interaction			Number of intermolecular interactions
	Hydrogen bond interaction	Hydrophobic bond interaction	Other bond interaction	
Ibuprofen (Control)	2	11	-	13
Glucomannan	3	8	-	11
Xylan	4	4	-	8
Galacturonic acid	4	3	-	7
Eugenol	1	9	-	10
Linalool	2	10	-	12

Table 6. Interaction of molecular docking simulation results between control and test ligand with deoxycytidylate deaminase (2HVW) and enzyme aspartic proteinases (2QZX) for antimicrobial potential.

Potential	Compound name	Intermolecular interaction			Number of intermolecular interactions
		Hydrogen bond interaction	Hydrophobic bond interaction	Other bond interaction	
Antibacterial	Amoxicillin (Control)	5	12	-	17
	Glucomannan	5	16	-	21
	Xylan	6	5	-	11
	Galacturonic acid	5	8	-	13
	Eugenol	4	10	-	14
	Linalool	3	13	-	16
Antifungal	Micafungin (Control)	9	13	-	22
	Glucomannan	11	16	1	28
	Xylan	3	5	-	8
	Galacturonic acid	2	6	-	8
	Eugenol	2	7	-	9
	Linalool	1	16	-	17

DISCUSSION

Physicochemical and administration properties

The physicochemical characteristics play an essential role in determining the pharmacokinetic feasibility of each compound for topical formulation. According to the obtained data, glucomannan exhibited the highest molecular weight (666.6 Da), followed by galacturonic acid (194.14 Da), xylan (166.12 Da), and eugenol (164.2 Da). The values demonstrate that, except for glucomannan, all compounds fulfilled the molecular weight criterion of Lipinski's Rule of Five (MW < 500 Da), which indicates better permeability and absorption potential (Ivanović et al., 2020).

Skin permeability is another vital factor in determining the ability of a compound to penetrate mucosal or dermal layers. The predicted skin permeability values ranged from −2.78 to 17.26, suggesting diverse diffusion capacities. Compounds with lower log permeability (e.g., eugenol −2.78, galacturonic acid −1.69) indicate a balance between hydrophilicity and lipophilicity, enabling them to diffuse efficiently through the oral mucosa. In contrast, the extremely high value of 17.26 observed for glucomannan suggests low diffusibility due to its large polysaccharide structure, which is consistent with previous findings that macromolecules above 500 Da have difficulty in passive diffusion across epithelial membranes (Wanasathop et al., 2021).

Furthermore, the logarithmic molecular weight (Log MW) of the five compounds ranged from 2.19 to 2.82. Current standards for mucosal drug delivery suggest that compounds with a Log MW < 2.5 are optimized for effective permeability. Xylan (2.22) and eugenol (2.22) fall within this optimal range, indicating

higher absorption efficiency through the oral mucosa than glucomannan (2.82). The results are consistent with studies on buccal drug delivery systems, in which molecules smaller than 300 Da have demonstrated efficient penetration through non-keratinized epithelial layers (Wanasathop et al., 2021).

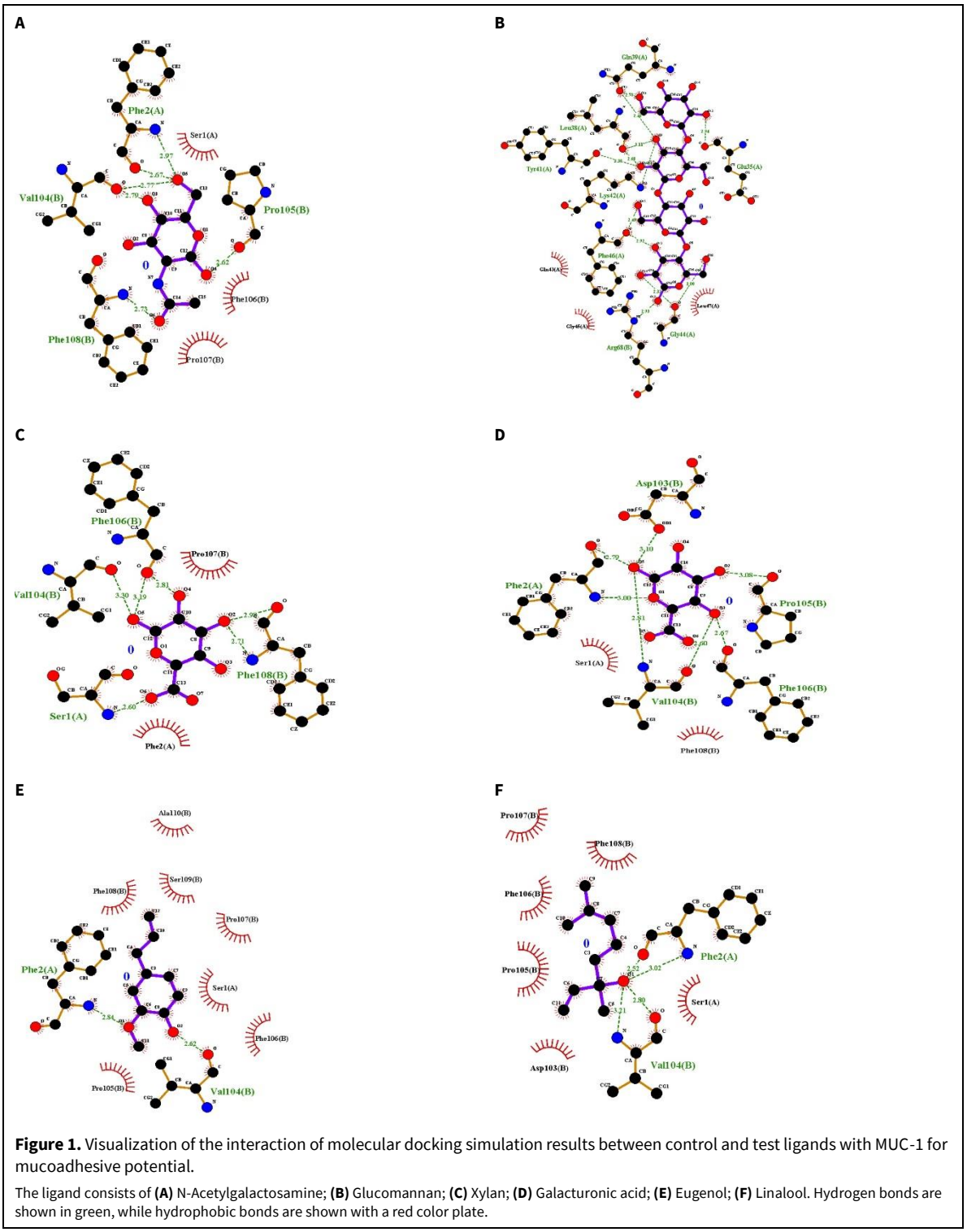


Figure 1. Visualization of the interaction of molecular docking simulation results between control and test ligands with MUC-1 for mucoadhesive potential.

The ligand consists of **(A)** N-Acetylgalactosamine; **(B)** Glucomannan; **(C)** Xylan; **(D)** Galacturonic acid; **(E)** Eugenol; **(F)** Linalool. Hydrogen bonds are shown in green, while hydrophobic bonds are shown with a red color plate.

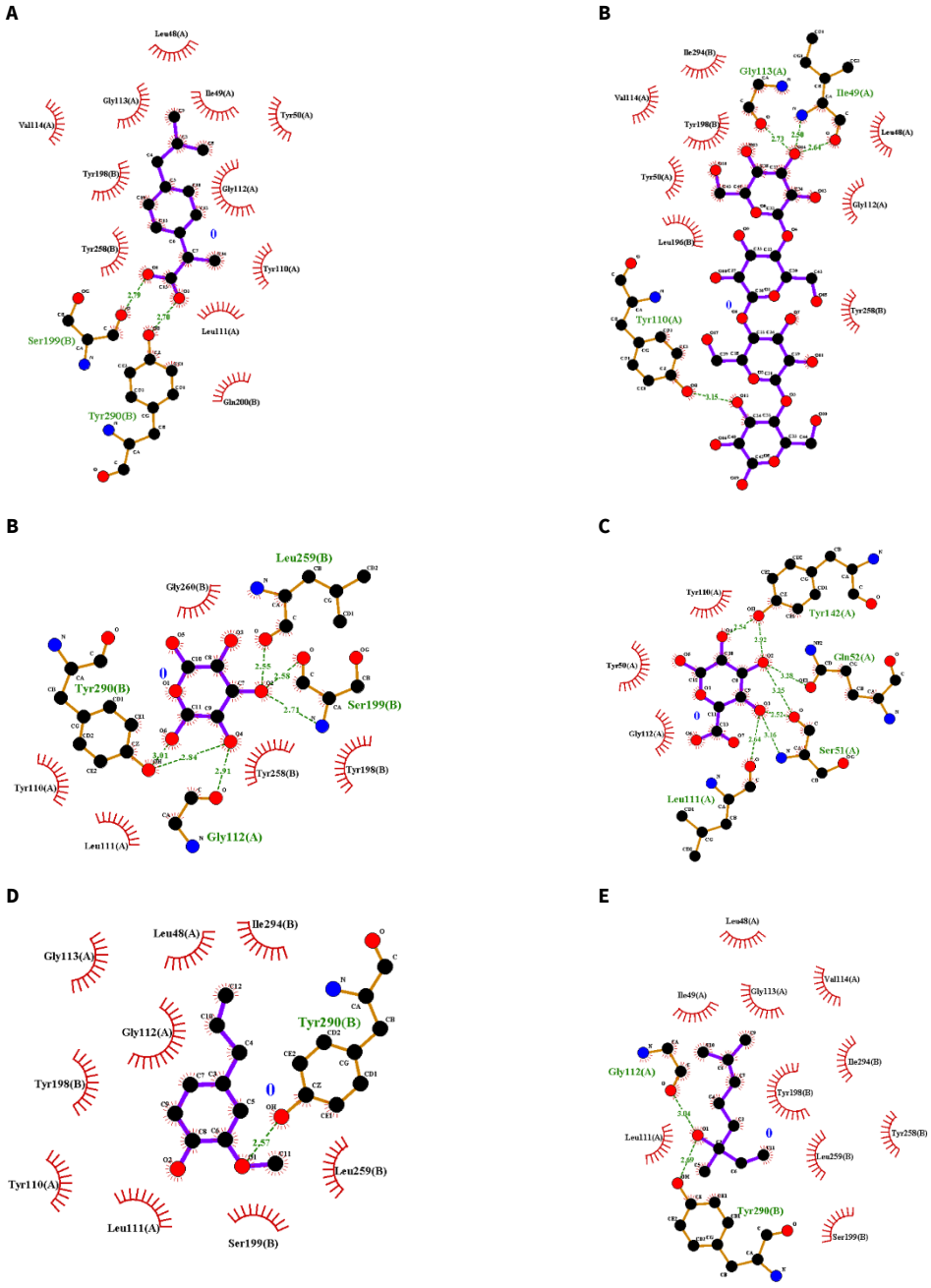


Figure 2. Visualization of the interaction of molecular docking simulation results between control and test ligands with TNF-α for anti-inflammatory potential.

The ligand consists of **(A)** Ibuprofen; **(B)** Glucomannan; **(C)** Xylan; **(D)** Galacturonic acid; **(E)** Eugenol; **(F)** Linalool. Hydrogen bonds are shown in green, while hydrophobic bonds are shown with a red color plate.

Distribution and plasma binding characteristics

The plasma protein binding (PPB) profiles of the examined compounds indicate moderate interactions with circulating plasma proteins. More specifically, the binding percentages of glucomannan and galacturonic acid were 38.57% and 38.65%, respectively, while the lowest affinity was observed for compound xylan, with a binding value of 22.97%. The fact that the tested compounds exhibit moderate protein binding is significant because moderate levels leave a considerable free fraction, which is responsible for their pharmacological activity. Moderate protein binding typically facilitates an equilibrium between systemic distribution and sustained plasma residence, potentially extending systemic exposure without compromising overall bioavailability (Ferreira & Andricopulo, 2019).

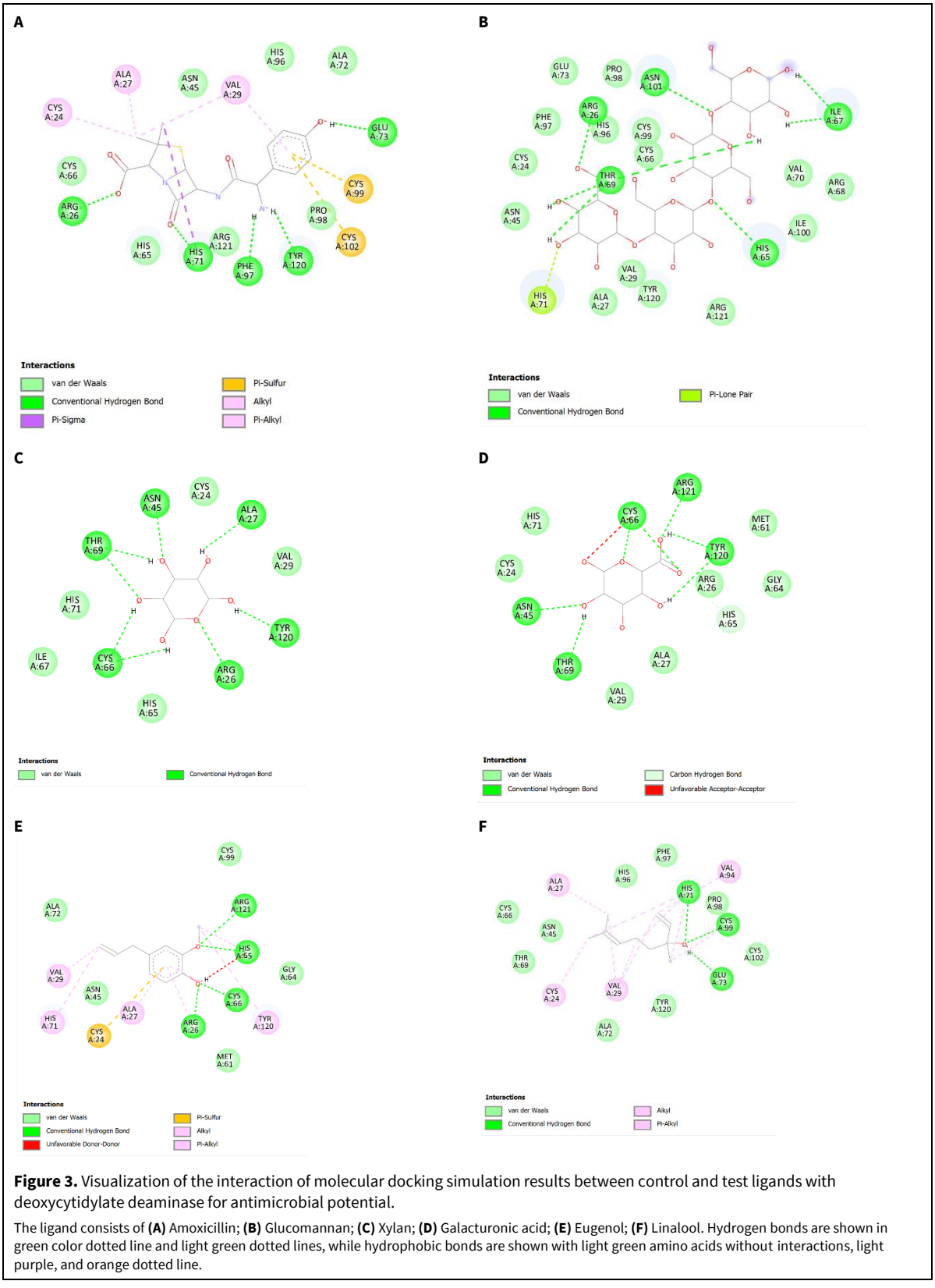


Figure 3. Visualization of the interaction of molecular docking simulation results between control and test ligands with deoxycytidylate deaminase for antimicrobial potential.

The ligand consists of **(A)** Amoxicillin; **(B)** Glucomannan; **(C)** Xylan; **(D)** Galacturonic acid; **(E)** Eugenol; **(F)** Linalool. Hydrogen bonds are shown in green color dotted line and light green dotted lines, while hydrophobic bonds are shown with light green amino acids without interactions, light purple, and orange dotted line.

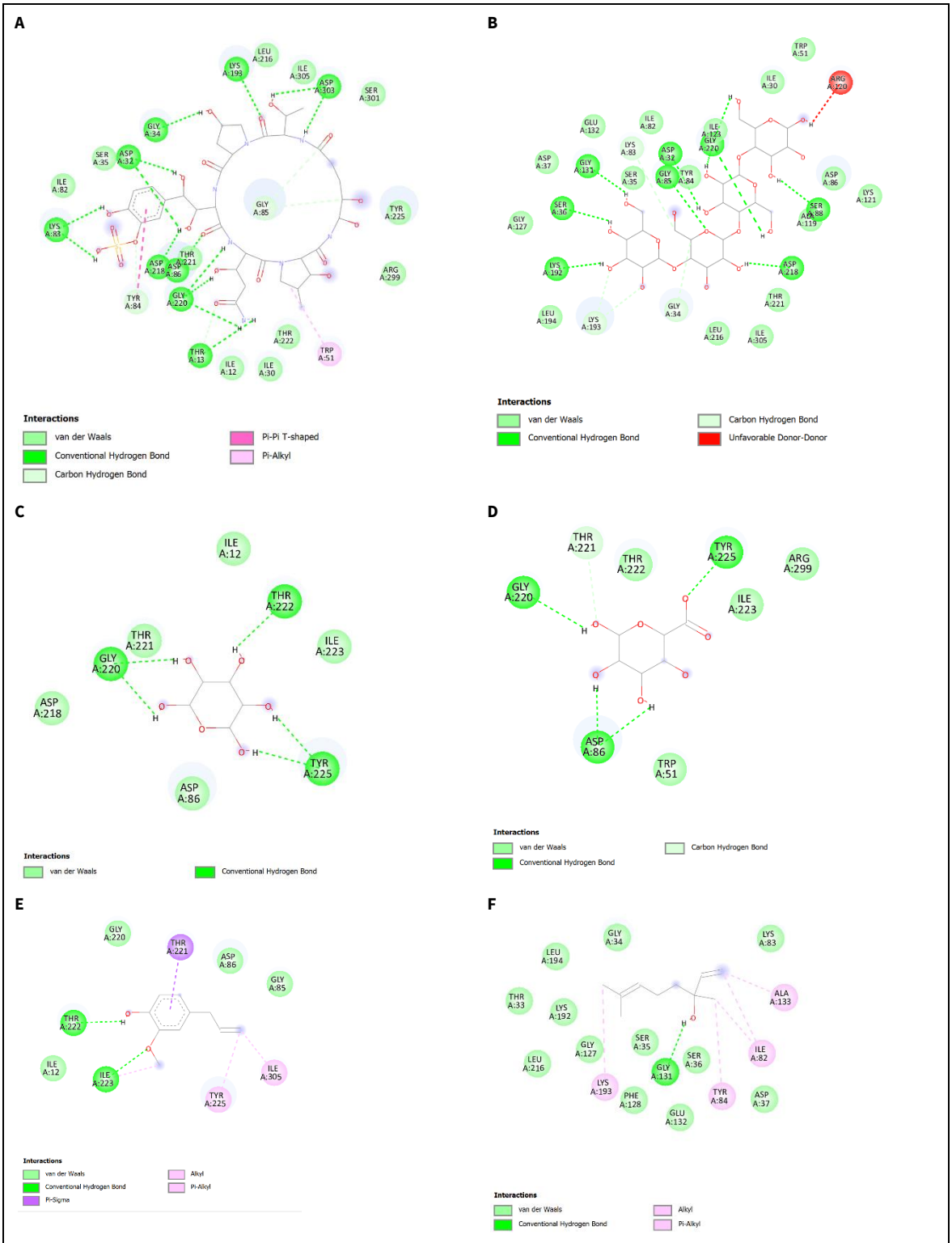


Figure 4. Visualization of the interaction of molecular docking simulation results between control and test ligands with aspartic proteinases (Saps) for antimicrobial potential.

The ligand consists of **(A)** Micafungin; **(B)** Glucomannan; **(C)** Xylan; **(D)** Galacturonic acid; **(E)** Eugenol; **(F)** Linalool. Hydrogen bonds are shown in green color dotted line and light green dotted lines; Hydrophobic bonds are shown with light green amino acids without interactions, light purple, and violet dotted line; Other interaction bond interaction (Unvorable Donor-Donor) is shown with red dotted line.

The fraction unbound (FU) is a critical parameter for achieving therapeutic concentrations at the target site. The higher the FU, the greater the potential of diffusion of the therapeutic agent across a biological membrane. Hence, xylan with the lowest binding percentage may demonstrate quicker onset of action and better tissue distribution. Nevertheless, for topical dosage forms such as orabase, the main concern is no longer systemic bioavailability. Rather, the retention of the local concentrations becomes the main priority. In this scenario, the therapeutic agent with moderate PPB (30%-50%) is preferable (Watanabe et al., 2018).

Metabolic stability and CYP2D6 interaction

Metabolism prediction through pkCSM showed that none of the tested compounds acted as substrates or inhibitors for the cytochrome P450 2D6 (CYP2D6) enzyme. This finding is significant as CYP2D6 is a key enzyme responsible for xenobiotic metabolism. The absence of substrate or inhibitory interaction suggests that these compounds are metabolically stable and unlikely to produce adverse drug–drug interactions (Shivanika et al., 2020).

Eugenol, in particular, is known for being metabolized primarily via glucuronidation rather than cytochrome-dependent oxidation, thereby reducing potential hepatotoxicity (Sripriya et al., 2021). Polysaccharide compounds such as glucomannan and xylan are typically resistant to hepatic metabolism due to their polymeric structure, instead undergoing partial degradation by intestinal microbiota (Chen et al., 2024). Consequently, their inclusion in topical formulations presents a low risk of metabolic interference.

Excretion dynamics

The clearance rates (CL) for the compounds varied notably, reflecting differences in molecular size and hydrophilicity. Glucomannan and galacturonic acid displayed moderate clearance values of 4.89 and 2.68 mL/min, respectively, while eugenol showed an exceptionally high clearance (9090 mL/min). The latter result is consistent with eugenol's small molecular size and high lipophilicity, leading to rapid elimination primarily via the renal and respiratory routes (Wang et al., 2026).

A drug's half-life also determines its residence time in the body. Most compounds, except eugenol, exhibited a predicted half-life ≥ 3 hours, indicating sufficient duration to exert pharmacological effects following topical application. For topical orabase systems, sustained drug retention within the mucosal surface is essential, as it allows prolonged contact and controlled drug release. Polysaccharides such as glucomannan and xylan, despite their slower permeability, may serve a dual function as bioadhesive agents that extend contact time and regulate local drug release (Yermak et al., 2022).

Toxicological evaluation

Toxicity assessment revealed that all compounds were negative for AMES mutagenicity and carcinogenicity, indicating no genetic or cellular mutation potential. Additionally, none demonstrated skin sensitization properties, confirming the biocompatibility and safety of these compounds for topical administration. These findings align with previous studies reporting that natural polysaccharides and phenolic compounds exhibit favorable cytocompatibility and minimal irritation (Sripriya et al., 2021; Stampfer et al., 2019).

Eugenol, while known for its strong biological activity, is classified as safe within the predicted concentration range used in topical formulations. Similarly, glucomannan and xylan, being plant-derived polysaccharides, have been widely recognized as non-toxic biomaterials used in pharmaceutical and food applications (Benalaya et al., 2024). The combined absence of mutagenic and irritative tendencies reinforces their potential use in mucosal drug delivery.

Integrated pharmacokinetic interpretation

When the ADMET parameters are evaluated collectively, the compounds demonstrate complementary pharmacological characteristics suitable for topical orabase development. Low-molecular-weight compounds such as eugenol and galacturonic acid provide effective penetration and anti-inflammatory activity due to their permeability and stability. Meanwhile, glucomannan and xylan serve as mucoadhesive matrices, thereby improving retention and the controlled release of active agents.

Such combination formulations have been suggested to optimize local delivery efficiency while maintaining minimal systemic absorption (Gao et al., 2023). These findings collectively indicate that the synergy between low-MW actives and polysaccharide excipients offers a promising pharmacokinetic profile for topical oral anti-inflammatory systems.

Molecular docking test analysis

Artificial saliva represents a critical therapeutic intervention for the management of xerostomia. To date, various focused approaches have been developed for the development of artificial saliva products, one of which leverages the potential of natural ingredients. The active compounds contained in BSM provide moisturizing, lubricating, and anti-irritating properties, so it allows saliva to adhere to artificial sticks longer on the surface of the oral mucosa, and effective

moisturization can last a long time (Kapourani et al., 2022; Manosroi et al., 2020; Tantiwatcharothai Prachayawarakorn, 2019). Additionally, *O. basilicum* seeds contain other useful active compounds for the development of artificial saliva, such as anti-inflammatory compounds, which help reduce inflammation in patients with dry oral mucous membranes (Dharsono et al., 2022; Łysik et al., 2019). *O. basilicum* seeds also have other pharmacological activities, such as antimicrobial (Calderón Bravo et al., 2021). Thus, this study investigated the mucoadhesive, anti-inflammatory, and antimicrobial potential of *O. basilicum* seeds using molecular docking simulations to develop an artificial saliva for xerostomia therapy.

The first analysis was carried out to determine that artificial saliva formulated with *O. basilicum* seed compounds demonstrates potential mucoadhesive activity. MUC-1 was identified as a membrane-bound mucin expressed in both major and minor salivary glands and the surface epithelial cells of the oral mucosa (Kashyap & Kullaa, 2020). Mucin glycoprotein is an important factor in the physical properties of artificial saliva, including mucoadhesivity (Manosroi et al., 2020). Therefore, MUC-1 is used as a protein or receptor target in therapeutic development to determine the mucoadhesive potential between mucin and molecules (Ukkonen et al., 2017).

In the first parameter, the docking result is the binding affinity value (Salman et al., 2023). Results molecular docking based on the best pose of each test ligand compound showed that four of the five test ligand compounds, namely galacturonic acid, eugenol, linalool, and xylan have binding affinity values that are close to N-acetylgalactosamine as an comparative ligand compound with each value -4.61 kcal/mol, -4.61 kcal/mol, -4.58 kcal/mol, and -4.57 kcal/mol. The more negative values, the better the binding affinity energy between MUC-1 and the ligands, so that the bond formed is more stable. The second parameter in molecular docking is the number of intermolecular bonds. Based on the approach using the number of intermolecular bonds as the parameter, all tested ligand compounds exhibit potential ligand-like activity control. The third parameter, in the visualization of the results of ligand molecular docking tests with MUC-1, identified four compounds as having matching amino acid residues with N-acetylgalactosamine as a control ligand. Based on visualization of docking results, the test ligands are galacturonic acid compounds, eugenol, linalool, and xylan, as well as a comparison ligand in the form of N-acetylgalactosamine, showing that there is an identity of amino acid residues in the active site of MUC-1, on the amino acid residues PHE2 and SER1.

The second analysis was to determine the anti-inflammatory potential. Ibuprofen is a commercial non-steroidal anti-inflammatory drug (NSAID) that is generally used to relieve pain, inflammation, and fever, so it has an anti-inflammatory effect. In this study, ibuprofen was used as a control ligand in molecular docking due to its ability to inhibit TNF-α (Salman et al., 2023). The docking results show that linalool, eugenol, xylan, and galacturonic acid have binding affinity energy values closer to the control, with values of -5.15 kcal/mol, -4.61 kcal/mol, -3.12 kcal/mol, and -2.83 kcal/mol, respectively. The more negative values, the better the binding affinity energy between TNF-α and the ligands, so that the bond formed is more stable. Based on the approach that uses the number of intermolecular bonds as the parameter, linalool, glucomannan, eugenol, and xylan have potential ligand-like activity. The test ligand is a compound of linalool, eugenol, and xylan, as well as a comparison ligand in the form of ibuprofen, which showed there is an identity in the amino acid residue in the active site of TNF-α, namely the amino acid residue Tyr290. The amino acid residue TYR or tyrosine is important in inhibiting TNF-α so that *O. basilicum* seed compounds have anti-inflammatory potential that resembles the control (Zia et al., 2020).

The third analysis was determined to have antimicrobial potential. Saliva contains antimicrobial proteins that play an important role in the body, but when the mouth is dry, this function decreases. In xerostomia, hyposalivation can increase the development of caries and tooth loss (Müller et al., 2023). In general, caries occurs in the cervical region. Plaque-dominant *Streptococcus mutans* bacteria promote caries development (Zhu et al., 2023). Therefore, the antibacterial receptor (deoxycytidylate deaminase) of *Streptococcus mutans* was used in an in-silico test (Hou et al., 2008). In addition, antimicrobial proteins such as histatins have antifungal activity, and salivary immunoglobulin A (IgA) can inhibit *Candida* adhesion (Nadig et al., 2017). However, in xerostomia, salivary function decreases, thereby increasing the risk of fungal infections. In the oral mucosa, oral candidiasis can occur, which is an opportunistic infection caused by the fungus *Candida albicans* (Radithia et al., 2023). *In silico* test for antifungal, five compounds identified in *O. basilicum* seeds, consisting of glucomannan, xylan, galacturonic acid, eugenol, and linalool, were docked with the enzyme aspartic proteinases (Saps). This proteolytic enzyme, produced by *Candida albicans*, plays a key role in the spread of infection (Borelli et al., 2008). The proteolytic properties of aspartic proteases enable *C. albicans* to adhere (Sulistyowaty et al., 2023).

In the antibacterial simulations, amoxicillin served as the reference standard. Except for glucomannan, all tested compounds exhibited binding affinities highly comparable to the control, with values of -6.81, -6.06,

-5.36, and -5.09 kcal/mol. While glucomannan demonstrated lower affinity, it possessed a higher frequency of intermolecular interactions exceeding the control. Regarding site specificity, all compounds successfully bound to amino acid residues identical to those of the Amoxicillin-receptor complex, specifically HIS71, CYS66, ASN45, CYS24, ALA27, and VAL29.

Micafungin was utilized as the antifungal control. Four compounds displayed binding affinities proximal to the control, ranging from -4.13 to -4.38 kcal/mol. Notably, glucomannan demonstrated a more negative binding affinity (-5.63 kcal/mol) than micafungin, suggesting a highly stable interaction. Furthermore, glucomannan exhibited superior intermolecular bonding profiles compared to the control, while linalool showed comparable interaction levels. Although xylan, galacturonic acid, and eugenol displayed relatively lower interaction scores, all five compounds demonstrated a high degree of residue matching with the control, confirming their affinity for the active site of the Sap enzyme.

Collectively, these findings demonstrate that *O. basilicum* seed compounds offer a multifaceted approach to xerostomia management. The capacity of glucomannan, xylan, and eugenol to inhibit key enzymatic targets in *S. mutans* and *C. albicans* provides essential protection against the opportunistic infections typically associated with hyposalivation. Crucially, this antimicrobial potential is augmented by the previously discussed mucoadhesive characteristics; the enhanced retention of these compounds on the oral mucosa, mediated by their interaction with MUC-1 proteins, ensures that the bioactive agents remain at the target site for an extended duration. The synergy between stable ligand-receptor binding and prolonged contact time suggests that basil-seed-based formulations function not merely as mechanical moisture substitutes but as therapeutically active biological protective barriers within the oral cavity.

CONCLUSION

Compounds isolated from *O. basilicum* seeds, including xylan, galacturonic acid, eugenol, and linalool, exhibit favorable in silico interactions with key biological targets associated with xerostomia. These findings support the potential development of a plant-based, halal-compliant artificial saliva formulation, although further experimental and clinical validation is required to confirm efficacy and safety.

CONFLICT OF INTEREST

The research was conducted entirely free from any involvement in commercial, financial, or personal matters that might be perceived as a possible conflict of interest or that could have influenced the outcomes or interpretation of the study.

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GENERATIVE ARTIFICIAL INTELLIGENCE (AI)

The authors used Grammarly (Superhuman Platform Inc.) and Perplexity (perplexity.ai) to improve the language and readability of the manuscript. The authors reviewed and edited the content and take full responsibility for its accuracy. No images were generated or manipulated using AI tools.

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AUTHOR CONTRIBUTION:

Contribution	Mahdani FY	Wati SM	Kurniawan A	Ayuningtyas NF	Darojah Z	Hussaini HM
Concepts or ideas	x	x				
Design	x	x				
Definition of intellectual content	x			x		
Literature search	x	x				x
Experimental studies			x		x	
Data acquisition			x			
Data analysis				x	x	
Statistical analysis				x	x	
Manuscript preparation			x	x	x	
Manuscript editing	x	x				x
Manuscript review	x	x	x	x	x	x

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