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Comparative Molecular Docking Analysis of *Ocimum sanctum* Compounds and Anti-Allergic Drugs Against Allergic Rhinitis Targets

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Abstract

Allergic rhinitis, commonly referred to as hay fever, is a hypersensitivity reaction caused by exposure to small airborne allergens such as pollen, dust, or animal dander. It is one of the most prevalent allergic disorders worldwide and in the United Kingdom affects nearly one-fifth of the general population. The condition has been closely linked with asthma and allergic conjunctivitis, forming part of a broader spectrum of atopic diseases. Clinically, allergic rhinitis manifests with characteristic symptoms including persistent sneezing, nasal congestion, rhinorrhea, coughing, postnasal drip, and headaches, which can significantly impair quality of life and productivity if left untreated. In recent years, there has been growing interest in exploring natural therapeutic agents as alternatives or complements to conventional antihistaminic drugs. In our study, bioactive compounds from *Ocimum sanctum* (commonly known as holy basil) were assessed in comparison to selected anti-allergic drug molecules for their capacity to inhibit key biochemical targets associated with allergic inflammatory pathways. Specifically, molecular docking analyses were performed against the crystal structure of human DPP4 in complex with the chitotriosidase-1 (hCHIT) catalytic domain bound to compound 7g (PDB ID: 5NRA). Among the standards tested, Levocetirizine, a widely prescribed second-generation antihistamine, achieved a docking score of –7.2 kcal/mol. Notably, Isoaromadendrene epoxide, a phytoconstituent isolated from the methanolic extract of *O. sanctum*, demonstrated superior binding affinity with a docking score of –8.2 kcal/mol. These encouraging findings highlight the potential of Isoaromadendrene epoxide as a natural therapeutic lead in allergic rhinitis management. Nevertheless, comprehensive pharmacological investigations, including mechanistic studies, dose optimization, and clinical validation, remain essential before translating these outcomes into practical medical applications.

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1. Introduction

Allergic rhinitis, the most typical chronic rhinitis, impacts around 10 to 20 percent of individuals, with indications that its prevalence is on the rise (Small, Keith, and Kim 2018; Nur Husna *et al.* 2022). In this, the three main phases of allergic response are: IgE allergic sensitization, allergen challenge, and triggering of symptoms. Between 5 and 22 percent of people are thought to have allergic rhinitis, Rhinorrhea, nasal congestion, and nasal congestion also noticed, which is the most typical atopic disorder (Brozek *et al.* 2017). Also, the cross-sectional epidemiological studies suggest that a significant proportion, up to 78%, of asthma patients also experience allergic rhinitis. Most of the synthetics drug molecules have intolerable adverse effects, although it can be used in allergen immunotherapy leukotriene inhibitors (Valovirta 2012; Kim, Bouchard, and Renzi 2008). Diagnosis allergic rhinitis is one of the most challenging, hence the patients are not significantly recognizing the indication of driving to under some specific condition, which indicates the condition that are effectively influence the social, instructive and pro and proficient lives (Smallwood and Wei 2016). Asthma is most recognizable in allergic rhinitis; several studies have reported that this allergic reaction tends to proceed with asthma. This consecutive growth occurs in approximately 43% to 64% of cases, prominence the potential role of allergic rhinitis as a precursor or contributory factor to the development of asthma in these individuals. In this, allergic rhinitis is brought on by responses to inhaled allergens that are mediated mainly by immunoglobulin E (IgE) (Polosa *et al.* 2005). The IgE antibodies significantly interact with high-affinity receptor (FcεRI) on the surface of mast cells, basophils, and antigen-presenting cells, which can lead to sensitization to allergens (Kanagaratham *et al.* 2020). Thus, a study revealed that 50% ethanol extract of Mentha × piperita L., (peppermint), will prevent actively sensitized rats peritoneal mast cells from releasing histamine and that prevents Rhinitis (Inoue *et al.* 2001). Therefore, some plants may also consist of many effective compounds which can used as drug. Traditionally plants were used as a remedy for most diseases. Plants have valuable compounds which can be used to treat various diseases (Petrovska 2012; Sofowora, Ogunbodede, and Onayade 2013). The World Health Organization (WHO) estimates that 80 percent of people in some Asian and African countries already obtain primary healthcare in some capacity using herbal medicine (Kumar *et al.* 2021). In India, tulsi which belongs to the family Lamiaceae is regarded as the most sacred plant. *Ocimum sanctum*, or tulsi, is a well-known aromatic plant used in Ayurveda. Numerous medical systems, such as Ayurvedic, Siddha, Greek, Roman, and Unani medicine, use tulsi (Cohen 2014). Many ailments, including wounds, bronchitis, liver illnesses, catarrhal fever, coughing fits, stomach difficulties, skin conditions, can be effectively treated over the counter with tulsi (Jamshidi and Cohen 2017). Tulsi extract is hence sometimes called the "Extract of Life" and is believed to lengthen life. Chewing tulsi leaves and consuming boiled tulsi water can help reduce symptoms of colds and flu, soothe a sore throat, and even treat respiratory disorders (Bhattacharyya and Bishayee 2013). The genus Ocimum comprises approximately 160 species that are widely distributed across warm regions of the globe (Dharsono *et al.* 2022). Examples of important species within this genus include *Ocimum americanum*, *Ocimum sanctum*, *Ocimum killimandscharicum*, *Ocimum camphora*, *Ocimum gratissimum, Ocimum canum* and *Ocimum basilicum* (Jahanger *et al.* 2023). It can spread all over world and are well-known for its medicinal properties. It is believed that the essential oil exhibits insecticidal and antibacterial properties (Chouhan, Sharma, and Guleria 2017). Research has demonstrated that the oil exhibits antimicrobial properties, inhibiting the growth of certain bacteria, including *Micrococcus pyogenes var. aureus* and *Mycobacterium tuberculosis* (Winska *et al.* 2019).

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Several studies have been reported that Tulsi has antioxidant properties, owing to this possessions, tulsi leaves has been used to treat number of aliments, it significantly protects cells from damage caused by free radicals (Hasan *et al.* 2023). "Eugenol" is one of the most prominent compounds presents in Tulsi and acts as effective anti-inflammatory ingredient. It is critical in regulating blood sugar levels by activating the pancreatic beta cells to release insulin (Ansari *et al.* 2023). A study has described that the long-term intake of *Ocimum sanctum* enhances natural antioxidants in the heart and protects against isoproterenol-induced heart damage in rats. Identification of potential drug like molecules via experimental and traditional methods is time consuming and expensive (Sharma *et al.* 2001). According to Niazi and Marium (2023), computer-aided methodologies have been used as effective approach in the drug development and discovery process and gaining great attention and becoming more widely used (Niazi and Mariam 2023). Molecular docking is one of the widely used approaches to find and develop a potential and effective small molecule. By modulating the functional groups, it leads to identification of novel medications and learning about the molecular mechanisms may all possible in computer-aided drug discovery (CADD) (Meng *et al.* 2011). Molecular docking analysis has been widely used for studying comprehending the interactions between a ligand and a target molecule. By influential the most advantageous orientation that produces the lowest free binding energy, it forecasts the strength of binding between the ligand and the protein (Ferreira *et al.* 2015). In this study we have predicted the effective drug candidate from *Ocimum sanctum* leaf and two anti-allergic rhinitis drugs for the treatment of allergic rhinitis.

2. Materials and Methods

2.1. Collection and processing of plant material

The plant leaves were sourced from Namakkal, Tamil Nadu, India. The plant *Ocimum sanctum* Common name: Tulasi (Tamil): (Family: Lamiaceae) (Pattanayak *et al.* 2010). The leaves were rinsed with water and distilled water three times before being dried in the shade. A mechanical grinder was employed to pulverize the leaves, and the powder was used for further investigation (Huang *et al.* 2025).

2.2. Sample extraction

The collected plant was washed thoroughly with flowing tap water and with distilled water to cleanse the dirt. The cleaned Tulasi leaves were shade dried for 7 days. Then the dried plant materials were grinded to make powder using mixer grinder. The powdered materials were stored in cool and dry place for future use. About 20 grams of plant sample were taken and soaked in 120 ml of methanol and shaken for 18 hours in a rotary shaker. Whatman filter paper Grade-1 was applied to filter, and the crude plant extract was collected. To investigate the presence of biological active phytochemical in the methanolic extract, phytochemical screening was performed. The extracts were transferred into pre-weighed sample containers and stored for future purpose (Oyedemi *et al.* 2017).

2.3. GC-MS analysis-identification of compounds

Gas chromatography-mass spectrometry (GC-MS) analysis (Agilent 7890 A) was Performed to investigate the biologically active components present in the extract. About 1 ml of methanolic extract was injected into GC-MS spectrometry with aid of micro syringe. While eluting the compound from the column, it produces prominent peak and each peak corresponds to signal of bioactive compounds (Kanthal *et al.* 2014). In the chromatogram, the x-axis denotes the retention time, and y-axis denotes the intensity of the signal to quantify the compounds present in the sample. The eluted compound from the chromatographic column were directed into mass spectrometry to detect the electron ionization, where a stream of electrons bombarded them and make compounds into fragments (Olayeriju *et al.* 2022). Then these fragments were charged with ions and produce specific masses. The conversion of mass-to-charge (M/Z) ration was calibrated and used in the graph obtained from mass spectrum, which acts molecular fingerprint of the eluted samples (Eckel-Passow *et al.* 2009). The gas chromatography and mass spectrometry were preset, with optimum temperature (100°C), with helium gas serving as the carrier, gas flow rate and electron gun were programmed. The flow rate of helium was set to 1 ml per minute, and the electron gun of the mass detector emitted electrons with an energy of approximately 70 eV. The column Elite 1 was used for component separation, which consisting of 100% dimethyl polysiloxane (Margolin Eren, Prest, and Amirav 2022). The association of retention directories and fragmentation pattern from mass spectrum of the sample were compared with those kept in the database, then compound present in the sample. The name, molecular weight, structure of the bioactive compounds presents in the methanolic extract, and were predicted (Yang *et al.* 2022).

2.4. Ligands Preparation

The chemical structure of bioactive compounds isolated from the GC-MS from *Ocimum sanctum* were retrieved from PubChem database. Based on the comprehensive literature review, the most prominent compounds were selected from *Ocimum sanctum* and studied its pharmacological activity (Beltran-Noboa *et al.* 2023; Gnanamurthy, Narasimhan, and Sabarathinam 2024). Several compounds, including Isoaromadendrene epoxide, eugenol, and ursolic acid have been previously reported for their anti-inflammatory, antioxidant, and immunomodulatory activities. Then the 3D structure of the selected compounds with similar chemical entities were searched in the PubChem database were downloaded in the form of structure-data format (SDF) (Arulnangai *et al.* 2025).

2.5. Target Protein Preparation

Two target protein structure were selected in this study to investigate the molecular binding mechanism of bioactive compounds identified from the plant extracts. Crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) was downloaded in the form PDB format from Protein Data Bank (PDB) (Ali *et al.* 2025). The PDB ID 5NRA corresponds to the crystal structure of the human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (1.27 Å resolution) (Mazur *et al.* 2018). This structure was selected for molecular docking due to its high resolution and relevance to allergic inflammation. hCHIT, a glycoside hydrolase (family 18), is pre-eminent in allergic airway diseases like asthma and allergic rhinitis and is intricate in chitin degradation, making it a potential therapeutic target. DPP4 (dipeptidyl peptidase-4) is involved in immune regulation and Th2-type inflammation, and its role in allergic rhinitis has also been reported (Duan *et al.* 2018). Both targets were selected due to their complementary roles in allergic inflammation, supporting a dual-target strategy. The 5NRA structure was used as a model for hCHIT due to its co-crystallized ligand and suitability for structure-based design (Mazur *et al.* 2018).

2.6. Molecular Docking

Multiple simultaneous molecular docking between the compounds and 5NRA were performed using the autodock vina program which was available in pyrx 0.8 version molecular docking software (Trott and Olson 2010). Prior to docking, the grid box was set to cover the entire protein surface area with the grid size at centre: X: -98.1058 Y:29.9197 Z:15.5717 and with the dimension: X:58.1940 Y: 73.7005 Z: 61.0362. The compounds with error notifications, due to the presence of heavy atoms, were removed from the docking list (Eberhardt *et al.* 2021).

2.7. Screening of the Docked Complexes

Upon completion of molecular docking, the inclusion criterion was used to select the compounds. The criterion was: the ligand-binding affinity

should be more than the binding affinity of the control ligand; fulfilment of the Lipinski's rule, based on molinspiration cheminformatics, which includes: The compound should contain fewer than 5 hydrogen bond donors and no more than 10 hydrogen bond acceptors. Its molecular weight must be under 500 g/mol, and the calculated Log P (CLog P) should be below 5 (Pantsar and Poso 2018; Agu *et al.* 2023).

2.8. Ligand-Protein Interaction Visualization

The docked complex files were exported from the pyrx software, in zip format. The zip file was then unzipped and the docked 5NRA and the compound script was combined together using TextEdit software and saved as in PDBQT files. Biovia Discover Studio 3.5, LigPlot + v.2.2, UCSF Chimera 1.13.1, and PyMOL 2.3 were applied to analyses and study 2D, 3D, and surface labeling of ligand-protein interactions (Vujovic *et al.* 2025).

2.9. ADMET analysis

ADMET (Adsorption, Distribution, Metabolism, Excretion, and Toxicity) study assumes pivotal functions in the process of discovering and developing drugs. Swiss ADME was used to predict the ADMET score of the compounds (Wu *et al.* 2020). The Swiss ADME web tool facilitates the computation of crucial physicochemical, pharmacokinetic, drug-like, and related characteristics for one or more compounds. The smiles of the ligands were obtained from the PubChem were uploaded in the Swiss ADME (Guan *et al.* 2019).

2.9. Toxicity analysis

ProTox II was used to predict the oral acute toxicity such as, immunotoxicity, mutagenicity, carcinogenicity, hepatotoxicity and cytotoxicity of the compounds. The ProTox-II web server, which is created by Drwal *et al.* (2014) and Banerjee *et al.* (2018), that helps to predict the toxicity and various harmful effects of different chemical compounds (Banerjee *et al.* 2018; Drwal *et al.* 2014).

3. Results

3.1. GC-MS Analysis

The different compounds present in the methanol extract of *Ocimum sanctum* were examined using GC-MS analysis (**Figure 1**). The list of phytocompounds is shown in **Table 1 and Supplementary Table 1**. The analysis conducted using GC-MS on the extract indicated the existence of multiple bioactive compounds. From the chromatogram, a total of 12 identified compounds were selected for docking studies. The selection of these compounds was based on the availability of structural data and their potential pharmacological activity. Importantly, compounds like Isoaromadendrene epoxide have been documented in prior studies to exhibit anti-inflammatory or immune-modulatory effects, thereby reinforcing their potential significance in the management of allergic rhinitis.

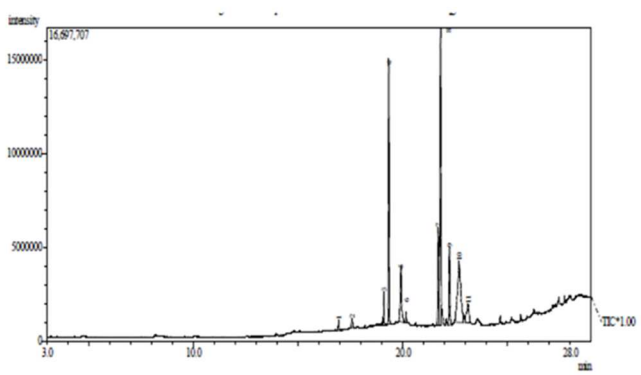

Figure 1: The GC-MS chromatogram spectrum of methanol leaf extract of *Ocimum sanctum*

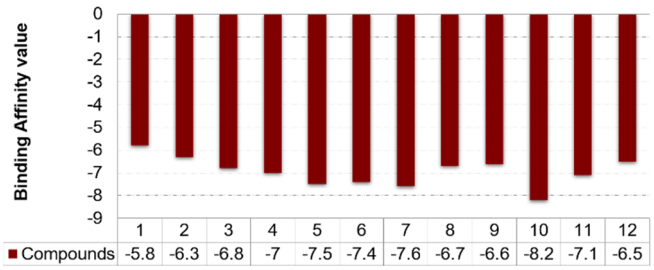

Figure 2: Docking result of target protein crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (PDB ID: 5NRA) with methanol extract of *Ocimum sanctum*

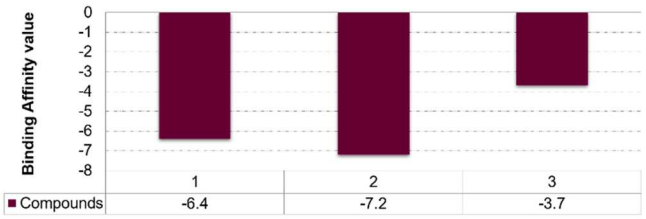

Figure 3: Docking of target protein crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) with standard drugs

3.2. Docking study

In this current study, we examined the affinity of twelve ligands with allergic rhinitis - crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) by molecular docking using PyRx. The screening of a small molecule library through docking with PyRx suggests that higher numerical values for binding affinity correlate with improved predicted interactions between a ligand and a macromolecule. In (5NRA) protein dock with Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1s-endo)- (CID 439569) binding energy was found to be -5.8 kcal/mol, Eugenol (CID 3314) binding energy was found to be -6.3 kcal/mol, Cyclohexane, 1-ethenyl-1-methyl-2,4-bis (1-methylethenyl)-, [1S-(1.alpha., 2.beta., 4.beta.)]- (CID 6431151) binding energy was found to be -6.8 kcal/mol, bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1r-(1r*,4e,9s) (CID 5322111) binding energy was found to be -7.0 kcal/mol, 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(e,e)] (CID 5373727) binding energy was found to be -7.5 kcal/mol (**Figure 2**), Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethenyl), (CID 442393) binding energy was found to be -7.4 kcal/mol, alpha.-selinene (CID 10123) binding energy was found to be -7.6 kcal/mol, (-)-5 Oxatricyclo[8.2.0.0(4,6)] dodecane,,12-trimethyl-9-methylene-, [1r] (CID 14350) binding energy was found to be -6.7 kcal/mol, (1R, 3E, 7E, 11R)-1,5,5,8-Tetramethyl-12-oxabicyclo [9.1.0]dodeca-3,7-diene (CID 5318104) binding energy was found to be -6.6 kcal/mol, Isoaromadendrene epoxide (CID 534398) binding energy was found to be -8.2 kcal/mol, 2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)prop-2-en-1-ol (CID-12304104) binding affinity was found to be -7.1 kcal/mol, 1,1,4,7-Tetramethyldecahydro-1H cyclopropa [e]azulene-4,7-dio (CID 178322) binding was found to be -6.5 kcal/mol. In this particular case of screening 5NRA with are 12 ligands predicted to have the best binding affinity of Isoaromadendrene epoxide (-8.2 kcal/mol), whereas the best binding mode allergic rhinitis - crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) is predicted to have binding affinity. The docking score of Isoaromadendrene epoxide (-8.2 kcal/mol)

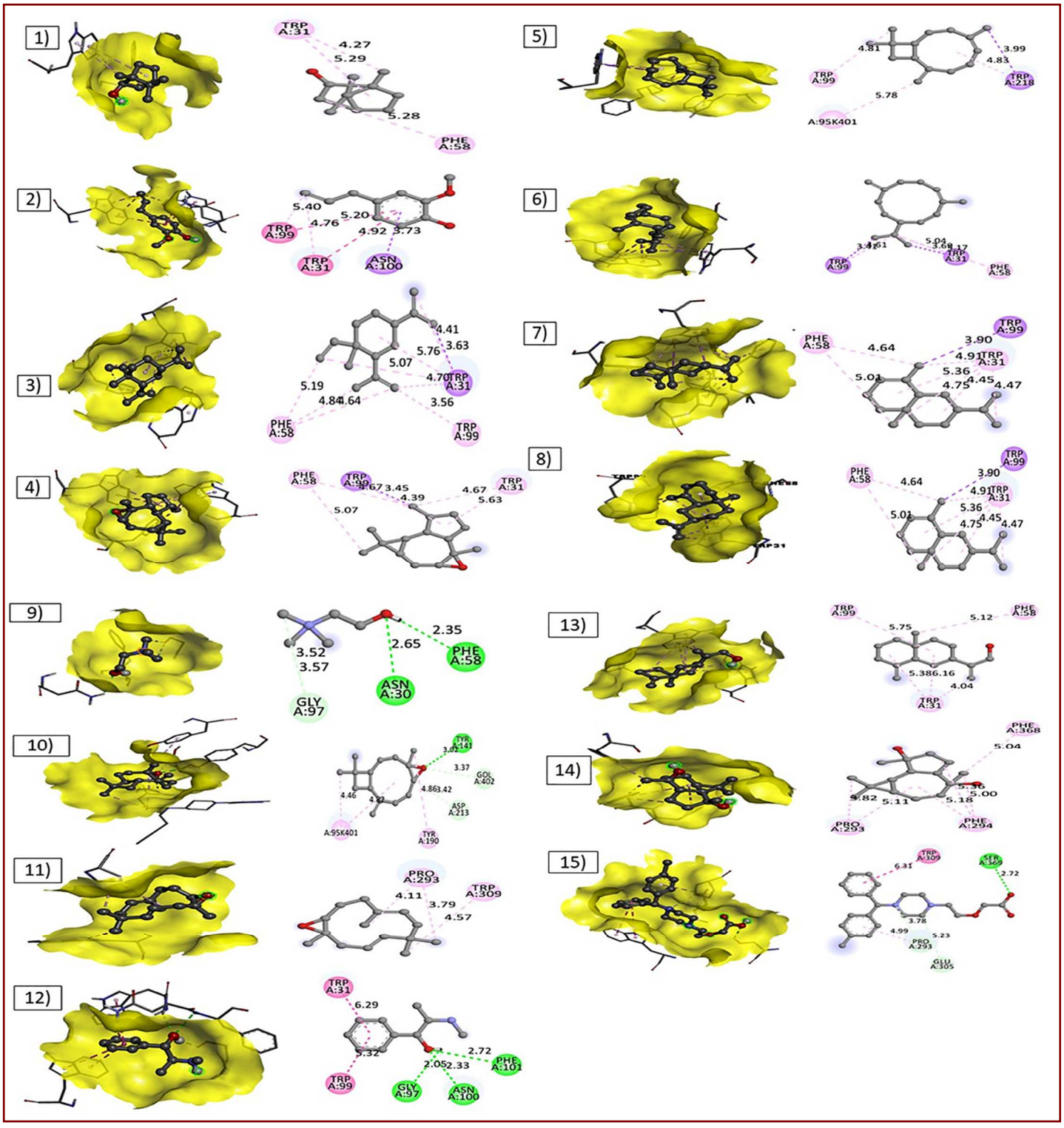

Figure 4: Docking complex and amino acids interactions of target proteins allergic rhinitis - crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) with all the phytocompounds identified from GCMS (1-15)

compared to Levocetirizine (-7.2 kcal/mol) indicates a potentially stronger binding affinity to the active site of the allergic rhinitis-related target (CHIT1/DPP4). This suggests that Isoaromadendrene epoxide may effectively inhibit or modulate target activity, offering therapeutic potential. In this current study, we examined the affinity of two anti-allergic drug compounds for allergic rhinitis which can be used as control by performing molecular docking using PyRx. The crystal structure of human DPP4 in complex with the catalytic domain of human chitotriosidase-1 (hCHIT) in complex with compound 7g (5NRA) was used with phytocompounds. From the docking of the 5NRA protein with pseudoephedrine (CID 7028), the binding energy was found to be -6.4 kcal/mol; for levocetirizine (CID 1549000), the binding energy was -7.2 kcal/mol. Among the screened compounds, levocetirizine exhibited the best binding affinity with a binding energy of -7.2 kcal/mol (**Table 1**).

3.3. Amino acid Interaction

The amino acids interaction was analyzed and tabulated shown in **Table 2**. Amino Acids That Frequently Interact: Tryptophan (Trp): Interacts with all four compounds between positions 31 and 99 in a variety of ways, including Pi-alkyl, Pi-alkyl, Pi-sigma, and Pi-sigma interactions. Phenylalanine (Phe): It engages in Pi-alkyl and Pi-sigma interaction types with three distinct molecules and conventional hydrogen bond with the one control drug molecule at position 58 (**Figure 3** and **Figure 4**).

Other Amino Acid Interactions: At position 293, proline (Pro) interacts with a single chemical, while at position 100, asparagine (Asn) also interacts with one chemical. Additionally, at position 30, asparagine (Asn) forms a similar interaction with a single chemical. Position 369 features an interaction between serine (Ser) and one molecule, and at position 305, glutamic acid (Glu) engages with a single molecule. Notably, at position 97, glycine (Gly) interacts with two molecules.

Table 1. List of PubChem ID's and docking scores of the phytocompounds for protein crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (PDB ID: 5NRA)

	PubChem id	Chemical formula	Docking Results
1.	439569	C10H18O	-5.8
2.	3314	C10H12O2	-6.3
3.	6431151	C15H24	-6.8
4.	534398	C15H24O	-8.2
5.	5322111	C15H24	-7.0
6.	5373727	C15H24	-7.5
7.	442393	C15H24	-7.4
8.	10123	C15H24	-7.6
9.	305	C5H14NO+	-3.7
10.	14350	C15H24O	-6.7
11.	5318104	C15H24O	-6.6
12.	12304104	C15H24O	-7.1
13.	178322	C15H26O	-6.5
14.	7028	C10H15NO	-6.4
15.	1549000	C21H25ClN2O3	-7.2

*Chemical Names are provided in supplementary table 1

Table 2: Amino acids favoring the interactions in the binding sites of receptor surface antigen from - crystal structure of human DPP4 in complex with a Crystal structure of human chitotriosidase-1 (hCHIT) catalytic domain in complex with compound 7g (5NRA) with methanol extract of *Ocimum sanctum* and anti-allergic rhinitis drug. Three compounds of *Ocimum sanctum* (Isoaromadendrene epoxide (CID:534398), Alpha-selinene (CID 10123), 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyl)-, [s-(e,e)] (CID 5373727) and with control drugs Pseudoephedrine (CID:7028) and choline (CID 305).

PubChem ID ➡	5373727	10123	534398	305	7028
	Trp31 (Pi-sigma)	Trp31 (Pi alkyl)	Trp 31 (Pi-alkyl)		Trp31
	Trp99 (Pi-sigma)	Trp99 (Pi sigma)	Trp 99 (Pi sigma)		Trp99
	Phe58 (Pi-alkyl)	Phe58 (Pi sigma)	Phe58 (Pi-alkyl)	*Phe58	
				*Asn30	
					*Asn100
					*Phe101
				#Gly97	*Gly97

*Indicates as Conventional H-bond residues
#indicates as carbon H-bond interaction

3.4. Toxicity prediction

ProTox-II is used to analyze the toxicity of the compounds which is the central part of the development process of drug designing (**Supplementary Table 2**). This is used to predict the types of toxicity that may be taken place after consuming the compounds as drugs. In the present study, various properties such as predicted toxicity class, immunotoxicity, LD50, hepatotoxicity, mutagenicity, carcinogenicity and cytotoxicity were considered. It is observed that the all three best compounds no active hepatotoxicity, carcinogenicity, cytotoxicity, mutagenicity and immunogenicity. The predicted toxicity of Isoaromadendrene epoxide, Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-selinene were class V.

3.5. ADMET analysis

In the study, ADME properties of the three best docked compounds and control drugs were done (**Supplementary Table 3**). Isoaromadendrene epoxide meets the criteria of Lipinski's rule of five. Whereas, 1,6-Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-selinene showed one violation. Isoaromadendrene epoxide showed high gastrointestinal adsorption (GI), while Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-selinene showed low GI adsorption. It is observed that all the three compounds have the bioavailability score of 0.55 which indicating that the 55% of the administered dose is expected to be absorbed into the bloodstream, making them promising candidates for further pharmacokinetic studies. In the study, the synthetic accessibility scores of Isoaromadendrene epoxide, Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-selinene were 3.96, 4.22, and 4.55.

4. Discussion

Allergic rhinitis is a widespread allergic condition that emerges when the immune system reacts to airborne allergens, causing inflammation in the nasal passages. It is marked by symptoms including sneezing, nasal congestion, a runny nose, and irritation of the eyes, nose, or throat. In the initial stage of the response, elevated levels of histamine seem linked to the activation of mast cells (Small, Keith, and Kim 2018). Provoking the nose with histamine results in symptoms like sneezing, itching, a runny nose, and nasal congestion. Mast cells play a significant role in mediating allergic reactions and the degranulation of mast cells which is crucial for determining activation of the extent of mast cell (Zoabi, Levi-Schaffer, and Eliashar 2022). Previous study has reported that the aqueous extracts of *Ocimum tenuiflorum* Linn has significant anti-allergic activity and regulate histamine induced mast cell activation by defeating the release of cytokines such as IL13, which leads inhibition of intracellular calcium and downregulation of NF-κB (Dharmani *et al.* 2004). Owing to the toxicity of most of the drug candidates, the safety concerns is critical to enlightening the accomplishment rates of drug development. Toxicity refers to the extent to which a substance can harm an organism or its components, such as cells and organs, and continues to be one of the most important concerns aims for late-stage drug development catastrophe and early documentation of toxicity would thus be very valuable (Amorim *et al.* 2024). In the present study, observed that the three best compounds of *Ocimum sanctum* (Isoaromadendrene epoxide, Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-selinene) and standard drugs (levocetirizine & choline) showed inactive on hepatotoxicity, carcinogenicity, cytotoxicity, mutagenicity and immunogenicity.

ADMET addresses pharmacokinetic factors that determine whether a drug molecule will reach its target protein in the body and how long it will remain in the bloodstream. The simultaneous assessment of the effectiveness and biopharmaceutical characteristics of drug molecule has been standardized. Comprehensive investigations into ADMET processes are now routinely conducted in the early phases of drug discovery to minimize the attrition rate (Shah 2015; Lagorce *et al.* 2017). Due to current resource and time constraints, these validations have not been completed yet. However, we plan to perform a comprehensive docking validation, including redocking of the co-crystallized ligand (compound 7g from 5NRA) and comparison with known inhibitors, as part of further studies (C *et al.* 2022). This will help further strengthen the predictive reliability of our docking strategy. Most clinical trial failures are caused by ADMET issues rather than a lack of efficacy, and since this is the costliest

stage for failures, ADMET-related research could save significant time and money by preventing even one clinical trial failure (Abraham and Myers, 2021). In our study, observed that three compounds of *Ocimum sanctum* (Isoaromadendrene epoxide, Cyclodecadiene, 1-methyl-5-methylene-8-(1-methylethyle)-[s-(e,e)] and Alpha-seline) have the bioavailability score of 0.55 which indicating that the 55% of the administered dose is expected to be absorbed into the bloodstream and the synthetic accessibility scores are 3.96, 4.22, and 4.55 (Sun *et al*. 2022; Fogel 2018).

Moreover, A study was made to investigate the mast cell stabilizing activity of the Ocimum sanctum. Twenty-eight albino rats were sensitized by injecting horse serum along with triple antigen containing Bordetella pertussis organisms, when the rats administered *Ocimum sanctum* leaves it shows inhibitory effects on mast cell degranulation and the observed inhibitory effects on mast cell degranulation indicate the potential therapeutic value of *Ocimum sanctum* in conditions involving mast cell activation, such as allergic reactions. the findings suggest that both the ethanolic extract and the flavonoidal fraction of *Ocimum sanctum* possess mast cell stabilizing properties. Furthermore, *Ocimum tenuiflorum*, have also been revealed to alleviate mast cell and cause inhibition of the allergic markers such as histamine, IL-4, and β-hexosaminidase in IgE-mediated allergic reaction. A study revealed that the extracts of *Ocimum sanctum* boast antibacterial, antifungal, and antiviral properties. Notably, they hinder the growth of various pathogens like *E. coli*, *B. anthracis*, and *M. tuberculosis*. This underscores their potential significance in addressing a range of health concerns.

5. Conclusion

The present investigation comprehensively evaluated the potential of *Ocimum sanctum* compounds for their anti-allergic rhinitis effects by targeting specific human proteins implicated in allergic pathways, particularly the crystal structure of human DPP4 and the catalytic domain of human chitotriosidase-1 (hCHIT) complexed with compound 7g. Advanced molecular docking techniques were employed to assess the binding affinities of various phytochemicals from *Ocimum sanctum* in comparison with established anti-allergic rhinitis drugs. Notably, Levocetirizine exhibited a docking score of -7.2 kcal/mol and Pseudoephedrine showed -6.4 kcal/mol, indicating moderate binding affinities with the targeted protein structure. However, among the tested compounds, Isoaromadendrene epoxide, a phytochemical found in Ocimum sanctum, displayed a superior docking score of -8.2 kcal/mol against the target protein, suggesting a stronger binding and potentially heightened biological activity in modulating allergic rhinitis mechanisms. This enhanced binding affinity underscores the possibility that Isoaromadendrene epoxide may more effectively inhibit the molecular interactions responsible for allergic inflammation compared to conventional drugs. The significance of these findings lies in the identification of Isoaromadendrene epoxide as a promising natural lead compound for further development as a therapeutic agent in allergic rhinitis. Despite these encouraging docking results, it is important to recognize that molecular docking provides only predictive evidence of efficacy. Therefore, additional investigations, including experimental validation, mechanistic pathway elucidation, and clinical dosage optimization, are imperative to confirm the practical therapeutic potential and establish a safe, effective dosage regimen for the treatment of allergic rhinitis.

6. Disclosure Statements

6.1. Author Contribution

NB: Writing-Original Draft Preparation; **TT:** Methodology; Software; Writing-Review and Editing; **SS:** Validation; Conceptualization; Supervision. All the authors have read and approved the final manuscript.

6.2. Declaration of Generative AI

The authors declare that no generative AI tools were used in the drafting, writing, or editing of the manuscript. All scientific interpretations and conclusions are the authors own. AI-based tools were used only for language grammar refinement and formatting purposes, and the final content was verified and approved by the authors.

6.3. Ethics approval (for clinical/animal studies)

This study does not involve the participation of human subjects, the use of identifiable human data or tissue, or any experiments on live animals. Consequently, the requirement for ethical approval or informed consent did not apply.

6.4. Informed Consent Statement

Not applicable.

6.5. Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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6.8. Conflicts of Interest

The authors declare that they have no known financial, personal, academic, or other relationships that could inappropriately influence, or be perceived to influence, the work reported in this manuscript. All authors confirm that there are no competing interests to declare.

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