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In-silico assessment of anti-asthmatic potential of Hydroalcoholic Extract of *Corallocarpus Epigaeus* rhizome (HAECER) phytoconstituents targeting β2-adrenergic receptor and phosphodiesterase enzyme

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Abstract
Asthma is a chronic inflammatory disorder of the airways characterized by bronchoconstriction and oxidative stress. The present *in silico* study was designed to explore the anti-asthmatic and antioxidant potential of phytoconstituents from the hydroalcoholic extract of *Corallocarpus epigaeus* rhizome (HAECER). Five major bioactive compounds—γ-Sitostenone, Ergosterol peroxide acetate derivative, Neophytadiene, Phenol (3,5-bis(1,1-dimethylethyl)-), and 1,2,3-Benzenetriol triacetate—were subjected to molecular docking against β2-adrenergic receptor (PDB ID: 2RH1) and cyclic nucleotide phosphodiesterase (PDB ID: 1ZKL) using PyRx AutoDock Vina. The docking analysis revealed that γ-Sitostenone and Ergosterol peroxide acetate derivative exhibited the strongest binding affinities (–9.4 and –9.7 kcal/mol) with the lowest inhibition constants (0.13 µM and 0.079 µM), suggesting potent dual activity through receptor activation and enzyme inhibition. Drug-likeness analysis using Molinspiration confirmed that all compounds satisfied Lipinski's Rule of Five, indicating favorable pharmacokinetic and oral bioavailability profiles. The strong correlation between binding energy and physicochemical parameters supports their potential as lead compounds for anti-asthmatic drug development. This study provides a computational basis for the traditional use of *C. epigaeus* and encourages further *in vitro* and *in vivo* validation.

Keywords: *Corallocarpus epigaeus*, β2-adrenergic receptor, cyclic nucleotide phosphodiesterase, molecular docking, drug-likeness, anti-asthmatic activity

Introduction

Medicinal plants are a source of valuable therapeutic assistance for the alleviation of human diseases. According to the World Health Organization (WHO), more than 80 per cent of the world's population, mainly in developing countries, relies on conventional plant-based medicines for their primary health needs. Scientific confirmation concerns the screening of bioactive compounds from plants and has contributed to the creation of new medicines with successful roles in the defence and treatment of various diseases [1].

Asthma: is a chronic inflammatory disease of the airways, about 262 million people are affected by asthma and caused 461,000 deaths in the year 2019 (WHO, 2020), and poses a significant burden on healthcare systems and quality of life. The disease is characterized by airway hyperresponsiveness, inflammation, and remodeling, driven by complex molecular pathways involving cytokines, enzymes, and oxidative stress [2]. Chronic asthma develops in approximately 70% of affected individuals, with a range of 50–85%, and can lead to severe complications such as airway remodeling and respiratory failure [3]. Despite advancements in asthma management, current therapies, including corticosteroids and β2-agonists, are associated with side effects such as immunosuppression, osteoporosis, and drug resistance [4]. These limitations highlight the urgent need for novel therapeutic agents with improved efficacy and safety profiles.

Corallocarpus epigaeus: (Rottl.) Hook.f. is a species in the Cucurbitaceae family, characterized as an herbaceous plant with a trailing or climbing growth habit, commonly found in tropical and subtropical regions. It is widely distributed across India—including states like Andhra Pradesh, Karnataka, Tamil Nadu, Maharashtra, and West Bengal—as well as in tropical Africa and parts of the Persian Gulf [5]. In folk medicine this rhizome is especially used for the treatment of various ailments, including, lateral stage of dysentery, enteritis, laxative, rheumatism, syphilis and venereal complaints. It is used as a remedy for snake bites [6]. It exhibited Analgesic, Antipyretic, Anti-inflammatory [7, 8], Anthelmintic [9, 10], Anti-fungal [11], Anti-diabetic [12,13], Anti-bacterial [14, 15], Hepatoprotective [16]. In recent years much attention has been devoted to natural antioxidant and their association with health benefits [17]. Antioxidant compounds like phenolic acids, polyphenols and flavonoids scavenge free radicals such as peroxide, hydro peroxide of lipid hydroxyl and thus inhibit the oxidative mechanisms that lead to degenerative diseases [18]. The phytochemical reported the presence of carbohydrates, flavonoids, alkaloids, mucilage, proteins and amino acids [19]. However, a systematic investigation into its potential molecular interactions with key asthma-related targets is crucial to understanding its therapeutic potential.

Among the molecular targets implicated in asthma pathogenesis, Beta 2 Adrenergic G- protein coupled receptor (PDB ID: 2RH1) and Cyclic Nucleotide Phosphodiesterase (PDB ID: 1ZKL) play crucial roles.

Advances in *in silico* drug discovery, particularly Computer-Aided Drug Design (CADD), have enabled rapid identification of promising drug candidates by integrating molecular docking, virtual screening, and pharmacokinetic analysis [20]. Molecular docking predicts the binding affinity and interactions of bioactive compounds within target proteins, providing insights into their potential therapeutic effects. ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis and drug-likeness analysis ensures that candidate compounds possess favorable

pharmacokinetic properties, reducing the likelihood of drug failure in later development stages [21].

Therefore, this study employs *in silico* approaches, including molecular docking and drug-likeness evaluation to investigate the potential of *Corallocarpus epigaeus* phytochemicals against β2-AR (PDB ID: 2RH1) and PDE (PDB ID: 1ZKL).

Materials and Methods

Collection of rhizome and Authentication

Rhizomes were collected from the foot of Sirumalai, Sadaiyandipuram village, Dindigul district, Tamil Nadu in the month of March 2025. The Rhizome was identified and authenticated by Dr. Stephen, Professor, Department of Botany, American College, Madurai-625020.

Powder preparation

The dust and debris on the collected rhizomes were washed using running tap water followed by distilled water. The rhizome skin was peeled off. The peeled rhizome was chopped into small pieces and then they were dried well in shade and converted into moderately coarse powder by mechanical grinder. Then the powder was sieved with a commercial sieve of mesh size approximately 60mm to make the particle size uniform. Finally, stored in air tight containers for further use.

Preparation of hydroalcoholic extract of *Corallocarpus epigaeus* (HAECE$_R$)

About 30g of air-dried coarse powder of rhizome of *Corallocarpus epigaeus* was macerated with 500ml of hydro alcoholic solvent (75:25) in the closed flask for 72hrs. The flask was shaken frequently. The extracts were then filtered through whatmann filter paper No.42 (125 mm) to remove all non- extractable matter, including cellular materials and other constituents that are insoluble in the extraction solvent. The entire extracts were concentrated to dryness and stored in sterile bottles for further use.

Gas Chromatography–Mass Spectrometry (GC–MS) Analysis

GC–MS analysis of the hydroalcoholic extract was performed using a Shimadzu QP 2020 NX system equipped with a fused silica SH-I-5 Sil MS column (30 m × 0.25 mm ID × 0.25 µm df). Helium was used as the carrier gas at a constant flow rate of 1 mL/min, with the injector temperature set at 250°C. The oven temperature was programmed from 50°C (1 min hold) to 280°C at a rate of 10°C/min. The mass spectrometer operated in electron impact mode (70 eV) with an ion source temperature of 230°C and a transfer line temperature of 270°C. Fragment ions were scanned over 50–600 Da, and the obtained spectra were compared with the NIST (2017) library for compound identification.

1. Preparation of Ligand

A total of 95 compounds were identified, representing major classes such as terpenoids, esters, alcohols and polyols, hydrocarbons, fatty acids, phenolics, and steroids. Among these, five bioactive compounds—γ-Sitostenone, Ergosterol peroxide acetate derivative, Neophytadiene, Phenol, 3,5-bis(1,1-dimethylethyl)-, and 1,2,3-Benzenetriol, triacetate—were selected for in silico molecular docking based on their pharmacological relevance. The selected phytoconstituents were subsequently docked with the target protein to predict their possible binding interactions and biological significance. The 2D/3D structures of the ligands and standard drugs were retrieved from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/).

2. Preparation of Target Protein

The crystal structures of Beta 2 Adrenergic G- protein coupled receptor (PDB ID: 2RH1) and Cyclic Nucleotide Phosphodiesterase (PDB ID: 1ZKL) were retrieved from the Protein Data Bank (RCSB) (https://www.rcsb.org/pdb). The β2-adrenergic receptor (β2-AR), a G-protein coupled receptor on airway smooth muscle cells, mediates bronchodilation by activating adenylate cyclase and increasing cAMP, which triggers PKA-induced muscle relaxation. Its activation also suppresses inflammatory mediator release. Cyclic nucleotide phosphodiesterases (PDEs) degrade cAMP and cGMP, regulating intracellular signaling. Inhibition of PDEs elevates cAMP levels, promoting bronchodilation and reducing inflammation. Thus, β2-AR agonists and PDE inhibitors serve as potential therapeutic agents in asthma management.

3. Molecular Docking Protocol

Water molecules, heteroatoms, and other non-protein complexes were removed from the receptor structures (PDB IDs: 2RH1 and 1ZKL) using Biovia Discovery Studio 4.5 Client. Molecular docking simulations were performed using PyRx, a virtual screening tool equipped with Open Babel and AutoDock Vina. The grid box dimensions were set to 36.37 Å × 42.07 Å × 61.93 Å (x, y, z axes), with a grid center at 23.00 Å × 47.19 Å × 59.35 Å and a spacing of 1.000 Å. The inhibition constants (Ki) in µM of the ligands and the standard method were obtained using their binding affinities (ΔG) in kcal/mol as shown in (equation 1) below, thus showing their potency against the target receptors (2RH1 and 1ZKL).

$$Ki = \exp\left(\frac{\Delta G}{RT}\right) \quad \text{.....(1)}$$

Where R= Gas constant (1.987×10-3 kcal/mol); T=298.15K (absolute temperature); Ki= Inhibition constant and ΔG = Binding energy.

Drug- Likeness Analysis

The drug-like properties of the phytochemicals were evaluated using the MOLINSPIRATION® web server (https://www.molinspiration.com/). Lipinski's rule of five (RO5) was applied to assess drug-likeness, allowing no more than one violation of the following criteria: molecular weight (MW) ≤ 500 Da, hydrogen bond donors (HBDs) ≤ 5, hydrogen bond acceptors (HBAs) ≤ 10, and octanol-water partition coefficient (log P) ≤ 5 (Lipinski, 2004).

Result and Discussion

1. Structural and Active Site Analysis of The Target Receptors

Beta 2 Adrenergic G- protein coupled receptor

The β2-adrenergic receptor (β2-AR) is a G-protein coupled receptor (GPCR) whose X-ray crystallographic structure (PDB ID: 2RH1) was resolved at 2.4 Å resolution. The structure represents the receptor in complex with an inverse agonist, carazolol, and provides key insights into ligand binding and receptor activation. The receptor consists of seven transmembrane α-helices (TM I–VII), connected by extracellular and intracellular loops, typical of GPCR topology. The active (binding) site lies within the

transmembrane region, primarily formed by residues from TM3, TM5, TM6, and TM7. Important amino acids involved in ligand recognition and binding include, Asp113 (TM3**)** – forms ionic interaction with the ligand's amine group, Asn312 (TM7) – participates in hydrogen bonding, Ser203, Ser204, Ser207 (TM5**)** – interact with hydroxyl groups of agonists, Phe290 and Tyr308 (TM6–TM7) – contribute to hydrophobic and π–π stacking interactions. These residues stabilize ligand binding and play a central role in signal transduction leading to bronchodilation when β_2-AR agonists are activated.

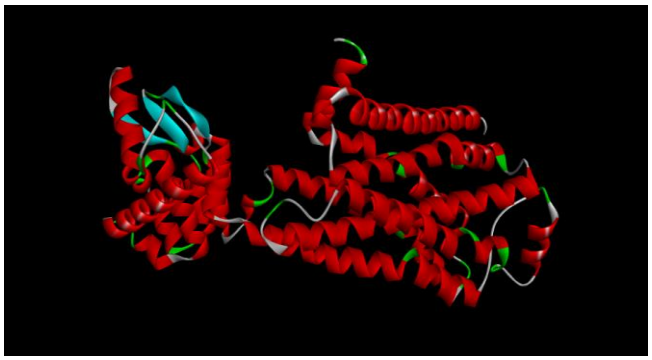


Fig 1: Beta 2 Adrenergic G- protein coupled receptor

Cyclic Nucleotide Phosphodiesterase

Crystallographic parameters: space group and unit cell: a = 115.751 Å, b = 115.751 Å, c = 64.29 Å; α = β = 90°, γ = 120° (so likely hexagonal/trigonal system). The active sities are the xanthine ring of IBMX stacks against Phe-416 (in PDE numbering) via π–π or aromatic stacking. A hydrogen-bond from the oxygen (O6) of the xanthine to Gln-413 (the invariant glutamine in PDE catalytic sites) is crucial for binding. Van der Waals / hydrophobic contacts with residues: Tyr-211, Val-380, Phe-384 (contacting xanthine portion) and hydrophobic contacts with Phe-384, Ile-412, Phe-416 (isopropyl group of IBMX) in PDE. Residue Ile-412 (neighbouring Gln-413) plays a role in shaping the size/shape of the binding pocket, and is part of the selectivity determinant (versus other PDE families). Residue **Ser-377** helps stabilize the "cAMP-selective" state of the glutamine switch (i.e., the conformation of Gln-413) via hydrogen-bonding.

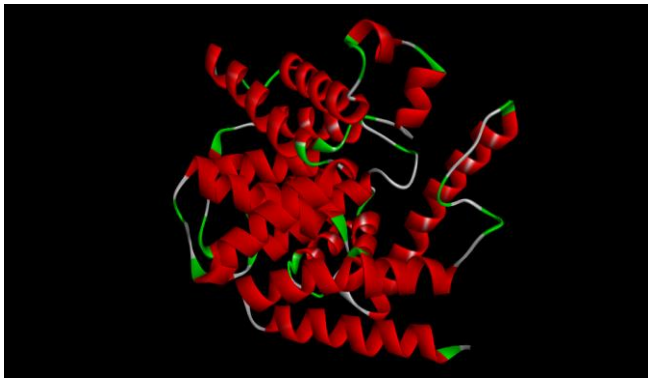


Fig 2: Cyclic Nucleotide Phosphodiesterase

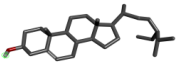
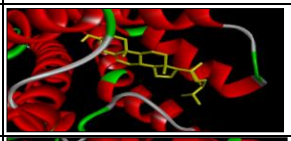
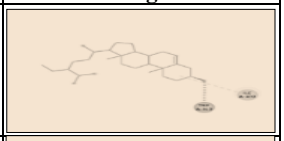
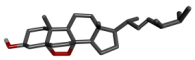
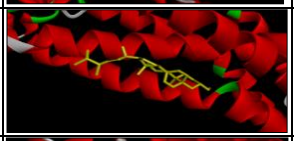
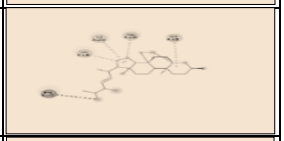
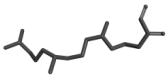
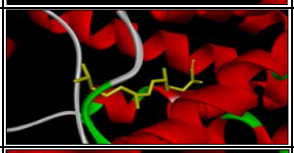
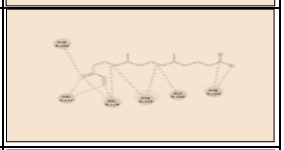
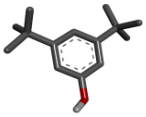
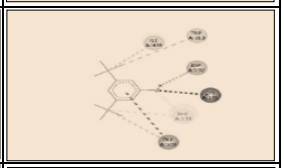
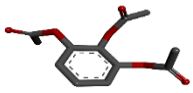
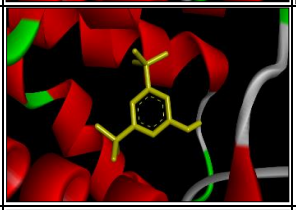
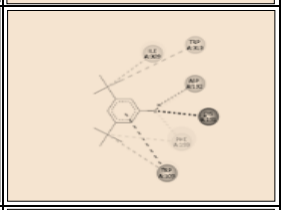
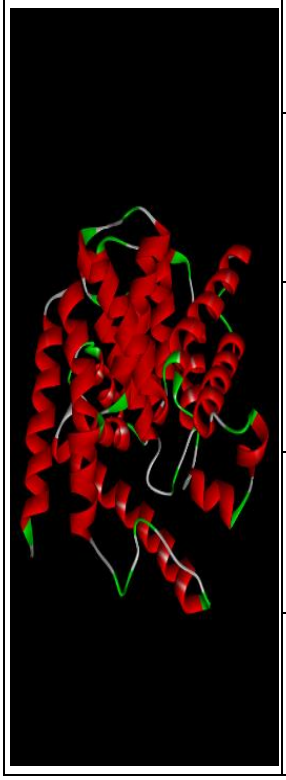
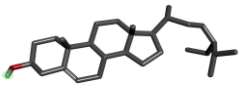
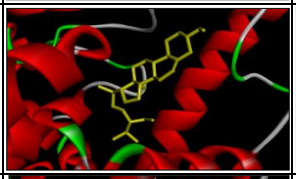
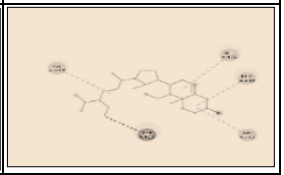
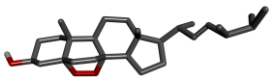
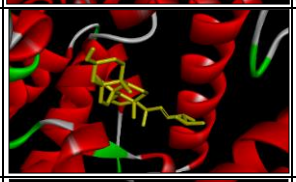
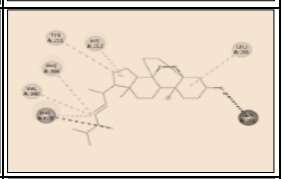
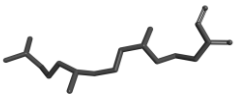
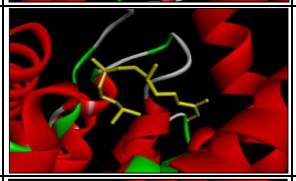
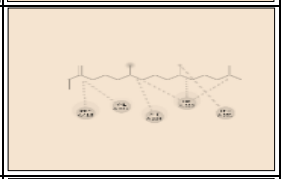
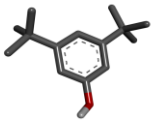
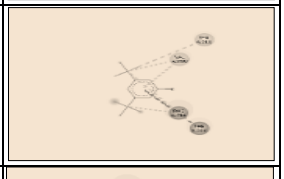
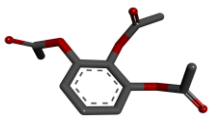
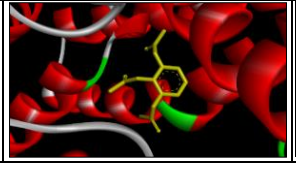
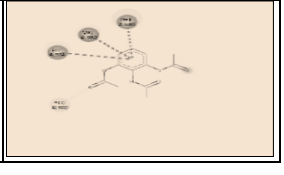
2. Molecular Docking Analysis of Phytochemicals Against B_2-Ar And Pde

Five ligands were screened against Beta 2 Adrenergic G-protein coupled receptor (PDB ID: 2RH1) and Cyclic Nucleotide Phosphodiesterase **(**PDB ID: 1ZKL) to evaluate their binding affinity using molecular docking.

Table 1: Molecular docking of phytochemicals against β_2-AR and PDE

Ligand	Receptor	Binding Affinity	Inhibition Constant (KI) IN µM
Docking with beta 2 adrenergic g- protein coupled receptor			
gamma. -Sitostenone	PDB ID 2RH1	-9.4	0.13
Ergosterol peroxide Ac derivative		-8.7	0.43
Neophytadiene		-6.8	10.4
Phenol, 3,5-bis(1,1-dimethylethyl)-		-6.8	10.4
1,2,3-Benzenetriol, triacetate		-6.7	12.3
Docking with cyclic nucleotide phosphodiesterase			
gamma. -Sitostenone	PDB ID 1ZKL	-8.9	0.30
Ergosterol peroxide Ac derivative		-9.7	0.079
Neophytadiene		-6.1	34.2
Phenol, 3,5-bis(1,1-dimethylethyl)-		-8.0	1.4
1,2,3-Benzenetriol, triacetate		-6.5	17.4

Table 2: Molecular Docking Interactions and 2D Ligand–Receptor Binding Diagrams of Phytoconstituents with β₂-Adrenergic G-Protein Coupled Receptor (2RH1) and Cyclic Nucleotide Phosphodiesterase (1ZKL)

Receptor	Ligand	Interaction	2d diagram
PDB ID 2RH1 	gamma. -Sitostenone 		
	Ergosterol peroxide Ac derivative 		
	Neophytadiene 		
	Phenol, 3,5-bis(1,1-dimethylethyl)- 		
	1,2,3-Benzenetriol, triacetate 		
PDB ID 1ZKL 	gamma. -Sitostenone 		
	Ergosterol peroxide Ac derivative 		
	Neophytadiene 		
	Phenol, 3,5-bis(1,1-dimethylethyl)- 		
	1,2,3-Benzenetriol, triacetate 		

Molecular Docking with β₂-Adrenergic G-Protein Coupled Receptor (PDB 2RH1)

Molecular docking of the selected phytoconstituents with the β₂-adrenergic receptor (β₂-AR) revealed varying binding affinities, indicating their potential to act as agonists or modulators of receptor function. Among the tested ligands, γ-Sitostenone exhibited the highest binding affinity (–9.4 kcal/mol) with a corresponding Ki = 0.13 µM, suggesting a strong and stable interaction with the receptor. Ergosterol peroxide acetate derivative also showed significant affinity (–8.7 kcal/mol; Ki = 0.43 µM), while Neophytadiene, Phenol, 3,5-bis(1,1-dimethylethyl)-, and 1,2,3-Benzenetriol triacetate displayed moderate binding energies ranging between –6.7 to –6.8 kcal/mol, corresponding to Ki values between 10.4 and 12.3 µM. The higher binding affinity of γ-Sitostenone and Ergosterol peroxide acetate derivative

implies that these compounds may effectively activate or stabilize β2-AR, enhancing cAMP production through Gs-protein coupling.

Molecular Docking with Cyclic Nucleotide Phosphodiesterase (PDB 1ZKL)

Docking with the catalytic domain of cyclic nucleotide phosphodiesterase (PDE) demonstrated that all selected ligands bind within the conserved catalytic pocket containing the key residues (Gln-413, Phe-416, Ile-412) and metal ions involved in substrate hydrolysis. Among them, Ergosterol peroxide acetate derivative exhibited the strongest binding affinity (–9.7 kcal/mol; Ki = 0.079 μM), followed closely by γ-Sitostenone (–8.9 kcal/mol; Ki = 0.30 μM). These low Ki values indicate strong inhibition potential toward PDE7A1, suggesting that both compounds may effectively prevent the breakdown of intracellular cAMP, thereby potentiating bronchodilatory and anti-inflammatory responses. Phenol, 3,5-bis(1,1-dimethylethyl)- displayed moderate affinity (–8.0 kcal/mol; Ki = 1.4 μM), while Neophytadiene (–6.1 kcal/mol; Ki = 34.2 μM) and 1,2,3-Benzenetriol triacetate (–6.5 kcal/mol; Ki = 17.4 μM) showed comparatively weak interactions, indicating limited PDE inhibition. The difference in binding energies reflects variations in the steric and electronic compatibility of each ligand with the PDE active site.

Comparative Interpretation

When comparing both receptor targets, Ergosterol peroxide acetate derivative and **γ-**Sitostenone consistently demonstrated the most favorable docking scores and lowest Ki values across both β2-AR and PDE7A1, implying dual activity potential. Such dual modulation — receptor activation and enzyme inhibition — could synergistically enhance intracellular cAMP levels, leading to smooth muscle relaxation and anti-asthmatic effects. Overall, the docking analysis supports the hypothesis that the hydroalcoholic extract of *Corallocarpus epigaeus* rhizome ($HAECE_R$) may exert its antiasthmatic potential through multi-target mechanisms involving β2-AR activation and PDE inhibition.

Drug- Likeness Analysis Lipinski's Rule of Five

The selected phytoconstituents from *Corallocarpus epigaeus* were evaluated for their drug-likeness based on Lipinski's Rule of Five, which predicts the oral bioavailability of potential therapeutic agents. The parameters analyzed included molecular weight, hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), partition coefficient (Log P), and molar refractivity (MR). The results are presented in Table 1.

Table 3: Lipinski's rule for phytoconstituents in $HAECE_R$

Compound Name	Mol. weight	H-Bond acceptors	H-Bond Donors	Log P	M.R (cm3/mol)	No. of Criteria
Rule	**<500**	**<10**	**<5**	**<5**	**<150**	**Atleast 3**
Gamma. –sitostenone	384.4	1	0	4.71	122.65	5
Ergosterol peroxide ac derivative	382.54	3	0	3.63	111.74	5
Neophytadiene	262.47	0	0	4.88	92.03	5
Phenol, 3,5-bis(1,1-dimethylethyl)-	206.32	1	1	4.64	-	4
1,2,3-benzenetriol, triacetate	274.27	7	1	2.07	62.70	5

The optimal lipophilicity–polarity balance observed in γ–Sitostenone and Ergosterol peroxide acetate derivative indicates strong potential for cell membrane penetration and target binding, consistent with their high docking affinities against β2-adrenergic receptor and cyclic nucleotide phosphodiesterase (PDE) reported earlier. The strong correlation between favorable physicochemical profiles and binding affinities supports the hypothesis that these compounds contribute significantly to the anti-asthmatic and antioxidant activity of *Corallocarpus epigaeus* rhizome ($HAECE_R$) through multi-target molecular interactions.

Conclusion

The present *in silico* investigation demonstrates that the hydroalcoholic extract of *Corallocarpus epigaeus* rhizome ($HAECE_R$) contains bioactive phytoconstituents with significant antiasthmatic potential. Molecular docking studies revealed that γ-Sitostenone and Ergosterol peroxide acetate derivative exhibited the strongest binding affinities and lowest inhibitory constants against both β2-adrenergic receptor (PDB ID: 2RH1) and cyclic nucleotide phosphodiesterase (PDB ID: 1ZKL), suggesting dual activity through receptor activation and enzyme inhibition. This dual mechanism may synergistically elevate intracellular cAMP levels, promoting bronchodilation and reducing airway inflammation. Drug-likeness analysis based on Lipinski's Rule of Five confirmed that all tested phytocompounds possess favorable physicochemical properties, indicating good oral bioavailability and pharmacokinetic feasibility. The correlation between docking scores and drug-likeness parameters supports the potential of these compounds as lead molecules for further development. Overall, the findings provide a strong computational basis for the anti-asthmatic and antioxidant efficacy of *Corallocarpus epigaeus*. Future *in-vitro* and *in-vivo* studies are recommended to validate these results and to advance these compounds as promising natural therapeutic candidates for asthma management.

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