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Unveiling the anti-inflammatory and wound-healing potential of *Hedyotis purpurascens* through integrated phytochemical and computational evaluation

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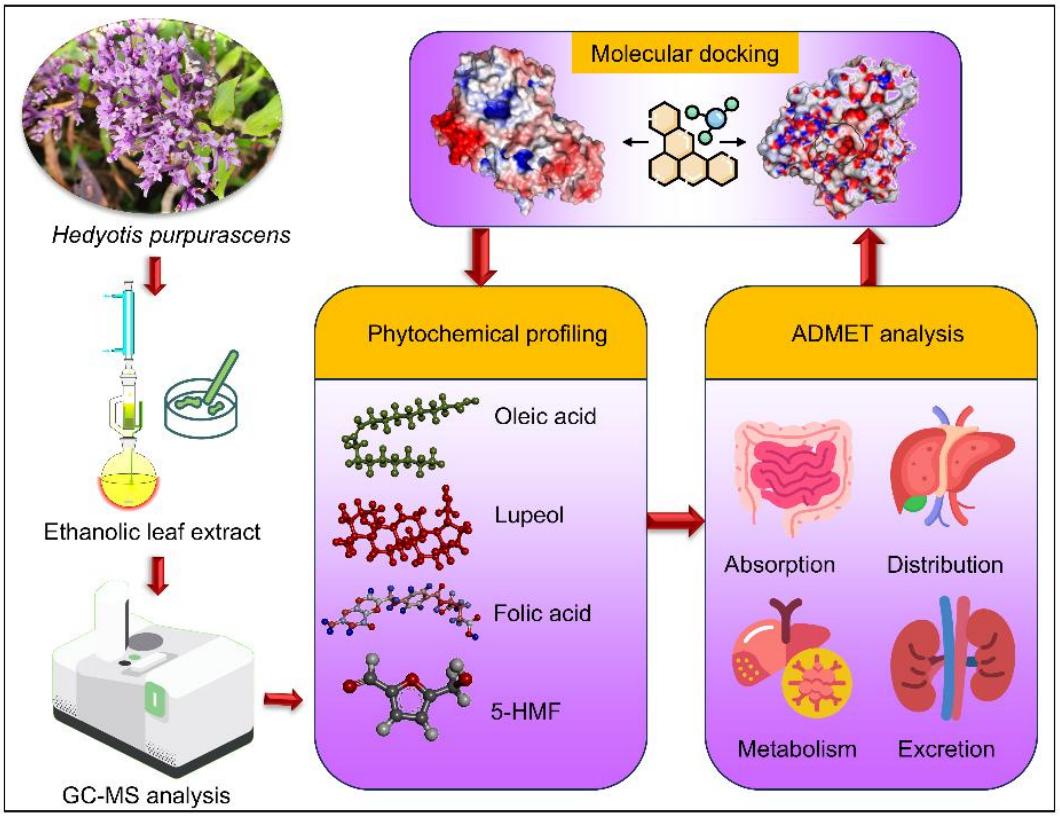
Abstract

Medicinal plants are prolific sources of bioactive compounds with therapeutic potential for combating inflammation and promoting wound healing. *Hedyotis purpurascens* (Rubiaceae) is an ethnomedicinal plant from the Southern Western Ghats that remains underexplored for its phytochemical composition and pharmacological relevance. In the present study, the ethanolic leaf extract of H. purpurascens was subjected to gas chromatography-mass spectrometry (GC-MS) analysis to profile its phytochemical constituents, followed by in silico molecular docking to evaluate the anti-inflammatory and wound-healing potential of the identified compounds. GC-MS analysis revealed a chemically diverse profile comprising sugars, organic acids, fatty acids, esters, phenolics, and triterpenoids, with oleic acid, triethyl citrate, 5-hydroxymethylfurfural, and lupeol identified as major constituents. In silico ADMET analysis indicated acceptable pharmacokinetic properties for most of the compounds, supporting their potential drug-likeness. Molecular docking studies against inflammation and wound-healing-related protein targets (PDB IDs: 1T4Q and 2AZ5) demonstrated that several compounds, particularly lupeol, folic acid, and betulin, exhibited strong binding affinities, suggesting favorable ligand-protein interactions. Overall, this integrated GC-MS and molecular docking approach highlights *H. purpurascens* as a promising source of bioactive phytochemicals with potential anti-inflammatory and wound-healing applications, warranting further experimental validation.

GRAPHICAL ABSTRACT



1.INTRODUCTION

Medicinal plants are important reservoirs of structurally diverse compounds with pharmacological activities, frequently serving as leads in drug discovery (Betty *et al.*, 2024; Arunkumar *et al.*, 2024). Phytochemicals such as flavonoids, terpenoids, and phenolics have been widely associated with anti-inflammatory and wound-healing activities due to their ability to modulate oxidative stress and cytokine-mediated pathways (Atanasov *et al.*, 2021; Malini et al., 2024).

Inflammation is a complex biological response that, while protective in acute stages, can delay wound resolution when chronically overstimulated (Medzhitov, 2008). Key mediators such as COX-2, tumor necrosis factor-α (TNF-α), and interleukins play critical roles in propagating inflammatory cascades, making them prominent targets for therapeutic intervention (Ricciotti and FitzGerald, 2011). Concurrently, wound healing is regulated by interactions between growth factors, extracellular matrix components, and immune signals that coordinate tissue regeneration (Eming et al., 2014).

Hedyotis purpurascens (Rubiaceae) is an ethnomedicinal species from the Southern Western Ghats valued in traditional medicine but lacking a comprehensive phytochemical and pharmacological evaluation. GC-MS profiling enables the sensitive identification of volatile and semi-volatile plant metabolites from extracts, allowing for focused bioactivity investigations (Chen et al., 2013). However, verifying the therapeutic relevance of each detected compound through in vitro assays alone can be a resource-intensive process.

Molecular docking is a widely used *in silico* technique that predicts binding interactions between small molecules and target proteins, providing insights into possible mechanisms of action before experimental studies (Ferreira et al., 2015; Arunkumar *et al.*, 2025). Recent studies have successfully combined GC-MS profiling with molecular docking to screen plant metabolites for their anti-inflammatory and wound-healing potential. For example, GC-MS identified phytocompounds that docked with COX-2 and TGF-ß receptors, correlating with experimental anti-inflammatory and wound-healing effects (Hasan et al., 2025; Saleem et al., 2025). Additionally, the *in-silico* identification of COX-2 inhibitory phytochemicals using docking and molecular dynamics has been reported, further supporting the use of computational approaches in screening natural products (Abdollahi et al., 2025).

In this study, we aim to profile phytochemicals from *H. purpurascens* ethanolic leaf extracts using GC–MS and to evaluate their binding potential with anti-inflammatory and wound healing targets through *in silico* molecular docking. This integrated approach may accelerate the identification of lead candidates for natural therapeutic development.

2. MATERIALS AND METHODS

Plant Material and Extraction

Leaf samples of *Hedyotis purpurascens* were collected, authenticated, washed, shade-dried, and powdered. The ethanolic leaf extract of *H. purpurascens* was obtained using a Soxhlet apparatus. Extracts were concentrated using a rotary

evaporator and stored at 4°C until analysis (Palanisamy *et al.*, 2025).

GC-MS Analysis

The Trace GC Ultra and DSQII model MS from Thermo Fisher Scientific Limited were engaged for analysis. The instrument was set as follows: Injector port temperature set to 250 °C, Interface temperature set to 250 °C, source kept at 200 °C. The oven temperature is programmed as available, 70 °C for 2 mins, 150 ºC @ 8 °C/min, up to 260 °C @ 10 °C/min. Split ratio set as1:50 and the injector used was in splitless mode. The DB-35 MS Nonpolar column was used, the dimensions were 0.25 mm OD x 0.25 µm ID x 30 meters length procured from Agilent Co., USA. Helium was used as the carrier gas at 1 mL/min. The MS was set to scan from 50 to 650 Da. The source was maintained at 200 °C and <40 mtorr vacuum pressure. The ionization energy was -70eV. The MS was also having an inbuilt pre-filter, which reduced the neutral particles. The data system has two inbuilt libraries for searching and matching the spectrum. NIST4 and WILEY9 each contain more than five million references. Only those compounds with spectral fit values equal to or greater than 700 were considered for identification.

Identification of compounds

Interpretation of the mass spectrum of GC-MS was done using the database of the National Institute of Standards and Technology (NIST4) and WILEY9. The spectrum of the known component was compared with the spectrum of the known components stored in the inbuilt library (Priya et al., 2024).

***In silico* ADME Evaluation**

The ADME (absorption, distribution, metabolism, excretion) properties were determined using online prediction tools SwissADME (https://www.swissadme.ch/) and pkCSM (https://biosig.lab.uq.edu.au/pkcsm/) (Arunkumar *et al.*, 2026).

Molecular Docking

Key proteins implicated in inflammation (COX-2) and wound healing (TGF-ß receptor) were selected based on literature relevance. The Protein Data Bank (PDB) provided the target proteins for this study: Interleukin 1 beta F101W (PDB ID: 1T4Q) and the crystal structure of TNF-alpha with a small molecule inhibitor (PDB ID: 2AZ5). The CASTp tool was used to identify the active binding sites of the target proteins. Molegro Molecular Viewer was used for protein preparation, where water molecules and heteroatoms were removed (Prameela *et al.*, 2026). Molecular docking analysis was executed using PyRx software. Protein and ligand structures were prepared by adding hydrogens, removing water molecules, and assigning charges. Binding affinity scores (kcal/mol) and interaction modes (hydrogen bonds, hydrophobic contacts) were analyzed. The two-dimensional and three-dimensional interactions of protein and ligand were visualized through Biovia Discovery Studio software (Prameela et al., 2025).

3. RESULTS AND DISCUSSION

GC-MS Profiling

A total of twenty-six phytoconstituents were detected in the leaf ethanolic *H. purpurascens* extract, and the chromatogram is shown in Figure 1. The results enabled the identification of 28 chemical constituents in the analyzed sample, characterized by their retention time (RT), molecular formula, molecular weight, probability score, and peak area percentage (Table 1). The biological activity of the compounds was obtained using Dr. Duke's Phytochemical and Ethnobotanical Databases (Table 2). The detected compounds represent a diverse group of sugars, organic acids, esters, fatty acids, phenolic compounds, terpenoids, and steroidal derivatives, indicating the chemical complexity of the sample. Oleic acid (25.42%), Triethyl citrate (8.43%), 5-hydroxymethylfurfural (8.10%), and lupeol (6.11%) emerged as dominant constituents, suggesting their significant presence in the extract. Additionally, carbohydrate-related compounds such as D-allose (4.37%), 2,7-anhydro-l-galacto-heptulofuranose (4.62%), and maltose (2.72%) were detected in appreciable amounts, highlighting the prevalence of sugar derivatives. Moderate peak areas were observed for tridecanoic acid (2.36%), ethyl α-d-glucopyranoside (1.94%), d-glucosamine (1.36%), and 2,3-dipropyl-cyclopropanecarboxylic acid, ethyl ester (1.06%), whereas several compounds, such as hexane, 3-bromo-, cyclohexyl isovalerate, and pregnan-20-one derivatives, appeared as minor constituents with lower peak area percentages. Several identified compounds are widely reported in the literature for their biological and pharmacological relevance. For instance, lupeol and betulin are known triterpenes associated with anti-inflammatory and anticancer properties (Saleem, 2009; Hordyjewska et al., 2018), while oleic acid and tridecanoic acid are fatty acids implicated in metabolic and membrane-related functions (Ghanem et all., 2015; Baer-Dubowska et al., 2021). 5-hydroxymethylfurfural and phenolic compounds may contribute to antioxidant potential (El Bohi et al., 2020), whereas sugars and sugar alcohols may play supportive roles in solubility and bioavailability. The presence of compounds with diverse molecular weights and functional groups suggests the extract's multifunctional chemical profile, which may underlie its observed or proposed biological activities.

ADMET analysis

In the present study, we conducted a comprehensive analysis of the ADMET properties of *H. purpurascens* compounds using SwissADME and pkCSM tools. In terms of physicochemical properties (Table 3), the molecular weight of each compound is within an acceptable range (MW ≤ 500), except for melezitose, which has a molecular weight of 504.44 g/mol. All showed the hydrogen bond donors (nHBD ≤ 5) and the hydrogen bond acceptors (nHBA ≤ 10), suggesting the compound's potential in drug-likeness (Maliehe et al., 2020), except for the maltose, melezitose, and folic acid. These parameters comply with Lipinski's rule of five. The molar refractivity of compounds between 40 to 140 displays an acceptable range. In the topological polar surface area (TPSA), all values less than 140 Å indicate good oral bioavailability, and less than 90 Å show significant blood-brain barrier permeability (Khare et al., 2023). Water solubility is a critical factor of a drug's pharmacological response after oral administration. The water solubility of the compounds was predicted using three versatile models, such as ESOL, Ali, and Silicos-IT (Kumar et al., 2023). All the compounds are soluble across three models, exhibiting an optimal solubility level, with log S greater than -6, indicating a highly soluble nature, except for lupeol and betulin (Table 4). The lipophilicity of the compounds adhered to the limited range (cLogP > 5) except for lupeol, leading to an increase in the probability of binding the hydrophobic protein targets (Maliehe et al., 2020). The consumption of modern and novel drugs has become easier and more available to mankind after the interventions on checking and increasing the absorption factor of oral drugs. The calibration of the compounds taken under study shows a bioavailability score above 0.55, indicating that they all have potent and influential standards, except for melezitose, maltose, and folic acid (Table 5).

In pharmacokinetic properties (Table 6), most of the compounds have exceptional human gastrointestinal absorption (GIA) and

the ability to cross the blood-brain barrier (BBB). Some compounds, including betulin, melezitose, lupeol, maltose, l-arabinose, d-glucosamine, 2,7-anhydro-1-galacto-heptulofuranose, and folic acid, do not have the capacity to traverse the gastrointestinal and BBB. Few compounds, such as 2-hydroxy-3-methylsuccinic acid, d-allose, oleic acid, and ethyl a-d-glucopyranoside, have only passed the GIA rates and not the BBB permeability. The compounds' metabolism was appraised by examining the restraining capability of primary Cytochromes (CYPs) P450 detoxifying enzymes, including CYP1A2, CYP2C19, CYP2C9, CYP2D6, and CYP3A4, and the results are summarized in Table X. Suppressing these enzymes may increase the toxicity level of the compound (Ha et al., 2023). Almost all the compounds do not inhibit the CYP enzymes, highlighting their ability to reduce the risk of drug-drug interactions (Radhakrishnan et al., 2026). Skin permeability (Log Kp) is a crucial trait for determining the compounds that could necessitate topical application (Hammami et al., 2023). Most of the compounds' Log Kp values are > -5 cm/s, suggesting good skin permeability.

Drug clearance is the rate at which a drug is eliminated from the plasma in the vascular compartment per unit time. Total clearance signifies the elimination of a drug from the primary compartment, regardless of the mechanism involved. The excretion rates of all compounds were assessed, ranging from 0.2 to 1.692 log mL/min/kg. These ranges are closely associated with the compounds' impending virulence in the internal mechanisms. Toxicity testing is crucial in drug development, as it necessitates a high therapeutic index to ensure that the drug's effective dose remains significantly lower than its toxic limit, thereby ensuring both effectiveness and safety (Mishra et al., 2016). All the compounds exhibited non-mutagenic properties, except for triethyl citrate, d-allose, and ethyl a-d-glucopyranoside, which were observed to be positive in the AMES toxicity test. The human maximum tolerated dose values and oral rat acute toxicity span greater than zero (log MTD ≥ 0) and (LD_{50} > 0.01 mol/kg), with the oral rat chronic toxicity log LOAEL > 2, implying the favorable toxicological characteristics. Additionally, the *Tetrahymena pyriformis* toxicity ($pIGC_{50}$ < -1) further indicates the lower environmental toxicity (Table 7). These findings align with recent studies employing the pkCSM method, which demonstrates that a diverse range of compounds have outstanding safety qualities, highlighting potential therapeutic effects (Ha et al., 2023).

Molecular Docking

Molecular docking was performed to evaluate the binding affinity of 26 selected bioactive compounds against two target proteins (PDB IDs: 1T4Q and 2AZ5). The docking scores, expressed as binding affinity (kcal/mol), are summarized in Table 8, and interactions are visualized in Figures 2 and 3. Out of the 28 identified compounds, only 26 compounds possessed well-defined three-dimensional (3D) structures suitable for molecular docking analysis; therefore, docking studies were performed exclusively on these 26 compounds, except for 2-Myristynoyl pantetheine and Pregnan-20-one, 5,6-epoxy-3-hydroxy-, (3á,5á,6á)-. Lower (more negative) binding energy values indicate stronger predicted ligand-protein interactions (Arunkumar et al., 2026). Against the 1T4Q target, several compounds demonstrated moderate to strong binding affinities. Among all ligands, Folic acid (-7.4 kcal/mol) exhibited the strongest interaction, followed closely by Lupeol (-7.3 kcal/mol) and Betulin (-6.8 kcal/mol). These compounds showed notably better binding compared to smaller aliphatic acids and esters, indicating that larger, structurally complex molecules may favor stronger interactions with the 1T4Q binding pocket. Moderate binding affinities were observed for Maltose (-6.1 kcal/mol), Melezitose (-6.0 kcal/mol), and Valerenic acid (-5.8 kcal/mol). In contrast, compounds such as Hexane, 3-bromo- (-3.0 kcal/mol) and Propane,1,1-diethoxy-2-methyl- (-3.5 kcal/mol) showed weaker interactions, suggesting limited binding stability.

Docking against the 2AZ5 protein revealed an overall trend of stronger binding affinities compared to 1T4Q for several compounds. Lupeol (-9.7 kcal/mol) emerged as the top-ranking ligand, followed by Folic acid (-9.3 kcal/mol) and Betulin (-9.2 kcal/mol). The enhanced binding energies suggest that these compounds fit more favorably within the active site architecture of 2AZ5. Other compounds, such as Valerenic acid (-7.2 kcal/mol), Maltose (-6.6 kcal/mol), Melezitose (-6.4 kcal/mol), and 2,4-di-tert-butylphenol (-6.4 kcal/mol), also showed appreciable interactions, indicating their potential as multi-target ligands. Overall, the docking results revealed considerable variation in binding affinity among the tested compounds, suggesting differences in molecular compatibility and interaction strength with the active sites of both target proteins.

4. CONCLUSION

The present study provides a comprehensive phytochemical and *in silico* evaluation of the ethanolic leaf extract of *H. purpurascens*. GC-MS profiling revealed the presence of a wide array of bioactive compounds, with oleic acid identified as the most abundant constituent, alongside notable levels of triethyl citrate, 5-hydroxymethylfurfural, and triterpenoids such as lupeol and betulin. The chemical diversity observed suggests a multifaceted phytochemical composition that may contribute to the ethnomedicinal relevance of the plant. Molecular docking analysis demonstrated that several identified compounds exhibited strong binding affinities toward key protein targets associated with inflammation and wound healing. Furthermore, *in silico* ADMET evaluation suggested that the compounds possess acceptable pharmacokinetic and drug-likeness characteristics, strengthening their suitability for further drug development considerations. Overall, this study provides a rational framework for prioritizing bioactive phytochemicals and lays the foundation for future *in vitro* and *in vivo* studies to validate their pharmacological efficacy.

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Conflict of interest

All the authors declare that there is no conflict of interest.

Table 1: Phytocomponents identified by GC-MS analysis for the ethanolic leaf extract of *H. purpurascens*

S. no	Retention time	Name of the compound	Molecular formula	Molecular weight	Probability	Peak area
1	3.013	Melezitose	$C_{18}H_{32}O_{16}$	504.43	4.13	0.614
2	3.389	d-Glucosamine	$C_6H_{13}NO_5$	179.17	9.17	1.364
3	4.814	Hexanoic acid, ethyl ester	$C_8H_{16}O_2$	144.21	2.82	0.419
4	5.975	3,3-Diethoxy-1-propanol, 3-methylbutyl ether	$C_7H_{16}O_3$	148.20	3.36	0.500
5	6.385	Propane, 1,1-diethoxy-2-methyl-	C8H18O2	146.23	5.59	0.832
6	6.955	L-Arabinose	$C_5H_{10}O_5$	150.13	8.31	1.236
7	7.045	Alprenolol	$C_{21}H_{39}NO_2Si_2$	393.71	6.38	0.949
8	8.050	Hexane, 3-bromo-	$C_6H_{13}Br$	165.07	2.73	0.406
9	8.235	5-Hydroxymethylfurfural	$C_6H_6O_3$	126.11	54.46	8.101
10	8.431	Cyclohexyl isovalerate	$C_{11}H_{20}O_2$	184.27	3.14	0.468
11	9.791	2-Hydroxy-3-methylsuccinic acid	$C_8H_{14}O_5$	190.19	3.92	0.584
12	10.821	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	$C_{12}H_{22}O_2$	198.30	7.09	1.055
13	11.562	Maltose	$C_{12}H_{22}O_{11}$	342.12	18.27	2.719
14	12.482	D-Allose	$C_6H_{12}O_6$	180.16	29.34	4.365
15	12.997	2,4-Di-tert-butylphenol	$C_{14}H_{22}O$	206.32	4.66	0.693
16	14.628	2,7-Anhydro-l-galacto-heptulofuranose	$C_7H_{12}O_6$	192.17	31.04	4.617
17	15.328	Éthyl à-d-glucopyranoside	$C_8H_{16}O_6$	208.21	13.04	1.940
18	16.149	Triethyl citrate	$C_{12}H_{20}O_7$	276.28	56.66	8.429
19	17.559	2-Myristynoyl pantetheine	$C_{25}H_{44}N_2O_5S$	484.7	3.78	0.562
20	17.794	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	$C_{11}H_{12}O_3$	192.2	5.26	0.783
21	21.120	Lidocaine	$C_{14}H_{22}N_2O$	234.34	4.53	0.674

22	22.146	Tridecanoic acid	$C_{13}H_{26}O_2$	214.34	15.88	2.362
23	23.056	Valerenic acid	$C_{18}H_{30}O_2Si$	306.51	3.92	0.583
24	25.327	Betulin	$C_{30}H_{50}O_2$	442.7	6.54	0.973
25	25.417	Oleic Acid	$C_{18}H_{34}O_2$	282.5	7.24	25.417
26	25.512	Folic Acid	$C_{19}H_{19}N_7O_6$	441.4	4.90	0.729
27	25.667	Pregnan-20-one, 5,6-epoxy-3-hydroxy-, (3á,5á,6á)-	$C_{21}H_{32}O_3$	332.47	2.96	0.440
28	29.464	Lupeol	$C_{30}H_{50}O$	426.7	41.09	6.113

Table 2: Biological activity of the compounds

S.no	Name of the compound	Class of compound	Biological activity
1	Melezitose	Carbohydrate	Sugar moiety and preservative
2	d-Glucosamine	Carbohydrate	Anticholinesterase activity, Anti-cancer, Antimutagenic.
3	Hexanoic acid, ethyl ester	Fatty Acid Methyl Ester	Treatment of oral diseases, antimicrobial, Anti-inflammatory, Antineoplastic, Antiurolithic, Antiobesity, Antiprotozoal, Antifibrinolytic, antialcoholic, Antipsoriatic, Antioxidant.
4	3,3-Diethoxy-1-propanol, 3-methylbutyl ether	Organic Compound	No bioactivity
5	Propane, 1,1-diethoxy-2-methyl-	Alkane	Antineoplastic, Antineurotoxic, Antiviral, Antibiotic, Antiprotozoal, Antihemorrhagic, Antiseptic
6	L-Arabinose	Aldehyde	Anti-inflammatory, Antibacterial, Antiseptic, Anticataract, Antidiarrheal, Antileprosy
7	Alprenolol	Alpheprol	Antihypertensive, Antiadrenergic
8	Hexane, 3-bromo-	Organic Compound	No bioactivity
9	5-Hydroxymethylfurfural	Organic Compound	Dehydrating of sugars
10	Cyclohexyl isovalerate	Fatty acid methyl ester	Food additive for flavor and fragrance
11	2-Hydroxy-3-methylsuccinic acid	Carboxylic acid	Antioxidant, anticancer
12	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	Carboxylic acid	Antioxidant, anticancer
13	Maltose	Carbohydrate	Sugar moiety and preservative
14	D-Allose	Monosaccharide	Sugar moiety and preservative
15	2,4-Di-tert-butylphenol	Phenol	Analgesic, Anesthetic, Antibacterial, Antioxidant, Antiprostatitic, Antipyretic, Antiseptic, Antiviral
16	2,7-Anhydro-l-galacto-heptulofuranose	Enzyme	Antibacterial

17	Ethyl à-d-glucopyranoside	Carbohydrate	Anticholinesterase activity, Anti-cancer, Antagonistic, Antineurotoxic, Antianemic, Antimutagenic
18	Triethyl citrate	Ester of citric acid	Antioxidant, Anticoagulant blood preservative
19	2-Myristynoyl pantetheine	Vitamin B5	Anti-inflammatory
20	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	Phenol	Analgesic, Anesthetic, Antibacterial, Antioxidant, Antiprostatitic, Antipyretic, Antiseptic, Antiviral
21	Lidocaine	Amino acid	Anti-inflammatory, Antioxidant
22	Tridecanoic acid	Fatty acid	Antimicrobial activity, Anti-inflammatory, Antineoplastic, Antiurolithic
23	Valerenic acid	Carboxylic acid	Anesthetic
24	Betulin	Triterpenoid	Antiretroviral, Anti-malarial, and Anti-inflammatory
25	Oleic Acid	Fatty acid	Antimicrobial, Anticarcinogenic, Antimalarials, Antineoplastics, Treatment of cancer, Antipruritic, Antihypercholesterolemic, Antiprotozoal, Antineurogenic, Anti-inflammatory, Antiviral, Antiseborrheic, Menopausal disorders treatment
26	Folic Acid	Vitamin B9	Nutritional therapy
27	Pregnan-20-one, 5,6-epoxy-3-hydroxy-, (3á,5á,6á)-	Steroids	Anti-inflammatory, used to treat several bone-degenerative diseases, antibiotics, mainly used as a female hormone
28	Lupeol	Triterpenoid	Anticancer and Anti-inflammatory

Table 3: Physicochemical properties

S. no.	Compounds	Mol. weight (g/mol)	No. of Heavy atoms	No. of arom. Heavy atoms	Fraction Csp^3	No. of Rotatable bonds	No. of H-bond acceptors	No. of H-bond donors	Molar refractivity	TPSA ($Å^2$)
1	Alprenolol	249.35	18	6	0.47	8	3	2	75.04	41.49
2	Lidocaine	234.34	17	6	0.5	6	2	1	72.81	32.34
3	Triethyl citrate	276.28	19	0	0.75	11	7	1	64.85	99.13
4	2,4-Di-tert-butylphenol	206.32	15	6	0.57	2	1	1	67.01	20.23
5	Tridecanoic acid	214.34	15	0	0.92	11	2	1	66.38	37.3
6	Hexane, 3-bromo-	165.07	7	0	1	3	0	0	38.83	0
7	2-Hydroxy-3-methylsuccinic acid	148.11	10	0	0.6	3	5	3	30.85	94.83
8	Hexanoic acid, ethyl ester	144.21	10	0	0.88	6	2	0	41.85	26.3
9	Betulin	442.72	32	0	0.93	2	2	2	136.30	40.46
10	Melezitose	504.44	34	0	1	8	16	11	100.54	268.68
11	Lupeol	426.72	31	0	0.93	1	1	1	135.14	20.23
12	Cyclohexyl isovalerate	184.28	13	0	0.91	4	2	0	54.16	26.3
13	Maltose	342.30	23	0	1.00	4	11	8	68.12	189.53
14	L-Arabinose	150.13	10	0	1	0	5	4	29.77	90.15
15	d-Glucosamine	179.17	12	0	1	1	6	5	37.28	116.17
16	D-Allose	162.14	11	0	1	1	5	3	32.38	82.45
17	Oleic acid	282.46	20	0	0.83	15	2	1	89.94	37.3
18	Propane,1,1-diethoxy-2-methyl-	146.23	10	0	1	5	2	0	42.74	18.46
19	2,7-anhydro-1-galacto-heptulofuranose	192.17	13	0	1	1	6	4	38.39	99.38
20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	198.3	14	0	0.92	7	2	0	58.97	26.3
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	180.2	13	6	0.2	3	3	2	51.02	49.69
22	Valerenic acid	234.33	17	0	0.67	2	2	1	70.81	37.3
23	Ethyl a-d-glucopyranoside	208.21	14	0	1	3	6	4	45.27	99.38
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	218.33	15	0	1	10	3	0	63.05	27.69
25	Folic acid	441.4	32	16	0.21	10	9	6	111.92	213.28
26	5-Hydroxymethylfurfural	126.11	9	5	0.17	1	3	1	31.08	50.44

1*Abbreviations: No.-number; arom.-aromatic; Fraction Csp3-fracton of carbon atoms in a molecule that are sp3 hybridized; H-bond-hydrogen bond; TPSA-topological polar surface area

Table 4: Water Solubility

S. no	Compounds	ESOL				Ali				SILICOS-IT			
			Solubility		Class		Solubility		Class		Solubility		Class
		Log S (ESOL)	mg/mL	mol/L		Log S (Ali)	mg/mL	mol/L		Log S (SILICOS-IT)	mg/mL	mol/L	
1	Alprenolol	-3.06	2.18E-01	8.76E-04	S	-3.64	5.72E-02	2.29E-04	S	-4.15	1.76E-02	7.05E-05	MS
2	Lidocaine	-2.58	6.14E-01	2.62E-03	S	-2.58	6.23E-01	2.66E-03	S	-4.5	7.33E-03	3.13E-05	MS
3	Triethyl citrate	-0.87	3.72E+01	1.35E-01	VS	-1.71	5.44E+00	1.97E-02	VS	-1.61	6.84E+00	2.48E-02	S
4	2,4-Di-tert-butylphenol	-4.55	5.78E-03	2.80E-05	MS	-5.36	8.97E-04	4.35E-06	MS	-4.25	1.16E-02	5.64E-05	MS
5	Tridecanoic acid	-3.95	2.39E-02	1.12E-04	S	-6.11	1.65E-04	7.68E-07	PS	-4.1	1.70E-02	7.93E-05	MS
6	Hexane, 3-bromo-	-2.68	3.44E-01	2.08E-03	S	-2.87	2.22E-01	1.34E-03	S	-2.76	2.86E-01	1.73E-03	S
7	2-Hydroxy-3-methylsuccinic acid	-0.08	1.23E+02	8.29E-01	VS	-0.75	2.61E+01	1.76E-01	VS	1.48	4.50E+03	3.04E+01	S
8	Hexanoic acid, ethyl ester	-1.89	1.87E+00	1.29E-02	VS	-2.66	3.18E-01	2.21E-03	S	-2.34	6.53E-01	4.53E-03	S
9	Betulin	-7.67	9.48E-06	2.14E-08	PS	-8.99	4.50E-07	1.02E-09	PS	-6.17	2.99E-04	6.75E-07	PS
10	Melezitose	1.25	8.89E+03	1.76E+01	HS	0.88	3.80E+03	7.53E+00	HS	5.43	1.35E+08	2.68E+05	S
11	Lupeol	-8.64	9.83E-07	2.30E-09	PS	-10.22	2.58E-08	6.05E-11	PS	-6.74	7.69E-05	1.80E-07	PS
12	Cyclohexyl isovalerate	-2.73	3.45E-01	1.87E-03	S	-3.41	7.11E-02	3.86E-04	S	-2.23	1.08E+00	5.83E-03	S
13	Maltose	0.55	1.22E+03	3.56E+00	HS	0.17	5.10E+02	1.49E+00	HS	4.25	6.10E+06	1.78E+04	S
14	L-Arabinose	1.13	2.03E+03	1.35E+01	HS	1.69	7.34E+03	4.89E+01	HS	2.23	2.56E+04	1.71E+02	S
15	d-Glucosamine	1.32	3.74E+03	2.09E+01	HS	1.64	7.84E+03	4.38E+01	HS	2.4	4.49E+04	2.51E+02	S
16	D-Allose	0.22	2.71E+02	1.67E+00	HS	0.37	3.78E+02	2.33E+00	HS	1.74	8.93E+03	5.51E+01	S
17	Oleic acid	-5.41	1.09E-03	3.85E-06	MS	-8.26	1.54E-06	5.46E-09	PS	-5.39	1.14E-03	4.04E-06	MS
18	Propane,1,1-diethoxy-2-methyl-	-1.78	2.44E+00	1.67E-02	VS	-2.18	9.65E-01	6.60E-03	S	-1.79	2.34E+00	1.60E-02	S
19	2,7-anhydro-1-galacto-heptulofuranose	0.58	7.38E+02	3.84E+00	HS	0.91	1.58E+03	8.21E+00	HS	1.8	1.22E+04	6.37E+01	S
20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	-3.11	1.52E-01	7.68E-04	S	-4.23	1.16E-02	5.84E-05	MS	-2.9	2.51E-01	1.26E-03	S
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	-2.23	1.06E+00	5.91E-03	S	-2.45	6.36E-01	3.53E-03	S	-1.87	2.44E+00	1.35E-02	S
22	Valerenic acid	-3.2	1.47E-01	6.28E-04	S	-3.7	4.71E-02	2.01E-04	S	-2.29	1.21E+00	5.15E-03	S
23	Ethyl a-d-glucopyranoside	0.5	6.64E+02	3.19E+0	HS	0.73	1.11E+03	5.34E+00	HS	1.5	6.58E+03	3.16E+01	S
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	-2.25	1.24E+00	5.66E-03	S	-2.96	2.42E-01	1.11E-03	S	-3.18	1.43E-01	6.55E-04	S
25	Folic acid	-1.61	1.09E+01	2.48E-02	VS	-2.91	5.44E-01	1.23E-03	S	-4.6	1.12E-02	2.54E-05	MS
26	5-Hydroxymethylfurfural	-1.68	2.64E+00	2.09E-02	VS	-1.78	2.08E+00	1.65E-02	VS	-1.33	5.90E+00	4.68E-02	S

Table 5: Lipophilicity, Drug likeness rule, and Bioavailability score

S. no	Compounds	iLOGP	XLOGP3	WLOGP	MLOGP	SILICOS-IT	Con Sensus Log $P_{o/w}$	Lipinski's rule	Bioavail Ability score
1	Alprenolol	3.29	3.1	2.15	2.23	3.17	2.79	Yes; 0 violation	0.55
2	Lidocaine	2.86	2.26	2.39	2.38	2.64	2.5	Yes; 0 violation	0.55
3	Triethyl citrate	2.8	0.07	0.19	0.4	1.19	0.93	Yes; 0 violation	0.55
4	2,4-Di-tert-butylphenol	3.08	5.19	3.99	3.87	3.81	3.99	Yes; 0 violation	0.55
5	Tridecanoic acid	3.21	5.57	4.38	3.42	3.94	4.1	Yes; 0 violation	0.85
6	Hexane, 3-bromo-	2.51	3.2	2.96	3.13	2.26	2.81	Yes; 0 violation	0.55
7	2-Hydroxy-3-methylsuccinic acid	-0.13	-0.76	-0.85	-0.96	-1.12	-0.76	Yes; 0 violation	0.56
8	Hexanoic acid, ethyl ester	2.33	2.46	2.13	1.96	1.92	2.16	Yes; 0 violation	0.55
9	Betulin	4.47	8.28	7	6	6.21	6.39	Yes; 1 violation; MLOGP>4.15	0.55
10	Melezitose	0.14	-5.85	-7.57	-6.15	-5.93	-5.07	No; 3 violations: MW>500, NorO>10, NHorOH>5	0.17
11	Lupeol	4.72	9.87	8.02	6.92	6.82	7.27	Yes; 1 violation: MLOGP>4.15	0.55
12	Cyclohexyl isovalerate	3.01	3.19	2.91	2.48	2.68	2.85	Yes; 0 violation	0.55
13	Maltose	0.42	-3.57	-5.4	-4.37	-4.4	-3.46	No; 2 violations: NorO>10, NHorOH>5	0.17
14	L-Arabinose	0.59	-3.02	-2.58	-2.32	-1.7	-1.8	Yes; 0 violation	0.55
15	d-Glucosamine	-0.66	-3.5	-3.25	-2.75	-2.54	-2.54	Yes; 0 violation	0.55
16	D-Allose	1.16	-1.59	-2.18	-1.94	-1	-1.11	Yes; 0 violation	0.55
17	Oleic acid	4.01	7.64	6.11	4.57	5.95	5.65	Yes; 1 violation: MLOGP>4.15	0.85
18	Propane,1,1-diethoxy-2-methyl-	2.64	2.16	2.04	1.7	1.57	2.02	Yes; 0 violation	0.55
19	2,7-anhydro-1-galacto-heptulofuranose	0.46	-2.46	-2.81	-2.4	-1.53	-1.75	Yes; 0 violation	0.55
20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	3.35	3.98	3.01	2.76	2.93	3.21	Yes; 0 violation	0.55
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	2.16	1.79	1.3	1.13	1.71	1.62	Yes; 0 violation	0.55
22	Valerenic acid	2.63	3.24	3.79	3.35	2.99	3.2	Yes; 0 violation	0.85
23	Ethyl a-d-glucopyranoside	1.53	-2.28	-2.18	-2.07	-1.52	-1.3	Yes; 0 violation	0.55
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	3.71	2.72	2.84	2.01	2.9	2.84	Yes; 0 violation	0.55
25	Folic acid	0.04	-1.08	-0.38	-0.62	0.24	-0.36	No; 2 violations: NorO>10, 26NHorOH>5	0.11
26	5-Hydroxymethylfurfural	1.14	1.13	1.11	-0.39	1.38	0.87	Yes; 0 violation	0.55

Table 6: Pharmacokinetic parameters

S. no	Compounds	Intestinal Absorption (%)	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation) (cm/s)	Excretion (Total clearance) log ml/min/kg
1	Alprenolol	High	Yes	No	Yes	No	No	Yes	No	-5.62	0.913
2	Lidocaine	High	Yes	No	No	No	No	Yes	No	-6.12	0.866
3	Triethyl citrate	High	No	No	No	No	No	No	No	-7.94	1.194
4	2,4-Di-tert-butylphenol	High	Yes	No	No	No	No	Yes	No	-3.87	0.71
5	Tridecanoic acid	High	Yes	No	Yes	No	No	No	No	-3.65	1.453
6	Hexane, 3-bromo-	Low	Yes	No	No	No	No	No	No	-5.03	0.382
7	2-Hydroxy-3-methylsuccinic acid	High	No	No	No	No	No	No	No	-7.74	0.787
8	Hexanoic acid, ethyl ester	High	Yes	No	No	No	No	No	No	-5.43	0.565
9	Betulin	Low	No	No	No	No	No	No	No	-3.12	0.2
10	Melezitose	Low	No	Yes	No	No	No	No	No	-13.53	1.357
11	Lupeol	Low	No	No	No	No	No	No	No	-1.9	0.116
12	Cyclohexyl isovalerate	High	Yes	No	No	No	No	No	No	-5.16	1.031
13	Maltose	Low	No	Yes	No	No	No	No	No	-10.92	1.294
14	L-Arabinose	Low	No	No	No	No	No	No	No	-9.36	0.553
15	d-Glucosamine	Low	No	Yes	No	No	No	No	No	-9.88	0.766
16	D-Allose	High	No	Yes	No	No	No	No	No	-8.42	0.472
17	Oleic acid	High	No	No	Yes	No	Yes	No	No	-2.6	1.692
18	Propane,1,1-diethoxy-2-methyl-	High	Yes	No	No	No	No	No	No	-5.66	0.67
19	2,7-anhydro-1-galacto-heptulofuranose	Low	No	Yes	No	No	No	No	No	-9.22	0.463
20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	High	Yes	No	No	No	Yes	No	No	-4.68	1.239
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	High	Yes	No	No	No	No	No	No	-6.13	0.239
22	Valerenic acid	High	Yes	No	No	No	Yes	No	No	-5.43	0.991
23	Ethyl a-d-glucopyranoside	High	No	Yes	No	No	No	No	No	-9.19	0.706
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	High	Yes	No	No	No	No	No	No	-5.7	1.468
25	Folic acid	Low	No	No	No	No	No	No	No	-9.76	0.519
26	5-Hydroxymethylfurfural	High	Yes	No	No	No	No	No	No	-6.27	0.622

Table 7: Toxicity prediction

S. no	Compounds	AMES toxicity	Maximum tolerated dose (Human) (Log mg/kg/day)	Oral Rat Acute Toxicity (LD_{50}) (mol/kg)	Oral Rat Chronic Toxicity (LOAEL) (Log mg/kg_bw/day)	*T. pyriformis* toxicity ($pIGC_{50}$) (Log ug/mL)
1	Alprenolol	No	0.811	2.468	1.719	1.143
2	Lidocaine	No	1.128	2.504	0.833	1.805
3	Triethyl citrate	Yes	0.833	1.789	1.119	-0.243
4	2,4-Di-tert-butylphenol	No	1.756	1.821	1.764	2.268
5	Tridecanoic acid	No	1.283	1.984	2.9	1.608
6	Hexane, 3-bromo-	No	1.577	2.276	1.928	0.465
7	2-Hydroxy-3-methylsuccinic acid	No	0.973	1.693	1.086	-0.012
8	Hexanoic acid, ethyl ester	No	1.455	2.067	2.225	-0.311
9	Betulin	No	0.239	2.15	2.151	0.539
10	Melezitose	No	0.688	0.825	1.484	0.285
11	Lupeol	No	0.454	2.065	1.021	0.574
12	Cyclohexyl isovalerate	No	1.116	2.202	2.068	0.377
13	Maltose	No	0.66	0.979	1.36	0.273
14	L-Arabinose	No	1.251	1.504	1.181	-0.852
15	d-Glucosamine	No	1.108	1.405	1.194	-0.5
16	D-Allose	Yes	0.94	2.32	1.112	-0.844
17	Oleic acid	No	1.224	1.849	3.2	1.615
18	Propane,1,1-diethoxy-2-methyl-	No	1.392	2.12	2.14	-0.179
19	2,7-anhydro-1-galacto-heptulofuranose	No	0.858	1.542	1.174	-0.405
20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	No	1.218	2.045	2.244	1.001
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	No	1.636	1.899	2.809	0.292
22	Valerenic acid	No	0.804	2.174	2.249	1.444
23	Ethyl a-d-glucopyranoside	Yes	0.972	1.537	1.145	-0.598
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	No	1.22	2.09	2.066	0.98
25	Folic acid	No	0.672	1.966	1.574	0.285
26	5-Hydroxymethylfurfural	No	1.423	2.383	2.44	-1.157

Table 8: Docking scores of secondary metabolites of *H. purpurascens* on 1T4Q and 2AZ5

S. No	Compound Name	Pubchem ID	Binding affinity kcal/mol	
			1T4Q	2AZ5
1	Alprenolol	2119	-5.3	-6
2	Lidocaine	3676	-5.2	-6.2
3	Triethyl citrate	6506	-5.1	-5.1
4	2,4-Di-tert-butylphenol	7311	-5.2	-6.4
5	Tridecanoic acid	12530	-4.3	-5
6	Hexane, 3-bromo-	18806	-3	-3.9
7	2-Hydroxy-3-methylsuccinic acid	24197	-4.8	-5
8	Hexanoic acid, ethyl ester	31265	-3.9	-4.8
9	Betulin	72326	-6.8	-9.2
10	Melezitose	92817	-6	-6.4
11	Lupeol	259846	-7.3	-9.7
12	Cyclohexyl isovalerate	287439	-4.8	-6
13	Maltose	439186	-6.1	-6.6
14	L-Arabinose	439195	-4.8	-5
15	d-Glucosamine	439213	-4.9	-5.1
16	D-Allose	439507	-5.5	-5.2
17	Oleic acid	445639	-4.1	-5.4
18	Propane,1,1-diethoxy-2-methyl-	519415	-3.5	-4.5
19	2,7-anhydro-1-galacto-heptulofuranose	552320	-5.1	-5.4

20	2,3-Dipropyl-cyclopropanecarboxylic acid, ethyl ester	593089	-4.1	-5.6
21	4-[(E)-3-hydroxyprop-1-enyl]-2-methoxyphenol	1549095	-5.1	-6.3
22	Valerenic acid	6440940	-5.8	-7.2
23	Ethyl a-d-glucopyranoside	9815668	-4.9	-5.3
24	3,3-Diethoxy-1-propanol, 3-methylbutyl ester	63629802	-4.2	-4.7
25	Folic acid	135398658	-7.4	-9.3
26	5-Hydroxymethylfurfural	136360357	-4.6	-4.7

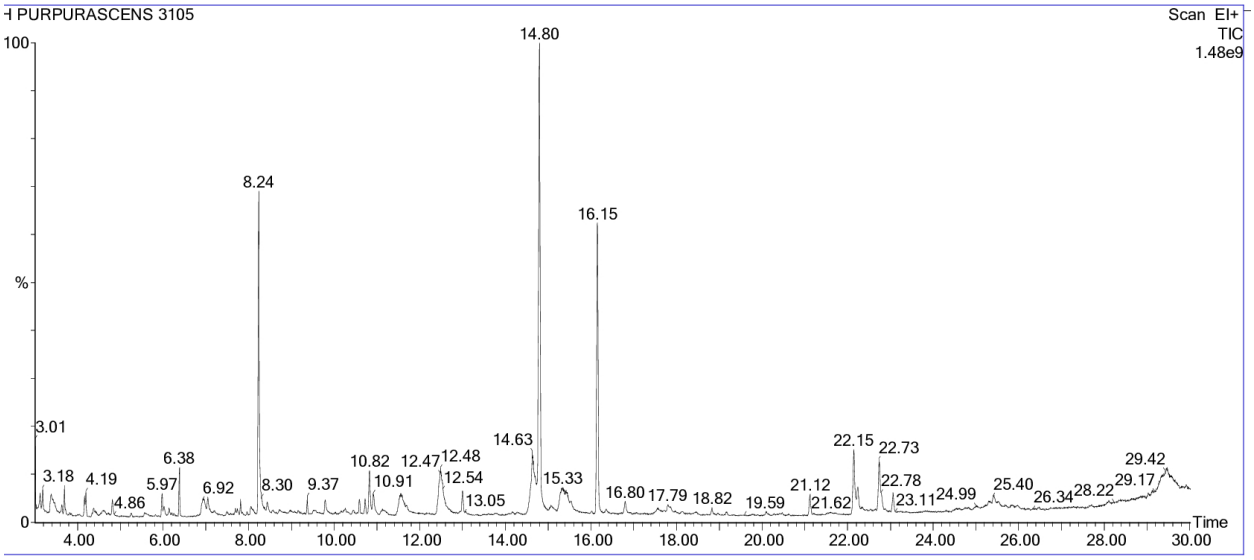

Figure 1: GC-MS chromatogram of ethanolic leaf extract of *H. purpurascens*

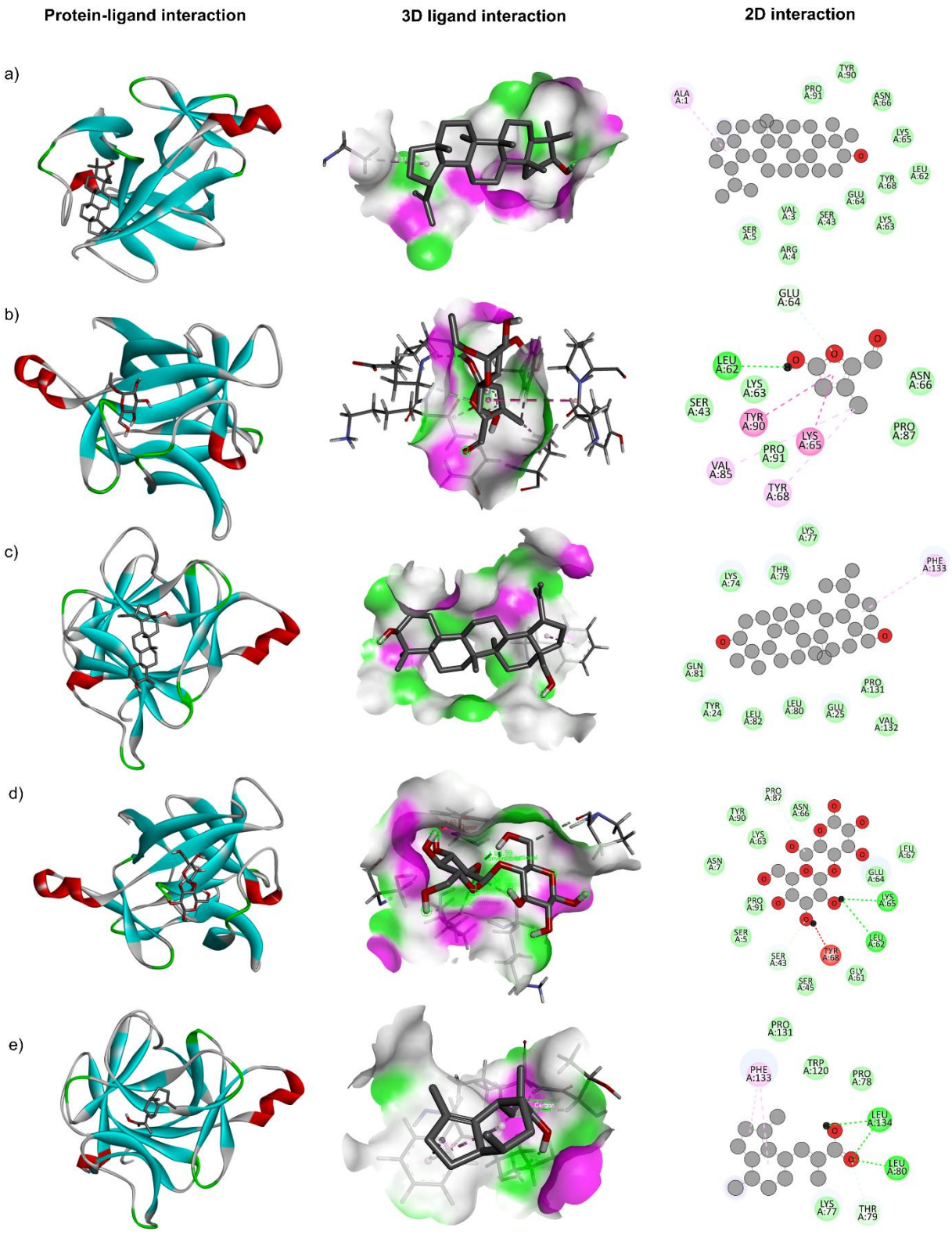

Figure 2: Interaction between the target protein (1T4Q) and the top interacting compounds: a) Folic acid, b) Lupeol, c) Betulin, d) Maltose, and e) Valerenic acid

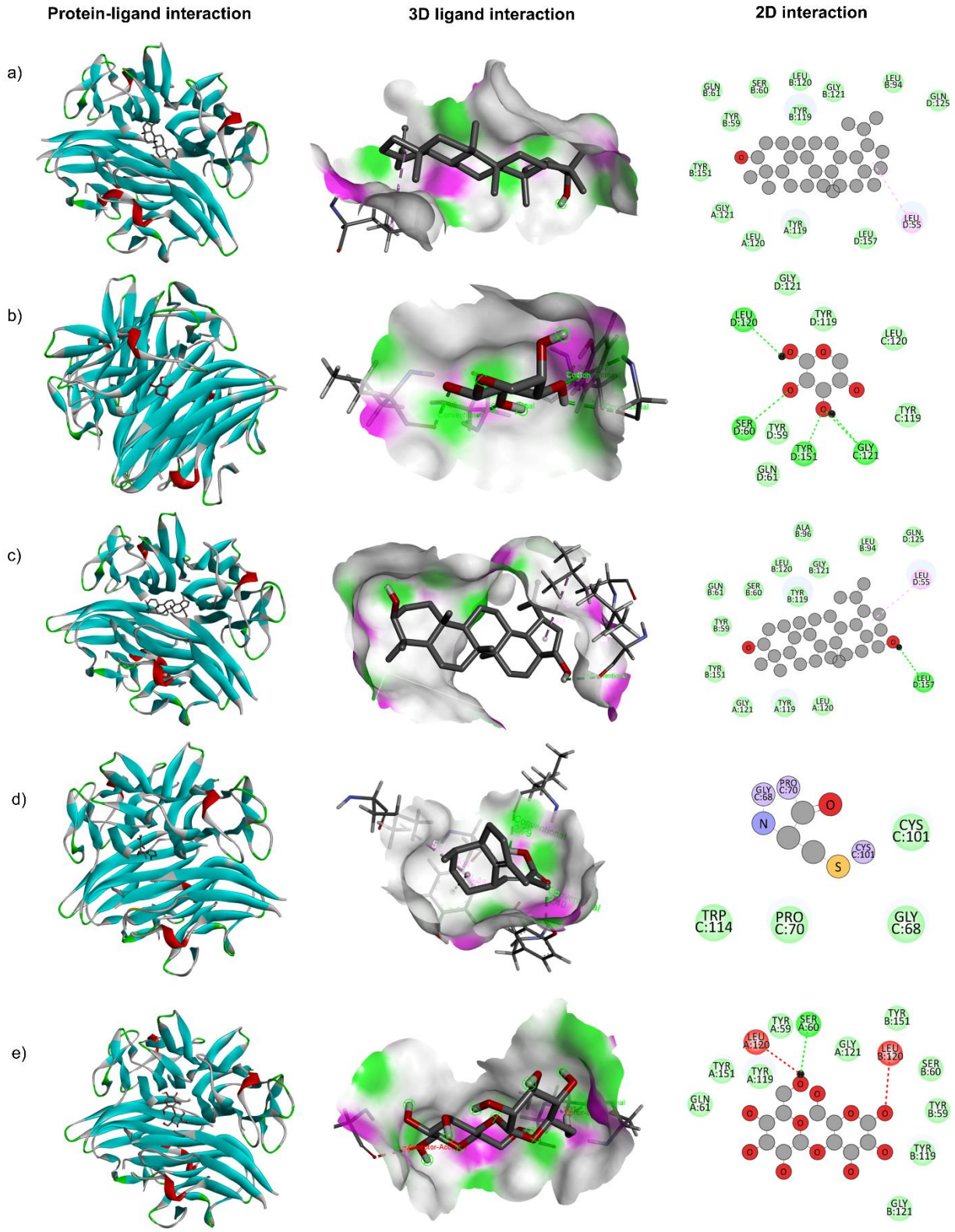

Figure 2: Interaction between the target protein (1T4Q) and the top interacting compounds: a) Lupeol, b) Folic acid, c) Betulin, d) Valerenic acid, and e) Maltose

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