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Insilico Screening of Nature Resin Phytoconstituents for Drug – Likeness and ADMET Profiling Against Dual Disease Targets.

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Abstract: Boswellia serrata, belonging to the Burseraceae family, is a tree native of India and the Arabian Peninsula. Commonly known as Indian frankincense, this medicinal plant is recognized for its numerous health benefits, particularly in inflammation. The Euphorbia resinifera, belonging to the family Euphorbiaceae, also known as the spurge family, drug discovery because of their therapeutic applications, such as cytotoxic, multi-drug-resistance-reversing, and anti-inflammatory activities the compounds were evaluated by in silico methods for drug-likeness, ADMET, bioactivity, and physicochemical properties. Most of the molecules shows favourable Lipinski compliance, acceptable pharmacokinetic profiles, and promising binding potential.

Keywords: Boswellia serrata, Euphorbia resinifera, Diabetes Mellitus, Gout, Alpha-Glucosidase, Xanthine Oxidase, Molecular Docking, In Silico Analysis, ADMET Prediction, Drug Likeness, Bioactivity, Anti inflammatory Activity.

INTRODUCTION:

Boswellia species and Euphorbia resinifera species have beneficial effects to control metabolic disorders like diabetes and gout[1]. Alpha-glucosidase activity accelerates intestinal glucose absorption, and this dual regulation of this enzyme represents control of the gout and diabetes[2]. Xanthine oxidase is an enzyme that helps the conversion of purine to the end product, uric acid[3]. Type 1 diabetes is characterized by autoimmune destruction of pancreatic beta cells, leading to a deficiency of insulin secretion, which results in metabolic rearrangement[4]. The result from insulin deficiency in type 1 diabetes are impaired glucose, lipid, and protein metabolism. Type 2 diabetes is impaired insulin secretion through dysfunction of the pancreatic beta cells and impaired insulin action through insulin resistance[5]. The plasma insulin concentration is insufficient to maintain normal glucose homeostasis[6].

MATERIALS AND METHOD:

Receptor protein preparation: The crystal structure of the kinase domain of 4B5P, 1FIQ along with cocrystallized ligand ((PDB ID: 4B5P, 1.60Å) (PDB ID :1FIQ, 2.50Å) were downloaded from RCSB protein data bank in pdb format. It is viewed and water molecules and ligands were removed using Biovia Discovery Studio 2024 software while retaining chainA and chainB for docking study[7].

Screening for compounds: SWISS-ADME web server was used for the screening of compounds. The compounds were filtered Lipinski's rule of five (RO5). Then druglikeness, pharmacokinetics, medicinal chemistry and physicochemical properties were analyzed for the prediction of absorption, distribution metabolism and excretion (ADME) of compound [8].

Ligand preparation : The two dimensional structures of resin diterpenoids , triterpenoids derivatives were drawn with the help of Chems sketch and then, convert to 3D structure using chem3D pro 12.0 software. The ligands molecular geometry optimization was achieved with energy minimization applying molecular mechanics force fields and saved in PDB format[9] .

Molecular docking using PYRx: AutoDock Vina integrated into PyRx was used for the molecular docking. The optimization was done with Open Babel and PyRx to prepare them for docking. The grid was arranged to cover only the active site of the 4B5P,1FIQZ protein. Visualization of docking results was done using Biovia Discovery Studio 2024. Docking result analysis mostly focused on binding affinity and binding site[10,11].

RESULTAND DISCUSSION

The insilico ADME studies are carried out in SWISSADME web server There are five different types of rule-based filters, namely Lipinski filter, Ghose filter, Veber filter, Egan and Muegge filter. Lipinski filter includes Molecular weight 500, MLOGP (lipophilicity) 4.15, hydrogen bond acceptors 10, and hydrogen bond donors 5 [12]. Ghose's filter has a molecular weight of 480, a lipophilicity of 0.4 WLOGP (5.6), a molar refractivity of 40, and a number of atoms of 20 [13] . The number of rotatable bonds is 10 and the total polar surface area is 140 in Veber's filter[14] .WLOGP (Lipophilicity) 5.88 and total polar surface area 131.6 are included in Egan's filter[15] . Muegge's filter contains the following parameters: 200 molecular weight 600, 2 XLOGP3 (lipophilicity) 5, total polar surface area 150, number of rings 7, number of carbon > 4, number of heteroatoms > 1, number of rotatable bonds 15, hydrogen bond acceptors 10, and hydrogen bond donors 5[16]. All the compounds obey all these filter and show drug likeness. Different physicochemical properties are tabulated. These shows that all the compounds are promising drug candidates, having improved ADME properties than the standard drug.

Table 1different physiochemical properties of drug

	COMPO UND	MOL WEIG HT (g/mol)	LIPOPHI LI CITY (log P)	HYDR O GEN BOND DONA RS	HYDR OG EN BOND ACCEP T ORS	TPSA (Å ²)	R O T B	NO OF LIPINS RU LES VIOLAT IO NS	NO.OF VEB ER'S RULES VIOLATI ON S
1.	Beta Boswellic acid	470.68 g/mol	3.96	2	4	74.60 Å ²	1	2	1
2.	Alpha- Boswellic acid	456.70 g/mol	3.96	2	3	57.53 Å ²	1	1	1
3.	11-Keto- Beta- Boswellic acid	470.68 g/mol	3.32	2	4	74.60 Å ²	1	2	2
4.	3-Acetyl- 11-Keto- Beta- Boswellic acid	512.72 g/mol	3.65	1	5	80.67 Å ²	3	2	1
5.	Acetyl- Beta Boswellic acid	498.74 g/mol	4.24	1	4	63.60 Å ²	3	1	3
6.	Acetyl- Alpha-	498.74 g/mol	4.24	1	4	63.60 Å ²	3	1	3

	Boswellic acid								
7.	Lupeolic acid	456.70 g/mol	3.98	2	3	57.53 Å ²	1	1	1
8.	Ursolic acid	302.19 g/mol	3.95	4	8	141.34 Å ²	0	1	1
9.	Myrcene	456.70 g/mol	3.99	2	3	57.53 Å ²	1	0	0
10.	Alpha-pinene	136.23 g/mol	2.63	0	0	0.00 Å ²	4	1	0
11.	Isocembrol	136.23 g/mol	5.81	0	0	0.00 Å ²	0	-	4
12.	P-cymene	426.72 g/mol	3.90	1	1	20.23 Å ²	4	1	0
13.	Limonene	290.48 g/mol	2.72	1	1	20.23 Å ²	1	0	1
14.	Beta-pinene	170.12 g/mol	2.59	4	5	97.99 Å ²	1	0	0
15.	Linalool	133.21 g/mol	3.21	0	0	0.00 Å ²	1	0	0
16.	Phorbol	136.23 g/mol	2.67	0	0	0.00 Å ²	1	0	0
17.	12-Deoxyphorbol 13-Acetate	180.16 g/mol	4.19	3	4	77.76 Å ²	2	0	0
18.	Ingenol	136.23 g/mol	2.30	0	0	0.00 Å ²	0	0	4
19.	Ingenol-3-Angelate	194.18 g/mol	2.33	2	4	66.76 Å ²	3		0
20.	Beta Amyrine	154.25 g/mol	4.63	1	1	20.23 Å ²	4	1	1
21.	Alpha Amyrin e	628.71 g/mol	4.80	2	9	120.75 Å ²	9	1	1
22.	Iupel	364.43 g/mol	4.72	5	6	118.22 Å ²	1	1	1
23.	Taraxerol	460.56 g/mol	4.73	2	7	110.13 Å ²	6	1	1
24.	Cycloartenol	348.43 g/mol	5.16	4	5	97.99 Å ²	1	1	1
25.	Ellagic acid	821.00 g/mol	0.79	6	12	208.12 Å ²	1	0	0
26.	Caffeic acid	556.65 g/mol	0.97	2	7	110.13 Å ²	7	0	0
27.	Ferulic acid	426.72 g/mol	1.62	1	1	20.23 Å ²	0	0	0
28.	Beta sitosterol	426.72 g/mol	5.05	1	1	20.23 Å ²	0	1	1
29.	Stigmasterol	426.72 g/mol	5.08	1	1	20.23 Å ²	1	1	1

30.	Campesterol	426.72 g/mol	4.97	1	1	20.23 Å²	0	1	1
S.N O	COMPOUND	MOLECULAR FORMULA	MOLECULAR WEIGHT(g/mol)	WATER SOLUBILITY CLASS	GI ABSORPTION	BBB PERM			
1.	Beta Boswellic acid	C30H46O4	470.68 g/mol	Moderately soluble	Low	No			
2.	Alpha-Boswellic acid	C30H48O3	456.70 g/mol	Moderately soluble	Low	No			
3.	11-Keto-Beta-Boswellic acid	C30H46O4	470.68 g/mol	Moderately soluble	High	No			
4.	3-Acetyl-11-Keto-Beta-Boswellic acid	C32H48O5	512.72g/mol	Poorly soluble	Low	No			
5.	Acetyl-Beta Boswellic acid	C32H50O4	498.74 g/mol	Poorly soluble	Low	No			
6.	Acetyl-Alpha-Boswellic acid	C32H50O4	498.74 g/mol	Poorly soluble	Low	No			
7.	Lupeolic acid	C30H48O3	456.70 g/mol	Moderately soluble	Low	No			
8.	Ursolic acid	C14H6O8	302.19 g/mol	Moderately soluble	Low	No			
9.	Myrcene	C30H48O3	456.70 g/mol	Soluble	Low	Yes			
10.	Alpha-pinene	C10H16	136.23 g/mol	Soluble	Low	Yes			
11.	Isocembrol	C10H16	136.23g/mol		-	-			
12.	P-cymene	C30H50O	426.72 g/mol	Soluble	Low	Yes			
13.	Limonene	C20H34O	290.48g/mol	Soluble	Low	Yes			
14.	Beta-pinene	C7H6O5	170.12 g/mol	Soluble	Low	Yes			
15.	Linalool	C10H13	133.21g/mol	Soluble	High	Yes			
16.	Phorbol	C10H16	136.23g/mol	Soluble	High	No			
17.	12-Deoxyphorbol 13-Acetate	C9H8O4	180.16 g/mol	Soluble	High	No			
18.	Ingenol	C10H16	136.23g/mol	Soluble	High	No			
19.	Ingenol-3-Angelate	C10H10O4	194.18 g/mol		-	-			
20.	Beta Amyrine	C10 H18O	154.25g/mol	Poorly soluble	Low	No			
21.	Alpha Amyrine	C37H40O9	628.71 g/mol	Poorly soluble	Low	No			
22.	Iupel	C20H28O6	364.43 g/mol	Poorly soluble	Low	No			
23.	Taraxerol	C26H36O7	460.56 g/mol	Poorly soluble	Low	No			

24.	Cycloartenol	C20H28O5	348.43 g/mol	Poorly soluble	Low	No
25.	Ellagic acid	C47H64O12	821.00 g/mol	Soluble	High	No
26.	Caffeic acid	C34H36O7	556.65 g/mol	Soluble	High	No
27.	Ferulic acid	C30H50O	426.72 g/mol	Soluble	High	Yes
28.	Beta sitosterol	C30H50O	426.72 g/mol	Poorly soluble	Low	No
29.	Stigmasterol	C30H50O	426.72 g/mol	Moderately soluble	Low	No
30.	Campesterol	C30H50O	426.72 g/mol	Moderately soluble	Low	No

COMPOUNDS	TARGET(PDBID)	DOCKING SCORE (kcal/mol)	INTERACTING AMINO ACID RESIDUES
FERULLIC ACID	4B5P	-7.8	PHE128,ALAB61,GLNB135,LYSB166
CAFFEIC ACID	4B5P	-7.9	TYRB129
ELLAGIC ACID	4B5P	-9.7	PHEB170,ILEB130,HISB139,GLYB138,HISB174
LINALOOL	4B5P	-6.8	ALAB62
ALPHA PINENE	4B5P	-7.5	PHEB128,PHEB170,LYSB166,LEUB167
BETA PINENE	4B5P	-7.6	PHEB128,PHEB170,LYSB166,LEUB167
P-CYMENE	4B5P	-7.5	PHEB128,PHEB170,LYSB166,LEUB167

COMPOUNDS	TARGET (PDBID)	DOCKING SCORE (kcal/mol)	INTERACTING AMINO ACID RESIDUES
FERULLIC ACID	1FIQ	-6.2	LEUB:352
CAFFEIC ACID	1FIQ	-6.5	LEUB:352
ELLAGIC ACID	1FIQ	-8.3	LEUA:127,ALAA:142,SERA:69,LYSB:340
LINALOOL	1FIQ	-5.3	ALAB:301,ILEB:407,LEUB:372,ILEB:3374,ILEB:352
ALPHA PINENE	1FIQ	-6	ILEB:352,ILEB:374,LEUB:372,LEUB:398,ALAB:301
BETA PINENE	1FIQ	-6.4	LEUB:398,ALAB:301,LEUB:372,ILEB:352,ILEB:407
P-CYMENE	1FIQ	-6.3	ILEB:352,ILEB:374,LEUB372,LEUB398,ILEB407,ALAB301

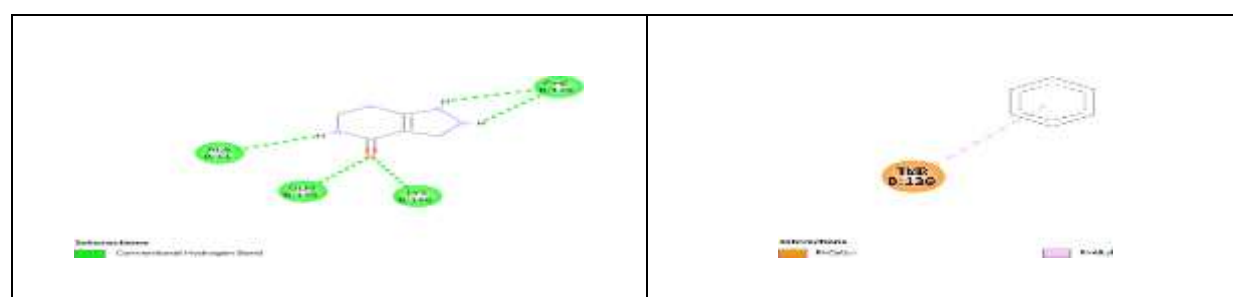
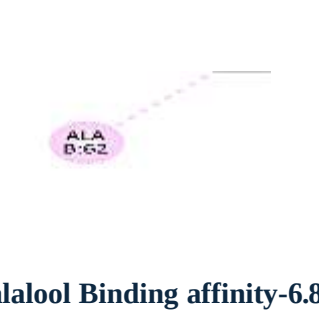
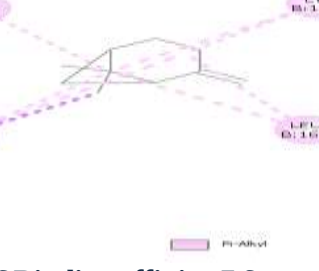
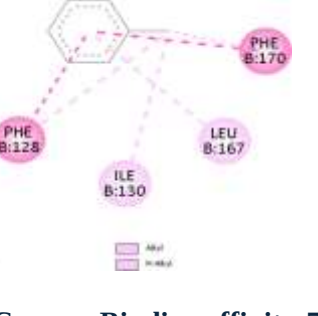
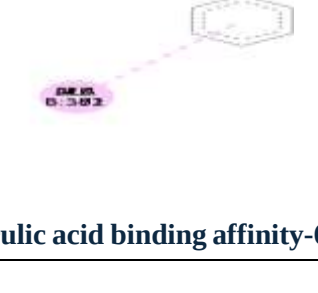
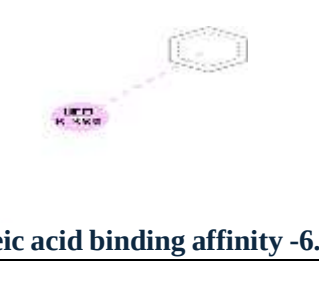
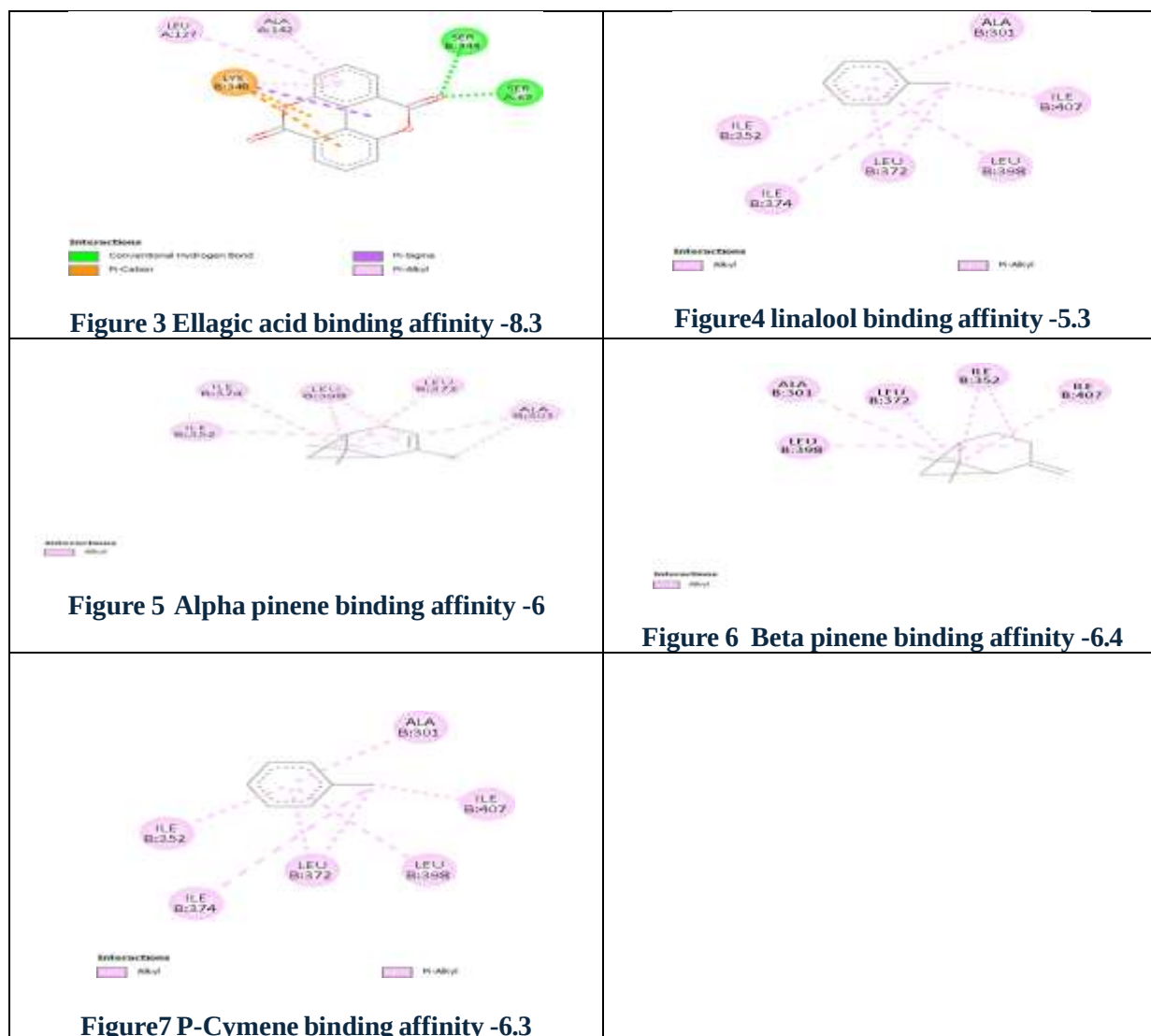


Figure 1 Ferullic acid Binding affinity-7.8	Figure 2 Caffeic acid Binding affinity-7.9
 Figure 3 Ellagic acid Binding affinity-9.7	 Figure 4 Linalool Binding affinity-6.8
 Figure 5 Alphapinene Binding affinity-7.5	 Figure 6 Binding affinity-7.6
 Figure 7 P-Cymene Binding affinity-7.5	
 Figure 1 Ferulic acid binding affinity-6.2	 Figure 2 Caffeic acid binding affinity -6.5



REFERENCE

1. Atta-ur-Rahman, Naz H, Fadimatou, Makhmoor T, Yasin A, Fatima N, et al. Bioactive constituents from *Boswellia papyrifera*. *J Nat Prod*. 2005; 68(2):189–193.
2. Althaher AR. Natural Products as Xanthine Oxidase Inhibitors: A Promising Approach for Hyperuricemia and Gout Management. *Current Traditional Medicine* [Internet]. 2026 Feb 13; 12.
3. Jung SW, Kim SM, Kim YG, et al. Uric acid and inflammation in kidney disease. *Am J Physiol Renal Physiol*. 2020.
4. Holt RI. Diagnosis, epidemiology and pathogenesis of diabetes mellitus: an update for psychiatrists. *Br J Psychiatry Suppl*. 2004; 47:S55–63.
5. American Diabetes Association. Diagnosis and classification of diabetes mellitus. *Diabetes Care*. 2010; 33(Suppl 1):S62–69.
6. Kumar PJ, Clark M. *Textbook of Clinical Medicine*. London: Saunders; 2002. p.1099–1121.
7. Dubey K, Dubey R, Gupta R, Gupta A. Insilico Reverse Docking Studies for the identification of potential of Betanin on some enzymes involved in diabetes and its complications. *Journal of Drug Delivery and Therapeutics*. 2019 Apr 24; 9 (2-A):72-4.
8. Sohrab SS, Kamal MA. Screening, docking, and molecular dynamics study of natural compound as an anti-HER2 for the management of breast cancer. *Life*. 2022 Oct 28;12(11):1729.

9. Katari NK, Gundla R, Reddy PK, Vanam A, Talatam A, Motohashi N, Gollapudi R. Human Epidermal Growth Factor Receptor Kinase.
10. Widyananda MH, Muhammad Ansori AN, Kharisam VD, Rizky WC, Antonius Dings TG, Rebezov M, Maksimiuk N, Denisenko A, Nugraha AP. Investigating The Potential of Curcumin, Demethoxycurcumin And Bisdemethoxycurcumin As Wildtype And Mutant Her2 Inhibitors Against Various Cancer Types Using Bioinformatics Analysis. *Biochemical& cellular Archives*.2021Oct1:21(2).
11. Ukonu CU, Alagamba EA. In silico Anticancer Assessment of the Bioactive compounds of Afromonium Melengueta on HER2 protein Associated with Breast Cancer. *International Journal of Women in Techinal Education and Employment* 2023;4(2):1-5.
12. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Adv. Drug Deliv. Rev.*2001March. 46(1-3):3-26.
13. Ghose AK, Viswanadhan VN, Wendoloski JJ. A knowledge- based approach in designing combinatorial or medical chemistry libraries for drug discovery. 1. A qualitative and quantitative characterization of known drug databases. *J Comb Chem.*1999 January.1 (1):55-68.
14. Veber DF, Johnson SR, Cheng HY, Smith BR, Ward KW Kopple KD. Molecular properties that influence the oral bioavailability of drug candidates. *J. Med.Chem.*2002 June. 45 (12):2615-23.
15. Egan WJ, Merz KM Jr, Baldwin JJ. Prediction of drug absorption using multivariate statistics. *J Med Chem.*2000 Oct 19; 43(21):3867-77.
16. Muegge I, Heald SL, Brittelli D. Simple selection criteria for drug-like chemical matter. *J Med Chem.*2001 Jun 7;44(12):1841-6. [doi : 10.1021/jm015507e] PMID: 11384230.