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Research Article

Investigating Drug Properties of Bioactive Compounds of *Cymbopogon citratus* by Absorption, Distribution, Metabolism, Excretion/Toxicity and Molecular Docking Analysis Against Apolipoprotein N-Acyl Transferase

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ABSTRACT

Delivering a potential drug is a predominant challenge in medicinal chemistry. In this study, bio-organic compounds of *Cymbopogon citratus* was screened by analysing physiochemical properties like solubility, permeability, efficacy, toxicity, and metabolic stability. The optimization of drug potential against virulent protein was calculated by using docking algorithm Autodock 4.2.3. Structure-based ligand docking reveals that the compounds had better inhibition potential against virulent enzymes with insoluble and impermeable activities. The organic compounds of *Cymbopogon citratus* were screened using Lipinski rule of five and absorption, distribution, metabolism, excretion/toxicity (ADME/T) prediction for drug likeliness. The structure-based ligand docking was done between bioactive compounds of plant and virulent protein that cause diseases. The interaction was visualized using Discovery studio and were studies. The molecular docking of bioactive compounds resulted in better inhibition potential with controlled lipophilicity level, without causing toxicity that harms the natural habitat of humans. The compounds, 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde, exhibit binding energy -4.70 Kcal/mol followed by β-myrcene –4.35 Kcal/mol and Geraniol –4.35 Kcal/mol. Hence, structure-based ligand docking and *in silico* ADME/T studies revealed that the compounds have better inhibition potential against Apolipoprotein by improving the prediction of drug compounds.

Introduction

Lipoproteins assumes a significant job in layer biogenesis correspondingly as a few diverse cells work in the cellular functions. In microorganisms, lipoproteins are engaged with orchestrating pre-prolipoproteins inside the cytoplasm.[1] Each prolipoprotein contains partner degree N-terminal sign amide that has a cysteine-containing 'lipobox' that contains amino alkanoic corrosive grouping of Leu–Ala–Gly–Cys. At the point when it is being co-translationally translocated by Sec/Tat translocon frameworks to the periplasm, the lipidation of pre-prolipoprotein is successively catalyzed by the resulting three chemicals to make a develop conjugated protein. The chemicals are (I) diacylglycerol (DAG) adjustment of pre-prolipoproteins by phosphatidylglycerol (PG): prolipoprotein DAG transferase (Lgt) to frame prolipoproteins; (ii) cleavage of sign peptide from prolipoproteins by lipoprotein signal peptidase (LspA) to shape Apolipoprotein N-acyl Transferases; and (iii) N-acylation of Apolipoprotein by Apolipoprotein N-acyl Transferase (Lnt).[2]

Cymbopogon citratus belongs to the family of Poaceae, which is an aromatic grass of 1.5 m tall. This plant is not known in a wild situation habitat and is widely cultivated in tropics and gardens, especially near South Asia. This tropic plant is probably originating in Sri Lanka and Malaysia. *Cymbopogon citratus* is widely found at an elevation up to 1,400 meters. This plant may be killed at a temperature below 10°C.[3,4] *Cymbopogon citratus* is eaten as a vegetable with rice and also a refreshing tea which can be brewed from these leaves. These leaves are

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also used to treat fever, cold, cough, and stomach upset. The tea has diuretic properties and can help in curing urination difficulties and water retention. This plant is used for the cellulose and production of paper. *Cymbopogon citratus* is a plant considered for economic importance, which forms a bedrock farming system in the United States of America and the south part of Asia. *Cymbopogon citratus* is used as a scent in many products like soap, perfume, candle, mosquito, and another insect repellent. Fresh leaves of this species are crushed and used as a shampoo, and the annual foliage yield is 30–50 tons per hectare. This plant exhibits to be a fungicide in treating pathogenic fungi on the cultivated jatropha curcas plant. This plant contains many phytochemical compounds such as flavonoids and phenolic compounds which consist of luteolin, quercetin, isoorientin, kaempferol, and apigenin. The compounds are mainly alcohol, ketones, aldehyde, and esters. The plant was used for pharmacological activities like anti-bacterial, anti-filarial, anti-fungal, and some other properties. Lemongrass is a bitter, aromatic, and a cooling herb that increases the perspiration and relieves spasms. The extracted oil from the plant is used in the effective treatment of skin conditions including athlete's foot, ringworm, and scabies.[5] The pain at the arthritic joints also treated using this plant. In this research, the bioactive compounds of lemongrass will be structurally docked against the virulent enzymes of Apolipoprotein n-acyl transferase that causes urine infectious disease. [6]

Materials and Methods

Bioactive Compounds of Obtained from Gas Chromatography-mass Spectroscopy (GC-MS) Analysis of *Cymbopogon citratus*

From the plant of *Cymbopogon citratus* 43 compounds were revealed by using GC-MS in which 8 compounds were selected as that were expected their presence in essential oil. It is commonly known that grass plants produce terpenoid hydrocarbons that can be used in medicinal, industrial, and perfumery. The major compounds reported are citral (34.8%), neral (30.72%), β-myrcene (11.28%), Geranyl acetate (0.57%), Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl (0.23%), geraniol (5.54%), 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde (2.20%), citronellol (1.34%) and D-limonene (0.03%). [7,8] its citral content mainly determined the lemon grass quality. Citral (3,7- dimethyl-2,6-octadienal) consists of the cis-isomer geranial and also the trans-isomer neral. These bioactive compounds were screened using Lipinski rule of five and ADME/T properties for knowing the drug likeliness.

Protein Target Confirmation

The apolipoprotein N-acyl transferase (PDB ID: 5XHQ) was utilized as a medication focus in this examination work with goals 2.587 Å and X beam diffraction technique. The protein was recovered from Protein Information Bank that comprises of two chains A and B. This chemical contains an exo-layer nitrilase space melded to a transmembrane (TM) area. The TM space of Lnt contains eight TM helices, which structure a layer installed pit with a sidelong opening and a periplasmic exit. The hydrophobic particles were evacuated for better ligand restricting proclivity that meddles in the crystallographic structures. The protein structure with the dynamic site appeared in Fig. 1. The ligand library was recovered from pubchem (https://pubchem.ncbi.nlm.nih.gov/), which was kept up by the National Focus of Biotechnology Data. The ligand was additionally screened for Lipinski rule of five by

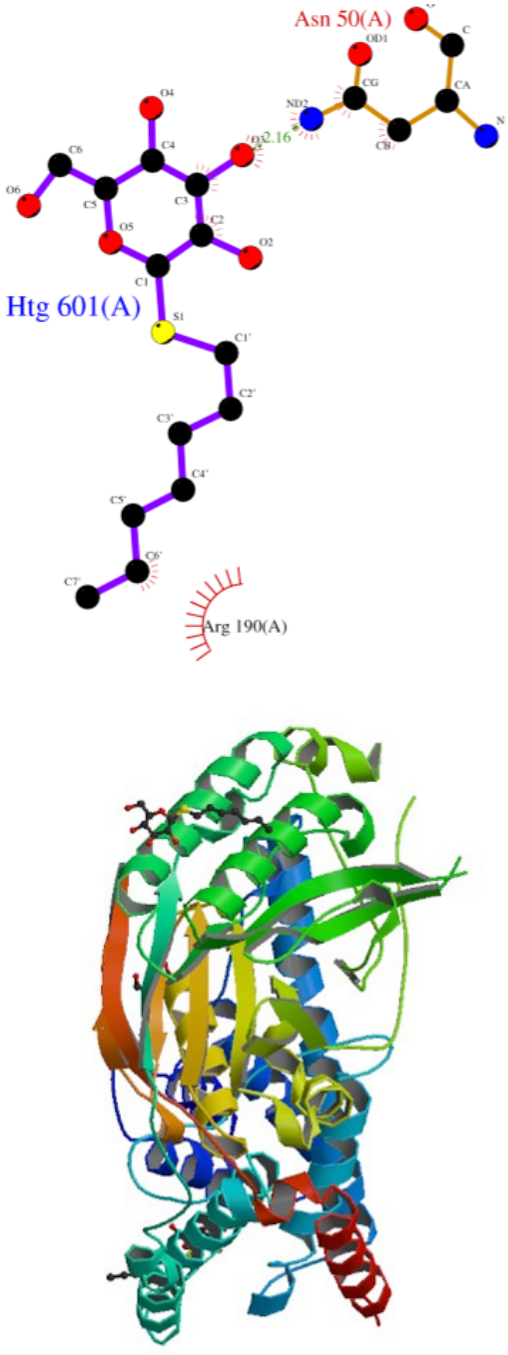

Fig. 1: Ligplot and 3D structure of Apolipoprotein N-acyl Transferase

following certain criteria like rotatable bonds <10, logP <5, hydrogen bond contributor <5, hydrogen bond acceptor <10 Molecular mass (<500) and molar refractivity (<130).

Absorption, Distribution, Metabolism, Excretion and Toxicity properties of Bioactive Compounds from Essential Oil

The expectation of ADME/T quality of the bioactive mixes were finished utilizing swiss ADME. These properties characterize the real condition of ligand by breaking down water solvency, gastrointestinal retention, infiltration of a ligand in blood mind obstruction, and focal sensory system. The danger level of the medication atoms was additionally screened with dose level for humans and rodents. These properties fundamentally run dependent on the guideline of vector-based calculation that can without much of a stretch break down informational collections of referred to inhibitor/non-inhibitor just as substrate/non-substrate.[9-11]

Molecular Docking Analysis using Autodock 4.2.6 Software

Molecular docking is a computational method of chemistry that plays a major role in designing drug molecules. The docking was done with virulent protein against bioactive compounds. The enzymes and receptors are chiral in a form that comprises of enantiomers with same or different biological activities. The rigid form docking was used in which the binding position of the ligand will be stable and binded with different types of amino acids. A default grid size of 20 Å was set. Total grid points per map were 64,000. Grid spacing was 0.375 Å (default). The center grid box sizes were x center: –16.302, y center: –23.34, and –16.245, respectively. The structure-based ligand docking was done using Autodock 4.2.6 software and was visualized using Discovery Studio 3.1.[12,13]

Result And Discussion

The following bioactive compounds obtained from *Cymbopogon citratus* were citral (34.8%), neral (30.72%), β-myrcene (11.28%), geraniol (5.54%), 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde (2.20%), citronellol (1.34%). Geranyl acetate (0.57%), bicyclo [3.1.1]heptane-2carboxaldehyde-6,6-dimethyl (0.23%) and D-limonene (0.03%). The bioactive compounds were unique in which no reports are available against the apolipoprotein N-acyl transferase, which paves the way for the discovery of novel phytomedicine. The bioactive compounds were screened using Lipinski rule five in which various parameters were checked like molecular weight, lipophilicity, hydrogen acceptor, and donor.

All the compounds satisfy the Lipinski rule of five, which means compounds do not have virulent factors that may disturb the normal microflora in the human intestine system.

Absorption, Distribution, Metabolism, Excretion and Toxicity Properties

The bioactive compounds were screened for physiochemical activities by using swiss ADME software. The compounds consist of less water solubility due to oil content in the lemongrass. The intestinal absorption in the oil of lemongrass shows a better result from 92–96%. The values of each property for all the compounds were tabulated in Table 2. The compounds β-myrcene has better absorption

Table 1: Compounds analyzed in Lipinski rule of five

Compound name	*Mass*	*Hydrogen bond donor*	*Hydrogen bond acceptor*	*LOGp*	*Molar refractivity*
Citral	152	0	1	2.87	48.48
Neral	152	0	1	2.87	48.48
β-myrcene	136	0	0	3.47	48.11
Geraniol	154	1	1	2.67	49.50
1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde	138	0	1	2.32	41.77
Citronellol	156	1	1	2.75	49.53
Geranyl acetate	196	0	2	3.24	59.05
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	152	0	1	2.25	44.16
D-limonene	136	0	0	3.30	45.91

Table 2: Absorption properties of compounds

Compound name	*Water solubility (log mol/L)*	*$CaCo_2$ permeability (Log Pabb in 10^{-6} cm/Sec)*	*GI absorption (%)*	*Skin permeability (Log Kp)*	*P-glyco-protein substrate*	*P-glyco-protein I inhibitor*
Citral	-3.337	1.504	95.31	-2.413	No	No
Neral	-3.337	1.504	95.31	-2.413	No	No
β-myrcene	-4.497	1.4	96.69	-1.043	No	No
Geraniol	-2.866	1.49	92.78	-1.511	No	No
1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde	-1.957	1.41	97.15	-2.309	No	No
Citronellol	-2.957	1.489	92.83	-1.525	No	No
Geranyl acetate	-3.446	1.627	94.9	-1.665	No	No
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	-3.221	1.476	95.74	-1.951	No	No
D-limonene	-3.568	1.401	95.89	-1.721	No	No

rate in gastrointestinal fluid with less water solubility and less skin permeability.

The essential oil of lemongrass does not have any harmful factors that can cross the blood-brain barrier (BBB) and central neuro system (CNS) as shown in Table 3. All the values are negative in the CNS permeability, which is understood that the compounds have better inhibition potential. The volume of distribution in human is a major parameter which measures the number of drug molecules distributes throughout the body. All the compounds are stable and will not penetrate in the immune system.

The enzymatic transformation in the body plays a major role in the conversion of drugs at a particular active site. These compounds are not involved in any metabolic activities with any substrate and inhibitor of cytochrome P450 that catalyzes the oxidation reaction, which was shown in Table 4.

The excretion and the toxicity level of the compounds were checked as tabulated in Table 5, and the tolerated dosage of human and rats were noted. While consuming the essential oil of lemongrass, it may be cause little irritation on the skin. The dosage level given for rats and humans can help to perform *in silico* studies. The dosage level for human as well as a rat was screened using the ADMET modeler™ module in ADMET Predictor in which the computational toxicology was built.

The bioactive compounds of *Cymbopogon citratus* were docked against apolipoprotein N-acyl transferase to identify novel therapeutic activities with selective targets and reasonable ADMET properties. The binding structure-

Table 3: Distribution properties of compounds

Compound name	*VDss (human) (Log L/kg)*	*Fraction unbound (human) (Fu)*	*BBB permeability (Log BB)*	*CNS permeability (Log PS)*
Citral	0.166	0.42	0.626	–1.986
Neral	0.166	0.42	0.626	–1.986
β-myrcene	0.363	0.39	0.781	–1.902
Geraniol	0.17	0.447	0.606	–2.159
1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde	0.133	0.568	0.262	–2.539
Citronellol	0.195	0.447	0.627	–2.222
Geranyl acetate	0.103	0.395	0.566	–2.199
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	0.497	0.392	0.838	–1.985
D-limonene	0.396	0.48	0.732	–2.37

Table 4: Metabolism properties of compounds

Compound name	*CYP2D6 substrate*	*CYP3A4 substrate*	*CYP1A2 inhibitor*	*CYP2C19 inhibitor*	*CYP2C9 inhibitor*	*CYP2D6 inhibitor*	*CYP3A4 inhibitor*
Citral	No	No	No	No	No	No	No
Neral	No	No	No	No	No	No	No
β-myrcene	No	No	No	No	No	No	No
Geraniol	No	No	No	No	No	No	No
1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde	No	No	No	No	No	No	No
Citronellol	No	No	No	No	No	No	No
Geranyl acetate	No	No	No	No	No	No	No
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	No	No	No	No	No	No	No
D-limonene	No	No	No	No	No	No	No

Table 5: Excretion and toxicity properties of compounds

Compound name	*Renal OCT2 substrate*	*AMES toxicity*	*Max. tolerated dose (human) (Log mg/kg/ day)*	*hERG I inhibitor*	*Oral rat acute toxicity (LD50) (mol/kg)*	*Oral rat chronic toxicity (LOAEL) (Log mg/kg)*	*Liver toxicity*	*Skin sensitization*
Citral	No	No	0.543	No	1.815	2.133	No	Yes
Neral	No	No	0.543	No	1.815	2.133	No	Yes
β-myrcene	No	No	0.617	No	1.643	2.406	No	No
Geraniol	No	No	0.65	No	1.636	2.03	No	Yes
1,3,4-trimethyl -3cyclohexene 1-carboxaldehyde	No	No	0.882	No	1.928	1.993	No	Yes
Citronellol	No	No	0.7	No	1.669	2.025	No	Yes
Geranyl acetate	No	No	0.474	No	1.683	2.272	No	Yes
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	No	No	0.16	No	1.589	1.896	No	Yes
D-limonene	No	No	0.777	No	1.88	2.336	No	Yes

based ligand docking was predicted using Autodock 4.2.3. The crystal structure of the targeted protein (PDB ID: 5XHQ) was retrieved from Protein Data Bank and was docked against the targeted ligand molecule. The binding site of the amino acids was visualized using the discovery studio, in which hydrostatic bonds will be visualized. The detailed interaction of molecules was shown in Figs. 2–3 and the free binding energy was shown in Table 6. As a

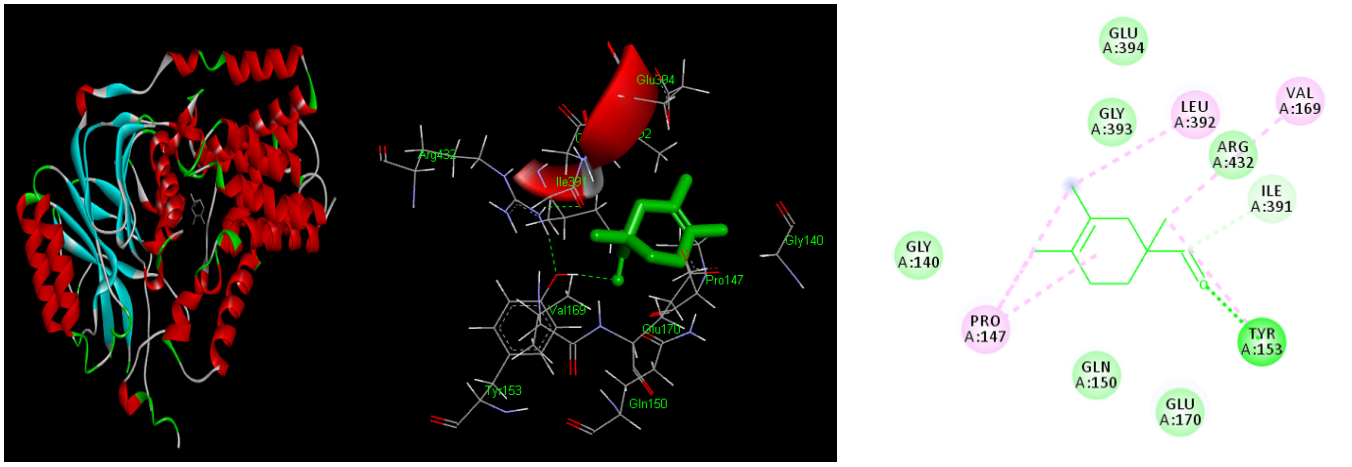

Fig. 2: 2D and 3D interaction of 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde

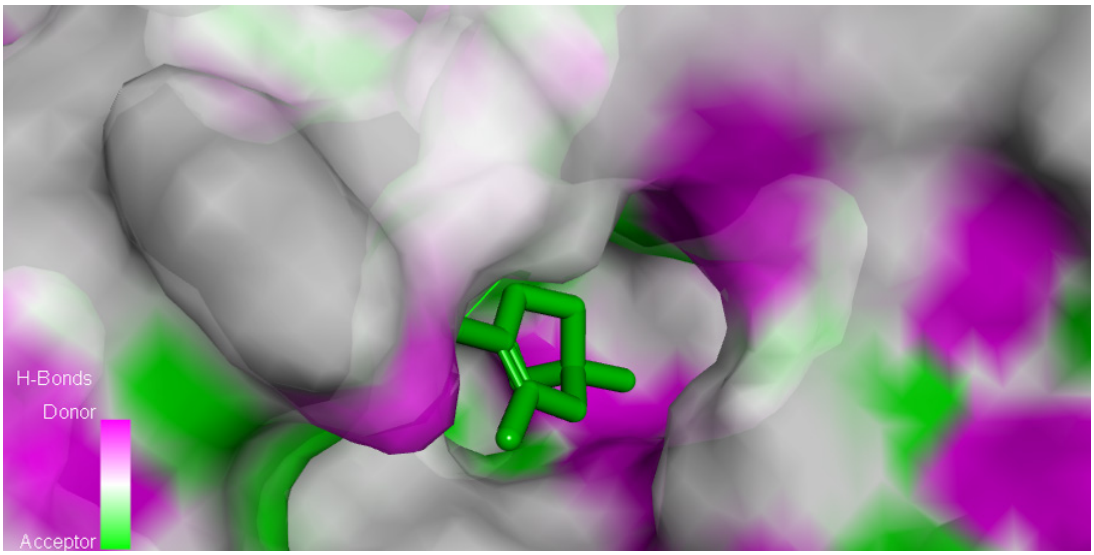

Fig. 3: Hydrogen bond interaction of 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde

Table 6: Interactions of various bioactive compounds

Compound name	*Binding energy*	*Vanderwaals interaction*	*No. of hydrogen bonds*	*Hydrogen interactions*	*Total no of residues*
Citral	-4.16	VAL 75, PHE 146, VAL 339, HIS 425, CYS 387, TRP 148, PHE 416, TYR 388, TRP 74	0	0	VAL 75, PHE 146, VAL 339, HIS 425, CYS 387, TRP 148, PHE 416, TYR 388, TRP 74
Neral	-3.91	VAL 339, TYR 388, TRP 148, GLY 421, PRO 422, CYS 387, PHE 416, HIS 425, ASP 413, TRP 74, PHE 146	0	0	VAL 339, TYR 388, TRP 148, GLY 421, PRO 422, CYS 387, PHE 416, HIS 425, ASP 413, TRP 74, PHE 146
β-myrcene	-4.35	VAL 339, GLY 421, PHE 146, TYR 388, TRP 148, TRP 74, PRO 422, HIS 425, CYS 387, ASP 413, PHE 416, GLY 421	0	0	VAL 339, GLY 421, PHE 146, TYR 388, TRP 148, TRP 74, PRO 422, HIS 425, CYS 387, ASP 413, PHE 416, GLY 421
Geraniol	-4.35	VAL 339, PHE 146, VAL 75, TYR 388, TRP 148, TRP 74, HIS 425, PHE 416, CYS 387, PRO 422, GLY 421	0	0	VAL 339, PHE 146, VAL 75, TYR 388, TRP 148, TRP 74, HIS 425, PHE 416, CYS 387, PRO 422, GLY 421

Contt.

Contt.

1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde	-4.72	GLU 170, GLN 150, PRO 147, GLY 140, GLY 393, GLU 394, LEU 392, ARG 432, ILE 391, VAL 169	1	TYR 153	TYR 153, GLU 170, GLN 150, PRO 147, GLY 140, GLY 393, GLU 394, LEU 392, ARG 432, ILE 391, VAL 169
Citronellol	-3.29	GLY 393, ARG 432, GLU 394, VAL 169, TYR 153, GLU 170, ASN 488, PHE 137, GLU 136, GLY 140, PRO 147, LEU 392	1	ILE 391	ILE 391, GLY 393, ARG 432, GLU 394, VAL 169, TYR 153, GLU 170, ASN 488, PHE 137, GLU 136, GLY 140, PRO 147, LEU 392
Geranyl acetate	-3.02	GLN 150, VAL 169, GLU 170, GLY 393, GLU 394, ARG 432, PRO 147, GLY 140, LEU 392, ILE 391, MET 428, TRP 148	1	TYR 153	TYR 153, GLN 150, VAL 169, GLU 170, GLY 393, GLU 394, ARG 432, PRO 147, GLY 140, LEU 392, ILE 391, MET 428, TRP 148
Bicyclo[3.1.1]heptane-2Carboxaldehyde-6,6-dimethyl	-3.45	GLU 170, GLY 393, GLU 394, ARG 432, PRO 147, GLY 140, LEU 392, ILE 391	0	0	GLU 170, GLY 393, GLU 394, ARG 432, PRO 147, GLY 140, LEU 392, ILE 391,
D-limonene	-4.30	GLY 421, PRO 422, PHE 416, ASP 413, TRP 74, HIS 425, PHE 146, VAL 339, TYR 388, TRP 148, CYS 387	0	**0**	GLY 421, PRO 422, PHE 416, ASP 413, TRP 74, HIS 425, PHE 146, VAL 339, TYR 388, TRP 148, CYS 387

result, these compounds have better inhibition potential against the virulent protein.

Conclusion

Planning the novel medication is a difficult issue that can be sifted through utilizing progressed computational advances (Bioinformatics). Structure-based ligand docking is a propelled apparatus being utilized for planning or contemplating the character of medication when corresponds with the destructive catalysts. The unrefined information of Apolipoprotein N-acyl Transferase was recovered from PDB and was investigated by expelling hydrophobic particles. The medication mixes of Cymbopogon citratus were assessed utilizing ADME/T and Lipinski rule of five. Our examination uncovers that the bioactive mixes present in Cymbopogon citratus can be utilized as medication in light of the fact that these mixes won't bring about any unsafe impacts in the inside organ of human just as creature. Among all the studies compounds, 1,3,4-trimethyl -3cyclohexene-1-carboxaldehyde exhibit binding energy -4.70 Kcal/mol followed by β-myrcene – 4.35 Kcal/mol and Geraniol -4.35 Kcal/mol. The common three-letter coding amino acids involved or attached with ligand molecules are VAL 75, PHE 146, VAL 339, HIS 425, CYS 387, TRP 148, PHE 416, TYR 388, TRP 74, TYR 153, GLN 150, VAL 169, GLU 170, GLY 393, GLU 394, ARG 432, PRO 147, GLY 140, LEU 392, ILE 391, GLY 421, PRO 422, PHE 416, ASP 413, TRP 74, HIS 425, PHE 146, VAL 339, TYR 388, TRP 148, CYS 387. We conclude that a combination of molecular docking and physiochemical properties of compounds helps to improve the potential inhibitor of the drug. For further studies, *in vitro,* and *silico* studies can be performed for developing the multiple drug target ability of *Cymbopogon citratus* against Apolipoprotein N-acyl transferase.

References

1. Poirier J, Bertrand P, Kogan S, Gauthier S, Davignon J, Bouthillier D. Apolipoprotein E polymorphism and Alzheimer's disease. The Lancet. 1993 Sep 18;342(8873):697-699.
2. Pitas RE, Boyles JK, Lee SH, Foss D, Mahley RW. Astrocytes synthesize apolipoprotein E and metabolize apolipoprotein E-containing lipoproteins. Biochimica et Biophysica Acta (BBA)-Lipids and Lipid Metabolism. 1987 Jan 13;917(1):148-161.
3. Shah G, Shri R, Panchal V, Sharma N, Singh B, Mann AS. Scientific basis for the therapeutic use of Cymbopogon citratus, stapf (Lemon grass). Journal of advanced pharmaceutical technology & research. 2011;2(1):3.
4. Negrelle RR, Gomes EC. Cymbopogon citratus (DC.) Stapf: chemical composition and biological activities. Revista Brasileira de Plantas Medicinais. 2007;9(1):80-92.
5. Carlini EA, De D.P. Contar J, Silva-Filho AR, Da Silveira-Filho NG, Frochtengarten ML, Bueno OFA. Pharmacology of lemongrass (Cymbopogon citratus Stapf). I. Effects of teas prepared from the leaves on laboratory animals. Journal of Ethnopharmacology. Elsevier BV; 1986 Jul;17(1):37–64.
6. Asaolu MF, Oyeyemi OA, Olanlokun JO. Chemical compositions, phytochemical constituents and in vitro biological activity of various extracts of Cymbopogon citratus. Pakistan Journal of Nutrition. 2009;8(12):1920-1922.
7. Gbenou JD, Ahounou JF, Akakpo HB, Laleye A, Yayi E, Gbaguidi F, Baba-Moussa L, Darboux R, Dansou P, Moudachirou M, Kotchoni SO. Phytochemical composition of Cymbopogon citratus and Eucalyptus citriodora essential oils and their anti-inflammatory and analgesic properties on Wistar rats. Molecular biology reports. 2013 Feb 1; 40(2):1127-1134.
8. Ajayi EO, Sadimenko AP, Afolayan AJ. GC–MS evaluation of Cymbopogon citratus (DC) Stapf oil obtained using modified hydrodistillation and microwave extraction methods. Food chemistry. 2016 Oct 15;209:262-266.
9. Biswal A, Aishwariya A, Sharma A, Pazhamalai V. 2D QSAR, ADMET prediction and multiple receptor molecular docking strategy in bioactive compounds of Gracilaria corticata against Plasmodium falciparum (contractile protein). Informatics in Medicine Unlocked. 2019 Jan 1;17:100258.
10. Meenambiga SS, Venkataraghavan R, Biswal RA. In silico analysis of plant phytochemicals against secreted aspartic proteinase enzyme of Candida albicans. J Appl Pharm Sci. 2018 Nov;8(11):140-150.

11. Biswal AR, Mirunalini K, Jayshree P, Pazhamalai V. Molecular Docking Analysis of Bioactive Compounds of Acacia Concinna against Fungal Protein. Journal of Pharmaceutical Sciences and Research. 2019 Apr 1;11(4):1216-1222.
12. Biswal A, Venkataraghavan R, Pazhamalai V. Molecular docking of various bioactive compounds from essential oil of Trachyaspermum ammi against the fungal enzyme Candidapepsin-1. Journal of Applied Pharmaceutical Science. 2019 May;9(05):021-032.
13. Biswal RA, Jayashree P, Mirunaalini K, Pazhamalai V. Molecular docking studies of bioactive compounds from the leaves of Epiphyllum oxypetalum against Treponema pallidum, Zika virus and liver cirrhosis. Journal of Applied Pharmaceutical Science. 2019 Nov;9(11):069-077.

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