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Research Article

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In Silico Molecular Docking and Admet Profiling of Eugenol (Bioactive Component of *Alstonia Boonei*) on 7E3F Protein of *Trypanosoma Brucei*

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Abstract

Molecular Docking techniques and ADMET study procedures were used to investigate the therapeutic potency and drug candidacy of the ethanolic root extract of *Alstonia boonei* against the 7E3F protein of *Trypanosoma brucei.* Auto dock and Auto dock Vina 1.5.6 software's were used for the virtual screening. The Gaussian 16 program was used for all computations. Results showed that a major bioactive ingredient in the plant extract, Eugenol, projects drug like potency with considerable significant ($P<0.05$) binding affinity value of -5.8kcal/mol. on the protein of interest, 7E3F, in the parasite. This value is high enough to qualify the A. boonei component, eugenol as a potential drug for treating African Trypanosomiasis. Eugenol was also examined for their drug likeness via ADMET studies and it demonstrated potency to serve as drug with good adsorption properties, good metabolism and other very favorable properties. The cytochrome 7E3F protein which plays very crucial roles in metabolism, was found to be compatible with the components of eugenol. It is recommended that other extracts of this plant be investigated to ascertain their binding affinities to the 7E3F protein and possible drug formulation potentials.

Keywords: *Alstonia boonei, Trypanosoma brucei*, Eugenol, Molecular docking, Drug formulation, ADMET study, Auto Dock vina, binding affinity, 7E3F protein

Introduction

Sleeping sickness, African trypanosomiasis, is endemic across sub-Saharan Africa, and is gaining worldwide attention. It is prevalent in sub-Saharan Africa, posing a significant public health threat in the region [1]. Current treatment options for African trypanosomiasis are limited and often associated with severe side effects, highlighting the need for new and effective therapeutic agents [2]. *Trypanosoma brucei*, a species of parasitic kinetoplast belonging to the genus Trypanosoma is identified as the causative agent of this parasitic infection. The parasite is transmitted to humans and animals through the bite of infected tsetse flies [3]. *Alstonia boonei* (Plate 1) is a medicinal plant native to West Africa that has been traditionally used in the treatment of various ailments, including malaria and gastrointestinal disorders. Previous studies

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have shown that extracts from the roots of *Alstonia boonei* possess antiparasitic properties against a range of pathogens, including *Trypanosoma brucei*. However, the specific compounds responsible for this activity and their inhibitory potency against the parasite remain largely unknown [4].

The main objective of this investigation was to evaluate the inhibitory potency of Eugrnol, a bioactive extract from A. boonei root, against *Trypanosoma brucei* and compare the inhibitory potency of the modified bioactive compound with existing drugs used for the treatment of Africa trypanosomiasis using molecular docking simulation methods and ADMET studies.

Molecular interactions play a crucial role in advancing our understanding of parasitology especially in developing new therapeutic studies. Docking techniques are essential in drug discovery, enabling researchers to predict the interactions between compounds and biological targets effectively.

Materials and Methods

Molecular Docking and ADMET studies were employed [5]. Auto dock tools and Auto Dock Vina 1.5.6 [6] are the software's used for performing molecular docking simulations.

In this protocol, the compound of interest, eugenol derivative from *Alstonia boonei* root was docked with the protein of interest with code 7E3F which is a *Trypanosoma brucei* receptor protein obtained from the RCSB protein data bank [7]. The standard drug Nifurtimox was also docked with the protein to compare the binding affinity of the studied compound with that of the standard drug [8]. ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) studies too were carried out. We drew the eugenol using a chemical structure drawing program (PubChem). Then translated it into the notation of the Simplified Molecular Input Line Entry System (SMILES) and examine for toxicity and drug-likeness.

Crucially, we validated the compound's compliance to the Lipinski rule for therapeutic viability and evaluated its potential against *Trypanosoma brucei*.

Results and Discussion

The result for the interaction of the studied compound (Eugenol) and the standard drug Nifurtimox (NFTMOX) with the receptor (7E3F) is presented in Table 1. On interaction with the protein (7E3F), eugenol recorded a binding affinity of -5.6 Kcal/Mol with significantly two conventional hydrogens (SER: 129, and VAL: 125), whereas, NFTMOX showed a slightly higher binding affinity value of -6.6Kcal/Mol with outstanding four hydrogen bonds (ALA: 114, ASP: 115, ASP: 182, ARG 285) (Table 1). The result for the analysis showed compatible predictions with green indication on the Caco-2 Permeability with 73.159% probability (Figure 1), indicating that the substance is able to pass through the blood stream to reach the target site.

Table 1: Showing the binding affinities in the interaction of studied compound and the Standard.

Interactions	Binding Affinity (Kcal/Mol)	Conventional Hydrogen
Eugenol/7E3F	-5.8	SER: 129, VAL: 125
NFTMOX/7E3F	-6.6	ALA: 114, ASP: 115, ASP: 182, ARG 285

Similarly, green prediction on Mardin-Darby Canine Kidney (MDCK) permeability (Figure 1, Table 2), suggests high or significant permeability across cells and membrane and hence it would imply good oral absorption owing to free transport of the compounds crossing the intestinal epithelium. More so, the Pgp-inhibitor parameter is shown to be favorable with the studied compound, indicating that the compound will not reduce the functionality of the P-glycoprotein (Pgp) as an efflux transporter protein.

Table 2: ADMET study for the bioactive compound Eugenol.

Compound: Eugenol	Characteristic	Probability	Prediction
Parameters: Absorption	Caco-2 Permeability MDCK	-4.938	Green
	Permeability Pgp-inhibitor	0.000046	Green
		---	Green
Distribution	PPB	73.159%	Green
	VDss	0.975	Green
	BBB Penetration	+++	Red

Metabolism	CYP1A2 inhibitor	---	Green
	CYP2C19 inhibitor	---	Green
	CYP2C9 inhibitor	---	Green
	CYP2D6 inhibitor	---	Green
	CYP3A4 inhibitor	---	Green
	Gastrointestinal absorption	High	
Excretion	Clearance	5.932 mL/min	Green
	T1/2	0.465s	
Toxicity	Hepatotoxicity	0.69%	Active
	Carcinogenicity	0.62%	Inactive
	Immunotoxicity	0.96%	Active
	Mutagenicity	0.97%	Inactive
	Cytotoxicity	0.93%	Inactive
Physicochemical properties	Formula	C10H12O2	
	Molecular weight	164.20 g/mol	
	Num. of heavy atoms TPSA	12 29.46Å2	
	Lipinski Rule of 5	Accepted	
	Ghose Rule	Accepted	

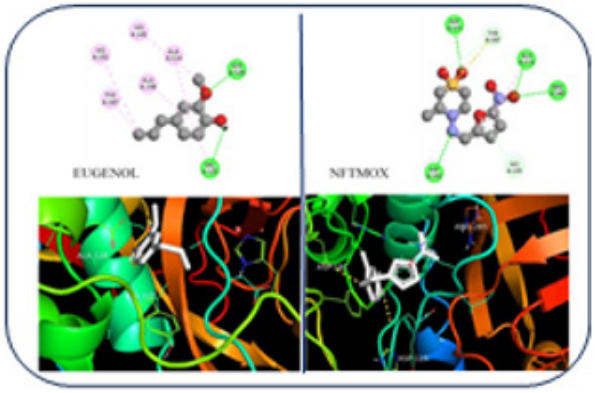


Figure 1: 2D and 3D visualization of Eugenol and the standard.

Consequently, eugenol showed green predictions on the Distribution parameter with favorable values for Plasma Protein Binding (PPB), (Table 2) inferring high binding and stability to function at target sites and good Volume of Distribution at Steady State (VDss), hence, the compound won't inhibit the functions of the proteins if administered as drug.

ADMET Study

Adsorption, Distribution, Metabolisms, Excretion, and Toxicity are only a few of the important factors that are carefully evaluated in ADMET studies, which are used to predict the pharmacokinetics of researched compounds and identify their therapeutic potency [9].

Notably, the studied compound showed compatible prediction on the Cytochrome 7E3F proteins which plays very crucial roles in metabolism, coupled with high gastrointestinal absorption, hence, the compound won't inhibit the functions of the proteins if administered as drug. More so, the compound exhibits good clearance with significant half-life under the Excretion parameter. Finally, on the Toxicity parameter, different organs of the human body were captured and the investigation of this compound's effect was also carried out and recorded as shown in the Table 1. Herein, Eugenol depicts active predictions on hepatotoxicity and immunogenicity implying that the liver and the immune system

can be negatively affected by the substance, hence, the least safe dose (LSD), needs to be established. More so, the substance shows inactive prediction on the gene and no trait of being cancerous, neither being toxic to the cells [10]. Wherefore, based on this evaluation from the ADMET studies and obedience to the Lipinski and Ghose rule of drug efficacy, the studied compound, eugenol, projects drug-like potency in its inhibitory effect against 7E3F protein in *Trypanosoma brucei*.

Conclusion

This research was carried out as preliminary studies to identify drug likeness of components of a locally acclaimed highly potent and medicinal plant, *Alstonia boonei*. The root extract contains a bioactive component Eugenol, which was used in this investigation against the cytochrome 7E3F proteins of Trypanasomiasis brucei and was found to contribute extensively to the observed inhibitory effects of the plant on *Trypanosoma brucei*, suggesting that *Alstonia boonei* could serve as a valuable source of natural anti trypanosomal agents. However, as is expected, further studies are recommended to establish these findings.

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Conflict of Interest

There is no conflict of interest to declare.

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