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Research Article

Physicochemical, ADMET Profiling and Anti-TB potential of Afzelin and Quercitrin derived from Euphorbia hirta L.

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ABSTRACT

Over the past few years, there has been an increased interest among scientists and researchers globally to discover alternative sources of sustainable materials to satisfy the development of ecosystems based on human factors, safety, versatility, efficacy, and environmental compatibility. In the present work, we investigated physicochemical, ADMET Profiling and Anti-TB potential of Afzelin and Quercitrin derived from *Euphorbia hirta L.* (PDB:6ACA). To assess the ADMET analysis and antidiabetic properties, *in silico* approach was used. The results have shown that the targeted drug molecules showed very good ADMET profiling and remarkable anti-TB ability and can be considered as novel therapeutic agent for TB cure after further clinical studies.

1. Introduction

Approximately 10 million people develop active TB every year, making it a serious public health issue that exists globally and is widespread. Despite being fully treatable and preventable, an average of 1.5 million people die from TB each year (the number one cause of death by an infectious disease). TB is an even greater problem for people with HIV because, without a strong immune system, it's the number one cause of death. Additionally, TB is a major and growing contributor to antibiotic resistance (as many multidrug-resistant and extensively drug-resistant strains of TB are emerging), making treatment and control efforts more difficult [1]. The burden of TB in South Asia is particularly significant. About 856,000 people developed TB in South Asia in 2022, and about 84,000 deaths were attributed to TB. The South Asian region represents nearly 8% of global TB cases and about 7% of TB-related deaths worldwide [2,3], indicating that the South Asian region requires increased surveillance of TB, early diagnosis of TB, improved adherence to treatment, and increased public health efforts to stem the burden of TB. The combined trends in these areas suggest that sustained global efforts, innovative therapies, and integrated health approaches.

Bioactive compounds from natural products have been used for thousands of years in medicine. Natural products are rich sources of diversity; this means that there are many naturally produced bioactive compounds with many different effects (i.e., antimicrobial, anti-inflammatory, anticancer and immunomodulatory) [4-6]. For this reason, the use of natural product-derived compounds has been an integral part of health care for centuries and has been shown to greatly impact people's health. Examples of these traditional systems include Ayurveda and Traditional Chinese Medicine. Given the limited health-care infrastructure and services in developing countries, natural product-derived compounds continue to provide a primary method of meeting the basic health care needs of individuals living in these regions [7-9].

In addition to the historical context, modern scientific studies provide evidence for the pharmaceutical development of natural products and their continued relevance within drug discovery programs. Approximately 30 percent of the currently available pharmaceutical products in the world were developed using some form of natural source (i.e., plants, microbiological organisms, marine organisms). Many of the most popular drugs, including many antibiotics and anticancer agents, contain naturally occurring compounds and have been chemically modified for use as pharmaceuticals. The long-standing tradition of using natural product-derived compounds coupled with the large number of scientific studies demonstrating the validity of using natural products as therapeutic products continues to generate significant interest in finding new therapeutic agents from natural products [10].

The medicinal herb *Euphorbia hirta* is common in humid, warm, areas of the world and has historically been used as a treatment for respiratory diseases, gastrointestinal issues, skin infections, and other inflammatory conditions. The numerous beneficial effects attributed to this plant can be contributed to the wide variety of biologically-active chemicals contained within its tissues; these include phytochemicals such as flavonoids, tannins, alkaloids, terpenoids and phenolic compounds. The activities exhibited by these active ingredients provide the basis for *Euphorbia hirta* being defined as an antimicrobial, antioxidant, anti-inflammatory, bronchodilator and antidiarrheal agent [11,12]. Consequently, due to the range of pharmacological effects associated with this species have led to increasing interest from current researchers who are seeking natural sources of products capable of producing beneficial effects in humans.

The therapeutic efficacy of plant-derived natural products has been well recognised in curing several health ailments/disorders,

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particularly obesity, cardiovascular diseases, diabetes, osteoporosis, arthritis, cancer, hypercholesterolemia, and age-related degenerative conditions. For example, curcumin from turmeric shows strong anti-inflammatory and anticancer properties; resveratrol from grapes provides cardioprotective and anti-aging benefits; catechins from green tea are powerful antioxidants, etc. reduce inflammation and supporting heart and brain health; while probiotics enhance gut microbiota and improve immunity [7-10]. These bioactive compounds exert their effects through diverse biochemical pathways such as free radical scavenging, modulation of inflammatory mediators, regulation of metabolic enzymes, inhibition of tumour cell proliferation, and protection of cellular components from oxidative damage. A number of plants are known for their therapeutic potential as well as their parts enriched with nutritious compounds such as *Emblica officinalis* (amla), *Curcuma longa* (turmeric), *Ocimum sanctum* (tulsi), *Linum usitatissimum* (Flaxseed/Linseed), *Camellia sinensis* (green tea), *Allium sativum* (garlic), *Zingiber officinale* (ginger), *Euphorbia hirta* (Dudhi), *Withania somnifera* (ashwagandha), *Rubia cordifolia* (Madder), *Vitis vinifera* (grapes) etc [11-19]. The present study is to investigate *E. hirta* L. derived phytocompounds for their pharmaco-chemical, ADMET analysis and their anti-TB potential using CADD-based *in silico* approach.

2. Materials and methods

2.1 Protein and Ligands preparation

The crystal structure of Mycobacterium tuberculosis at 3.6 A resolution Receptor Protein (6ACA) under R-Value Free: 0.295 (Depositor), 0.300 (DCC); R-Value Work: 0.249 (Depositor), 0.250 (DCC); R-Value Observed: 0.252 (Depositor) was obtained from the RCSB Protein Data Bank (https://www.rcsb.org/). The Ligands (Table 1), Ethambutol (ETM) as a standard drug reference, Afzelin (AFZ) and Quercitrin (QUE) were prepared using chemdraw software, obtained SMILES and. mol2 files. The energy minimization of the modeled structures were done using Avogadro Software v1.2.0.

2.2 Pharmaco-chemical, ADMET and anti-TB Assessment

Drug target and pharmacological assessments (physicochemical, lipophilicity, water solubility, pharmacokinetics, druglikeness) and ADMET and drug target assessments were investigated using http://www.swisstargetprediction.ch/ and ADMETLab 3.0 (https://admetlab3.scbdd.com/) online web platforms [20-24].

2.3 Molecular docking studies and Anti-TB prediction

For the deep machine learning (dML)-enabled prediction of binding energies and molecular docking studies, we have utilized CB-Dock Online platform (http://cadd.labshare.cn/cb-dock2/), a user-friendly and blind docking web server that offers an interactive 3D visualisation of results. [25,26]. Further, anti-TB potential of the targeted compounds **L1-L7** was assessed using mycoCSM Platform, The University of Melbourne (https://biosig.lab.uq.edu.au/myco_csm/) [27].

3. Results and discussion

3.1 Pharmaco-chemical characteristics and ADMET properties evaluation

The biological activities of selected **Compounds 1-3** were assessed and shown in Table 2. With reference to the biological activities, the selected compounds 1 and 2 demonstrated pronounced bioactive profiles. For novel drug discovery, considering pharmacokinetic and pharmacodynamic characteristics, drug validation is strongly recommended by researchers using computer aided drug design manner [18]. The ADMET profiles for **Compounds 1-3** have been assessed and presented in Tables 2-4 in silico, computed with Admet 3.0 and Swissdock ADME (**Supplementary Materials**) platforms integrated with multi-component-biological Alogarithms. The ADMET profiling shows significant variations among the three ligands (ETM, AFZ, and QUE) in terms of physicochemical and pharmacokinetic characteristics. ETM has low lipophilicity and permeability (Caco-2, MDCK, and PAMPA values), indicating poor absorption, but moderate plasma protein binding (PPB) and good fraction unbound (Fu). By contrast, AFZ and QUE have higher permeability and absorption, with QUE having slight improvements in human intestinal absorption (HIA) and fraction absorbed (f20-f50) (Table 2 and **Supplementary Materials**). None of the compounds show significant P-glycoprotein inhibition, but AFZ has higher substrate affinity. Generally, high transporter affinity (OATP1B1, OATP1B3, BCRP) and low blood-brain barrier (BBB) penetration is demonstrated by the ligands, suggesting poor central nervous system (CNS) distribution. Moreover, AFZ and QUE have higher PPB than ETM, indicating greater plasma protein binding. Thus, AFZ and QUE show better absorption and distribution profiles than ETM, and would be better drug candidates in terms of pharmacokinetics (Table 2 and **Supplementary Materials**).

The metabolism and excretion data (Table 3) suggest that ETM has lower inhibition of major CYP enzymes (lower propensity to drug–drug interactions) but higher plasma clearance values (~9.85), suggesting that the compound will be cleared quickly and will have a shorter half-life. By contrast, AFZ and QUE show moderate CYP3A4 inhibition (~0.9), which could increase the risk of interactions, but have lower clearance values (~2.92 and 3.60), and longer half-lives, indicating higher metabolic stability and longer duration of action. The toxicity results (Table 4) indicate satisfactory profiles for all three compounds with low hERG inhibition, suggesting low risk for cardiovascular toxicity. In summary, AFZ and QUE show better metabolic retention while ETM has high clearance but is safer in terms of CYP inhibition. Toxicity analysis suggests (Table 4) that the three ligands have different toxicity profiles. ETM displays lower Ames mutagenicity, carcinogenicity and genotoxicity indices, thus a safer profile, but higher prediction for skin sensitization and hepatotoxicity (H-HT). In contrast, AFZ and QUE show higher Ames and genotoxicity values (i.e. ~0.7 and ~0.95, respectively), suggesting a higher tendency towards mutagenic and genetic toxicity effects. But both show lower neurotoxicity and nephrotoxicity values than ETM, indicating lower risk for the nervous system and kidney. Respiratory toxicity and drug-induced liver injury (DILI) indices for all ligands are moderate, while cytotoxicity for the three cell lines (RPMI 8226, A549 and HEK293) is variable, with AFZ and QUE exhibiting relatively higher toxicity. Hence, ETM is safer with respect to genetic toxicity, while AFZ and QUE may be more genotoxic but have lower target organ toxicities.

3.2 Molecular Docking Studies and Anti-TB Potential

Molecular docking is employed to simulate and predict the most considerable orientation and interaction of selected ligands within the target protein's active site, providing insights into binding energy and potential binding mechanisms [28-31]. In the molecular docking analysis against the 6ACA receptor, it was observed that the three compounds exhibited stable binding interactions, as reflected by their negative docking scores (Fig. 1 and Fig. 2).

The molecular docking results against the 6ACA target show a clear difference in binding affinities among the compounds studied. Ethambutol (ETM) has a weak binding score of −5.2 kcal/mol, which indicates lower interaction strength with the target protein. In contrast, both Afzelin (AFZ) and Quercitrin (QUE) have much stronger binding affinities, each with a docking score of −9.7 kcal/mol. This suggests that AFZ and QUE have a higher potential to form stable ligand-protein complexes (Fig. 1-3). Their better fitting within the active site and stronger intermolecular interactions, like hydrogen bonding and hydrophobic contacts, likely contribute to this. Thus, AFZ and QUE seem more promising candidates than ETM for effectively inhibiting the 6ACA target.

Table 1: Selected targets as ligands.

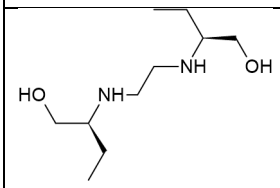
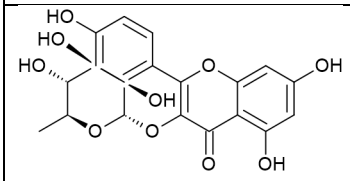
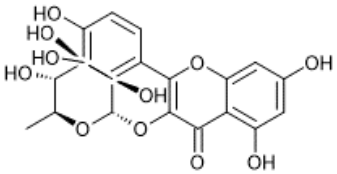
Chemical structures	**Name of Compounds/Smile Codes**	**Molecular formula**	**Molecular weight (g/mol)**	**Docking Score against 6ACA (kcal/mol)**
	Ethambutol (**ETM**) CC[C@@H](CO)NCCN[C@@H](CC)CO	$C_{10}H_{24}N_2O_2$	204.31	-5.2
	Afzelin (**AFZ**) C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC=C(C=C4)O)O)O)O	$C_{21}H_{20}O_{10}$	432.4	-9.7
	Quercitrin (**QUE**) C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC2=C(OC3=CC(=CC(=C3C2=O)O)O)C4=CC(=C(C=C4)O)O)O)O)O	$C_{21}H_{20}O_{11}$	448.4	-9.7

Table 2: Physicochemical, Absorption and Distribution parameters for selected drugs calculated with Admet3.0.

Ligands	logS	caco2	MDCK	PAMPA	pgp_inh	pgp_sub	hia	f20	f30	f50	OATP1B1	OATP1B3	BCRP	BSEP	BBB	MRP1	PPB	log VDss	Fu
ETM	-0.62	-5.24	-5.10	0.49	0.05	0.58	0.0	0.0	0.0	0.03	0.995	0.99	0.60	0.13	0.13	0.16	26.0	0.25	74.36
AFZ	-3.42	-6.09	-5.02	0.99	0.0	0.69	0.0	0.0	0.9	0.99	0.992	0.99	0.95	0.29	0.0	0.11	88.4	-0.05	10.83
QUE	-3.13	-6.04	-4.97	0.98	0.0	0.27	0.1	0.6	0.9	0.99	0.993	0.99	0.95	0.02	0.0	0.07	86.1	-0.06	12.88

Table 3: Metabolism and Excretion parameters for selected drugs calculated with Admet3.0.

CYP1A2 -inh	CYP1A2 -sub	CYP2C1 9-inh	CYP2C1 9-sub	CYP2C9 -inh	CYP2C9 -sub	CYP2D6 -inh	CYP2D6 -sub	CYP3A4 -inh	CYP3A4 -sub	CYP2C8 -inh	LM-human	cl-plasma	t 1/2	BCF	IGC50	LC50 DM	LC50FM	hERG	hERG-10um
0.040	0.241	0.0	0.0	0.0	0.257	0.014	0.292	0.0	0.0	0.0	0.0	9.85	0.8	0.0	1.80	3.27	2.27	0.4	0.45
0.282	0.049	0.0	0.0	0.0	0.017	0.027	0.136	0.9	0.0	0.9	0.96	2.92	3.3	0.8	3.57	4.53	3.98	0.0	0.27
0.261	0.030	0.0	0.0	0.0	0.002	0.0	0.006	0.9	0.0	0.9	0.98	3.60	3.7	0.8	3.52	4.63	4.08	0.0	0.34

Table 4: Toxicity parameters for selected drugs calculated with Admet3.0.

DILI	Ames	ROA	FDAMDD	SkinSen	Carcino genicity	EC	EI	Respiratory	H-HT	Neuro toxicity-DI	Nephro toxicity-DI	Genotoxicity	RPMI 8226	A549	HEK 293
0.093	0.13	0.02	0.147	0.99	0.128	0.44	0.34	0.311	0.936	0.519	0.6307	0.0004	0.09	0.06	0.077
0.902	0.7	0.21	0.397	0.97	0.165	0	0.98	0.319	0.496	0.017	0.1156	0.9514	0.12	0.71	0.762
0.928	0.7	0.2	0.372	0.99	0.1	0	0.98	0.288	0.437	0.003	0.0684	0.946	0.07	0.91	0.558

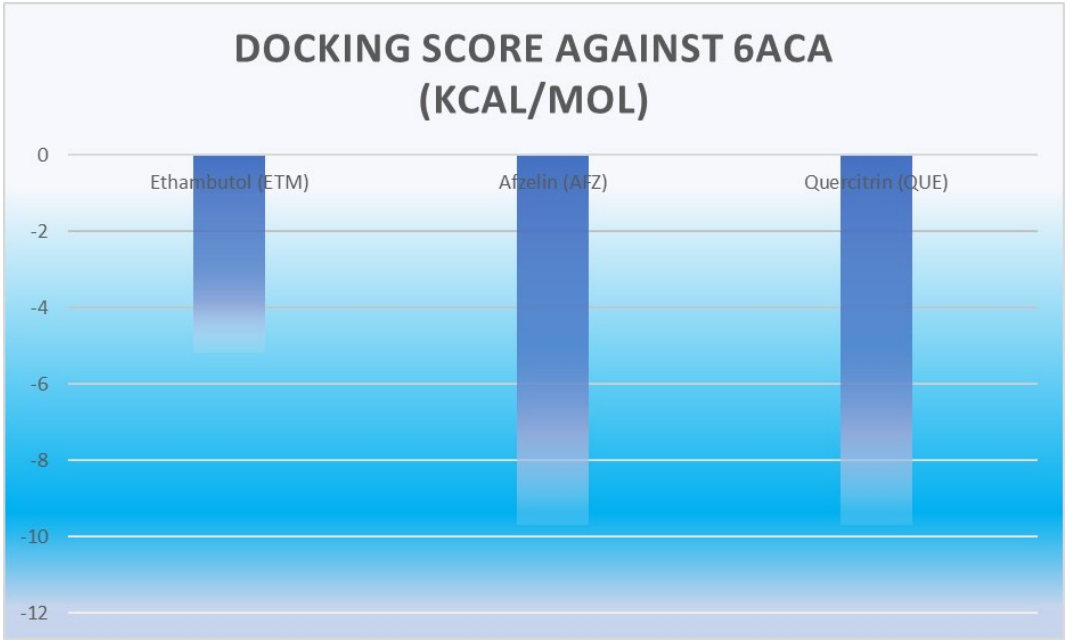


Figure 1: Comparative molecular docking score of selected compounds **1-3**.

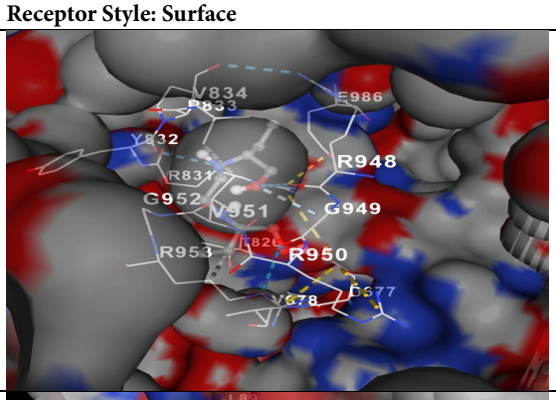
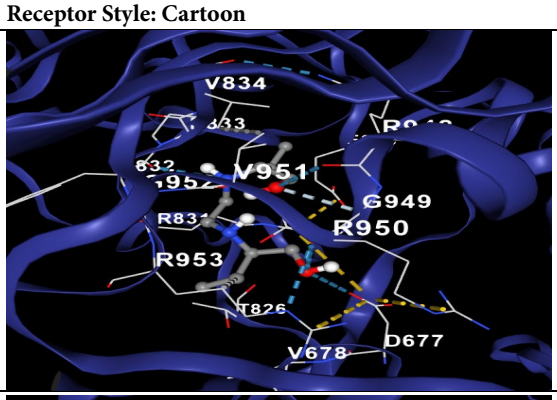
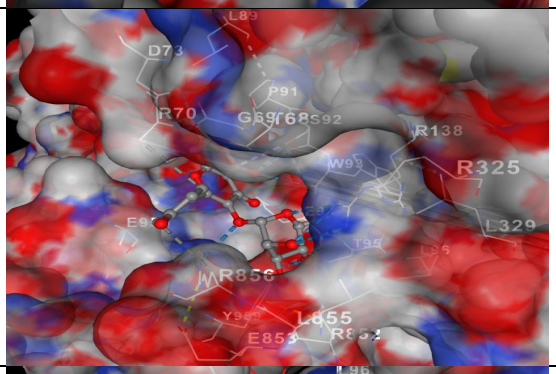
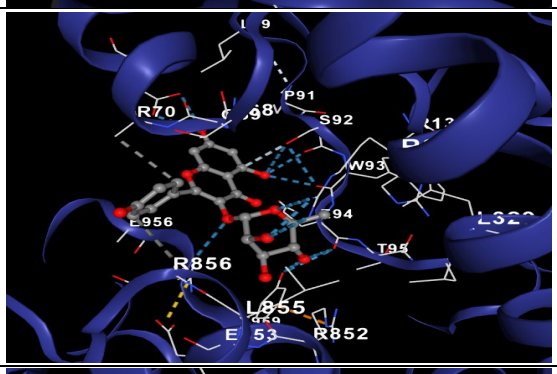
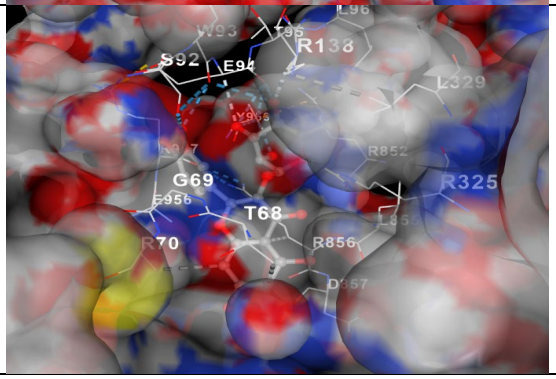
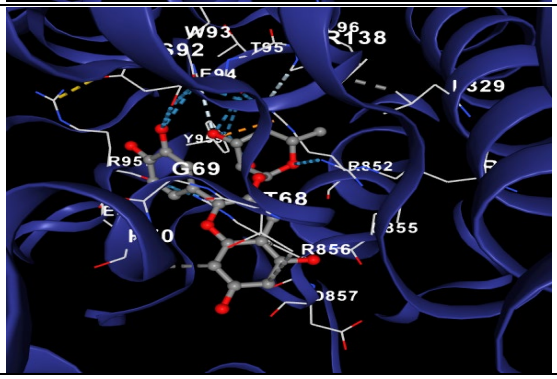
Drug target	Molecular docking pattern	
	Receptor Style: Surface	Receptor Style: Cartoon
ETM		
AFZ		
QUE		

Figure 2: Molecular docking pattern of selected target compounds **1-3** against 6ACA.

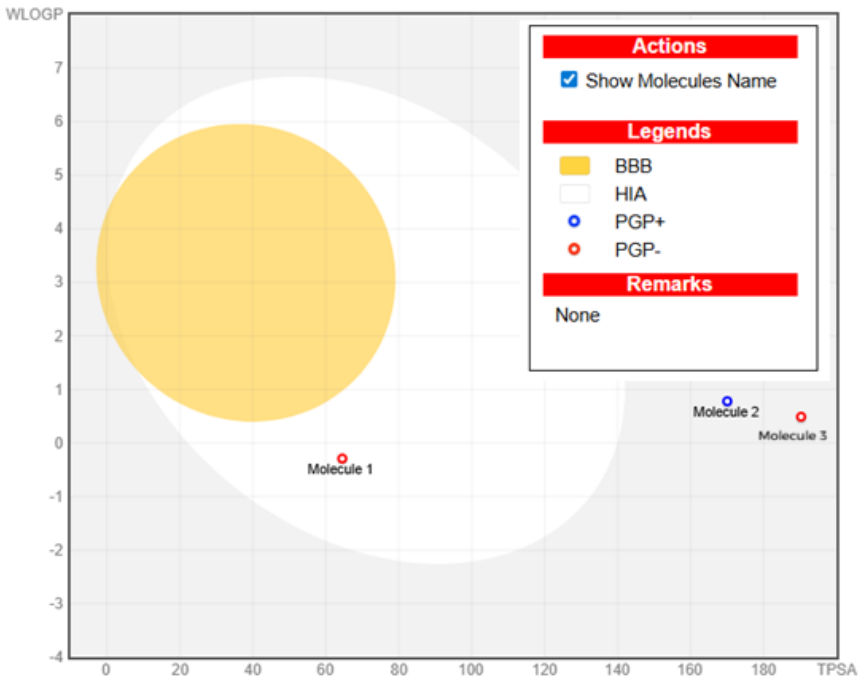


Figure 3: Boiled egg diagram for selected drug targets.

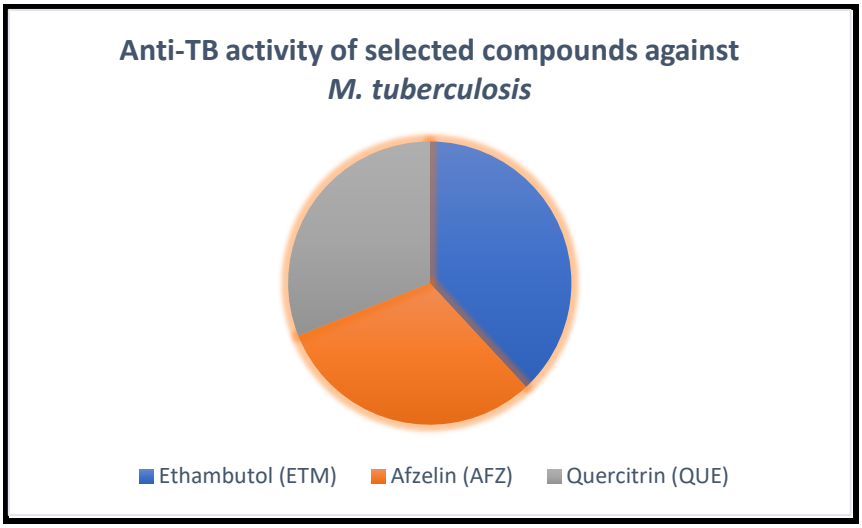


Figure 4: Anti-TB activity of selected compounds against *M. tuberculosis*.

The docking results against M. tuberculosis show that Ethambutol (ETM) has the strongest binding affinity, with a score of −4.895. This suggests more favorable interactions with the target compared to the other compounds. On the other hand, Afzelin (AFZ) and Quercitrin (QUE) have relatively weaker binding energies at −3.958 and −3.992, respectively, indicating lower interaction strength. Although the differences are not very large, ETM stands out as the more effective ligand against *M. tuberculosis* in this analysis (Fig. 4). AFZ and QUE may still have moderate inhibitory potential, but they are less potent than the standard drug. In the search for new anti-tuberculosis drugs, natural products from plants have gained significant interest in the pharmaceutical field [32-38]. This is due to their natural biological activities, especially their antimicrobial and antioxidant effects that can help fight Tuberculosis. Their wide therapeutic benefits, along with eco-friendliness, compatibility with living organisms, and lower environmental impact, make them strong candidates for creating safer and more effective anti-TB drugs. This is particularly important given the increasing issue of antibiotic resistance.

4. Conclusion

Euphorbia hirta is an important medicinal plant that contains a variety of beneficial compounds. It shows a wide range of biological and health benefits, including antimicrobial, anticancer, and antidiabetic effects. Traditionally, it has been used to manage various health issues. In this study, we evaluated Afzelin (AFZ) and Quercitrin (QUE), which are naturally derived from the aerial parts of *E. hirta*. We looked at their physical and chemical properties, therapeutic potential, ADMET characteristics, and anti-tuberculosis activity against Tuberculosis. The results showed that both compounds have good physical and chemical properties, notable biological activity, and acceptable ADMET profiles. This supports their potential as drug candidates. Moreover, molecular docking studies against the 6ACA target indicated promising anti-TB potential, suggesting they could act as antibacterial agents. However, more in vitro, in vivo, and

clinical studies are needed to confirm these results. If clinical evaluations are successful, these compounds could become viable oral treatments. Additionally, modifying the structures and developing derivatives of AFZ and QUE might widen their use in various biomedical areas. This could help advance nature-based drug discovery, not just for tuberculosis but also for metabolic disorders like diabetes, though further validation is required.

Supplementary Materials

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Contribution

Rashmi: Concept, literature review, data interpretation, drafting the manuscript and approval for final submission.

Awadhesh Kumar: Data analysis, editing and approval for final submission

Mohd Yusuf: Concept, data analysis, editing, technical support, drafting the manuscript and approval for final submission and correspondence.

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Conflicts of Interest

The authors declare no conflict of interest.

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