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Molecular Docking and ADME Analysis of the novel compound [(Z)-1a,5-dimethyl-9-methylene-8-oxo1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa bicyclo(8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate] isolated from *Tanacetum dolicophyllum* (Kitam.) Kitam

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Abstract
In contemporary drug design, molecular docking is essential for understanding drug-receptor interactions. The present study aimed to use molecular docking to determine the anticancer potential of the bioactive compound [(Z)-1a,5-dimethyl-9-methylene -8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate] isolated from *Tanacetum dolicophyllum* (Kitam.) Kitam. The outcome demonstrated that the molecule obtained from *T. dolicophyllum* binds with a stronger affinity and lower free energy than roflumilast (the control ligand), with 1XMU exhibiting a glide score of -6.379 Kcal/mol and -6.14 Kcal/mol, respectively. When the binding energy is negative, the ligand and target protein are well aligned, which may have therapeutic benefits in suppressing microbial activity. Additionally, as determined by *in-silico* Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) calculations, the synthesized compound validates the drug-likeness within the specified ranges: molecular weight between 150 and 500g/mol, Topological Surface Area (TPSA) polarity between 20 and 130 Å2, lipophilicity between -0.7 and +5.0, Log S not exceeding 6, flexibility not exceeding 9, and saturation not less than 0.25. An evaluation of docking score and ADME properties reveals that the synthesized compound exhibits notable characteristics, positioning it as a promising candidate for drug development. The compound showed adherence to these requirements, indicating favorable *in-vivo* drug penetration and absorption properties.

Keywords: Anticancer, Drug penetration, Lipinski's rule of five, Molecular docking, Roflumilast.

INTRODUCTION

The crucial procedure known as "molecular docking" determines the ideal alignment—also called the "best-fit"—between a ligand and its target protein, making intermolecular complex prediction easier. Molecular docking, which is widely used in contemporary drug design, provides a deep comprehension of drug-receptor interactions (Lee and Kim 2019). Molecular docking is an essential method in drug research because it can anticipate the binding affinity of these interactions and provide information about the binding orientation of medicines and their target proteins, which helps to predict affinity (Sharma *et al.*, 2010).
Similarly, bio-informatics has advanced alongside improved drug discovery techniques, making it possible to

test compounds based on constituents present in medicinal plants (Vijesh *et al.*, 2011). One economical method for the development and analysis of medications is molecular docking. It details the interactions between pharmaceuticals and receptors, explaining how the target proteins will bind to the medications to produce a strong binding at the ligand's binding site. Extensive research efforts have been directed towards the fight against life-threatening disease due to the pressing need for new anticancer drugs. There is an urgent need for anticancer agents that are more accurate and effective than existing drugs and less hazardous (Sliwoski *et al.*, 2014; Ndombera *et al.*, 2019).

These days, computational techniques are essential for predicting the ADME characteristics of pharmaceuticals and offer useful information in addition to experimental findings (Sean *et al.*, 2024). These computer models provide information about the pharmacokinetics, physiochemical characteristics, and therapeutic potential of many substances. Of these tools, Swiss ADME is a well-known platform run by the Swiss Institute for Bioinformatics that helps with drug discovery decision-making by making it easier to analyze ADME parameters for medicinal compounds (Luca *et al.*, 2025). It makes it possible to assess Lipinski's concept of 5, crucial in determining oral bioavailability and drug-likeness (Lipinski *et al.*, 2012).

A variety of traits are included in the concept of drug-likeness, such as molecular flexibility, hydrophobicity, electron distribution, molecular weight, and hydrogen bonding qualities. The features of Swiss ADME include gastrointestinal absorption, glycoprotein efflux/retention prediction, and BOILED-Egg evaluation (Daina *et al.*, 2016). Additionally, it provides predictions regarding blood-brain barrier penetration and substrate inhibition of the Cytochrome P450 enzyme, addressing pseudo-affirmative outcomes that are frequently contested in biochemical evaluation with an objective degree of accuracy (Matlock *et al.*, 2018; Ndombera *et al.*, 2019).

Similarly, bio-informatics has advanced alongside improved drug discovery techniques, making it possible to test compounds based on constituents present in medicinal plants. One economical method for the development and analysis of medications is molecular docking. It details the interactions between pharmaceuticals and receptors, explaining how the target proteins will bind to the medications to produce a strong binding at the ligand's binding site.

The synthesized chemical in this research study was evaluated in silico by the Swiss ADME website (https://www.swissadme.ch/). The screening aimed to analyze several ADME behaviours, such as pharmacokinetics, lipophilicity, physiochemical properties, water solubility, medicinal chemistry, and drug-likeness of the produced compounds.

MATERIALS AND METHODS

Bioinformatics

In present study docking studies with target protein 1XMU (Catalytic Domain of Human Phosphodiesterase 4b [PDE4B] in Complex with Roflumilast) to investigate the anticancer property of the plant compound [(Z)-1a,5-dimethyl-9-methylene-8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate]. For this study, the Schrodinger molecular drug discovery suite's glide tool was employed (Schrodinger, 2018; Sliwoski *et al.*, 2014).

Data Given-

Protein: 1XMU

Control Ligand: Roflumilast

Target Ligand: [(Z)-1a,5-dimethyl-9-methylene-8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate]

Protein preparation and receptor grid generation

The protein was improved and tweaked as part of the protein preparation process, which was done using the Protein Preparation Wizard in the Schrödinger software (Bharathi *et al.*, 2014). Any hydrogen atoms and side chains are found and filled in during the procedure using the prime tool. In addition, it corrects metal ions, cofactors, water molecules, and heavy atoms. With a sequence length of 398 and a structural weight of 92.6 kDa, the 1XMU (Catalytic Domain of Human Phosphodiesterase 4B in Complex with Roflumilast) is categorized as a hydrolase enzyme. To find the most stable energy state, the protein was subjected to energy minimization using the OPLS4 force field (Ndombera *et al.*, 2019; Alland *et al.*, 2005; Lipinski *et al.*, 2012). A cubicle grid was created around the active portion of the attached amino acid to hold all of the residues of the functional amino acid.

Ligand preparation

The docking study's ligands were chosen from the literature. Using ACD/ChemSketch 2019.1.2, the structure of the plant chemical of *T. dolicophyllum* was modeled. The ligand structures underwent three-dimensional optimizations stored as ".mol files." Studies on molecular docking made use of this improved structure. The phytochemicals were produced using the LigPrep interface in Schrodinger with an OPLS4 force field (Friesner *et al.*, 2006; Adane *et al.*, 2011).

Molecular docking

Molecular docking investigations were conducted using the GLIDE ligand docking program. It considers the ready-made ligands and was screened using the receptor gird using the extra precision approach, which includes a variety of structural characteristics and ligand-

specific modifications. The best-docked score, docked position, and additional GLIDE scores were generated for every ligand. The relative binding energies and energy characteristics of specific ligands, receptors, and complex structures that contribute to the total binding energies are ascertained using this method (Sable and Ahire, 2024; Ndombera *et al.*, 2019).

Swiss ADME

Swiss ADME software was used to evaluate each compound's unique ADME properties. The software incorporates a chemical sketcher driven by ChemAxon's Marvin JS enabling us to sketch and change 2D chemical structures (Tajane *et al.*, 2024), as readily demonstrated in Fig. 1. The produced compounds' structures were then transformed into the standard SMILES format and sent for computation (Sable and Ahire, 2024; Egan *et al.*, 2000).

Structure and bioavailability radar

The bioavailability radar provides a preliminary indication of how drug-like the chemical is. The optimal physicochemical area inside this radar, where characteristics favorable to oral bioavailability are anticipated to dwell, is represented by the pink region. As indicated in Table 1, six important physicochemical properties are taken into account: SIZE, Flexibility (FLEX), Insolubility (INSOLU), Polarity (POLAR), Lipophilicity (LIPO), Insaturation (INSATU), and SIZE. Based on how well the compounds correspond with these important characteristics, this graphic helps evaluate the molecules' possible oral bioavailability (Sable and Ahire, 2024; Baell and Holloway, 2010).

Physiochemical characteristics

Details such as molecular weight, molecular formula, number of heavy and aromatic heavy atoms, number of donors and acceptors of hydrogen bonds, number of rotatable bonds, molar refractivity, csp3 hybridization, and Topological Polar Surface Area (TPSA) are provided. By computing these values, the properties of the compounds were analyzed with accuracy and dependability (Sable and Ahire, 2024; Boyle *et al.*, 2011).

Lipophilicity

Among the essential physiochemical characteristics (Testa *et al.*, 2000; Arnott *et al.*, 2012), lipophilicity (Leeson *et al.*, 2007) is a complementary component in drug designing and medicinal chemistry discovery. Five freely accessible models—iLOGP, MLOGP, XLOGP3, WLOGP, and SILICOS-IT—are provided by Swiss ADME to evaluate a compound's lipophilicity profile. A thorough evaluation of the compound's lipophilicity is provided by the Consensus log Po/w value obtained from all of these techniques by the arithmetic mean (Baell and Holloway, 2010).

Water solubility

Drugs are divided into four types based on their permeability and solubility: 1) very permeable and very soluble 2) Low solubility and very permeable 3) Very soluble and low permeability 4) According to Savjani *et al.* (2012), low soluble and low permeable. Two techniques are integrated into the Swiss ADME tool to assess water solubility. Firstly, it utilizes the ESOL model, and secondly, it applies the Ali model (Amidon *et al.*, 1995). These techniques deviate from the fundamental general solubility equation (Yalkowsky *et al.*, 1980). Swiss ADME also includes a third predictor that was created by SILICOS-IT. This predictor has an enhanced correlation coefficient of R2=0.75 after the linear coefficient is modified by the molecular weight.

Pharmacokinetics

A clear distinction between two computed descriptors that are favorable for gastrointestinal (GI) absorption—pharmacokinetics ALOGP and PSA—emerges. Well-absorbed molecules tend to group together in an oval pattern within this defined region, which is also known as the Egan egg. The Egan egg is a helpful tool for assessing the prognostic potential of models for GI absorption and passive diffusion-mediated brain access. The BOILED-Egg (Brain or IntestinaL Estimate D penetration prognostic model) was created as a result of this idea (Daina and Zoete, 2016; Di *et al.*, 2012; Brito *et al.*, 2015; Montanari *et al.*, 2015). Between 50% and 90% of medicinal compounds undergo biotransformation, and cytochrome P450 isoenzymes play a critical role in this process. Five key isozymes—CYP2D6, CYP3A4, CYP2C9, CYP1A2, and CYP2C19—are primarily involved in this process (Ndombera *et al.*, 2019; Ogu *et al.*, 2000). Swiss ADME uses the support vector machine (SVM) algorithm to deal with this complexity. SVM is especially used for datasets identified as substrates or non-substrates, making it easier to perform binary categorization tasks

Table 1. Standards for describing bio-availability of drugs in radar via SwissADME (Baell and Holloway 2010; Boyle *et al.,*2011; Lipinski *et al.,* 2001; Egan *et al.,* 2000; Brenk *et al.,* 2008).

Radar	The area marked in the coloured zone represents the optimal physiochemical environment for ensuring oral bioavailability
Lipophilicity	-0.7<XLogP3<+5.0
Size	mol<MV<500 g/mol
Polarity	20Å^2<TPSA<130 Å^2
Insolubility	-6<LogS (ESol)<0
Insaturation	0.25<Fraction Csp3<1
Flexibility	0<No. of rotable bonds<9

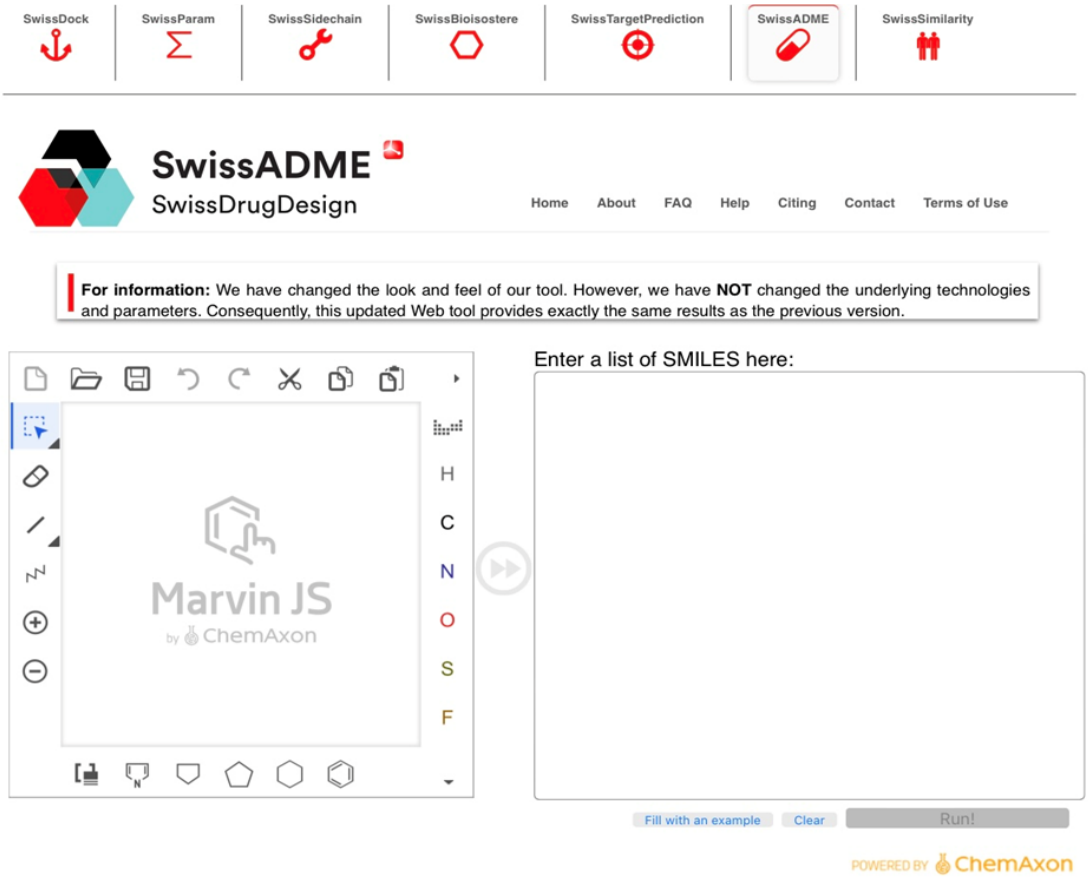

Fig. 1. *Swiss ADME software to evaluate the ADME characteristics of the compound*

crucial for comprehending drug interactions and metabolism.

Drug-likeness

It assesses the likelihood that a chemical will be bioavailable enough to be taken orally. Pfizer created the Lipinski model, which is the groundwork for the groundbreaking rule of 5 (Sable and Ahire, 2024; Lipinski *et al.*, 2001) for the physicochemical profile-based characterization of small compounds. These characteristics include an estimated partition coefficient (MLOGP) of ≤ 4.15 and a molecular weight of less than 500 Da (Baell and Holloway, 2010; Sable and Ahire, 2024).

Medicinal chemistry

This seeks to encourage and assist medicinal chemists in their drug discovery efforts. Regardless of the protein targets under investigation, Pan Assay INterference compounds (PAINS) are the chemicals that exhibit strong responses in research. Using an alternative strategy, Brenk *et al.* (2008) concentrate on substances that have low hydrophobicity (Lipinski *et al.*, 2001; Mujawar *et al.*, 2023) to increase the likelihood of lead optimization (Hann and Keseru, 2012; Sable and Ahire, 2024; Mujawar *et al.*, 2023; Teague *et al.*, 1999).

RESULTS AND DISCUSSION

Molecular docking

The minimal potential energy-enhanced NPACT databases were used to choose the ligand, and the LigPrep program was used to construct several conformers. The ligands were estimated for molecular docking and synthesized following the necessary standards.

Using Protein Preparation Wizard, the 3-D structure or ribbon model of 1XMU was examined and arranged. The grid was created using the glide tool so that receptor 1XMU could locate the active site (Gnana *et al.*, 2024; Mujawar *et al.*, 2023). The non-covalent interactions between the docked protein and ligand are estimated by the docking score, which also indicates their binding affinity or strength. The Glide tool from the Schrodinger Suite, which is depicted in Fig. 2, was used to evaluate the stability and binding of the 1XMU ligand interaction.

The outcomes of the docking simulation, are displayed in Table 2. The strong binding of the ligand to the target protein was indicated by the negative docking score (Tajane *et al.*, 2024; Schrodinger, 2018; Sliwoski *et al.*, 2014). The unit of energy is Kcal/mol. The plant molecule "[(Z)-1a,5-dimethyl-9-methylene-8-oxo

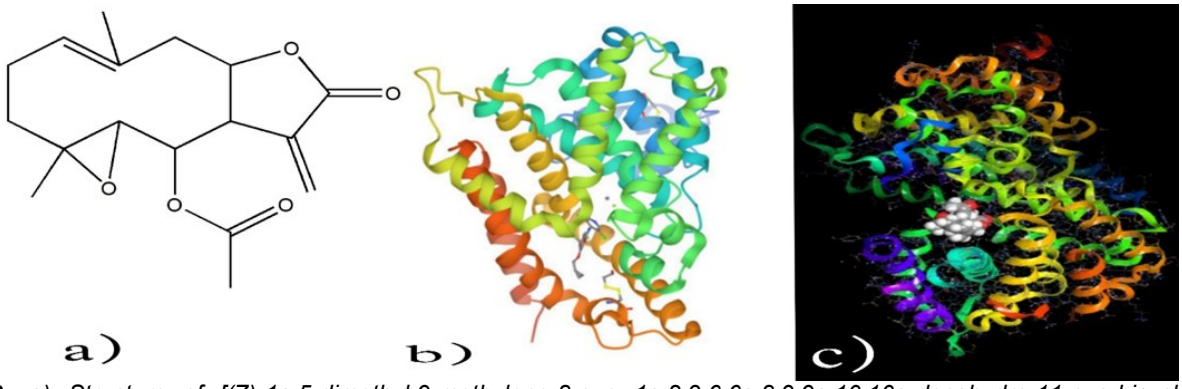

Fig. 2. *a) Structure of [(Z)-1a,5-dimethyl-9-methylene-8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate] compound isolated from T. dolicophyllum; b) Protein target 1XMU; c) Ribbon model illustrating the binding posture of compound into the 1XMU site*

1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate]" has the lowest binding energy, with a docking and glide score of -6.379 Kcal/mol for roflumilast. Glide Ligand Efficiency is the ratio of the compound's non-hydrogen atom count to its Gibbs free energy (G.E.). The compound's glide ligand efficiency was -0.279, while the ligand's was -0.29. The glide Van der Walls Energy (evdw) of the ligand was -28.124 and the compound was -27.659.Table 2 displays the glide coulomb energy (ecoul) of roflumilast as -9.189 and the plant compound as -7.784.

In-silico ADME analysis

The physiochemical properties, lipophilicity, water solubility parameters, pharmacokinetic features, drug-likeness and bioavailability score, medicinal chemistry characteristics, and the bioavailability radar for drug-likeness of compound were all studied using the Swiss ADME web tool (Egan *et al.*, 2000), in that order. The produced chemical completely agrees with Lipinski's *et al.*'s guidelines for finding drug-like characteristics in small molecules. The compound satisfies the reference's requirements for appropriate molecular flexibility, as evidenced by the presence of less than 10 rotatable bonds, a molecular weight of less than 500 Da, H-bond acceptors <10, H-bond donors <5, and a topological surface area <140 Å² (Boyle *et al.*, 2011).

Specifically, the chemical [(Z)-1a,5-dimethyl-9-methylene-8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate] Its chemical formula is $C_{17}H_{22}O_5$, its number of heavy atoms is 22, its fraction Csp3 is 0.65, its number of rotable bonds is 2, its number of H-bond acceptors is 5, its number of H-bond donors is 0, its molar refractivity is 80.24, and its TPSA is 65.13 $Å^2$. Its molecular weight is 306.35 g/mol (Boyle *et al.*, 2011).

For the chemical to have good oral action, its lipophilicity—measured as the consensus Log P—must be less than 5. The produced molecule fits this criterion, showing its potential as an orally active medication. iLOGP.83, XLOGP3 was 1.93, WLOGP was 2.30, MLOGP was 2.00, and SILICOS-IT was 2.65 (Leeson *et al.*, 2007; Mujawar *et al.*, 2023) were the lipophilicity values. Consensus Log Po/w, or the average of the five projections, was 2.34 (Baell and Holloway, 2010; Liu *et al.*, 2011; Mujawar *et al.*, 2023;).

Additionally, the molecule demonstrates perfect solubility in the ESOL, Ali models, and SILICOS-IT model with an ESOL score of -2.82, Ali score of -2.92, and SILICOS-IT score of -2.62 (Daina *et al.*, 2014; Gnana *et al.*, 2024; Liu *et al.*, 2011; Yalkowsky *et al.*, 1980), further indicating its eligibility for development as an oral medication candidate. All of these results point to the compound's desirable drug-like qualities and potential for further advancement in the medicinal chemistry de-

Table 2. Docking results of plant compound and control ligand (Roflumilast) with 1XMU

Title	Docking score	Glide ligand efficiency	Glide ligand efficiency surface area (SA)	Glide ligand efficiency natural log (ln)	Glide gscore	glide evdw	Glide ecoul	Glide energy	glide einternal	Glide emodel
1XMU										
Roflumilast	-6.379	-0.29	-0.813	-1.559	-6.379	-28.124	-9.189	-37.313	2.531	-48.16
Isolated compound	-6.14	-0.279	-0.782	-1.501	-6.14	-27.659	-7.784	-35.443	5.811	-40.952

Table 3. Physiochemical, lipophilicity characteristics and water solubility of the compound(Z)-1a,5-dimethyl-9-methylene-8-oxo1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate

Compound	Canonical SMILES	Physiochemical characteristics		Lipophilicity		Water solubility	
(Z)-1a,5-dimethyl-9-methylene-8-oxo1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno (7,8-b) furan-10-yl acetate	CC(=O)OC1C2C(CC(=CCCC3(C1O3)C)C)OC(=O)C2=C	Molecular formula	$C_{17}H_{22}O_5$	iLOGP	2.83	ESOL	
		Molecular weight	306.35 g/mol	XLOGP3	1.93	Log S	-2.82
		Num. Heavy atoms	22	WLOGP	2.30	Solubility	4.60e-01 mg/ml;1.50 e-03 mol/l
		Num. arom. heavy atoms	0	MLOGP	2.00	Class	Soluble
		Fraction Csp3	0.65	SILICOS-IT	2.65	Ali	
		Num. rotable bonds	2	Consen-sus Log $P_{o/w}$	2.34	Log S	-2.92
		Num. H-bond acceptors	5			Solubility	3.67e-01 mg/ml; 1.20e-03 mol/l
		Num. H-bond donors	0			Class	Soluble
		Molar refrac-tivity	80.24			SILICOS-IT	
		TPSA	65.13Å^2			Log S	-2.62
						Solubility	7.38e-01 mg/ml ; 2.41e-03 mol/l
						Class	Soluble

Num- Number, H-bond-Hydrogen bond, Arom.-Aromatic, TPSA-Topological Polar Surface Area

scribed in Table 3.

Swiss ADME also sheds light on the compound's potential to inhibit different Cytochrome isoforms and its propensity to function as a substrate or non-substrate of BBB permeant (Daina *et al.*, 2014; Liu *et al.*, 2011; Cho and Park, 2008). Additionally, it is computed that the skin permeability coefficient, or Log Kp, is -6.80 cm/s, indicating comparatively lower skin permeability (Gnana *et al.*, 2024; Mujawar *et al.*, 2023; Ndombera *et al.*, 2019; Daina *et al.*, 2014; Liu *et al.*, 2011; Ogu *et al.*, 2000). The chemical has a bioavailability score of 0.55 and is rated positively by all five criteria. Based on the evaluations made by Swiss ADME, these results imply that the molecule has desirable drug-like qualities.

The Swiss ADME study did not identify any PAINS signals for the chemical under investigation. On the other hand, four warning signs were found in the molecule as per Brenk's guidelines: more than two esters, isolated alkenes, Michael acceptor 1, and three membered heterocycles (Lipinski *et al.*, 2001). The bioavailability ra-

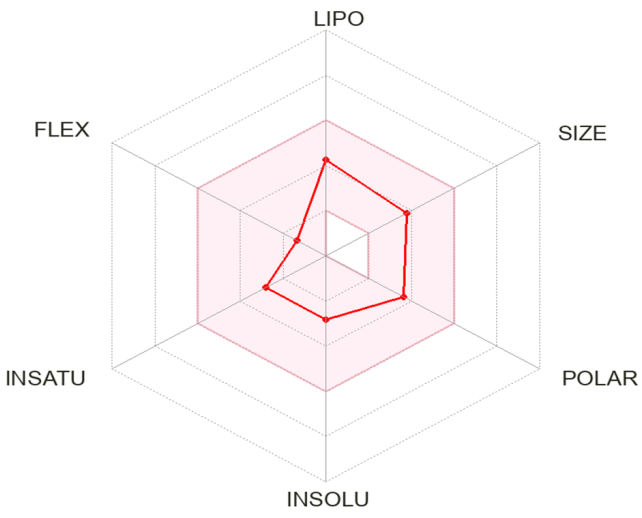

Fig. 3. *Schematic diagram of Bioavailability Radar for Drug likeness of the compound*

Table 4. Pharmacokinetics, Druglikeness rule, Bioavailability score and Medicinal chemistry of the compound (Z)-1a,5-dimethyl-9-methylene-8-oxo1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate

Compound	Pharmacokinetics		Drug likeness & Bioavailability		Medicinal chemistry	
(Z)-1a,5-dimethyl-9-methylene-8-oxo1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate	GI absorption	High	Lipinski	Yes; 0 viola-	PAINS	0 alert
	BBB permeant	Yes	Ghose	Yes	Brenk	4 alerts: three-membered_heterocycle, isolated_alkene, Michael_acceptor_1, more_than_2_ester
	P-gp substrate	No	Veber	Yes	Leadlikeness	Yes
	CYP1A2 inhibitor	No	Egan	Yes	Synthetic accessibility	5.06
	CYP2C19 inhibitor	No	Muegge	Yes		
	CYP2C9 inhibitor	No	Bioavailability Score	0.55		
	CYP2D6 inhibitor	No				
	CYP3A4 in-	No				
	Log K_p (skin permeation)	-6.80 cm/s				

dar was used to assess the drug similarity of the molecule, as indicated in Table 4. As shown in Fig. 3, the pink area on this radar chart represents the optimal reach for certain qualities that are important for drug development. A molecule's potential as a medicine is assessed using the following standards:

Lipophilicity (XLOGP3) within the range of -0.7 to ＋5.0.
Polarity (TPSA) between 20 to 130 $Å^2$.
Solubility (log S) not more than 6.
Molecular weight ranging 150 and 500 Da.
Flexibility not exceeding 9 rotatable bonds.
Saturation not lesser than 0.25.
Fulfilling this requirement contributes to the evaluating our compound's suitability for creating medications with advantageous in vivo drug absorption and penetration properties (Sable and Ahire, 2024; Baell and Holloway, 2010).
The *in-silico* ADME prediction analysis results supports the synthesized drug's computational evaluation and pharmacologically active structure. The feasibility of moving forward with possible hits found throughout the assessment process is highlighted by this alignment.

Conclusion

Promising binding affinity towards XMU was demonstrated by the bioactive molecule [(Z)-1a,5-dimethyl-9-methylene-8-oxo 1a,2,3,6,6a,8,9,9a,10,10a-decahydro-11-oxa-bicyclo (8.1.0) undeca-1(10),4-dieno(7,8-b) furan-10-yl acetate]. In the molecular docking studies, the plant molecule with the lowest binding energy, -6.14 Kcal/mol, was found to have the lowest glide score of roflumilast, -6.379 Kcal/mol. The ligand and target protein are more tightly bound or have a complicated, promising alignment when the binding energy is negative. An assessment of ADME qualities indicates that the synthesized compound possesses significant physicochemical and pharmacokinetic properties, making it a strong candidate for medicinal development. This work demonstrates how easily novel and fascinating structures can be identified using the docking and ADME method. The importance of the results in relation to the novel compounds' potential as anticancer drug. The results suggest that *T. dolicophyllum* could yield reliable and effective anti-cancer medications. Additional research is required to examine the bioactivity of novel medications and conduct clinical trials.

Conflict of interest

The authors declare that they have no conflict of interest.

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