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Exploring Anti-Angiogenic Potential of 1, 3, 4-Oxadiazole Derivatives of Substituted Benzoyl Chloride Via Swissadme Tool

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Abstract: Anti-angiogenic therapy, a traditional strategy in cancer treatment, functions by restricting the formation of new blood vessels, thereby cutting off the supply of oxygen and nutrients to tumor cells. It primarily targets the vascular endothelial growth factor (VEGF) pathway, helping to suppress angiogenesis and improve the outcomes of immunotherapy. The development of novel anti-angiogenic agents is crucial for advancing cancer therapy, and in silico tools have become essential for accelerating the drug discovery process. In this study, ten 1,3,4-oxadiazole derivatives of substituted benzoyl chloride were evaluated for their drug-likeness and pharmacokinetic properties using the Swiss ADME web tool. Key physicochemical descriptors—including molecular weight, topological polar surface area, hydrogen bonding capacity, lipophilicity, and molecular flexibility were assessed alongside drug-likeness filters such as Lipinski, Veber, and Muegge rules. All derivatives demonstrated favorable profiles, with minimal violations, no PAINS alerts, and moderate bioavailability scores (0.55). Despite minor alerts under Brenk and lead-likeness criteria, the compounds exhibited acceptable synthetic accessibility, suggesting good potential for further development. These findings highlight the utility of SwissADME in guiding the early-stage evaluation of drug-like properties, supporting the continued investigation of 1,3,4-oxadiazole scaffolds as promising candidates for anti-angiogenesis therapy.

Key Words – Anti-angiogenesis, VEGF(Vascular endothelial growth factor), SwissADME, 1,3,4-oxadiazole

I. Introduction

The process of angiogenesis, which creates new blood vessels from preexisting endothelium, is essential for many physiological and pathological processes, such as wound healing, embryonic development, chronic inflammation, tumor progression, and metastasis.[1]Current chemotherapeutic drugs have a number of drawbacks, such as chemoresistance, the emergence of unwanted side effects, and a lack of selectivity. The creation of innovative small compounds with few adverse effects and the capacity to target tumor cells specifically is therefore needed but unmet.[2]This highlights the need for novel molecules with enhanced pharmacokinetic properties and safety profiles to serve as potential future therapeutics for anti-angiogenic treatment The pharmacological actions of substituted 1,3,4-oxadiazoles have been found to be diverse and include antibacterial, antimycobacterial, antifungal, anti-inflammatory, analgesic, anticonvulsant and anticancer qualities. Recently shown that compounds containing oxadiazole have the ability to cause cytotoxicity and antiproliferative effects on a range of cancer cell lines .[3]In silico approaches offer a faster, more efficient, and cost-effective alternative to traditional drug discovery, significantly reducing time, labour, and expenses in developing new drugs.[4] In silico techniques have become increasingly popular in small molecule drug discovery, aiding hit generation, lead optimization, and property prediction. SwissADME, a free and accessible tool, efficiently predicts physicochemical, pharmacokinetic, and drug-likeness parameters, supporting reliable analysis in medicinal chemistry and early drug development stages.[5] SwissADME was used in this investigation to investigate a number of 1,3,4-oxadiazole derivatives of substituted benzoyl chloride . By forecasting their pharmacokinetic characteristics and ensuring that they adhere to drug-likeness guidelines, the objective is to assess their potential for the therapy of angiogenesis.

II. Materials and Method

Swiss ADME

SwissADME is a freely accessible web-based tool available at http://www.swissadme.ch, offering a comprehensive suite of fast and reliable predictive models for evaluating physicochemical properties, pharmacokinetics, drug-likeness, and medicinal chemistry friendliness. It features in-house developed methods such as the BOILED-Egg model, iLOGP, and the Bioavailability Radar, which provide valuable insights in the early stages of drug discovery. Designed with a user-friendly interface, the platform allows for easy input and interpretation of results without requiring any login. Both specialists and users without expertise in cheminformatics or computational chemistry can efficiently predict key parameters for a wide range of molecules, greatly aiding their drug development efforts.[6]

Structure and bioavailability radar:

The bioavailability radar chart is a valuable tool for assessing a molecule's physicochemical and drug-likeness properties by predicting six key descriptors. These include: lipophilicity (LIPO), where the log P (partition coefficient between n-octanol and water) should range between −0.7 and +5.0; molecular size, ideally within 150–500 Da; polarity (POLAR), measured by topological polar surface area (TPSA), which should lie between 20 and 130 Å²; insolubility (INSOL), with the water solubility (log S) not

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exceeding −6; unsaturation (UNSAT), requiring a minimum sp^3 carbon fraction of 0.25; and flexibility (FLEX), with no more than 9 rotatable bonds. The radar plot displays these parameters against an ideal range, shown as a pink area. For a compound to be classified as drug-like, its radar must entirely fall within this defined zone. Compounds that meet these requirements are more likely to have (Figure 1) excellent oral bioavailability characteristics[7]

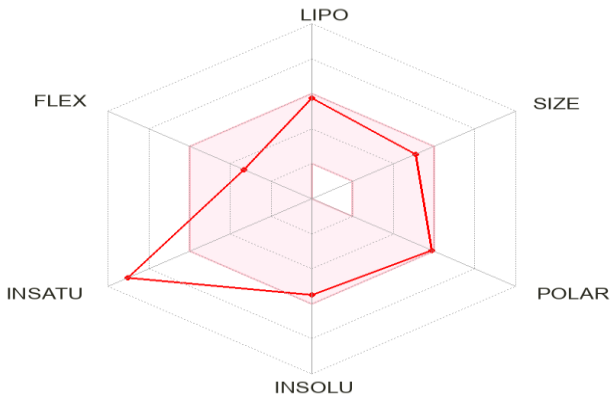

Figure 1 - Bioavailability Radar of Derivative 1

Physicochemical Properties.

This section includes fundamental molecular and physicochemical descriptors such as molecular weight (MW), molecular refractivity (MR), counts of certain atom types, and polar surface area (PSA). These parameters are computed using OpenBabel version 2.3.0.[8] PSA is estimated using a fragment-based approach called topological polar surface area (TPSA), which accounts for sulfur and phosphorus as polar atoms. TPSA has been widely recognized as an effective descriptor for predicting ADME-related properties, especially for assessing a molecule's ability to cross biological barriers like the intestinal lining and the blood–brain barrier.[9]

Lipophilicity.

The partition coefficient between n-octanol and water (log P o/w) is a classical and widely used descriptor for assessing lipophilicity, a key physicochemical property in pharmacokinetics and drug discovery. Due to its critical role, SwissADME features a dedicated section for (log P o/w) prediction. Numerous computational models have been developed to estimate this value, each showing varying degrees of performance across different chemical datasets. A commonly adopted strategy involves using multiple predictive models to either select the most appropriate one for a specific chemical series or to derive a consensus value, which enhances prediction reliability[10]. To ensure model diversity and increase accuracy, SwissADME incorporates five freely available and methodologically distinct models: XLOGP3, an atomistic method that uses corrective factors and a knowledge-based fragment library; WLOGP, a fragmental approach based on the Wildman and Crippen model; MLOGP, a topological method built on a linear relationship with 13 molecular descriptors; SILICOS-IT, a hybrid model combining 27 molecular fragments and 7 topological descriptors; and iLOGP, an in-house physics-based method that estimates free energy of solvation in n-octanol and water using the Generalized-Born and solvent-accessible surface area (GB/SA) model. The consensus (log P o/w) is calculated as the arithmetic mean of these five predictions, providing a balanced and reliable estimate of a compound's lipophilicity.[11]

Solubility

Having a soluble molecule significantly aids various stages of drug development, particularly in terms of ease of handling and formulation. For discovery programs aimed at oral administration, solubility is a key factor affecting drug absorption. Similarly, drugs intended for parenteral use must exhibit high water solubility to ensure delivery of an adequate dose in a small volume. SwissADME incorporates two topological approaches to predict water solubility. The first is based on the ESOL model, while the second is derived from the method proposed by Ali et al. Unlike the original general solubility equation—which includes the melting point parameter, a difficult property to predict—both methods omit this factor. They also show strong linear correlations with experimental solubility values (R^2 = 0.69 and 0.81, respectively). A third solubility predictor in SwissADME, developed by SILICOS-IT, employs a fragment-based approach adjusted by molecular weight and demonstrates a correlation coefficient of R^2 = 0.75.[12]

Pharmacokinetics

SwissADME features an intuitive two-dimensional graphical approach—plotting ALOGP against PSA—to visually represent the likelihood of passive gastrointestinal absorption and brain penetration, commonly referred to as the Egan egg and the BOILED-Egg model (Figure 2). The main elliptical "egg" zone highlights compounds with a high probability of intestinal absorption, while the yellow "yolk" denotes potential for blood–brain barrier penetration. This visualization tool enables quick and dependable

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predictions during early stages of drug discovery. In addition, SwissADME uses support vector machine (SVM) models to predict whether molecules are substrates or inhibitors of critical efflux transporters, such as P-glycoprotein, and key cytochrome P450 enzymes, including CYP1A2, CYP2C19, CYP2C9, CYP2D6, and CYP3A4. These classifiers are trained on extensive datasets and validated through cross-validation and external test sets, consistently showing strong predictive performance with accuracies around 0.7–0.8 and AUC scores between 0.8 and 0.9. Combined, the BOILED-Egg visualization and SVM-based predictions form a robust, integrated platform for evaluating oral bioavailability, CNS penetration, and potential metabolic interactions of drug candidates.[13]

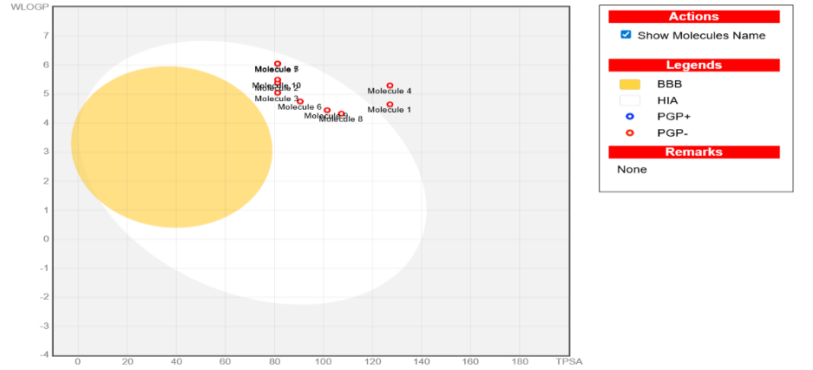

Figure 2 - Boiled Egg Model of 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Drug likeliness

Drug likeliness refers to the qualitative assessment of a molecule's potential to become an orally active drug, particularly in relation to bioavailability. This concept stems from structural and physicochemical evaluations of compounds that have progressed far enough in development to be considered viable oral drug candidates. Drug-likeness is widely used to screen chemical libraries by eliminating molecules that likely possess poor pharmacokinetic profiles. SwissADME provides access to five distinct rule-based filters, each defining a set of property ranges within which a molecule is considered drug-like. These filters were largely developed by major pharmaceutical companies to enhance the quality of their proprietary compound libraries. The Lipinski rule-of-five (Pfizer) was the first of its kind, followed by filters from Ghose (Amgen), Veber (GSK), Egan (Pharmacia), and Muegge (Bayer). By offering multiple criteria, SwissADME allows users to either adopt a consensus approach or choose the filter that best aligns with their project goals and chemical space. Any violation of these drug-likeness rules is clearly indicated in the output panel.[14]

Medicinal Chemistry

This section is designed to assist medicinal chemists in their routine drug discovery efforts. It uses two complementary pattern recognition approaches to identify potentially problematic molecular fragments. One such category is PAINS (pan-assay interference compounds), also known as frequent hitters or promiscuous compounds. These are molecules that contain substructures known to produce strong assay responses regardless of the target protein, often resulting in false-positive biological signals. Baell identified these fragments by analyzing six distinct assay systems and isolating 481 recurring substructures commonly found in compounds active across two or more assays. SwissADME flags a warning if any of these problematic moieties are detected in the compound being evaluated.[15]

III. Results

Chemdraw software version 16.0.1.4(77) was used to draw the structures of the 1,3,4-oxadiazole derivatives of substituted benzoyl chloride (Figure 3). The SMILES of these compounds were then retrieved and put into Swiss ADME software to predict their physicochemical properties. Table 1-7 presents the tabulated results.

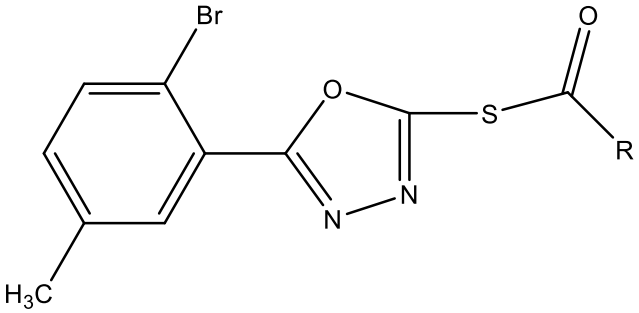

Figure 3- 1,3,4-Oxadiazole Derivatives of Substituted benzoyl Chloride

Where R = Substituted benzoyl chlorides.

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Table 1 -General characteristics of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl.no	Substituted benzoyl chloride (R)	Compound	Molecular Formula	SMILES	Molecular weight
1.	4-nitro benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-nitrobenzothioate	$C_{16}H_{10}BrN_3O_4S$	Cc1ccc(c(c1)c1nnc(o1)SC(=O)c1ccc(cc1)[N+](=O)[O-])Br	420.24 g/mol
2.	4-chloro benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-chlorobenzothioate	$C_{16}H_{10}BrClN_2O_2S$	Clc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	409.68 g/mol
3.	4-methyl benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-methylbenzothioate	$C_{17}H_{13}BrN_2O_2S$	Cc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	389.27 g/mol
4.	2-chloro-4-nitro benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 2-chloro-4-nitrobenzothioate	$C_{16}H_9BrClN_3O_4S$	Cc1ccc(c(c1)c1nnc(o1)SC(=O)c1ccc(cc1Cl)[N+](=O)[O-])Br	454.68 g/mol
5.	4-bromo-2-fluoro benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-bromo-2-fluorobenzothioate	$C_{16}H_9Br_2FN_2O_2S$	Brc1ccc(c(c1)F)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	472.13 g/mol
6.	4-methoxy benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-methoxybenzothioate	$C_{17}H_{13}BrN_2O_3S$	COc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	405.27 g/mol
7.	3,4-dichloro benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 3,4-dichlorobenzothioate	$C_{16}H_9BrCl_2N_2O_2S$	Cc1ccc(c(c1)c1nnc(o1)SC(=O)c1ccc(c(c1)Cl)Cl)Br	444.13 g/mo
8.	4-amino benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-aminobenzothioate	$C_{16}H_{12}BrN_3O_2S$	Nc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	390.25 g/mol
9.	4-hydroxy benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-hydroxybenzothioate	$C_{16}H_{11}BrN_2O_3S$	Oc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	391.24 g/mol
10.	4-bromo benzoyl chloride	S-(5-(2-bromo-5-methylphenyl)-1,3,4-oxadiazol-2-yl) 4-bromobenzothioate	$C_{16}H_{10}Br_2N_2O_2S$	Brc1ccc(cc1)C(=O)Sc1nnc(o1)c1cc(C)ccc1Br	454.14 g/mol

Table 2-Physicochemical Properties of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl No	Num. heavy atoms	Num. arom. heavy atoms	Fraction Csp3	Num. rotatable bonds	Num. H-bond acceptors	Num. H bond donors	Molar refractivity	TPSA ($^0A^2$)
1.	25	17	0.06	5	6	0	97.85	127.11
2.	23	17	0.06	4	4	0	94.04	81.29
3.	23	17	0.12	4	4	0	94.00	81.29
4.	26	17	0.06	5	6	0	102.86	127.11
5.	24	17	0.06	4	5	0	96.69	81.29
6.	24	17	0.12	5	5	0	95.52	90.52
7.	24	17	0.06	4	4	0	99.05	81.29
8.	23	17	0.06	4	4	1	93.43	107.31

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9.	23	17	0.06	4	5	1	91.05	101.52
10.	23	17	0.06	4	4	0	96.73	81.29

Table 3- Lipophilicity of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl no	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
1.	2.98	4.58	4.65	2.22	2.35	3.36
2.	3.31	5.38	5.39	3.68	5.16	4.58
3.	3.39	5.12	5.05	3.41	5.03	4.40
4.	3.20	5.21	5.30	2.45	3.00	3.83
5.	3.56	5.54	6.06	3.91	5.61	4.94
6.	3.37	4.72	4.75	2.85	4.56	4.05
7.	3.30	6.01	6.05	3.91	5.80	5.01
8.	2.79	4.07	4.33	2.62	3.80	3.52
9.	2.79	4.40	4.45	2.62	4.04	3.66
10.	3.49	5.44	5.50	3.80	5.19	4.68

Table 4- Water Solubility of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl No	ESOL				Ali				SILICOS-IT			
	Log s	Solubility		Class	Log s	Solubility		Class	Log s	Solubility		Class
		mg/mL	mol/L			mg/mL	mol/L			mg/mL	mol/L	
1.	-5.5	1.32e-03	3.13e-06	MS	-6.97	4.47e-05	1.06e-07	PS	-6.48	1.38e-04	3.29e-07	PS
2.	-6.05	3.63e-04	8.86e-07	PS	-6.84	5.91e-05	1.44e-07	PS	-7.73	7.66e-06	1.87e-08	PS
3.	-5.76	6.73e-04	1.73e-06	MS	-6.57	1.04e-04	2.68e-07	PS	-7.52	1.18e-05	3.04e-08	PS
4.	-6.1	3.65e-04	8.03e-07	PS	-7.63	1.07e-05	2.36e-08	PS	-7.07	3.91e-05	8.61e-08	PS
5.	-6.52	1.43e-04	3.04e-07	PS	-7.01	4.64e-05	9.84e-08	PS	-8.18	3.10e-06	6.56e-09	PS
6.	-5.52	1.22e-03	3.02e-06	MS	-6.35	1.81e-04	4.47e-07	PS	-7.24	2.31e-05	5.70e-08	PS
7.	-6.64	1.02e-04	2.29e-07	PS	-7.49	1.42e-05	3.20e-08	PS	-8.31	2.17e-06	4.88e-09	PS
8.	-5.11	3.05e-03	7.82e-06	MS	-6.03	3.66e-04	9.37e-07	PS	-6.77	6.63e-05	1.70e-07	PS
9.	-5.32	1.87e-03	4.78e-06	MS	-6.25	2.21e-04	5.64e-07	PS	-6.55	1.10e-04	2.80e-07	PS
10.	-6.37	1.96e-04	4.31e-07	PS	-6.9	5.67e-05	1.25e-07	PS	-7.92	5.43e-06	1.20e-08	PS

MS: Moderately soluble, PS: Poorly soluble

Table 5- Pharmacokinetics of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl no	GI absorption	BBB permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)
1.	Low	No	No	Yes	Yes	Yes	No	No	-5.61
2.	High	No	No	Yes	Yes	Yes	No	No	-4.98
3.	High	No	No	Yes	Yes	Yes	No	No	-5.04
4.	Low	No	No	Yes	Yes	Yes	No	No	-5.37
5.	High	No	No	Yes	Yes	Yes	No	No	-5.25

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6.	High	No	No	Yes	Yes	Yes	No	No	-5.42
7.	High	No	No	Yes	Yes	Yes	No	No	-4.74
8.	High	No	No	Yes	Yes	Yes	No	Yes	-5.79
9.	High	No	No	Yes	Yes	Yes	No	No	-5.56
10.	High	No	No	Yes	Yes	Yes	No	No	-5.21

Table 6- Drug likeness rule and Bioavailability score of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl no	Lipinski violations	Ghose violations	Veber violations	Egan violations	Muegge violations	Bioavailability Score
1.	0	0	0	0	0	0.55
2.	0	0	0	0	1	0.55
3.	0	0	0	0	1	0.55
4.	0	0	0	0	1	0.55
5.	0	1	0	1	1	0.55
6.	0	0	0	0	0	0.55
7.	0	1	0	1	1	0.55
8.	0	0	0	0	0	0.55
9.	0	0	0	0	0	0.55
10.	0	0	0	0	1	0.55

Table 7-Medicinal Chemistry properties of the 1,3,4 oxadiazole derivatives of substituted benzoyl chloride

Sl no	PAINS	Brenk	Leadlikeness	Synthetic Accessibility
1.	0	3	2	3.39
2.	0	1	2	3.26
3.	0	1	2	3.43
4.	0	3	2	3.36
5.	0	1	2	3.28
6.	0	1	2	3.36
7.	0	1	2	3.28
8.	0	2	2	3.36
9.	0	1	2	3.32
10.	0	1	2	3.33

IV. Discussion

The SwissADME-based in silico evaluation of ten 1,3,4-oxadiazole derivatives of substituted benzoyl chloride revealed that all compounds possessed favorable drug-like characteristics, including acceptable molecular weights (<500 Da), balanced lipophilicity (consensus log P: 3.36–5.01), and no violations of Lipinski's rule, indicating good oral drug-likeness. Most compounds showed moderate solubility and high gastrointestinal absorption, though none were predicted to penetrate the blood–brain barrier—suggesting limited CNS activity, which is beneficial for cancer therapy to avoid neurological side effects. All derivatives were non-substrates for P-glycoprotein and exhibited minimal cytochrome P450 interactions, suggesting low risk of efflux or metabolic instability, with the exception of compound 8, which inhibited CYP3A4. Additionally, the absence of PAINS alerts and acceptable synthetic accessibility scores support their suitability for further development. Although minor violations in Veber, Egan, or Muegge filters and low solubility were observed in a few compounds, the overall pharmacokinetic and medicinal chemistry profiles suggest that these derivatives hold significant promise as lead candidates for anti-angiogenic therapy.

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V. Conclusion

The SwissADME-guided in silico evaluation of 1,3,4-oxadiazole derivatives of substituted benzoyl chloride revealed promising drug-like characteristics, with favorable lipophilicity, oral bioavailability, synthetic accessibility, and no PAINS alerts. While poor solubility remains a limitation for some derivatives, their overall pharmacokinetic and medicinal chemistry profiles support further biological validation. These compounds are viable candidates for continued exploration as anti-angiogenic agents targeting the VEGF pathway in cancer therapy.

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