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SwissADME-Guided Drug-Likeness Evaluation of 1,3,4-Oxadiazole Mannich Derivatives for Parkinson's Disease

Gokul K[a], Anitha K N[b], Arun Kumar H S[a], Vani S Kumbar[a], Chaluvaraju K C[a]*

[*]Department of Pharmaceutical Chemistry, Government College of Pharmacy, Bengaluru-560 027, India.
[b]Department of Pharmacology, Government College of Pharmacy, Bengaluru-560 027, India.

Abstract

Parkinson's disease (PD) is a progressive neurodegenerative disorder marked by the degeneration of dopaminergic neurons in the substantia nigra, leading to motor and non-motor symptoms. MAO-B inhibitors have been studied for enhancing the dopamine levels and thus reduces the symptoms of PD. Various studies have been reported that 1,3,4-oxadiazole compound is potent MAO-B inhibitor. In this study, we designed some of the novel mannich based derivatives of 1,3,4-oxadiazole compounds and conducted an In-silico evaluation of its pharmacokinetic properties and drug-likeness using the SwissADME web-tool. The compound's SMILES notation was input into SwissADME to predict key parameters, including gastrointestinal (GI) absorption, blood-brain barrier (BBB) permeability, lipophilicity, and compliance with drug-likeness rules such as Lipinski's Rule of Five. The predictions indicated high GI absorption and BBB permeability, suggesting favourable oral bioavailability and central nervous system (CNS) penetration. The compound exhibited optimal lipophilicity and did not violate any of the evaluated drug-likeness rules, indicating good drug-like properties. Additionally, the synthetic accessibility score suggested that the compound is amenable to chemical synthesis. These in-silico findings support the potential of the novel oxadiazole derivative as a promising candidate for further development as a therapeutic agent for PD. Future studies will focus on the synthesis of the compound and experimental validation of its MAO-B inhibitory activity.

Key Words - Parkinsons disease, MAO-B inhibitors, SwissADME, SMILES notation, 1,3,4-oxadiazole

1. Introduction

Parkinson's disease (PD) is one of the most common neurological diseases that affects millions of people worldwide and it is characterized by motor dysfunction due to degeneration of dopamine in the substantia nigra.The degeneration is caused due to oxidative stress, α-synuclein aggregation and mitochondrial function (Christopher Kobylecki,2020). Current treatment strategies onlyoffers symptomatic relief and are often associated with several. adverse effects or diminishing efficacy over the time and also there is no permanent cure (Poewe W et.,al.2017). This demands a need for novel molecules with improved pharmacokinetic and safety profiles to serve as future therapeutics for PD.

1,3,4-Oxadiazole is a versatile heterocycle with proven bioactivity across a range of therapeutic areas, including antimicrobial, anticancer, and various CNS disorders (Marcin Luczynski et al., 2022).

Mannich bases are the highly reactive species which has been documented for several biological activities including Neurological activities (Senthil Kumar Raju et al.,2023).

As a matter of drug design before proceeding to synthesis and biological evaluationsof drugs it is good to predict its pharmacokinetic properties, oral bioavailability, drug-likeness, and CNS penetration by using in-silico methods(Badaway et al.,2021). SwissADME is an accessible computational tool that supports drug design by predicting a wide array of molecular and pharmacokinetic properties. It offers a suite of predictive models to evaluate lipophilicity, solubility, absorption, bioavailability, and overall drug-likeness. Among its unique features are internally developed models such as the BOILED-Egg, which predicts gastrointestinal absorption and brain access; iLOGP, which estimates partition coefficients; and the Bioavailability Radar, a visual tool for assessing oral bioavailability based on key physicochemical criteria(Antoine Daina et al., 2017).

In this study, a series of Mannich base derivatives of 1,3,4-oxadiazole were analyzed using SwissADME. The aim was to evaluate their potential as CNS-active agents for the treatment of Parkinsonism through the prediction of their pharmacokinetic properties and compliance with drug-likeness rules.

2.Materials and Method

2.1 Swiss ADME

SwissADME is a freely available web-based tool(http://www.swissadme.ch/) developed by the Swiss Institute of Bioinformatics, designed to predict pharmacokinetic parameters, physicochemical properties, drug-likeness, and medicinal chemistry friendliness of small molecules. It features an

intuitive interface that allows researchers to input chemical structures in SMILES (Simplified Molecular Input Line Entry System) format—one per line—to evaluate compounds of interest. The platform outputs result in multiple formats, including descriptive tables, interactive plots, and downloadable spreadsheets, enabling comprehensive assessment of absorption, distribution, metabolism, and excretion profiles (Antoine Daina et al., 2017).

2.2 Structure and bioavailability radar:

At the outset, the chemical structures of the selected compounds were represented using the SMILES (Simplified Molecular Input Line Entry System) format. To determine the drug-likeness of these molecules, the bioavailability radar approach was employed, which evaluates six essential physicochemical properties: lipophilicity, molecular size, polarity, water solubility, saturation, and flexibility. Each property is assessed based on specific thresholds that are considered optimal for oral bioavailability. Lipophilicity, predicted by the XLOGP3 model, should fall between –0.7 and +5.0. The ideal molecular weight is within the 150–500 g/mol range. Polarity, measured by the topological polar surface area (TPSA), is expected to range from 20 to 130 Å. A log S value no greater than 6 is preferred for adequate solubility. Saturation is represented by the fraction of sp^3-hybridized carbons, which should be at least 0.25. Lastly, the number of rotatable bonds, reflecting molecular flexibility, should not exceed nine. Compounds satisfying these criteria are more likely to possess (figure 1) favourable oral bioavailability profiles (Pooja A.Chimane et al., 2025).

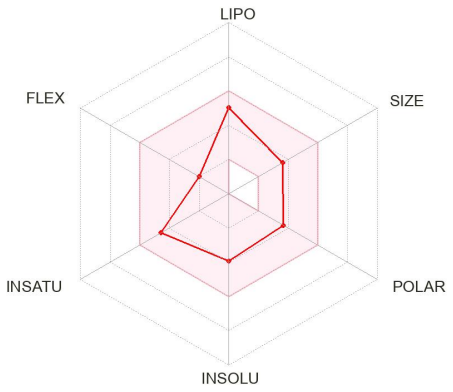

Figure 1 - Bioavailability Radar of Derivative 1

2.3 Physicochemical Properties.

This section describes the calculation of key molecular and physicochemical descriptors—such as molecular formula, molecular weight, heavy atoms (total and aromatic), fraction of sp^3-hybridized carbons, rotatable bond count, hydrogen bond acceptors and donors, molar refractivity, and topological polar surface area (TPSA)—using Open Babel v2.3.0. (Ranjith D et al., 2019).Polar surface area can be calculated using the TPSA for molecules which have at least on Sulphur, oxygen, phosphorus or nitrogen atom. This property can be used to calculate transport of molecule through a membrane (Peter Ertl et al., 2000)

2.4 Lipophilicity.

Lipophilicity is a key physicochemical characteristic in medicinal chemistry, playing a vital role in drug design and development. It affects the transport of drug through the lipid membrane and plays a major role in binding of drug to its target receptor and thus it's a crucial parameter in drug discovery and development (Ewelina Rutkowska et al., 2013). Lipophilicity significantly influences the ADMET properties of the drug and it is measured usually as Log P. According to Lipinski's rule of 5, a drug with lipophilicity with <5 is said to be a potent molecule with good ADMET properties (Arnott, J. A et al., 2012). SwissADME detects five log P values to evaluate the lipophilicity of the molecule —XLOGP3, an atom-based approach with empirically optimized parameters; WLOGP, which uses atomistic fragment contributions; MLOGP, a topological descriptor model based on 13 molecular features; SILICOS-IT, a hybrid technique combining fragment and topological data; and iLOGP, a physics-based method calculating solvation free energies via a GB/SA framework. Each model provides an independent estimate of n-octanol/water lipophilicity, and their arithmetic mean produces a consensus log P value, enhancing overall prediction accuracy by balancing the strengths and biases of individual methods(Tasmeem T. shaikh et al., 2025).

2.5 Solubility

Solubility can vary significantly depending on the solvent, temperature, and pressure, and is quantified by the saturation concentration—the point beyond which adding more solute no longer increases its concentration in solution (Krishnan A et.al.,). A compound is considered highly soluble if its maximum dose dissolves in 250 mL or less of aqueous medium across a pH range of 1 to 7.5, consistent with standard bioequivalence protocols. SwissADME utilizes three topological models to predict water solubility, all based on the logarithm of molar solubility (Log S): the ESOL model and

the Ali method both omit melting point input and classify solubility on a scale from very soluble to insoluble, showing strong linear agreement with experimental data, while the SILICOS-IT predictor incorporates molecular weight correction and achieves comparable accuracy. SwissADME reports predicted solubility values as Log S and also provides the corresponding concentrations in mol/L and mg/mL along with qualitative classifications, facilitating diverse formulation and drug development analyses (P H Riyadi et.al., 2021).

2.6 Pharmacokinetics

SwissADME integrates an intuitive two-dimensional graphical method—ALOGP versus PSA—to highlight regions associated with passive gastrointestinal absorption and brain permeability, commonly known as the Egan egg and BOILED-Egg model(figure 2). The central elliptical "egg" area identifies molecules likely to be absorbed via the intestine, while the yellow "yolk" indicates potential blood–brain barrier penetration. This visual tool supports rapid, reliable predictions in early drug discovery(Daina et al., 2016). Additionally, SwissADME employs support vector machine (SVM) classifiers to assess whether compounds act as substrates or inhibitors of key efflux transporters (such as P-glycoprotein) and cytochrome P450 isoforms (CYP1A2, CYP2C19, CYP2C9, CYP2D6, and CYP3A4). These models are trained on large datasets and validated through cross-validation and external testing, consistently achieving robust performance metrics (accuracy in the range of approximately 0.7–0.8 and AUC values of 0.8–0.9). Together, the BOILED-Egg framework and SVM-based classifiers provide a comprehensive, efficient platform for evaluating oral absorption, CNS access, and metabolic interaction risks of small molecules
(Miss Tasmeem T. shaikh et al., 2025).

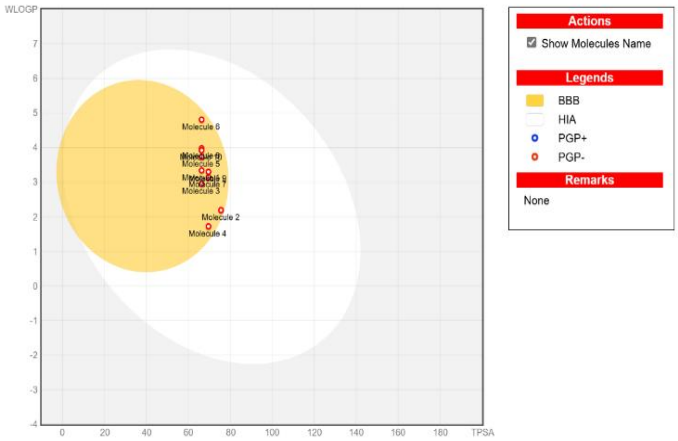

Figure 2 - Boiled Egg Model of 1,3,4-Oxadiazole Mannich Base derivatives.

2.7 Drug likeliness

SwissADME gauges a compound's oral drug potential—termed drug-likeness—using a Bioavailability Radar, where an ideal molecule fits within a pink hexagon overlay. It applies five pharmaceutical industry-derived rule sets—Lipinski, Ghose, Veber, Egan, and Muegge—each defining specific thresholds based on molecular weight, lipophilicity, polar surface area, hydrogen bonding capability, and molecular flexibility. Any deviation flags the compound as potentially problematic for pharmacokinetics. Additionally, SwissADME calculates a bioavailability score estimating the likelihood of achieving ~10% oral bioavailability in preclinical models. Together, these features offer a rapid, integrated assessment to prioritize small molecules for drug development. (Ranjith D et al., 2019)

2.8 Medicinal Chemistry

This segment focuses on the detection of harmful fragments.PAINS, or Pan Assay INterferencecompoundS, are chemical structures that often appear active in multiple biological tests—but not for the right reasons. Instead of genuinely targeting the biology of interest, these compounds interfere with the assay detection system itself. This interference can produce misleading "hits" during drug screening campaigns(Baell et al., 2010). Swiss ADME also integrates Brenk filters which also identifies the harmful fragments present in the compounds. It provides alerts if any of the suspicious fragments are detected in the molecule being analysed. With these two implementation and other Physicochemical filters Swiss ADME also analyses 'Leadlikeness' which aids in designing a Lead molecule (Daina et al., 2016). The objective of this lead-likeness concept is to generate high-affinity hits suitable for high-throughput screening (HTS), allowing for systematic structural modifications during the optimization phase. Typically, leads are refined using rule-based methods, prioritizing compounds with molecular weights between 100 and 350 Da and ClogP values ranging from 1 to 3. These criteria distinguish them from drug-like molecules and enhance their potential for successful development (Omkar J. Yadav et.al. 2024).

3. Results.

The structures of the 1,3,4-oxadiazole derivatives (figure 3) were drawn using Chemdraw software version 16.0.1.4(77) and its SMILES were extracted and pasted in Swiss ADME software to predicts its Physicochemical Properties. The results obtained are tabulated(Table 1-7).

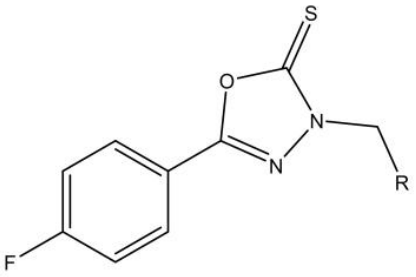

Figure 3- 1,3,4-Oxadiazole Mannich base

Where R = Different secondary amines

Table 1 -General characteristics of the compound

Sl.no	Secondary Amine (R)	Compound	Molecular Formula	SMILES	Molecular weight
1.	Piperidine	5-(4-fluorophenyl)-3-((piperidin-1-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C14H16FN3OS	Fc1ccc(cc1)c1oc(=S)n(n1)CN1CCCCC1	293.36 g/mol
2.	Morpholine	5-(4-fluorophenyl)-3-((morpholin-4-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C13H14FN3O2S	Fc1ccc(cc1)c1oc(=S)n(n1)CN1CCOCC1	295.33 g/mol
3.	Pyrrolidine	5-(4-fluorophenyl)-3-((pyrrolidin-1-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C13H14FN3OS	Fc1ccc(cc1)c1oc(=S)n(n1)CN1CCCC1	279.33 g/mol
4.	N-methylpiperazine	5-(4-fluorophenyl)-3-((4-methylpiperazin-1-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C14H17FN4OS	CN1CCN(CC1)Cn1nc(oc1=S)c1ccc(cc1)F	308.37 g/mol
5.	Azepane	5-(4-fluorophenyl)-3-((azepan-1-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C15H18FN3OS	Fc1ccc(cc1)c1oc(=S)n(n1)CN1CCCCCC1	307.39 g/mol
6.	Benzylpiperdine	3-((4-benzylpiperidin-1-yl)methyl)-5-(4-fluorophenyl)-1,3,4-oxadiazole-2(3H)-thione	C21H22FN3OS	Fc1ccc(cc1)c1nn(c(=S)o1)CN1CCC(CC1)Cc1ccccc1	383.48 g/mol
7.	Benzylpiperazin	3-((4-benzylpiperazin-1-yl)methyl)-5-(4-fluorophenyl)-1,3,4-oxadiazole-2(3H)-thione	C20H21FN4OS	Fc1ccc(cc1)c1nn(c(=S)o1)CN1CCN(CC1)Cc1ccccc1	384.47 g/mol
8.	Ethylpiperidine	3-((4-ethylpiperidin-1-yl)methyl)-5-(4-fluorophenyl)-1,3,4-oxadiazole-2(3H)-thione	C16H20FN3OS	CCC1CCN(CC1)Cn1nc(oc1=S)c1ccc(cc1)F	321.41 g/mol
9.	Phenylpiperazine	5-(4-fluorophenyl)-3-((4-phenylpiperazin-1-yl)methyl)-1,3,4-oxadiazole-2(3H)-thione	C19H19FN4OS	Fc1ccc(cc1)c1nn(c(=S)o1)CN1CCN(CC1)c1ccccc1	370.44 g/mol
10.	Indolin	5-(4-fluorophenyl)-3-(indolin-1-ylmethyl)-1,3,4-oxadiazole-2(3H)-thione	C17H14FN3OS	Fc1ccc(cc1)c1nn(c(=S)o1)CN1CCc2c1cccc2	327.38 g/mol

Table 2 - Physicochemical Properties

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.	20	11	0.43	3	4	0	80.71	66.29
2.	20	11	0.38	3	5	0	76.99	75.52
3.	19	11	0.38	3	4	0	75.91	66.29
4.	21	11	0.43	3	5	0	87.53	69.53
5.	21	11	0.47	3	4	0	85.52	66.29
6.	27	17	0.33	5	4	0	110.01	66.29
7.	27	17	0.3	5	5	0	112.01	69.53
8.	22	11	0.5	4	4	0	90.33	66.29
9.	26	17	0.26	4	4	0	107.76	69.53
10.	23	17	0.18	3	3	0	91.5	66.29

Table 3- Lipophilicity

Sl no	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
1.	3.29	3.29	3.34	2.54	3.7	3.23
2.	3.09	2.07	2.19	1.45	3.09	2.38
3.	3.09	2.93	2.95	2.28	3.48	2.95
4.	3.8	2.26	1.72	2.12	2.68	2.51
5.	3.39	3.65	3.73	2.79	3.92	3.5
6.	4.12	5.15	4.81	3.96	5.18	4.64
7.	4	3.75	3.14	2.91	4.06	3.57
8.	3.61	4.27	3.98	3.44	4.14	3.89
9.	3.58	4.04	3.3	2.95	3.68	3.51
10.	3.24	4.26	3.92	3.32	4.28	3.8

Table 4- Water Solubility

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.	-3.94	3.36e-02	1.15e-04	S	-4.36	1.29e-02	4.39e-05	MS	-4.07	2.50e-02	8.53e-05	MS
2.	-3.18	1.93e-01	6.54e-04	S	-3.29	1.53e-01	5.19e-04	S	-3.53	8.72e-02	2.95e-04	S
3.	-3.65	6.28e-02	2.25e-04	S	-3.98	2.90e-02	1.04e-04	S	-3.8	4.47e-02	1.60e-04	S
4.	-3.37	1.33e-01	4.31e-04	S	-3.36	1.36e-01	4.40e-04	S	-3.51	9.60e-02	3.11e-04	S
5.	-4.23	1.79e-02	5.82e-05	MS	-4.73	5.71e-03	1.86e-05	MS	-4.34	1.40e-02	4.55e-05	MS
6.	-5.6	9.68e-04	2.52e-06	MS	-6.29	1.98e-04	5.16e-07	PS	-6.7	7.58e-05	1.98e-07	PS
7.	-4.72	7.29e-03	1.90e-05	MS	-4.9	4.81e-03	1.25e-05	MS	-5.99	3.93e-04	1.02e-06	MS
8.	-4.63	7.55e-03	2.35e-05	MS	-5.37	1.36e-03	4.22e-06	MS	-4.62	7.76e-03	2.42e-05	MS
9.	-4.9	4.64e-03	1.25e-05	MS	-5.2	2.32e-03	6.26e-06	MS	-5.6	9.37e-04	2.53e-06	MS
10.	-4.9	4.10e-03	1.25e-05	MS	-5.36	1.42e-03	4.33e-06	MS	-5.73	6.07e-04	1.85e-06	MS

Table 5-Pharmacokinetics

Sl no	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor
1.	High	Yes	No	Yes	Yes	Yes	No
2.	High	Yes	No	Yes	Yes	No	No
3.	High	Yes	No	Yes	Yes	Yes	No
4.	High	Yes	No	Yes	Yes	Yes	No
5.	High	Yes	No	Yes	Yes	Yes	No
6.	High	Yes	No	Yes	Yes	Yes	No
7.	High	Yes	No	Yes	Yes	Yes	Yes
8.	High	Yes	No	Yes	Yes	Yes	No
9.	High	Yes	No	Yes	Yes	Yes	No
10.	High	Yes	No	Yes	Yes	Yes	No

Table 6-Drug likeness rule and Bioavailability score

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	0	0.55
3.	0	0	0	0	0	0.55
4.	0	0	0	0	0	0.55
5.	0	0	0	0	0	0.55
6.	0	0	0	0	1	0.55
7.	0	0	0	0	0	0.55
8.	0	0	0	0	0	0.55
9.	0	0	0	0	0	0.55
10.	0	0	0	0	0	0.55

Table 7-Medicinal Chemistry properties

Sl no	PAINS	Brenk	Leadlikeness	Synthetic Accessibility
1.	0	1	0	3.03
2.	0	1	0	3.09
3.	0	1	0	2.96
4.	0	1	0	3.23
5.	0	1	1	3.15
6.	0	1	2	3.44
7.	0	1	2	3.5
8.	0	1	1	3.24
9.	0	1	2	3.36
10.	0	1	1	3.03

4. Discussion

The in-silico evaluation of 1,3,4-oxadiazole Mannich base derivatives using the SwissADME platform revealed a promising pharmacokinetic profile and drug-likeness potential for all ten designed compounds. The physicochemical parameters—including molecular weight, topological polar surface area (TPSA), number of rotatable bonds, and hydrogen bonding capabilities—were within the optimal range, suggesting good oral bioavailability and membrane permeability. Notably, the consensus Log P values ranged between 2.3 and 4.6, indicating balanced lipophilicity favourable for both absorption and CNS penetration.

All compounds demonstrated high predicted gastrointestinal absorption and blood–brain barrier (BBB) permeability based on the BOILED-Egg model, indicating strong potential for CNS activity—critical for Parkinson's disease therapy. Additionally, none of the molecules were flagged as P-glycoprotein (P-gp) substrates, which minimizes concerns of efflux-related CNS exclusion. Most compounds were also predicted to inhibit key CYP450 enzymes (such as CYP1A2 and CYP2C19), an aspect that will need further in vitro verification due to the implications on drug–drug interaction potential. Drug-likeness assessment showed full compliance with Lipinski, Ghose, Veber, and Egan rules across all compounds. Only one compound (benzylpiperidine derivative) showed a violation in Muegge's rule, likely due to its higher molecular complexity. Nonetheless, all derivatives received a bioavailability score of 0.55, indicating moderate oral absorption potential in preclinical models. Importantly, the medicinal chemistry filters provide insights into the lead potential and safety of chemical scaffolds. None of the compounds triggered PAINS(Pan-Assay INterferencecompoundS) alerts, which is a significant positive indicator. PAINS-positive molecules often yield false-positive results in biological assays due to non-specific interactions. Their absence here supports the reliability of these molecules for downstream bioassays without a high risk of assay interference.

However, all compounds showed Brenk alerts, which flag substructures known to be associated with potential toxicity, instability, or poor pharmacokinetics. While a single Brenk alert is not necessarily disqualifying, it suggests that further optimization may be needed during lead refinement to eliminate or replace problematic moieties. These alerts serve as early warnings to guide medicinal chemists during the hit-to-lead transition. Finally, the synthetic accessibility (SA) scores ranged from 2.9 to 3.5, indicating that these molecules are moderately easy to synthesize—an essential consideration for future lab-scale production and optimization.

5. Conclusion.

The SwissADME-guided evaluation of the designed 1,3,4-oxadiazole Mannich base derivatives reveals that these compounds exhibit favourable pharmacokinetic and drug-likeness properties. All derivatives demonstrated high gastrointestinal absorption, good blood–brain barrier permeability, and compliance with major drug-likeness rules, making them strong candidates for CNS-related therapeutic development such as in Parkinson’s disease. The absence of PAINS alerts further strengthens their suitability by reducing the risk of false-positive assay results. While the presence of Brenk alerts suggests potential liabilities, these can be addressed through rational medicinal chemistry optimization. Overall, the study supports these compounds as promising leads for further synthesis and biological validation as MAO-B inhibitors.

6. ACKNOWLEDGMENT

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