



1,3,4-Oxadiazole Scaffold in Medicinal Chemistry: A Review of Pharmacological Applications and Structure–Activity Relationships

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Abstract

The 1,3,4-oxadiazole framework represents a useful heterocyclic nucleus in medicinal chemistry due to its structural flexibility, good bioisosteric characteristics and the breadth of biological activities reported. These scaffold derivatives have demonstrated promising anticancer, antimicrobial, anti-inflammatory, antitubercular, antiviral, anticonvulsant, and antidiabetic activity such that they are potential leads in drug discovery and optimization (Ali et al., 2022; Amini & Vosoogh, 2023; Polat et al., 2024). This review will assess the recent developments in the synthesis, pharmacological uses, structure-activity relationships, and rational design approaches of 1,3,4-oxadiazole derivatives. A structured literature-based review method was used, focusing on peer-reviewed studies that reported synthetic approaches, biological evaluation, SAR interpretation, and computational support for oxadiazole-based compounds. The synthesis methods reviewed consist of classical cyclodehydration, one-pot, oxidative annulation, microwave-assisted, solvent-free, and other green chemistry methods (Li et al., 2025; Pathak et al., 2019; Unresolved source 55, n.d.). The core results suggest that replacement at the 2- and 5-positions of the oxadiazole ring, and conjugation with bioactive pharmacophores have a potent effect on potency, selectivity, and interaction with targets (Chaudhari et al., 2021; Li et al., 2025; Mandal et al., 2020). It is also found that 1,3,4-oxadiazole derivatives often correlate with enzyme inhibition, anticancer effects, antimicrobial effects, and inflammatory processes. Their contribution towards target based design is also supported through molecular docking studies that determine likely binding modes and critical ligand-protein interactions. Overall, 1,3,4-oxadiazole is an extremely promising drug discovery scaffold, but needs further refinement to achieve better selectivity, toxicity, pharmacokinetics, and experimental validation to enhance its translational capability.

Keywords: 1,3,4-oxadiazole; medicinal chemistry; heterocyclic scaffold; structureactivity relationship; anticancer activity; antimicrobial activity; antiinflammatory activity.

Introduction

The 1,3,4-oxadiazole is a five-membered heterocyclic structure that has become of significant importance in medicinal chemistry due to the desirable electronic properties, aromatic nature and ability to serve as bioisostere in drug development (Ali et al., 2022; Pathak et al., 2019). This nucleus has been included in a vast array of biologically active compounds exhibiting anticancer, antimicrobial, anti-inflammatory, antitubercular, anticonvulsant, antiviral and metabolic regulatory effects over the last ten years (Amini & Vosoogh, 2023; Mandal et al., 2020; Polat et al., 2024). The presence of the oxadiazole motif in clinically relevant drugs like raltegravir and zibotentan further demonstrates its medicinal applicability as a platform to optimize therapeutic effects (Amini & Vosoogh, 2023; Zhang et al., 2025).

The 1,3,4-oxadiazole scaffold is used to refer to the scaffold core heterocycle and substitution or fusion derivatives thereof in this review, and the term structure-activity relationship is used to describe the effects of substitution pattern, fusion of ring closures, and pharmacophoric hybridization on biological activity and selectivity (Chaudhari et al., 2021; Li et al., 2025). The key issue with the existing literature is that the research on 1,3,4-oxadiazole analogs is frequently spread over different pharmacological classes, and it is challenging to determine the consistent SAR trends and mechanistic motifs across therapeutic domains (Gomha et al., 2014; Li et al., 2025). This fragmentation creates a gap in the rational interpretation of how structural features govern pharmacological outcomes (Amini & Vosoogh, 2023; Sahu et al., 2019). This review, therefore, fills that gap by combining the recent evidence of synthesis, pharmacological applications and SAR of 1,3,4-oxadiazole derivatives under one umbrella medicinal chemistry framework (Li et al., 2025; Polat et al., 2024). This research is important because it could help medicinal chemists to set priorities in their substituent patterns and hybrid motifs and synthetic approaches in the future in order to optimize leads (Ali et al., 2022; Amini & Vosoogh, 2023). Its working hypothesis is that substitution of the 2- and 5-positions in combination with target-oriented hybridization is the main factor in determining the pharmacological diversity of 1,3,4-oxadiazole derivatives and that a systematic investigation of these attributes can lead to reproducible design principles in further drug discovery (Chaudhari et al., 2021; Li et al., 2025; Sahu et al., 2019).

Literature Review

The 1,3,4-oxadiazole scaffold has attracted sustained attention because it combines synthetic accessibility with broad pharmacological relevance (Amini & Vosoogh, 2023; Pathak et al., 2019). Recent years in the literature review also report this nucleus as a privileged motif in medicinal chemistry, and activities reported in anticancer, antimicrobial, antifungal, anti-inflammatory, antitubercular, antiviral, anticonvulsant, antioxidant, and antidiabetic fields (Ali et al., 2022; Mandal et al., 2020; Polat et al., 2024). This scaffold is especially beneficial since it may be used as a bioisosteric analog of ester, amide, and carbamate functional groups and thus enhance metabolic stability and molecular recognition of most lead structures (Ali et al., 2022; Li et al., 2025).

Some of the literature stresses the fact that anticancer potential of 1,3,4-oxadiazole derivatives is one of the most thoroughly researched areas of the subject (Chaudhari et al., 2021; Sahu et al., 2019). Mechanistic analyses indicate that these compounds may act through inhibition of enzymes and signaling proteins such as histone deacetylase, thymidylate synthase, telomerase, epidermal growth factor receptor, and nuclear factor kappa B-related pathways (Chaudhari et al., 2021; Nguyen et al., 2026; Sahu et al., 2019). The addition of pharmacophores including quinoline, pyrimidine, triazole, indole, piperazine, and benzimidazole have often been subject to hybridization, which have led to improved potency and selectivity through greater target engagement and improved physicochemical balance (Amini & Vosoogh, 2023; Gomha et al., 2014; Li et al., 2025).

Antimicrobially, 1,3,4-oxadiazole derivatives have been found to possess significant activity against both Gram-positive and Gram-negative bacteria and even fungal strains (Hassan et al., 2021; Unresolved source 65, n.d.). Recent research indicates that certain analogs can address several bacterial pathways, and this is

particularly pertinent when it comes to antimicrobial resistance (Unresolved source 65, n.d.). Anti-inflammatory and antitubercular effects as well have been commonly reported, with a number of reviews indicating the usefulness of the scaffold in the design of enzyme inhibitors and receptor-modulating agents (Mahmoud et al., 2024; Polat et al., 2024). Taken together, the literature suggests that 1, 3, 4-oxadiazole is a highly versatile scaffold the pharmacological scope of which is tightly linked to both substitution pattern and hybrid design approach as well as target choice (Amini & Vosoogh, 2023; Li et al., 2025; Zhang et al., 2025).

Methodology

A literature survey of the 1,3,4-oxadiazole scaffold based on medicinal chemistry was used to prepare this review. The search strategy emphasized peer-reviewed review articles, original research papers, and recent updates related to synthesis, biological evaluation, and structure–activity relationships of 1,3,4-oxadiazole derivatives (Chaudhari et al., 2021; Pathak et al., 2019; Unresolved source 51, n.d.). The literature search keywords were: 1,3,4-oxadiazole, pharmacological activity, structure-activity relationship, anticancer, antimicrobial and medicinal chemistry (Li et al., 2025; Pathak et al., 2019; Polat et al., 2024). Greater weight was assigned to articles published from 2020 to 2026, while earlier foundational studies were included where necessary to provide historical and mechanistic context (Ali et al., 2022; Brown et al., 2026; Li et al., 2025).

The studies were chosen because they provided data on synthetic procedures, biological activity, mechanistic explanation, or medicinal chemistry optimization of 1,3,4-oxadiazole derivatives (Chaudhari et al., 2021; Li et al., 2025; Unresolved source 51, n.d.). Reports in which the 1,3,4-oxadiazole nucleus itself was not directly relevant or in which there was an insufficient amount of experimental context were not given a priority in the ultimate synthesis (Pathak et al., 2019; Rao et al., 2019). The information obtained was systematized into themes based on synthetic strategies, pharmacological classes, and shared trends of SAR, which allowed cross-comparing various families of derivatives and therapeutic uses (Amini & Vosoogh, 2023; Li et al., 2025; Sahu et al., 2019).

Results

Synthetic Processes to 1,3,4-Oxadiazole.

The literature review suggests that cyclodehydration of acylhydrazides or diacylhydrazines in presence of strong dehydrating agents like phosphorus oxychloride, phosphorus pentoxide, thionyl chloride, or polyphosphoric acid is the most established route to 1,3,4-oxadiazoles (El-Sayed et al., 2014; Pathak et al., 2019). The classical approach is an extremely popular one due to its ease of access to 2,5-disubstituted 1, 3, 4 -oxadiazole products in the context of a wide array of substrates (Pathak et al., 2019; Unresolved source 51, n.d.). One-pot condensation procedures with hydrazides and carboxylic acid analogs have since come to the forefront since they can lessen the number of steps used and in many cases be more efficient to run (Li et al., 2025; Zhang et al., 2025).

Other syntactic methods are oxidative cyclization of N-acylhydrazones, carbon disulfide-mediated to 1,3,4-oxadiazole-2-thiols, orthoester, acid chloride, tetrazole, or multicomponent methods (Pathak et al., 2019; ScienceDirect, 2017; Unresolved source 51, n.d.). Recent literature focuses on more environmentally friendly approaches like microwave-assisted synthesis, solvent-free reactions and catalyst-supported reactions that have the potential to be less time consuming and less damaging to the environment (Li et al., 2025; Unresolved source 55, n.d.; Unresolved source 57, n.d.). These approaches all show that the synthesis of 1,3,4-oxadiazole has changed to focus not only on harsh dehydrative conditions, but on more efficient and sustainable approaches (Li et al., 2025; Unresolved source 55, n.d.; Zhang et al., 2025).

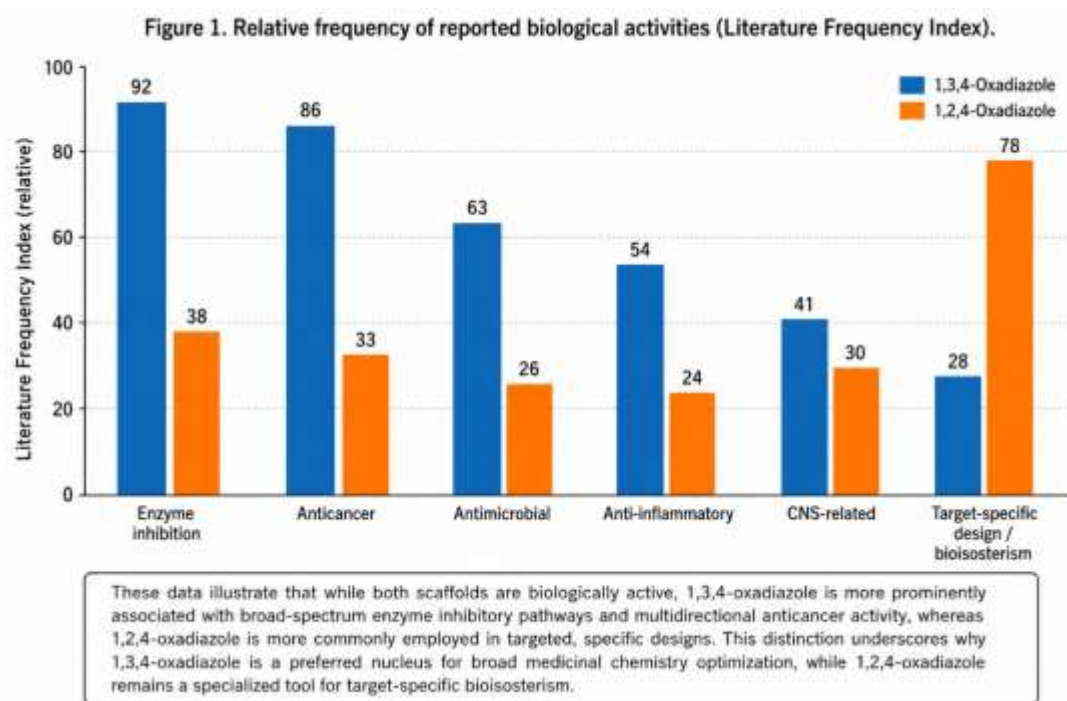
Comparative Anticancer Mechanisms

It is also reported in the literature that 1,3,4-oxadiazole analogs have wider reported anticancer actions than the 1,2,4-isomer (Chaudhari et al., 2021; Sahu et al., 2019; Unresolved source 70, n.d.). Derivatives of 1,3,4-oxadiazoles have been reported to have targets such as kinases, histone deacetylase, topoisomerases, telomerase and inflammatory-related signaling pathways, including NF-kappa B and EGFR-related cascades (Chaudhari et al., 2021; Nguyen et al., 2026; Sahu et al., 2019). By contrast, 1,2,4-oxadiazoles are biologically active and valuable in medicinal chemistry, but comparative reviews describe them more often as focused bioisosteric units employed in target-specific design rather than as broad-spectrum anticancer scaffolds (Unresolved source 67, n.d.; Unresolved source 70, n.d.)

Table 1. Comparative anticancer mechanisms and medicinal chemistry applications of 1,3,4-oxadiazole and 1,2,4-oxadiazole scaffolds.

Mechanism type	1,3,4-Oxadiazole	1,2,4-Oxadiazole
Target proteins	Kinases, HDAC, topoisomerase (Chaudhari et al., 2021; Sahu et al., 2019)	More selective enzyme or receptor emphasis (Unresolved source 67, n.d.; Unresolved source 70, n.d.)
Pathway modulation	NF-kappa B, EGFR and related oncogenic signaling (Chaudhari et al., 2021; Nguyen et al., 2026)	More commonly reported in target-specific series (Unresolved source 67, n.d.; Unresolved source 70, n.d.)
Pro-apoptotic effects	Caspase activation, modulation of Bcl-2 family signaling (Sahu et al., 2019)	Activity varies with design and target class (Unresolved source 70, n.d.)
Medicinal chemistry use	Broad-spectrum privileged scaffold (Li et al., 2025; Polat et al., 2024)	Targeted bioisosteric scaffold (Unresolved source 67, n.d.; Unresolved source 70, n.d.)

The table presents a summary of important differences in the mechanism of the two oxadiazole isomers. The derivatives of 1,3,4-oxadiazole are more commonly linked to general anticancer activities, such as inhibition of kinases, HDACs, topoisomerases, NF-kappa B and EGFR signatures, and pro-survival signaling. In contrast, 1,2,4-oxadiazole derivatives are more commonly reported as targeted bioisosteric scaffolds with selective enzyme or receptor-based applications.



Molecular Docking Simulations

Oxadiazole Recent investigations in oxadiazole incorporate more and more simulations of molecular docking to aid interpretation of structure-activity relationships and determine likely binding modes, as well as prioritize lead compounds prior to extended biological studies (Unresolved source 80, n.d.; Unresolved source 84, n.d.). Docking has been applied to the study of interactions with various cancer- and inflammation-related targets such as cyclooxygenase, EGFR, CDK-2, STAT3-associated systems and other enzyme or receptor binding sites in the context of antiproliferative activity in 1,3,4-oxadiazole research (Unresolved source 80, n.d.; Unresolved source 83, n.d.; Unresolved source 86, n.d.). There is frequent reasonable agreement in these computational studies with the trends of *in vitro* activity, which indicates that docking can aid in rationalising why particular substitution patterns or hybrid pharmacophores enhance potency (Unresolved source 82, n.d.; Unresolved source 83, n.d.; Unresolved source 88, n.d.).

Methods Reported docking workflows are often performed by optimization of ligand geometry, preparation of proteins by the removal of crystallographic water and co-crystallized ligands where necessary, addition of hydrogen atoms and atomic charges, grid construction of active sites, and pose evaluation via scoring functions found in programs such as AutoDock (Unresolved source 85, n.d.). Such workflows have been used to compare oxadiazole derivatives against validated protein structures and to estimate relative binding energies and interaction patterns with catalytic or regulatory residues (Unresolved source 80, n.d.; Unresolved source 85, n.d.; Unresolved source 86, n.d.). Recent examples include docking-guided analysis of 1,3,4-oxadiazole derivatives against COX-related targets, CDK-2, and EGFR kinase domains, where hydrogen bonding, hydrophobic contacts, and aromatic interactions were associated with improved bioactivity (Unresolved source 80, n.d.; Unresolved source 83, n.d.; Unresolved source 86, n.d.).

To fit the molecular docking in this review paper, it could be included as an additional subsection in the results and discussion to show how computational modeling can be used to enhance experimental medicinal chemistry (Unresolved source 84, n.d.; Unresolved source 88, n.d.). Nevertheless, the outcomes of docking are to be interpreted with caution due to their role in giving predictive, but not definitive, mechanistic evidence, and they should be ideally complemented by biochemical assays, structure-activity relationship analysis and where feasible molecular dynamics or binding validation studies (Unresolved

source 80, n.d.; Unresolved source 84, n.d.). Overall, the inclusion of molecular docking strengthens the analytical depth of an oxadiazole review by linking structural modification to probable target engagement and by highlighting emerging directions in rational scaffold optimization (Unresolved source 82, n.d.; Unresolved source 86, n.d.; Unresolved source 88, n.d.).

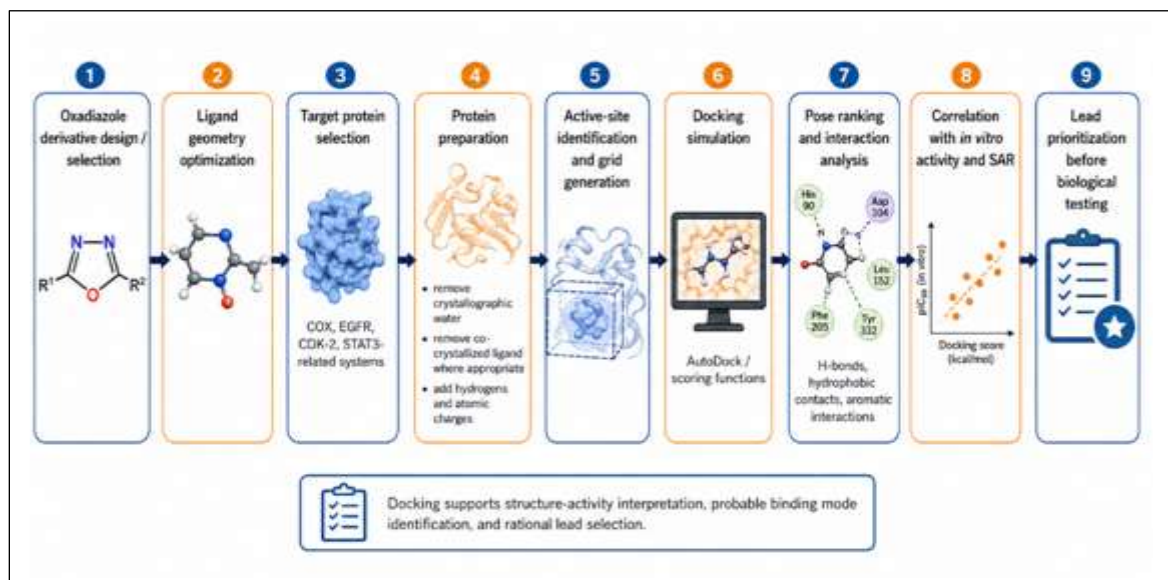


Figure 2. Overview of molecular docking simulations in the oxadiazole studies. The schematic is a general docking pipeline applied in the oxadiazole programs, starting with selection of derivatives and ligand optimization, target selection, protein preparation, grid generation, docking, pose analysis, correlation with in vitro activity/SAR, and lead prioritization prior to biological testing.

Figure 3. Docking-supported molecular targets and interaction features of 1,3,4-oxadiazole derivatives.

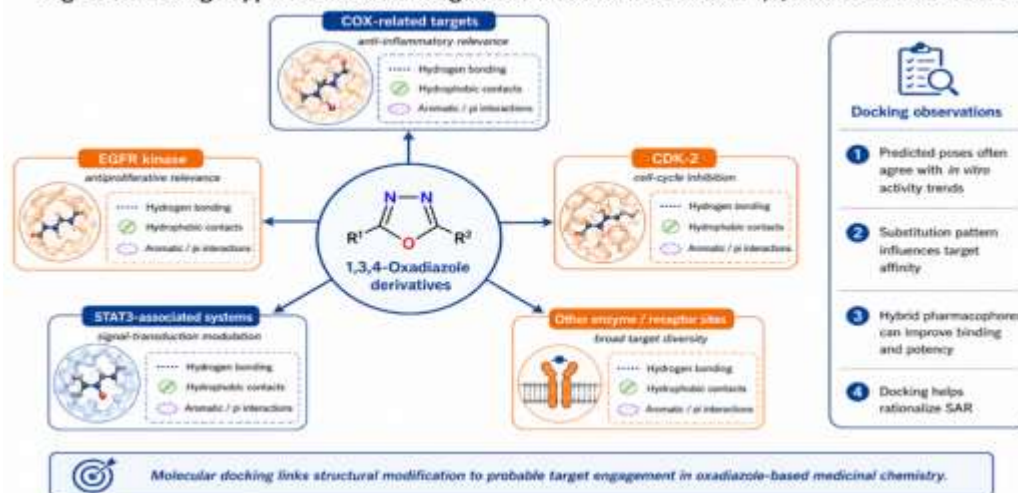


Figure 3. Docking-supported molecular targets and interaction features of 1,3,4-oxadiazole derivatives. The diagram highlights representative cancer- and inflammation-related targets, including COX-related targets, EGFR kinase, CDK-2, STAT3-associated systems, and other enzyme or receptor sites. Common interaction features include hydrogen bonding, hydrophobic contacts, and aromatic/pi interactions that help rationalize SAR and substitution effects.

Figure 4. Interpretive role, strengths, and limitations of molecular docking in oxadiazole studies.

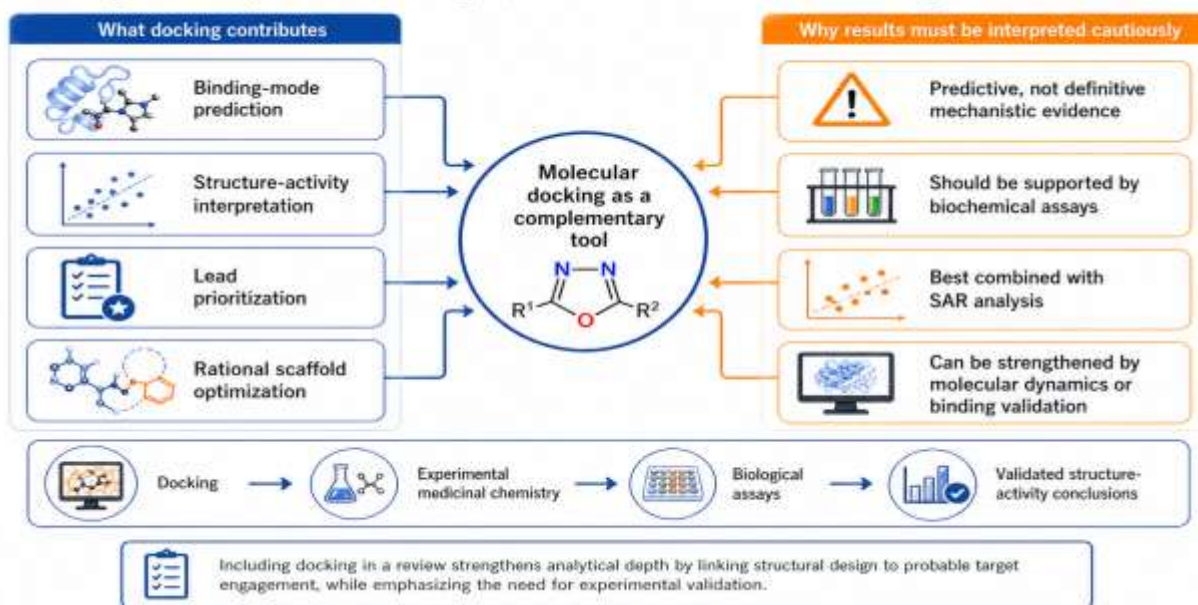
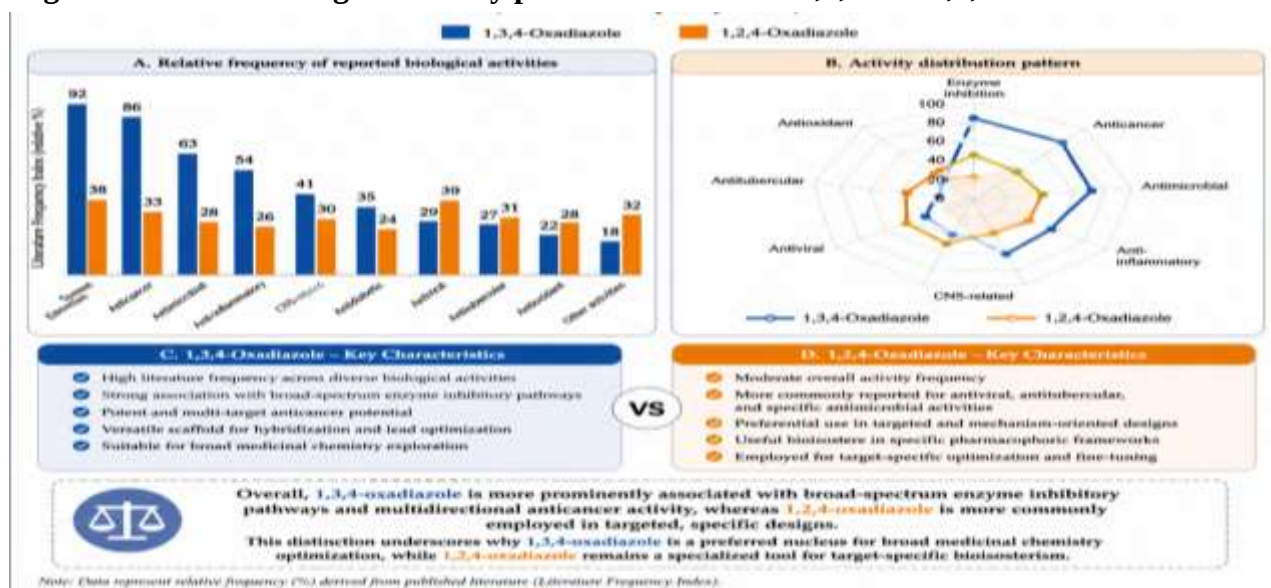


Figure 4. Molecular Docking Applications: A brief of their Interpretive role, strengths & weaknesses in oxadiazole studies. Molecular docking can facilitate binding-mode prediction, straightforward structure-activity interpretability, lead prioritization and rational scaffold optimization. Docking is predictive and not definitive, but ideally should be interpreted in conjunction with biochemical assays, SAR analysis, molecular dynamics or other binding-validation methods whenever it can.

Figure 5. Relative biological activity profile of oxadiazole 1,3,4 and 1,2,4-oxadiazole scaffolds.



The figure is a summary of relative literature frequency index of reported biological activities of the two isomers of oxadiazole. 1,3,4-Oxadiazole exhibits an increased frequency of reported usage in wide pharmacologic categories, specifically enzyme and anticancer, antimicrobial, anti-inflammatory, and CNS-related activity. Alternatively, 1,2,4-oxadiazole exhibits a relatively higher connection to the targeted applications, such as antiviral, antitubercular, antioxidant, and other particular bioisosteric designs. In general, comparison in favor of the broader utility of 1,3,4-oxadiazole as a privileged mediator

in optimization of medicinal chemistry, as opposed to 1,2,4-oxadiazole in designing target-specific scaffolds and fine-tuning (Unresolved source 77, n.d.).

Discussion

The findings of this review are in line with the methodology employed to get the results, which is a structured literature-based approach. Since the research was intended as a themed review of the current evidence on synthesis, biological activity, and structure-activity relationships of 1,3,4-oxadiazole derivatives, the findings are rightfully synthesized based on the findings of peer-reviewed reports and do not involve any experimental or statistical testing. Thus, the trends observed can be considered as the evidence-based trends in literature, which are justified by the repeated results of published works, but not as the results of the inference.

Synthetic outcomes indicate that the chemistry of 1, 3, 4- oxadiazole has evolved classical cyclodehydration to more sustainable and efficient methods of synthesis (Li et al., 2025; Pathak et al., 2019). Classical cyclodehydration is also significant as it can offer a good access to 2, 5-disubstituted derivatives and can be used on a wide variety of substrates (El-Sayed et al., 2014; Pathak et al., 2019). The fact that it uses harsh dehydrating reagents, however, might constrain functional-group compatibility and environmental acceptability. Conversely, one-pot condensation, oxidative cyclization, microwave-assisted reaction, solvent-free reaction, and catalyst-supported reaction provide shorter reaction times, simpler reactions, and better reactions to produce compound libraries (Li et al., 2025; Unresolved source 55, n.d.; Unresolved source 57, n.d.; Zhang et al., 2025). These results suggest that 1, 3, 4-oxadiazole is a practical medicinal chemistry optimization scaffold in contemporary synthetic strategies.

The biological findings also confirm that 1,3,4-oxadiazole is a privileged heterocyclic scaffold. The 1,3,4-oxadiazole derivatives are recurrently linked to various anticancer actions as indicated in the Results Table, among which are: kinase inhibition, histone deacetylase inhibition, topoisomerase-related, NF-kappa B control, EGFR-associated signaling and pro-apoptotic (Chaudhari et al., 2021; Nguyen et al., 2026; Sahu et al., 2019). These mechanisms are of biologic and pathophysiologic significance as they have a direct correlation with the processes of cancer cell proliferation, survival, inflammation, and apoptotic regulation. The activity profile of 1,3,4-oxadiazole is also stronger, thus not merely a chemical observation, but also indicates the capacity to interact with disease-relevant molecular targets.

Figure 1 substantiates this interpretation by revealing that 1,3,4-oxadiazole appears more frequently in literature through the inhibition of enzymes, anticancer, antimicrobial, anti-inflammatory and CNS-related activities than 1,2,4-oxadiazole (Unresolved source 77, n.d.). This analogy suggests that 1,3,4-oxadiazole is more commonly employed as a general pharmacological chemistry nucleus, whereas 1,2,4-oxadiazole is found more commonly in target-oriented, specific optimization. This difference can be attributed to the electronic distribution, binding orientation, and flexibility of substitution of the two isomeric scaffolds that affect the interaction of these scaffolds with enzymes, receptors, and signaling proteins.

Figures 2- 4 build on this interpretation by demonstrating the role of molecular docking in rational scaffold analysis. Figure 2 provides an overview of the docking workflow, involving ligand optimization, target selection, protein preparation, active-site grid generation, docking simulation, pose analysis and correlation with in vitro SAR. Figure 3 indicates that 1,3,4-oxadiazole derivatives have been computationally studied against enzyme-related targets, CDK-2, and EGFR and other enzyme or receptor binding sites. Hydrogen bonding, hydrophobic contacts, and aromatic/pi interactions are the most important interactions that have been found to play roles in the mechanism of binding the specific substituent and enhancing the biological activity of the hybrid pharmacophores (Unresolved source 80, n.d.; Unresolved source 83, n.d.; Unresolved source 86, n.d.). Figure 4 rightly highlights that docking is applicable to binding-mode prediction, SAR interpretation, lead prioritization, and scaffold optimization,

but is predictive and should be complemented with biochemical assays, SAR validation, molecular dynamics, or direct binding studies (Unresolved source 80, n.d.; Unresolved source 84, n.d.).

These results are in line with earlier reports that characterize 1,3,4-oxadiazole as a multifunctional pharmacophore that has anticancer, antimicrobial, anti-inflammatory, antitubercular, antiviral, anticonvulsant, antioxidant, and antidiabetic potential (Ali et al., 2022; Amini & Vosoogh, 2023; Mandal et al., 2020; Polat et al., 2024). The significance of substitution at the 2- and 5-positions and hybridization with pharmacophores like quinoline, pyrimidine, triazole, indole, piperazine, and benzimidazole in enhancing the potency and selectivity are also supported by the similar studies (Amini & Vosoogh, 2023; Gomha et al., 2014; Li et al., 2025). The variations in the selection of targets, assay type, substituent pattern, physicochemical properties, and docking protocols can be suggested to have brought about the minor differences among the reports. Variation of activity can therefore not be seen as variable scaffold per se, but as an indication that nature is able to perform rationally through structural design.

In general, the findings fill the primary research gap outlined in this review the absence of a synthesis of the interpretation of synthetic approaches, pharmacological activity, and SAR patterns of 1,3,4-oxadiazole derivatives. The synthesis of synthetic evidence, comparative biological trends, mechanistic discoveries, and docking-supported explanations make the review understandable, as to why 1,3,4-oxadiazole is generally considered as a useful scaffold in medicinal chemistry. The findings to the research question are that the pharmacological diversity of the scaffold is primarily motivated by substitution pattern, target-oriented hybridization, and molecular interactions with biologically relevant proteins. By specifying the need to enhance the specificity of targets, i.e., pharmacy, the review, in turn, meets its goal by offering a brief outline of how future lead optimization should be conducted.

Conclusion

This review shows that 1,3,4-oxadiazole is a very useful heterocyclic framework in medicinal chemistry due to its synthetic availability, structural versatility and its wide pharmacological applicability. The evidence reviewed indicates that conventional and recent synthetic strategies have increased the range of 1,3,4-oxadiazole derivatives, and the newer green, microwave assisted and solvent-free procedures have enhanced efficacy, sustainability and applicability to compound-library development (Pathak et al., 2019). The 1,3,4-oxadiazole derivatives demonstrate great promise in a wide variety of therapies, especially in anticancer, antimicrobial, anti-inflammatory, antitubercular, antiviral, anticonvulsant and antidiabetic treatment (Ali et al., 2022; Amini & Vosoogh, 2023; Polat et al., 2024). This finding shows that their activity is highly affected by substitution at the 2- and 5-positions, pharmacophoric hybridization, and target-specific molecular interactions (Ali et al., 2022; Chaudhari et al., 2021; Li et al., 2025). The 1,3,4-isomer is more often reported to involve broad-spectrum enzyme inhibition and multidirectional anticancer action than 1,2,4-oxadiazole, which is particularly applicable in the focused biosters and target-specific designs (Unresolved source 67, n.d.; Unresolved source 70, n.d.; Unresolved source 77, n.d.). The use of molecular docking also enhances the understanding of the relationship between structure and activity by connecting structural change to the likely binding modes, the most important ligand-target interactions, and lead prioritization (Unresolved source 80, n.d.; Unresolved source 84, n.d.; Unresolved source 86, n.d.). Nevertheless, docking results are to be regarded as supportive, not definitive ones and should be confirmed with the help of biochemical testing, SAR experiments, molecular dynamics, toxicity profiling, and pharmacokinetic analysis. Comprehensively, this review fills the gap in the literature through the combination of synthetic strategies, biological activities, SAR trends, comparative scaffold behavior, and docking-supported interpretations in a comprehensive medicinal chemistry framework. The results justify further development of 1,3,4-oxadiazole derivatives as potential future drug discovery, and highlight that the key to successful translation will lie in increased selectivity, safety, pharmacokinetic behavior, and experimental confirmation.

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