INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

OPEN ACCESS

Review Article

The Furan Nucleus: A Professional Assessment of its Pharmacological Significance

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ARTICLE INFO

Published: 30 Apr 2026
Keywords:
Furan; Heterocyclic compounds; Antibacterial; Antifungal; Antiviral; Anticancer; Anti-inflammatory; Cardioprotective; Biological activity; Drug discovery; Medicinal chemistry
DOI:
10.5281/zenodo.19920482

ABSTRACT

Furan, a five-membered aromatic heterocycle containing an oxygen atom, represents an important structural scaffold in medicinal and pharmaceutical research due to its electron-rich nature, planarity, and ability to participate in π–π stacking and hydrogen-bond interactions. The IUPAC name of furan is oxacyclopenta-2,4-diene, and it is isomeric with other five-membered heteroaromatic systems such as pyrrole and thiophene, which differ in the nature of the heteroatom. The furan nucleus plays a crucial role in modulating biological activity, metabolic stability, and pharmacokinetic behavior of drug candidates. Furan and its derivatives exhibit a wide spectrum of pharmacological activities, including antibacterial, antifungal, antiviral, anti-inflammatory, anticancer, and cardioprotective effects. Several antimicrobial studies have demonstrated potent antibacterial and antimycobacterial activities of substituted furan derivatives, with certain compounds showing low micromolar minimum inhibitory concentration (MIC) values against both Gram-positive and Gram-negative bacteria, as well as Mycobacterium tuberculosis. Antifungal investigations revealed significant inhibitory activity against pathogenic fungi such as Candida albicans, Aspergillus species, and Botrytis cinerea. Furan-based molecules have also shown promising antiviral properties, including activity against hepatitis B virus (HBV), hepatitis C virus (HCV), and human immunodeficiency virus (HIV), attributed to their ability to interact with viral enzymes and replication pathways. In anticancer research, several furan-containing compounds exhibited notable cytotoxicity against human cancer cell lines such as MCF-7, A549, HCT-116, and HeLa by inducing apoptosis and cell cycle arrest. Additionally, certain derivatives demonstrated anti-inflammatory and cardioprotective effects through modulation of oxidative stress and inflammatory mediators. Overall, furan represents a versatile and pharmacologically significant heterocyclic nucleus, offering substantial potential for the development of novel therapeutic agents across diverse disease areas.

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

INTRODUCTION

Furan is an aromatic five-membered heterocyclic compound containing one oxygen atom in the ring. Owing to its electron-rich nature and aromatic stability, furan serves as an important structural unit in medicinal chemistry and pharmaceutical research. The oxygen atom in the furan ring contributes two lone pairs of electrons, one of which participates in the aromatic sextet, thereby imparting aromaticity, planarity, and significant reactivity to the molecule. These electronic features allow furan and its derivatives to engage in hydrogen bonding, π–π interactions, and dipole-mediated binding with biological targets, making them valuable scaffolds in drug design.[1]

The IUPAC name of furan is oxacyclopenta-2,4-diene, and it is considered structurally related to other five-membered heteroaromatic compounds such as pyrrole and thiophene. Furan may be regarded as a heterocyclic analogue of cyclopentadiene, in which one methylene (–CH_2–) group is replaced by an oxygen atom. Although furan is less aromatic than benzene due to the higher electronegativity of oxygen, it still exhibits considerable aromatic stabilization and participates readily in electrophilic substitution reactions, predominantly at the 2-position[2]

Furan derivatives are widely employed as bioisosteric replacements for phenyl rings and other heterocycles such as thiophene and pyrrole in medicinal chemistry. The furan ring is planar, weakly basic, and moderately lipophilic, properties that favor membrane permeability and receptor binding. Substitution on the furan nucleus often results in improved pharmacokinetic profiles, enhanced biological activity, and reduced toxicity of drug molecules.[3]

Numerous furan-containing compounds have demonstrated a broad spectrum of biological activities, including antibacterial, antifungal, antiviral, anti-inflammatory, anticancer, and cardioprotective effects. Clinically important drugs such as nitrofurantoin, furazolidone, and nifuroxazide highlight the therapeutic relevance of the furan scaffold, particularly in antimicrobial chemotherapy. The biological activity of furan derivatives is attributed to their aromatic character, electronic distribution, and ability to interact with key enzymes and nucleic acids within biological systems.[4]

Overall, furan represents a versatile and pharmacologically significant heterocyclic nucleus. Its structural simplicity, chemical reactivity, and adaptability to substitution make it a valuable core in the rational design of novel therapeutic agents. Continued research on furan-based molecules is expected to contribute significantly to the development of safer and more effective drugs across multiple therapeutic domains.[5]

Anti-Microbial Activity :

Paul Ehrlich and co-workers first highlighted the therapeutic relevance of furan derivatives with the discovery of nitrofuran compounds, which later became clinically important antimicrobial agents. Nitrofurans exert their activity by enzymatic reduction within microbial cells, generating reactive intermediates that damage DNA and essential proteins.[6]

Several studies have reported potent antibacterial activity of substituted furan derivatives against both Gram-positive and Gram-negative bacteria. Dodd and Stillman demonstrated that nitrofurazone and related furan compounds exhibit strong bactericidal effects against *Staphylococcus aureus*, *Escherichia coli*, and *Salmonella* species by interfering with bacterial enzyme systems.[7]

Antimycobacterial activity has also been extensively reported for furan-containing compounds. Nitrofurantoin, a well-known furan-based drug, showed inhibitory activity against

Mycobacterium tuberculosis and remains an important urinary tract antimicrobial agent. Further synthetic modifications of the furan ring have resulted in compounds exhibiting low minimum inhibitory concentration (MIC) values against *Mycobacterium tuberculosis* H37Rv strains, highlighting their potential as antitubercular agents.[8]

In antifungal studies, furan derivatives demonstrated effective inhibition against pathogenic fungi such as *Candida albicans*, *Aspergillus niger*, and *Aspergillus fumigatus*. The antifungal mechanism is believed to involve disruption of fungal cell membrane integrity and inhibition of essential oxidative enzymes.[9]

The antimicrobial efficacy of furan derivatives is strongly influenced by the nature and position of substituents on the ring. Electron-withdrawing groups, particularly nitro substituents at the 5position, significantly enhance antimicrobial activity by increasing lipophilicity and intracellular accumulation. Due to these properties, the furan scaffold is widely utilized in the development of new antibacterial and antifungal agents, especially in cases of drug-resistant microbial infections.[10]

Overall, furan represents a pharmacologically important heterocyclic nucleus with proven antimicrobial significance. Continued structural modification and biological evaluation of furan derivatives are expected to yield novel antimicrobial agents with improved potency, selectivity, and safety profiles.

Derivative compounds of Furan having Anti-microbial Activity *:*

- Nitrofurantoin
- Furazolidone
- Nitrofurazone
- Nifuroxazide

Anti-Cancer Activity :

Zhang et al. synthesized a series of substituted furan derivatives and evaluated their cytotoxic activity against human cancer cell lines, including breast (MCF-7), lung (A549), colon (HCT116), and cervical (HeLa) cells using the MTT assay. Several compounds demonstrated significant anticancer activity, with IC_{50} values in the low micromolar range, attributed to the presence of electron-donating substituents on the furan ring that enhanced apoptotic induction.[11]

Kumar et al. reported the synthesis of furan-based chalcone derivatives and assessed their anticancer potential against MCF-7, DU-145 (prostate), and A549 cell lines. Among the synthesized compounds, those bearing nitro and methoxy groups on the aromatic moiety attached to the furan core exhibited potent cytotoxicity, with IC_{50} values comparable to standard anticancer agents. Structure–activity relationship (SAR) studies revealed that substitution at the 2-position of the furan ring played a crucial role in enhancing anticancer activity.[12]

In another study, El-Sayed et al. investigated a series of fused furan heterocycles for their anticancer activity against liver (HepG-2), colon (HT-29), and breast (MCF-7) cancer cell lines. The compounds exhibited dose-dependent cytotoxic effects, primarily through cell cycle arrest and induction of apoptosis. The presence of conjugated systems involving the furan nucleus

was found to significantly improve antiproliferative efficacy.[13]

Furan-containing natural products and synthetic analogues have also demonstrated promising anticancer effects. Raviña and co-workers reported that several bioactive furan derivatives interfere with tubulin polymerization and topoisomerase activity, leading to inhibition of cancer cell proliferation. These findings underscore the role of the furan scaffold as a privileged structure in anticancer drug development.[14]

Textbook literature further supports the anticancer relevance of furan derivatives. According to Wilson and Gisvold, incorporation of the furan ring into anticancer molecules often improves metabolic stability and receptor selectivity. Additionally, Burger's Medicinal Chemistry highlights furan as a bioisosteric replacement for phenyl rings in anticancer agents, contributing to improved pharmacodynamic and pharmacokinetic profiles.[15]

Overall, furan represents a pharmacologically significant heterocyclic nucleus with substantial anticancer potential. Continued exploration of furan-based compounds through rational design and SAR studies is expected to yield novel anticancer agents with enhanced efficacy and reduced toxicity.

Derivative compounds of Furan having Anti-Cancer Activity *:*

- Furan-chalcone derivatives
- Furan-thiosemicarbazones
- Benzofuran derivatives

Anti-Inflammatory Activity:

Inflammation is a complex biological response mediated by pro-inflammatory enzymes, cytokines, and signaling molecules such as cyclooxygenase (COX), lipoxygenase (LOX), nitric oxide synthase (NOS), tumor necrosis factor-α (TNF-α), and interleukins. Furan derivatives have demonstrated the ability to interfere with these inflammatory mediators, thereby exhibiting potent anti-inflammatory effects.[16]

Several synthetic furan-based compounds have been reported to possess significant antiinflammatory activity in both in vitro and in vivo models. Substituted furan derivatives were shown to inhibit COX-2 and suppress prostaglandin synthesis, leading to reduced edema and inflammatory pain. The presence of electron-withdrawing or electron-donating substituents at the 2- or 5-position of the furan ring plays a crucial role in enhancing anti-inflammatory efficacy.[17]

Furan-containing non-steroidal anti-inflammatory drugs (NSAIDs) and related analogues have also attracted attention due to their reduced gastrointestinal toxicity compared to traditional NSAIDs. According to Burger's Medicinal Chemistry, the furan ring acts as a bioisosteric replacement for phenyl rings in anti-inflammatory agents, contributing to improved safety and potency profiles.[18]

Natural and synthetic furan derivatives have further been reported to exhibit anti-inflammatory activity by inhibiting nitric oxide production and down-regulating pro-inflammatory cytokines such as TNF-α and IL-6. These mechanisms highlight the potential of furan-based compounds in the treatment of chronic inflammatory disorders, including arthritis, inflammatory bowel disease, and cardiovascular inflammation.[19]

Textbook evidence further supports the importance of furan in anti-inflammatory drug development. Wermuth highlighted the role of heterocyclic bioisosterism in improving drug

efficacy and safety, identifying furan as a valuable scaffold for rational drug design. Similarly, Foye's Principles of Medicinal Chemistry describes furan as a key heterocycle capable of enhancing receptor affinity and metabolic stability in anti-inflammatory agents.[20]

In summary, furan represents a pharmacologically significant heterocyclic nucleus with proven anti-inflammatory potential. Continued research on furan-based derivatives through rational drug design and structure–activity relationship (SAR) studies is expected to facilitate the development of safer and more effective anti-inflammatory therapeutics.

Derivative compounds of Furan having Anti-Inflammatory Activity *:*

- Furan-carboxylic acid derivative
- Benzofuran analogues
- Furan-pyrazole hybrids

Anti-HIV Activity :

HIV-1 RNase H, the ribonuclease H domain of reverse transcriptase (RT), has emerged as an attractive yet underexplored antiviral target because it is indispensable for viral replication and exhibits structural features that differ significantly from human RNase H enzymes, thereby allowing selective inhibition. As RNase H is responsible for degrading the RNA strand of RNA– DNA hybrids during reverse transcription, its inhibition leads to failure of viral DNA synthesis. Recent high-throughput screening campaigns and structure–function studies have therefore focused on identifying small-molecule scaffolds capable of chelating the catalytic divalent metal ions or otherwise disrupting the RNase H active site.[21]

A notable class of HIV-1 RNase H inhibitors incorporates a nitro-furan-2-carboxylate subunit as a key pharmacophoric element. In a high-throughput screening effort followed by systematic medicinal chemistry optimization, derivatives of 5-nitro-furan-2-carboxylic acid carbamoylmethyl esters were identified as potent inhibitors of RNase H activity associated with HIV-1 reverse transcriptase, as well as murine leukemia virus RT. These compounds exhibited IC_{50} values in the range of approximately 3–30 μM. Importantly, several nitro-furan derivatives selectively inhibited HIV-1 replication in cell-based assays at concentrations of ~20–25 μM, while displaying only weak inhibition of bacterial RNase H, thereby demonstrating a favorable selectivity window. The study concluded that the nitro-furan-2-carboxylate fragment represents a critical pharmacophore for RNase H inhibition.[22]

Subsequent structural and structure–activity relationship (SAR) investigations further refined this hit series. X-ray crystallography and molecular modelling studies revealed that the furan ring primarily functions as a rigid and planar scaffold, appropriately orienting the nitro and carboxylate (or ester/carbamoyl) groups for effective coordination with the RNase H metalbinding site and for optimal interactions within the active-site pocket. Rational optimization of substituents around the furan nucleus resulted in analogues with up to an order-of-magnitude improvement in potency, while maintaining low cytotoxicity in many cases. These findings clearly demonstrate that substituent positioning on the furan core is central to RNase H inhibitory activity.[23]

Beyond RNase H inhibition, furan motifs have also been identified in other non-nucleoside anti-HIV chemotypes, including NNRTI-like scaffolds and viral entry or replication inhibitors. In NNRTI frameworks, the furan ring contributes favorable hydrophobic contacts and π–π stacking

interactions within the reverse transcriptase allosteric binding pocket. In addition, furan and benzofuran fragments have been incorporated into sulfated-polysaccharide mimetics and related entry inhibitors to improve molecular recognition, cellular uptake, and antiviral efficacy. Collectively, these applications highlight furan as a versatile and pharmacologically valuable heterocyclic scaffold in anti-HIV medicinal chemistry.[24]

Derivative compounds of Furan having Anti-Inflammatory Activity *:*

- 5-Nitro-furan-2-carboxylate derivatives
- Nitro-furan carbamoylmethyl esters
- Furan-based NNRTI analogues

Anti-Diabetic Activity :

Persistent hyperglycemia brought on by decreased insulin production, insulin resistance, or both is a hallmark of diabetes mellitus, a chronic metabolic disease. Current therapeutic strategies focus on improving insulin sensitivity, enhancing insulin secretion, delaying carbohydrate absorption, and modulating glucose metabolism. In recent years, heterocyclic scaffolds have gained prominence in antidiabetic drug discovery due to their ability to interact with key metabolic enzymes and receptors.[25]

Several furan-based compounds have demonstrated antidiabetic activity through inhibition of carbohydrate-digesting enzymes such as α-glucosidase and α-amylase, which play a critical role in postprandial hyperglycemia. Inhibition of these enzymes delays glucose absorption in the intestine, thereby reducing post-meal blood glucose levels. According to Tripathi, enzyme inhibition remains a validated therapeutic approach in the management of type 2 diabetes, particularly in controlling postprandial glucose excursions.[26]

Structure–activity relationship (SAR) studies have revealed that substitution on the furan nucleus significantly influences antidiabetic potency. Electron-withdrawing and heteroaryl substituents on the furan ring enhance binding interactions with α-glucosidase and related enzymes through hydrogen bonding and π–π interactions. Silverman and Holladay reported that oxygencontaining heterocycles such as furan provide favorable spatial orientation for enzyme inhibition in metabolic disorders.[27]

Beyond enzyme inhibition, furan derivatives have also been investigated for their ability to improve insulin sensitivity and regulate glucose homeostasis through modulation of peroxisome proliferator-activated receptors (PPARs) and AMP-activated protein kinase (AMPK) pathways. These mechanisms contribute to enhanced glucose uptake in peripheral tissues and improved lipid metabolism. Rang and Dale highlighted the importance of targeting insulin resistance and metabolic signaling pathways in modern antidiabetic therapy.[28]

Natural and synthetic furan-containing compounds have further shown antioxidant properties that are beneficial in diabetes management, as oxidative stress plays a crucial role in the progression of diabetic complications. By scavenging reactive oxygen species and reducing inflammatory mediators, furan derivatives may offer dual antidiabetic and cytoprotective effects. Goodman and Gilman emphasized that agents with combined glucose-lowering and antioxidant activity are particularly valuable in preventing long-term diabetic complications.[29]

Derivative compounds of Furan having Anti-Inflammatory Activity:

- Furan-carboxylic acid derivatives
- Benzofuran analogues
- Furan-pyrazole hybrids

Anti-convulsant Activity :

Epilepsy is a chronic neurological disorder characterized by recurrent seizures resulting from abnormal neuronal excitability and synchronization in the brain. Anticonvulsant drug discovery primarily focuses on modulation of ion channels, enhancement of inhibitory neurotransmission, and suppression of excitatory pathways. In this context, heterocyclic compounds have gained considerable importance due to their ability to interact selectively with central nervous system (CNS) targets. [30]

Several furan-containing compounds have demonstrated anticonvulsant activity through modulation of γ-aminobutyric acid (GABA)-mediated inhibitory neurotransmission. Enhancement of GABAergic activity remains a major therapeutic strategy for seizure control. According to Goodman and Gilman, agents that increase GABA availability or enhance GABA receptor function are effective in reducing neuronal hyperexcitability associated with seizures.[31]

Structure–activity relationship (SAR) studies have revealed that substitution on the furan nucleus significantly influences anticonvulsant efficacy. Furan derivatives bearing aromatic or electronwithdrawing substituents exhibit improved binding to voltage-gated sodium channels and GABA_A receptors, thereby stabilizing neuronal membranes. Silverman emphasized that oxygen-containing heterocycles such as furan provide optimal electronic distribution for interaction with CNS ion channels and receptors.[32]

Furan-based compounds have also been reported to inhibit voltage-gated sodium and calcium channels, which play a crucial role in seizure initiation and propagation. Suppression of repetitive neuronal firing through sodium channel blockade is a well-established anticonvulsant mechanism. Katzung highlighted that heterocyclic anticonvulsants with appropriate lipophilicity and aromaticity demonstrate enhanced anticonvulsant activity by targeting these channels.[33]

Derivative compounds of Furan having Anti-Convulsant Activity:

- Furan-semicarbazones
- Furan-hydrazones
- Furan-benzodiazepine hybrids

Anti-Viral Activity :

Viral infections remain a major global health concern due to rapid viral mutation, drug resistance, and limited availability of broad-spectrum antiviral agents. Antiviral drug discovery primarily targets critical stages of the viral life cycle, including viral entry, genome replication, protein processing, and viral assembly. In recent years, heterocyclic compounds have played a pivotal role in antiviral chemotherapy.[34]

Furan derivatives have demonstrated antiviral activity against a wide range of viruses, including influenza virus, hepatitis viruses, herpes simplex virus (HSV), and emerging RNA viruses. The antiviral potential of furan-based compounds is largely attributed to their ability to inhibit viral polymerases, proteases, and helicases. According to De Clercq, small heterocyclic molecules capable of selectively inhibiting viral replication

enzymes represent a cornerstone of modern antiviral therapy.[35]

Structure–activity relationship (SAR) studies have revealed that substitution on the furan nucleus significantly influences antiviral efficacy. Electron-withdrawing groups, halogens, and heteroaryl substituents on the furan ring enhance antiviral potency by improving binding affinity to viral enzymes and increasing cellular uptake. Katsuno et al. emphasized that oxygen-containing heterocycles such as furan offer favorable geometry and electronic distribution for antiviral drug–target interactions.[36]

Furan-containing compounds have also been explored as nucleoside and non-nucleoside analogues capable of interfering with viral genome replication. Some furan-based antivirals act by mimicking natural substrates of viral polymerases, leading to premature chain termination or inhibition of viral RNA synthesis. Goodman and Gilman highlighted that heterocyclic scaffolds are central to the design of polymerase inhibitors used in antiviral therapy.[37]

In addition to direct enzyme inhibition, certain furan derivatives exhibit antiviral activity by modulating host-cell pathways involved in viral entry and replication. These include inhibition of viral fusion, interference with host proteases, and disruption of virus–host interactions. Ashutosh Kar described heterocyclic compounds such as furan as multifunctional scaffolds capable of exerting antiviral effects through both viral and host-directed mechanisms.[38]

Derivative compounds of Furan having Anti-Viral Activity:

- Furan-nucleoside analogues
- Furan-triazole hybrids
- Furan-quinazoline conjugates

Anti-Oxidant Activity :

Oxidative stress plays a crucial role in the pathogenesis of numerous diseases, including cancer, diabetes, neurodegenerative disorders, cardiovascular diseases, and inflammation. It arises from an imbalance between the generation of reactive oxygen species (ROS) and the antioxidant defense mechanisms of the body. Consequently, the development of effective antioxidant agents has become a major focus in medicinal chemistry. In this context, heterocyclic compounds have gained significant importance due to their ability to stabilize free radicals and modulate oxidative pathways.[39]

Furan and its derivatives exhibit antioxidant activity primarily through free-radical scavenging, metal ion chelation, and inhibition of lipid peroxidation. The presence of an oxygen atom within the aromatic ring facilitates electron donation, enabling furan derivatives to neutralize reactive oxygen and nitrogen species. According to Halliwell and Gutteridge, compounds capable of donating electrons or hydrogen atoms play a critical role in preventing oxidative damage at the cellular level.[40]

Structure–activity relationship (SAR) studies have demonstrated that substitution on the furan nucleus significantly influences antioxidant potential. Furan derivatives bearing hydroxyl, methoxy, or electron-donating aromatic substituents exhibit enhanced radical-scavenging activity by stabilizing the resulting radical intermediates. Leopoldini et al. emphasized that aromatic heterocycles with conjugated systems, such as furan, are particularly effective in delocalizing unpaired electrons, thereby improving antioxidant efficiency.[41]

In addition to direct free-radical scavenging, furan-based compounds have been reported to

modulate endogenous antioxidant defense systems by enhancing the activity of enzymes such as superoxide dismutase (SOD), catalase, and glutathione peroxidase. This dual mechanism—direct ROS neutralization and indirect enzymatic regulation—makes furan derivatives attractive candidates for the management of oxidative stress-related disorders. Sies highlighted that compounds capable of influencing redox signaling pathways offer therapeutic advantages beyond conventional antioxidants.[42]

Natural and synthetic furan-containing compounds, including furan derivatives found in plant secondary metabolites, have also demonstrated notable antioxidant properties. These compounds contribute to cellular protection by reducing oxidative damage to lipids, proteins, and nucleic acids. Harborne reported that heterocyclic constituents in natural products play an essential role in antioxidant defense mechanisms.[43]

Derivative compounds of Furan having Anti-Oxidant Activity:

- Hydroxyl-substituted furan derivatives
- Methoxy-furan derivatives
- Natural furan compounds (plant-derived)

CONCLUSION

Furan and its derivatives constitute an important class of heterocyclic compounds with substantial biological and pharmacological relevance. The presence of an oxygen atom within the five-membered aromatic ring imparts distinctive electronic characteristics, planarity, and reactivity, which collectively enhance molecular interactions with biological targets. These intrinsic properties make the furan scaffold highly adaptable and valuable in medicinal chemistry. Structural modification at key positions of the furan ring has been shown to significantly influence biological activity, stability, and pharmacokinetic behavior.

Extensive research has demonstrated that furan derivatives exhibit a broad spectrum of biological activities, including antimicrobial, antifungal, antiviral, anti-HIV, anticancer, anti-inflammatory, antidiabetic, antioxidant, anticonvulsant, and cardioprotective effects. Clinically established nitrofuran drugs such as nitrofurantoin, furazolidone, and nitrofurazone exemplify the therapeutic importance of the furan nucleus, particularly in antimicrobial therapy. Moreover, recent advances have highlighted the potential of furan-based compounds as inhibitors of critical biological targets such as HIV-1 RNase H, cyclooxygenase enzymes, α-glucosidase, and various cancer-related signaling pathways, often demonstrating high potency with acceptable safety profiles.

Overall, furan derivatives represent versatile and promising frameworks for the development of novel bioactive molecules. Their structural flexibility, compatibility with diverse pharmacophores, and broad pharmacological profile make them excellent candidates for continued exploration in drug discovery and development. Further research focused on rational design, structure–activity relationship studies, and toxicity optimization is expected to yield innovative furan-based therapeutics with improved efficacy, selectivity, and clinical applicability.

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HOW TO CITE: Dr. Sunayana Ghodgaonkar, Pragati Gharatkar, Purva Gambhirrao, Chaitali Gaikar, Sanchita Ghode, Aditi Ghadge, The Furan Nucleus: A Professional Assessment of its Pharmacological Significance, Int. J. of Pharm. Sci., 2026, Vol 4, Issue 4, 5028-5038. https://doi.org/10.5281/zenodo.19920482