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Pharmacological Evaluation of Metal–Organic Frameworks (MOFs): Emerging Nanocarriers in Modern Pharmaceutics

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Abstract:

Metal–organic frameworks (MOFs) have emerged as powerful next-generation nanocarriers in modern pharmaceutics, offering unique advantages over conventional delivery systems through their exceptional porosity, tunability, and modular architecture. This review provides a comprehensive evaluation of MOF-based drug delivery platforms, emphasizing their structural fundamentals, synthesis strategies, drug-loading mechanisms, pharmacokinetics, and therapeutic potential. Pharmaceutical-grade MOFs are now engineered through advanced solvothermal, microwave-assisted, mechanochemical, and microfluidic methods, supported by green chemistry innovations and precise post-synthetic modifications. Their versatile loading mechanisms accommodate small-molecule drugs, biomacromolecules, and nucleic acids, while physicochemical attributes—such as pore size, surface chemistry, and degradability—dictate in vivo biodistribution and release kinetics. MOFs demonstrated significant pharmacological applications in cancer therapy, antimicrobial and antiviral treatment, gene delivery, gas storage, and enzyme-based therapeutics. However, concerns regarding cytotoxicity, degradation products, immunogenicity, and long-term accumulation highlight the importance of rigorous toxicological evaluation and biosafety-focused design. Emerging trends—including biomimetic coatings, MOF–polymer hybrids, stimuli-responsive systems, AI-guided design, and theranostic platforms—are rapidly advancing their clinical relevance. Despite ongoing challenges related to scalability, reproducibility, and regulatory approval, MOF nanocarriers hold strong potential to revolutionize personalized and precision medicine through smart, adaptable, and multifunctional therapeutic delivery systems.

Keywords: Metal–Organic Frameworks (Mofs); Nanocarriers; Drug Delivery; Pharmacokinetics; Biodistribution; Nucleic Acid Delivery; Anticancer Therapy; Biomimetic Coatings; Stimuli-Responsive Systems; Theranostics; Pharmaceutical Nanotechnology.

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1. Introduction

The rapid evolution of nanocarrier-based drug delivery systems has reshaped modern pharmaceutics, particularly as conventional delivery platforms continue to show inherent limitations. Traditional systems such as liposomes, polymeric nanoparticles, and micelles often struggle with low drug-loading capacities, premature drug leakage, limited stability, and unpredictable pharmacokinetics [1-2]. These issues hinder the precise and sustained delivery required for advanced therapeutics like biologics, poorly soluble drugs, and combination treatments. In this context, the pharmaceutical field has been searching for materials that offer better control over drug encapsulation, tunable release behavior, and improved biocompatibility. This search has propelled the rise of Metal–Organic Frameworks (MOFs), a class of highly porous crystalline materials that combine the benefits of inorganic and organic chemistry. Unlike traditional nanocarriers, MOFs provide exceptionally high surface area, modular structural tunability, and the ability to engineer pore environments at the molecular scale, making them promising candidates for next-generation drug delivery [3].

Metal–Organic Frameworks have emerged as one of the most versatile platforms in materials science due to their distinctive architecture consisting of metal ion clusters coordinated with organic linkers. This unique arrangement creates periodic frameworks with ultra-high porosity and tailorable functionality. The pharmaceutical appeal of MOFs lies in their unparalleled tunability: researchers can fine-tune the pore size, modify the inner surface chemistry, and introduce stimuli-responsive elements to design highly specific drug delivery systems. Their capacity to encapsulate both hydrophilic and hydrophobic cargo, protect sensitive molecules like nucleic acids, and achieve controlled, sustained, or stimuli-triggered release adds to their therapeutic potential. Additionally, the possibility of engineering MOFs with biocompatible metals (e.g., Zn, Fe, Mg) and naturally derived linkers has sparked interest in their application for safe and degradable nanomedicines [4-5].

The clinical relevance of MOFs is rapidly growing as they transition from theoretical exploration to real biomedical applications. Recent preclinical studies have demonstrated their value in treating cancer, infectious diseases, inflammation, and genetic disorders, primarily due to their high loading capacity and ability to deliver drugs precisely to target tissues. MOFs can also operate as multifunctional platforms—combining imaging, drug delivery, and sensing in a single system—which positions them as strong contenders for theranostic applications. Despite promising progress, challenges such as toxicity, long-term biodegradation, and regulatory concerns must still be addressed [6-7]. This review provides a comprehensive examination of MOF-based nanocarriers, focusing on their structural fundamentals, physicochemical characteristics, pharmacological potential, and emerging innovations. By evaluating the current evidence and identifying future research directions, this review aims to highlight the transformative potential of MOFs in next-generation pharmaceutics and their realistic path toward clinical translation [8].

2. Fundamentals of Metal–Organic Frameworks

Metal–Organic Frameworks are crystalline materials composed of two essential building blocks: metal ions or metal-based clusters serving as nodes, and organic ligands acting as linkers. Together, these components form highly ordered structures with tunable pore networks. The metal nodes—including Zn^{2+}, Fe^{3+}, Zr^{4+}, Cu^{2+}, and Mg^{2+}—provide structural rigidity and offer coordination sites for drug loading or functionalization. The organic linkers, typically carboxylates, imidazolates, or aromatic polyfunctional molecules, dictate the geometry, connectivity, and chemical environment of the pores. By selecting appropriate metal–ligand combinations, researchers can engineer MOFs with desired

topologies, ranging from simple cubic structures to sophisticated three-dimensional architectures with intricate channels and binding pockets. This molecular precision distinguishes MOFs from classical porous materials and allows unprecedented control over drug encapsulation and release kinetics [9-10].

Based on structural principles and synthetic chemistry, MOFs can be broadly classified into several subclasses relevant to pharmaceutics. Zeolitic Imidazolate Frameworks (ZIFs) are among the most widely studied due to their high chemical stability, pH responsiveness, and biocompatibility. They mimic the topology of zeolites but offer organic-inorganic hybrid flexibility, making them ideal for encapsulating biomacromolecules such as proteins and nucleic acids. Porous Coordination Polymers (PCPs), another major subclass, consist of extended networks with diverse metal–ligand arrangements and tunable pore environments, enabling the development of drug-specific delivery platforms. Bio-MOFs and peptide-linked MOFs represent the newest generation, engineered using amino acids, peptides, or biologically derived ligands to enhance biocompatibility and biodegradability [11-12]. These systems are especially promising for in vivo applications because they degrade into non-toxic metabolites and can interact favorably with biological systems.

The physicochemical properties of MOFs play a central role in determining their pharmacological behavior. Their exceptionally high surface area—often exceeding that of traditional nanocarriers by several orders of magnitude—allows efficient encapsulation of therapeutic agents with minimal material consumption. Porosity and pore size distribution influence drug diffusion rates, loading capacity, and release kinetics. Morphological factors such as particle size, shape, and surface charge determine circulation time, cellular uptake, and biodistribution within the body. Degradability, governed by the nature of the metal–linker bond and environmental pH, ensures safe elimination after drug release, which is critical for biomedical translation. Additionally, surface chemistry can be engineered to introduce targeting ligands, stealth coatings, or stimuli-responsive functional groups that enhance therapeutic performance [13-14].

Overall, understanding the structural and physicochemical fundamentals of MOFs is essential for their rational design as nanocarriers. Their modularity, tunability, and unique porous architecture provide a strong foundation for developing next-generation pharmaceutical delivery systems tailored to the needs of precision medicine [15].

3. Synthesis Strategies for Pharmaceutical-Grade MOFs

Pharmaceutical-grade metal–organic frameworks (MOFs) are produced through a variety of advanced synthesis strategies designed to ensure precision, purity, and scalability. Conventional approaches such as solvothermal, microwave-assisted, and mechanochemical synthesis remain widely used due to their ability to yield highly crystalline structures with controlled porosity [16-17]. To meet modern sustainability demands, green synthesis techniques employing biocompatible and environmentally friendly solvents have gained traction, reducing toxic byproducts without compromising performance. Microfluidic-based fabrication offers another level of refinement by enabling precise control over particle size, morphology, and batch-to-batch uniformity—an essential requirement for drug delivery applications. Additionally, surface functionalization and post-synthetic modification strategies allow researchers to tailor MOF surfaces for enhanced drug loading efficiency, improved stability, and targeted delivery. Despite these advancements, significant challenges persist regarding quality control, reproducibility, and large-scale manufacturing, highlighting the need for standardized protocols to ensure consistent production of pharmaceutical-grade MOFs [19-20].

4. Drug Loading Mechanisms

Drug loading in metal–organic frameworks (MOFs) is governed by several interconnected mechanisms that determine how efficiently therapeutic agents are incorporated and retained within the material. The most common approach is adsorption-driven loading, where drugs are encapsulated inside the porous network or adsorbed onto the framework surface through physical interactions. Depending on the chemical nature of both the MOF and the therapeutic cargo, loading can occur through covalent bonding or more flexible noncovalent forces such as hydrogen bonding, electrostatic attraction, and π–π interactions. Diffusion-controlled entrapment also plays a crucial role, particularly for molecules that migrate gradually into internal pores during post-synthetic soaking. MOFs can encapsulate a wide range of therapeutic agents, including small molecules, peptides and proteins, and various nucleic acids such as siRNA, mRNA, and plasmid DNA [21-22]. Ultimately, loading efficiency is strongly influenced by factors such as pore size, surface chemistry, and the hydrophobic–hydrophilic balance of the framework, all of which must be optimized to achieve stable and high-capacity drug incorporation.

5. Pharmacokinetics and Biodistribution of MOF Nanocarriers

The pharmacokinetics and biodistribution of MOF nanocarriers are shaped by multiple physicochemical factors that govern how these systems behave in vivo. Their circulation time and plasma stability largely determine the extent of systemic exposure and therapeutic availability. Key structural attributes—including particle size, shape, and surface charge—play major roles in dictating biodistribution patterns and organ accumulation [23-24]. A persistent challenge is uptake by the reticuloendothelial system (RES), prompting the development of evasion strategies such as PEGylation and biomimetic surface coatings to prolong bloodstream persistence. Controlled degradation of the MOF framework further influences drug release kinetics, ensuring that cargo is liberated at the desired rate and location. Additionally, the choice of metal ions and organic linkers significantly affects biological interactions, stability, and overall in vivo fate, underscoring the importance of rational design for safe and effective MOF-based drug delivery [25-26].

6. Pharmacological Activities and Therapeutic Applications

Metal–organic frameworks (MOFs) exhibit diverse pharmacological activities and have emerged as versatile platforms for a wide range of therapeutic applications. In cancer therapy, MOF-based delivery systems enable efficient chemotherapy, combination treatments, and reactive oxygen species (ROS)-responsive drug release, while pH-sensitive frameworks provide highly targeted delivery to the acidic tumor microenvironment. Their antimicrobial and antiviral potential is equally significant, with metal-containing MOFs such as zinc-, copper-, and silver-based structures demonstrating strong intrinsic antimicrobial effects, complemented by MOF-enhanced photodynamic and photothermal therapies for pathogen eradication [27-28]. MOFs also serve as promising carriers for gene and nucleic acid therapeutics, where cationic frameworks facilitate the delivery of siRNA, mRNA, and CRISPR components while shielding these biomolecules from enzymatic degradation. Beyond drug and gene delivery, MOFs function as reservoirs for biologically active gases such as oxygen and nitric oxide, supporting gas-based therapies, and provide stable platforms for enzyme immobilization, enabling catalytic treatments with enhanced stability and specificity. Together, these capabilities highlight the expansive therapeutic potential of MOF nanocarriers across modern medicine [29-30].

7. Toxicological Considerations

Toxicological considerations play a critical role in evaluating the safety of MOF-based nanocarriers for clinical use. Potential cytotoxicity arising from metal ions and organic linkers remains a primary concern, as certain components may induce harmful cellular responses depending on their concentration

and release behavior. Equally important is the toxicity of degradation products, since incomplete breakdown or long-term accumulation of MOF fragments in organs can lead to chronic adverse effects. Immunogenicity and inflammatory responses also influence biocompatibility, with some MOFs triggering unwanted activation of immune pathways [31-32]. To accurately assess these risks, standardized in vitro and in vivo toxicity evaluation models are essential for determining safe exposure levels, degradation profiles, and organ-specific effects. Advancements in biosafety strategies, including the development of bio-MOFs and the incorporation of biodegradable linkers, offer promising solutions to minimize toxicity while maintaining therapeutic performance [33].

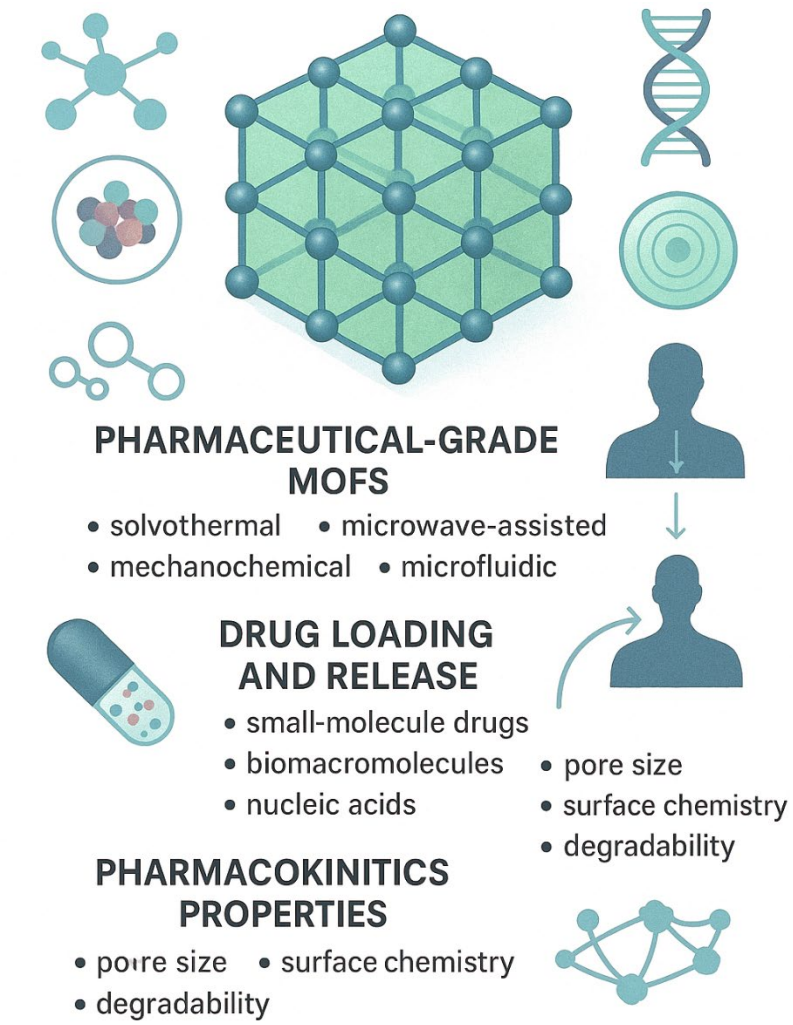

Figure-1 Pharmceutical Grade MOFS

8. Analytical and Characterization Techniques

A comprehensive understanding of MOF nanocarriers requires the use of advanced analytical and characterization techniques that reveal their structural, physicochemical, and biological properties. Structural and surface analyses are commonly performed using powder X-ray diffraction (PXRD), Brunauer–Emmett–Teller (BET) surface area measurements, Fourier-transform infrared spectroscopy (FTIR), and electron microscopy techniques such as SEM and TEM. Thermal stability is evaluated through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC), while inductively coupled plasma mass spectrometry (ICP-MS) enables precise quantification of metal ions within the framework [34-35]. To assess functional performance, in vitro release profiling and kinetic

modeling are employed to understand drug release mechanisms and predict behavior under physiological conditions. Biological compatibility and therapeutic potential are further verified using assays such as cell viability testing, cellular uptake studies, and hemolysis assays, providing essential insights into the safety and efficacy of MOF-based delivery systems [36-37].

9. Clinical and Regulatory Landscape

The clinical and regulatory landscape for MOF-based nanocarriers is evolving as these materials begin transitioning from laboratory research to translational and clinical settings. Although only a limited number of MOF-based systems have entered early-stage clinical evaluation, ongoing studies highlight their potential for targeted delivery, imaging, and therapeutic applications. However, significant regulatory hurdles remain, particularly regarding the use of metal-based components, which raise concerns related to long-term safety, biodegradation, and systemic exposure [38-39]. Meeting Good Manufacturing Practice (GMP) requirements is another major challenge, as MOF production must ensure strict batch consistency, high purity, and reproducibility—factors that are difficult to control given their complex architectures. Additionally, environmental and occupational safety issues must be addressed during large-scale manufacturing, since handling metal precursors, organic linkers, and nanoparticulate materials may pose risks to workers and surrounding ecosystems. Together, these considerations shape the path toward safe, standardized, and commercially viable MOF-based therapeutics [40-41].

10. Emerging Innovations

Emerging innovations in MOF-based nanomedicine are rapidly expanding the therapeutic potential of these systems. Biomimetic MOFs, particularly those coated with natural cell membranes, offer enhanced immune evasion, prolonged circulation, and improved targeting capabilities. Hybrid nanocarriers that integrate MOFs with polymers or lipids combine the structural tunability of MOFs with the biocompatibility of soft materials, creating highly versatile platforms for drug and gene delivery. Stimuli-responsive MOFs—activated by pH, enzymes, reactive oxygen species (ROS), or light—enable precise, on-demand drug release tailored to specific disease microenvironments. Advances in computational tools, including AI-driven design and predictive modeling, are accelerating the discovery of new MOF structures with optimized performance [42-43]. Additionally, theranostic MOFs capable of simultaneous imaging and therapy are paving the way for integrated diagnostic–therapeutic strategies that support real-time treatment monitoring.

11. Challenges and Future Directions

Despite significant progress, several challenges must be addressed before MOF nanocarriers can achieve widespread clinical adoption. Enhancing biostability while preserving the high porosity essential for effective drug loading remains a central hurdle, particularly under physiological conditions. Large-scale production also poses difficulties, as maintaining pharmaceutical-grade reproducibility and batch consistency is complex due to MOFs' structural sensitivity. Reducing toxicity—both from metal ions and degradation products—without compromising therapeutic performance is another ongoing priority. Looking ahead, integrating MOFs into personalized medicine frameworks and precision nanotherapy will require improved targeting strategies, deeper understanding of patient-specific responses, and alignment with evolving regulatory standards. Together, these efforts will shape the future trajectory of MOF-based therapeutics [44-45].

12. Conclusion

Metal–organic frameworks (MOFs) have rapidly emerged as one of the most promising classes of nanocarriers in modern pharmaceutics, offering an exceptional combination of structural tunability, high porosity, and functional versatility. Significant advances across synthesis, characterization, drug loading, and biomedical applications have demonstrated their capacity to enhance therapeutic delivery, improve pharmacokinetics, and enable controlled, stimuli-responsive release. Their broad pharmacological potential—spanning anticancer therapy, antimicrobial action, gene delivery, gas transport, and enzyme-based catalysis—highlights the adaptability of MOFs to diverse clinical needs. As innovations such as biomimetic coatings, hybrid nanocarriers, AI-guided design, and theranostic platforms continue to evolve, MOFs are increasingly positioned as smart, modular systems capable of integrating multiple therapeutic and diagnostic functions. Although challenges remain in biostability, toxicity reduction, regulatory approval, and large-scale manufacturing, ongoing research and technological refinement point toward a future in which MOF nanocarriers play a transformative role in personalized and precision medicine.

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