fortune Journals

JOURNAL OF PHARMACY AND PHARMACOLOGY RESEARCH

ISSN: 2578-1553

Research Article

Supramolecular Chemistry: Unveiling the Fascinating World of Non-Covalent Interactions and Complex Assemblies

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Abstract

Supramolecular chemistry is a captivating and interdisciplinary field that explores the interactions between molecules to form complex and functional assemblies through non-covalent forces. This review paper presents an in-depth exploration of the fundamental concepts, supramolecular assemblies and structures, applications in nanotechnology and biology, as well as challenges and future perspectives in supramolecular chemistry. The paper begins by elucidating the fundamental principles of supramolecular chemistry, emphasizing the significance of weak, non-covalent interactions such as hydrogen bonding, van der Waals forces, and π-π interactions. Molecular recognition, self-assembly, and host-guest interactions are highlighted as key concepts shaping the field.

Subsequently, the review delves into various supramolecular assemblies and structures, showcasing the diversity of nanoscale architectures that arise from self-assembly processes. From nanotubes and nanofibers to metal-organic frameworks and dynamic supramolecular systems, each structure's properties and potential applications are explored.

The application of supramolecular chemistry in nanotechnology and biology is a central focus of the paper. It covers the design of supramolecular materials for drug delivery, nanoelectronics, nanosensors, and biomimetic systems. Additionally, the integration of supramolecular approaches in biology, including molecular recognition, enzyme mimics, and bioimaging, is discussed in detail.

Furthermore, the challenges faced by supramolecular chemistry, such as predictability, stability, and scalability, are addressed. The paper also looks into the future perspectives of the field, envisioning adaptive materials, supramolecular machines, and data-driven design as exciting prospects. Overall, this comprehensive review offers a thorough understanding of the captivating world of supramolecular chemistry and its potential to revolutionize various scientific and technological domains. Through interdisciplinary efforts and a focus on sustainability, supramolecular chemistry holds promise for addressing real-world challenges and shaping a future defined by innovative materials and transformative applications.

Keywords: Supramolecular chemistry, non-covalent interactions, molecular recognition, self-assembly, supramolecular assemblies, nanotechnology, drug delivery, nanoelectronics, biomimetic materials, nanosensors, supramolecular machines, challenges, future perspectives.

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Citation: Shreya Talreja, Shashank Tiwari. Supramolecular Chemistry: Unveiling the Fascinating World of Non-Covalent Interactions and Complex Assemblies. Journal of Pharmacy and Pharmacology Research. 7 (2023): 133-139.

Received: August 01, 2023
Accepted: August 08, 2023
Published: August 10, 2023

Introduction

Supramolecular chemistry is a fascinating and interdisciplinary field that explores the interactions between molecules to create complex and functional assemblies. Unlike traditional covalent chemistry, which focuses on strong chemical bonds, supramolecular chemistry is concerned with weaker non-covalent forces, such as hydrogen bonding, van der Waals interactions, and electrostatic forces. These subtle interactions give rise to a wide array of supramolecular structures and materials with unique properties and applications. The term "supramolecular" comes from the Latin words "supra" (meaning above or beyond) and "molecula" (meaning molecule). It aptly describes the field's essence, as supramolecular chemistry involves the study of chemical species that are "beyond the molecule" – assemblies formed by the association of multiple molecules. The roots of supramolecular chemistry can be traced back to the late 19th and early 20th centuries with pioneering work by scientists such as J.W. McBain and Hermann Staudinger.

However, the field experienced significant growth and recognition in the latter half of the 20th century, especially with the groundbreaking work of Nobel laureate Jean-Marie Lehn, Donald J. Cram, and Charles J. Pedersen, who developed the concept of molecular recognition and supramolecular self-assembly. Since then, supramolecular chemistry has expanded into diverse areas, including materials science, nanotechnology, biology, and drug discovery. The ability to engineer and control these non-covalent interactions has led to the creation of smart materials, drug delivery systems, nanomachines, and molecular sensors, among other innovative applications. This review paper aims to provide a comprehensive exploration of supramolecular chemistry, covering fundamental concepts, supramolecular assemblies and structures, applications in nanotechnology and biology, challenges faced by the field, and exciting future perspectives. By understanding the principles and advancements in this dynamic field, we can appreciate the transformative potential of supramolecular chemistry in shaping the landscape of science and technology.

Fundamental Concepts

Supramolecular chemistry is built upon several key principles that govern the non-covalent interactions between molecules, leading to the formation of larger, more complex assemblies. Understanding these fundamental concepts is crucial to grasp the essence of supramolecular chemistry. Here are some of the key concepts:

Non-Covalent Interactions

Supramolecular chemistry relies on weak, non-covalent interactions between molecules, as opposed to the strong, directional bonds seen in covalent chemistry. The primary non-covalent interactions include hydrogen bonding, van der Waals forces (dispersion forces, dipole-dipole interactions, and dipole-induced dipole interactions), π-π interactions, electrostatic interactions, and metal-ligand coordination. These interactions are reversible, dynamic, and responsive to environmental changes, making them essential for the formation and modulation of supramolecular structures.

Molecular Recognition

Molecular recognition is a fundamental concept in supramolecular chemistry. It refers to the selective binding of one molecule (the guest) to another molecule (the host) through specific non-covalent interactions. This process is akin to a "lock and key" mechanism, where the host possesses a complementary binding site that fits the guest molecule. Molecular recognition plays a crucial role in biological processes, such as enzyme-substrate interactions and receptor-ligand recognition.

Self-Assembly

Self-assembly is the spontaneous formation of well-defined structures or patterns from individual components driven by non-covalent interactions. These components may be molecules, ions, or even nanoparticles. Self-assembly can lead to various supramolecular structures, such as aggregates, nanotubes, vesicles, and crystals. Understanding the factors that influence self-assembly, such as intermolecular forces, solubility, and molecular shape, is vital in designing functional supramolecular materials.

Supramolecular Complexes

Supramolecular complexes refer to assemblies of molecules held together by non-covalent interactions. These complexes are typically reversible and dynamic, allowing for adaptability and responsiveness to external stimuli. Supramolecular complexes can exhibit unique properties, such as host-guest interactions, chirality, and guest-induced transformations, making them essential for various applications, including drug delivery and catalysis.

Host-Guest Chemistry

Host-guest chemistry is a central theme in supramolecular chemistry, where a host molecule selectively accommodates a guest molecule within its cavity or binding site. The interaction between the host and guest is governed by complementary non-covalent interactions, leading to the formation of stable host-guest complexes. Host-guest systems find applications in molecular recognition, drug delivery, and the design of functional materials.

Supramolecular Polymers

Supramolecular polymers are macromolecular structures formed through non-covalent interactions. They differ

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from traditional covalently-bonded polymers and possess unique properties, such as dynamic reversibility and stimuli responsiveness. Understanding the principles governing the self-assembly and disassembly of supramolecular polymers is crucial for the design of adaptive materials and drug delivery systems.

Dynamic Supramolecular Systems

Dynamic supramolecular systems refer to assemblies that undergo reversible changes in their structures and properties in response to external stimuli. These stimuli can be physical (e.g., temperature, pH) or chemical (e.g., guest binding). Dynamic supramolecular systems exhibit intriguing behaviors, such as self-healing, self-sorting, and adaptive functions. Overall, these fundamental concepts of supramolecular chemistry provide the foundation for exploring the design, synthesis, and applications of complex and functional materials with wide-ranging implications in various scientific and technological fields.

Supramolecular Assemblies and Structures

Supramolecular assemblies and structures are complex arrangements of molecules held together by non-covalent interactions, resulting in higher-order architectures with unique properties and functionalities. These structures play a vital role in supramolecular chemistry and have applications in various fields, including materials science, nanotechnology, and drug delivery. Here are some common types of supramolecular assemblies and structures:

Aggregates

Supramolecular aggregates are formed when individual molecules or ions come together through non-covalent interactions. These aggregates can range from small clusters to larger assemblies, depending on the strength and nature of the interactions involved. Examples of aggregates include micelles, which are formed by amphiphilic molecules in a solvent, and colloidal particles, where nanoparticles or colloids assemble into larger structures.

Vesicles

Vesicles, also known as liposomes, are spherical structures composed of lipid bilayers. They are formed when amphiphilic molecules, such as phospholipids, self-assemble in an aqueous environment. Vesicles have a hydrophilic exterior and a hydrophobic interior, making them ideal for encapsulating hydrophobic drugs or molecules. They find applications in drug delivery and cell membrane mimics for biological studies.

Nanotubes and Nanofibers

Nanotubes and nanofibers are elongated supramolecular structures formed by the self-assembly of molecules or building blocks. They have nanoscale diameters and can vary in length. These structures often arise from the stacking or alignment of π-conjugated molecules, such as aromatic compounds or peptides. Nanotubes and nanofibers have unique electronic, mechanical, and optical properties, making them valuable for nanoelectronics and nanocomposite materials.

Metal-Organic Frameworks (MOFs)

MOFs are a class of porous materials formed by coordination bonds between metal ions or clusters and organic ligands. These structures have high surface areas and tunable pore sizes, making them ideal for gas storage, separation, and catalysis. MOFs can be engineered to have specific functionalities and are promising candidates for applications in environmental and energy-related fields.

Co-crystals

Co-crystals are crystalline structures formed by the association of two or more molecules through non-covalent interactions. Unlike traditional crystals, where a single compound forms the lattice, co-crystals involve multiple components that interact with each other. Co-crystals offer unique opportunities for modifying and improving the properties of active pharmaceutical ingredients (APIs) in drug formulation.

Dynamic Supramolecular Structures

Dynamic supramolecular structures refer to assemblies that undergo reversible changes in their structures in response to external stimuli, such as temperature, pH, or guest binding. These structures are often designed to be adaptive and responsive, and they can exhibit interesting behaviors, such as self-healing and shape memory effects.

Supramolecular Gels

Supramolecular gels are three-dimensional networks formed by the self-assembly of molecules in a solvent. These gels have a solid-like appearance but can be reversibly transformed into a sol state under specific conditions. Supramolecular gels find applications in drug delivery, tissue engineering, and soft robotics. Overall, supramolecular assemblies and structures offer a wide range of possibilities for designing new materials with tailored properties and functions. The ability to control and manipulate non-covalent interactions allows researchers to create complex and versatile architectures that hold significant promise in advancing various scientific and technological fields.

Supramolecular Materials and Nanotechnology

Supramolecular materials play a crucial role in nanotechnology, offering unique properties and functionalities that arise from their non-covalent interactions

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and self-assembly capabilities. These materials have diverse applications in nanotechnology, ranging from nanomedicine and nanoelectronics to nanocatalysis and nanosensors. Here are some key aspects of supramolecular materials in nanotechnology.

Self-Assembly of Nanomaterials

Supramolecular chemistry enables the controlled self-assembly of nanomaterials into specific structures and morphologies. By carefully designing the interactions between the building blocks, researchers can create nanoscale architectures with precise control over size, shape, and surface properties. Self-assembled nanostructures include nanotubes, nanofibers, nanocapsules, and nanosheets, among others.

Nanocarriers for Drug Delivery

Supramolecular materials are widely used as nanocarriers for drug delivery due to their biocompatibility and ability to encapsulate and protect therapeutic agents. Liposomes, micelles, and vesicles formed through self-assembly of amphiphilic molecules are examples of supramolecular nanocarriers. They can improve drug solubility, stability, and targeted delivery to specific tissues, enhancing therapeutic efficacy and reducing side effects.

Supramolecular Nanocomposites

Supramolecular materials can be combined with nanoparticles or other nanomaterials to create functional nanocomposites. These nanocomposites often possess synergistic properties derived from both the supramolecular structures and the incorporated nanoparticles. Supramolecular nanocomposites find applications in areas such as sensing, imaging, and catalysis.

Nanoelectronics and Nanophotonics

Supramolecular materials offer new opportunities for nanoelectronic and nanophotonic devices. Organic semiconductors and supramolecular nanowires can be integrated into electronic circuits and photonic devices. Their flexible and tunable properties make them attractive for next-generation nanoelectronics and organic optoelectronics.

Nano sensors and Molecular Probes

Supramolecular materials can act as nanosensors and molecular probes by selectively recognizing and responding to specific analytes or environmental changes. Functionalization of supramolecular structures with sensing units allows for the detection of ions, small molecules, and biomolecules with high sensitivity and selectivity. These nanosensors have applications in environmental monitoring, diagnostics, and biological imaging.

Nanocatalysis

Supramolecular catalysts can be designed by incorporating catalytically active moieties into supramolecular assemblies. These nanocatalysts offer advantages such as enhanced catalytic activity, substrate specificity, and easy recovery and recycling. Supramolecular nanocatalysis shows promise in green chemistry and energy-related applications.

Nanomaterials for Energy Conversion

Supramolecular materials are being explored for energy conversion and storage applications. For instance, supramolecular assemblies based on organic chromophores can be used in photovoltaics for efficient light absorption and charge transfer. Additionally, supramolecular nanomaterials are studied for their potential use in energy storage devices, such as batteries and supercapacitors. In summary, supramolecular materials have emerged as versatile building blocks in nanotechnology, offering a wide range of applications in drug delivery, nanoelectronics, nanosensors, catalysis, and energy conversion. The ability to engineer and control these materials at the molecular level holds tremendous potential for advancing various fields and addressing real-world challenges.

Supramolecular Approaches in Biology

Supramolecular approaches in biology have revolutionized our understanding of biological processes and provided valuable tools for various applications in biotechnology and medicine. By harnessing non-covalent interactions, researchers have developed innovative strategies to study, manipulate, and mimic biological systems. Here are some key areas where supramolecular approaches have made significant contributions in biology.

Molecular Recognition and Binding

Supramolecular chemistry plays a critical role in understanding molecular recognition and binding events in biological systems. By designing artificial receptors and host-guest systems, researchers can mimic the interactions between biomolecules, such as enzymes and substrates or proteins and ligands. These studies provide insights into the specificity and selectivity of biological processes and facilitate the development of new drugs and therapeutic approaches.

Drug Delivery

Supramolecular materials are extensively used as carriers for drug delivery. Nanocarriers based on self-assembled supramolecular structures, such as liposomes, micelles, and dendrimers, can efficiently encapsulate and transport therapeutic agents to target sites. This approach enhances drug stability, improves bioavailability, and enables targeted delivery, minimizing side effects and improving treatment efficacy.

Biomimetic Materials

Supramolecular chemistry allows researchers to

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create biomimetic materials that closely resemble biological structures and functions. For instance, synthetic supramolecular hydrogels can mimic the extracellular matrix and provide a suitable microenvironment for cell growth and tissue regeneration. The design of bioactive surfaces and coatings is another application, enabling better integration of biomedical implants and devices with surrounding tissues.

Enzyme Mimics and Catalysis

Supramolecular chemistry has led to the development of enzyme mimics or artificial enzymes. These synthetic structures can replicate enzyme-like catalysis, offering advantages such as increased stability and tunable reactivity. Supramolecular catalysts have been employed in applications ranging from organic synthesis to environmental remediation.

Bioimaging

Supramolecular probes and sensors are valuable tools in bioimaging studies. These probes can selectively interact with specific biomolecules or ions and emit detectable signals, such as fluorescence or luminescence. By attaching these probes to biological targets, researchers can visualize and monitor cellular processes in real-time, advancing our understanding of various biological phenomena.

Artificial Photosynthesis

Supramolecular complexes inspired by natural photosynthetic systems have been developed for artificial photosynthesis. These complexes can capture light energy and facilitate electron and energy transfer, mimicking the light-harvesting and energy conversion processes in plants. Artificial photosynthesis research aims to harness solar energy for the production of clean and renewable fuels.

Protein Engineering and Design

Supramolecular approaches are employed to engineer proteins and peptides with novel functions and properties. Through rational design and directed evolution, researchers can create new biomolecular assemblies with enhanced stability, activity, and specificity. These engineered proteins find applications in biocatalysis, biotherapeutics, and biosensors. Overall, supramolecular approaches in biology have paved the way for innovative solutions to biological challenges and have contributed significantly to advancements in biotechnology, medicine, and bioengineering. As the field of supramolecular biology continues to evolve, it holds great promise for addressing complex biological questions and driving transformative developments in various applications.

Challenges and Future Perspectives in Supramolecular Chemistry

Supramolecular chemistry has made remarkable strides in recent decades, but it also faces certain challenges and holds exciting prospects for the future. Addressing these challenges and exploring new directions will shape the evolution of this field. Here are some of the key challenges and future perspectives in supramolecular chemistry.

Challenges:

Complexity and Predictability: Designing supramolecular assemblies with specific functions and properties can be highly challenging due to the complexity of non-covalent interactions and the vast array of possible structures. Improving our ability to predict and control self-assembly processes is a significant challenge.

Stability and Robustness

Many supramolecular structures are sensitive to environmental changes, which can impact their stability and functionality. Achieving robust and stable supramolecular materials that retain their properties under various conditions remains a challenge.

Integration with Biology

While supramolecular approaches have shown promise in biology, translating these findings into practical biomedical applications faces hurdles. Ensuring biocompatibility, long-term stability, and efficient targeting in vivo are essential considerations.

Dynamic Systems

Understanding and controlling dynamic supramolecular systems, where structures constantly undergo rearrangements in response to stimuli, pose challenges for both fundamental research and practical applications. Scalability and Manufacturing: Developing scalable and cost-effective methods for the synthesis and production of supramolecular materials is crucial to their broader application in industry and technology.

Future Perspectives

Adaptive and Responsive Materials

Future supramolecular materials are expected to be more adaptive and responsive to external stimuli, leading to materials that can autonomously adjust their properties and functions in real-time.

Supramolecular Machines

Advances in supramolecular chemistry may lead to the development of artificial molecular machines and nanodevices that perform specific tasks, such as molecular transport, information processing, and mechanical work.

Artificial Intelligence and Data-Driven Design

The integration of artificial intelligence and machine learning into supramolecular chemistry can accelerate the

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discovery of novel supramolecular structures and their properties, enabling data-driven design and optimization.

Supramolecular Nanomedicine

The development of smart supramolecular nanocarriers for drug delivery, responsive therapeutics, and targeted imaging holds great potential for personalized medicine and disease treatment.

Sustainable Materials

Supramolecular chemistry can contribute to the creation of sustainable materials by exploring bio-based and environmentally friendly supramolecular systems.

Supramolecular Electronics

The development of supramolecular materials for advanced nanoelectronics and molecular-scale devices could lead to transformative breakthroughs in electronics and information processing.

Supramolecular Materials for Energy

Advances in supramolecular chemistry may lead to new materials for energy storage, conversion, and harvesting, contributing to the development of sustainable energy technologies. In conclusion, while supramolecular chemistry has made significant progress, challenges related to predictability, stability, and scalability remain to be addressed. Nevertheless, the field's future perspectives, including adaptive materials, molecular machines, and AI-driven design, hold great promise for solving complex scientific and technological problems and creating novel materials with diverse applications. Continued interdisciplinary research and collaboration will play a pivotal role in shaping the future of supramolecular chemistry.

Conclusion

In conclusion, supramolecular chemistry stands at the forefront of scientific research, offering a captivating world of non-covalent interactions and self-assembly that holds tremendous promise for various disciplines. Through the study of weak molecular forces, researchers have unlocked a wealth of possibilities for creating complex, functional, and adaptive materials with applications ranging from nanotechnology and materials science to biomedicine and energy.

This review has provided an overview of the fundamental concepts of supramolecular chemistry, exploring key principles such as non-covalent interactions, molecular recognition, and self-assembly. We have delved into the diverse array of supramolecular assemblies and structures, ranging from nanotubes and vesicles to metal-organic frameworks and dynamic supramolecular systems. These structures exhibit remarkable properties that make them invaluable in fields such as drug delivery, nanoelectronics, catalysis, and biomimetic materials. Furthermore, we have examined the crucial role of supramolecular approaches in biology, showcasing their impact on molecular recognition, drug delivery, biomimetic materials, and enzyme mimics. Supramolecular chemistry has provided essential tools for understanding complex biological processes and designing novel therapeutics and diagnostics.

As with any scientific discipline, supramolecular chemistry faces its share of challenges, including predictability, stability, scalability, and integration with biology. Overcoming these challenges will require continuous research and innovation, paving the way for exciting future perspectives. The development of adaptive and responsive materials, supramolecular machines, and AI-driven design holds great potential for advancing the field and addressing real-world problems. In conclusion, supramolecular chemistry represents a vibrant and dynamic frontier of science that continues to evolve and shape the way we interact with matter at the molecular level. With ongoing interdisciplinary efforts and a focus on sustainability and societal impact, the future of supramolecular chemistry looks promising, unlocking new opportunities for groundbreaking discoveries and transformative applications. As researchers venture further into the realm of supramolecular interactions, we can anticipate a world of advanced materials, nanotechnological wonders, and innovative solutions to some of humanity's most pressing challenges.

Source of Funding: Self-Funded

Conflict of Interest: Nil

Acknowledgement

The author would like to thank all his mentors. The notes compiled here are collected over a period of time and may have been reproduced verbatim. Apologize to all researchers if in-advertently failed to acknowledge them in the references.

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