Global Trends in Science and Technology

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

# Frontiers in Organic Chemistry: From Reaction Mechanisms to Molecular Design

**Javeriya Sayed**[1*]

[1]Independent Researcher, Maryland, United States

[1]javeriyasayed1985@gmail.com

open access

**Corresponding Author**

**Javeriya Sayed**
javeriyasayed1985@gmailcom

**Article History:**

Submitted: 08-11-2025

Accepted: 06-11-2025

**Published: 13-11-2025**

**Keywords**

Organic chemistry, Reaction mechanisms, Catalysis, Molecular design, Functionalization, Emerging technologies, Computational modeling.



## ABSTRACT

The field of organic chemistry is developing as one of the key areas of contemporary science serving as a connection between the mechanistic knowledge and the molecular design and usability. The current review outlines the most important developments between reaction mechanisms and catalytic approaches, green and sustainable techniques, and new technologies like machine learning and automated synthesis. The accurate control of reactivity is possible with the help of mechanistic insights, whereas complex molecules can be construscted with high efficiency with the help of catalysis and functionalization. Greener strategies reduce environmental impact and computer aided technologies are faster in predictive design. Collectively, these trends broaden the horizons of organic chemistry, with the growth and development of innovation in the pharmaceuticals, materials, and energy field. The future directions are on the emphasis on interdisciplinary collaboration, predictive modeling, and the use of environmentally friendly chemical practices.

## INTRODUCTION

Organic chemistry is in the center of the chemical science of today, the backbone of such diverse fields as medicinal chemistry and materials science, biotechnology and energy research. The field has grown over the last few decades in complexity to become a multidimensional science that involves a combination of mechanistic understanding, molecular design and computational forecasting. This combination has not only allowed chemists to know how reactions happen, but also to rationally

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

design new molecules and synthetic pathways with the functions and selectivity that they want [1]. The study of mechanisms of reaction is still at the heart of organic chemistry. Mechanistic studies enable chemists to determine the successive changes of molecules, identify reaction intermediates and regulate reaction pathways. This understanding is now being transformed with the development of spectroscopic, kinetic and computational tools, being able to obtain transient species and transition states previously unknown [2]. These innovations have enhanced our understanding of reaction formation and breaking processes, electron transfer and energy flow in chemical systems, therefore, facilitating a more accurate control of reactivity and selectivity [3].

In line with mechanistic developments, the idea of molecular design has become extremely significant. Synthesizing molecules efficiently is just one of the aims of organic chemists today, who also hope to create molecules with particular properties to serve a given purpose: either as pharmaceuticals, catalysts, electronic materials, or even supramolecular assemblies. Molecular design is based on strategic choice and control of functional groups, stereochemistry and molecular structures in order to obtain desired physical, chemical or biological properties. The increased synergy observed between synthetic methodology, computational modeling and materials chemistry has boosted the finding of functional organic systems with capability so new [4].

The new frontier of the organic chemistry is the intersection of the reaction mechanism and the molecular design. A profound mechanistic knowledge offers the explanation of how molecules can be made more effectively, whereas rational molecular design guides the synthetic strategies to the practical uses. This intersection forms the basis of catalysis progress, green chemistry and molecular innovation that is progressively reforming industries as well as research [5]. This review is aimed at delineating current advances in the illustration of such frontiers - in mechanistic breakthroughs, catalytic innovations, and strategies in molecular design that can be put together to define the future of organic chemistry. This article will offer a reflection of how organic chemistry is still being transformed as an innovative and dynamic science by balancing the classical concepts with the new developments in technology [6].

## REACTION MECHANISMS: THEORIES AND CONTEMPORARY UNDERSTANDINGS

The intellectual fundamental of organic chemistry is the comprehension of reaction mechanisms. Mechanistic investigations form the basis of predicting the chemical reactivity, selectivity control and developing new methods of synthesis. Reaction mechanism describes in detail how the products are formed out of the reactants by forming and breaking bonds showing the intermediates and transition states. Mechanistic organic chemistry has historically emerged as a result of classical observations of kinetics, substitution patterns, and stereochemical reactions resulting in the development of the

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

concepts of nucleophilicity, electrophilicity, and in situ reaction intermediates such as carbocations and carbanions [7].

In the modern age, it has become feasible, by spectroscopically, through the development of spectrometric methods (such as NMR, IR, UV Vis, and mass spectrometry) to observe and characterize short-lived species, providing a first-hand demonstration of mechanistic hypotheses [8]. In addition, the advent of computational chemistry has brought a revolution in mechanistic studies because chemists can now simulate reaction pathways, estimate the activation energies and visualize transition states in detail on an atomic scale. Theoretical techniques like Density Functional Theory (DFT) are very informative on the nature of potential energy surfaces and reaction coordinates that are valuable in supplementing experimental measurements and improving predictability [9].

Mechanisms of radical, ionic, and pericyclic reactions are increasingly studied and contribute to an enlarged synthetic arsenal of organic chemists. Radical reactions which were deemed hard to control are now exactly controlled using photoredox and electrochemical techniques. Orbital symmetry controlled pericyclic reactions continue to play a role in the study of concerted reactions and the design of stereospecific reactions. Equally, the clarification of transition-metal-catalyzed processes that include oxidative addition, migratory insertion, and reductive elimination reactions has set the stage of cross-coupling and C-H activation reactions that prevails in contemporary synthetic chemistry [10].

A mechanistic knowledge also offers an outline in formulating selective and sustainable transformations. Finding the important steps that determine the rate and selectivity allows chemists to optimize the reaction conditions to obtain as high a yield as possible and as little by-products and waste as possible. This strategy is in harmony with both green and sustainable synthesis [11]. The current mechanistic research combines experimental, theoretical, and computational methods to decipher the dynamics of organic reactions. Real-time analysis, predictive modeling, and data-driven provide insights into our conceptualization of molecular reactivity, and they continue to redefine the concept. Consequently, the study of reaction mechanisms is an active boundary, which directs the rational design of new organic reactions and the development of synthetic strategy in organic chemistry [12].

## STRATEGIES OF CATALYSIS AND ACTIVATION

Catalysis is a central theme of contemporary organic chemistry, as it is one of the primary methods of increasing reactivation, selectivity, and sustainability of reactions. A catalyst offers an alternate reaction route that has a lower activation energy allowing chemical transformations otherwise sluggish, unselective, or infeasible at more normal conditions. In recent decades, the science of

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

catalysis has developed the synthetic organic chemistry revolution, that is, there is a plethora of different catalytic systems, such as transition-metal catalysis, organocatalysis, photoredox catalysis, and biocatalysis, which revolutionize the very process of molecule assembly [13].

One of the most potent methods of organic synthesis has become transition-metal catalysis. Metals that facilitate a wide variety of reactions, the reactions that include cross-coupling, hydrogenation, C -H activation, and olefin metathesis, include palladium, nickel, ruthenium, and copper. These reactions enable chemists to make carbon-carbon and carbon-heteroatom bonded molecules with high precision, simplifying the process of making complex molecules. Megaproductive knowledge of major processes, including oxidative addition, migratory insertion and reductive elimination, has played a crucial role in streamlining the design of catalysts and enhancing their efficiency [14].

A more sustainable and generalized approach has been the emergence of organocatalysis, or the use of small organic molecules as catalysts, instead of a system utilizing metals. Organocatalysts like Proline, imidazolidinones and cinchona alkaloids facilitate enantioselective asymmetric transformations usually in mild and environmentally friendly conditions. Organocatalysts are required to have a simplicity, tunability and a non-toxic attribute that makes them particularly attractive in green chemistry applications and pharmaceutical synthesis [15]. Photoredox and electrochemical catalysis is another disruptive technology that uses light and electricity to catalyze a redox or radical transformation that is redox neutral. The methods enlarge the chemical space available to organic chemistry by producing highly reactive intermediates in mild conditions, and usually with excellent functional group tolerance. In addition, organic chemistry is connected to biology through biocatalysis and enzyme-inspired catalysis which allow selective transformations to be performed to resemble natural enzyme processes [16].

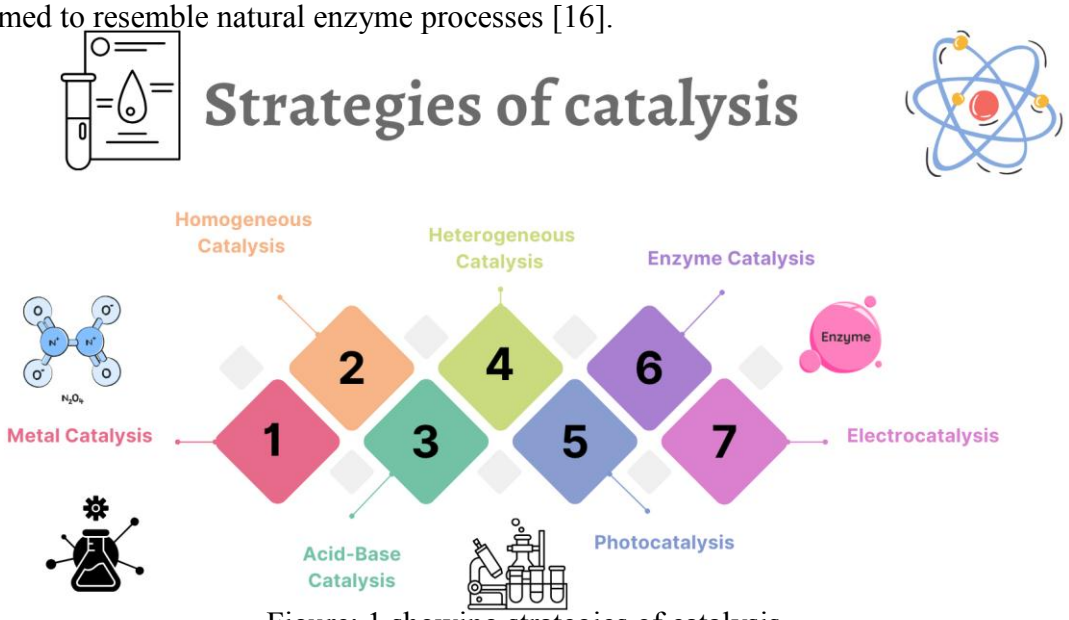


Figure: 1 showing strategies of catalysis

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

New frontiers in molecular activation are coming up in the form of emerging dual and cooperative catalysis strategies in which the catalytic mode of two reactions interacts with each other synergistically. These methods are the integration of the strengths of various catalytic systems such that the reactivity and selectivity of these systems cannot be attained in isolated catalysts [17]. The development of projects in catalysis and activation methods keeps changing the boundaries of organic synthesis. Combinating mechanistic knowledge and new catalyst design chemists are obtaining greater efficiency, sustainability, and specificity- the future of molecular building in organic chemistry [18].

## GREEN AND SUSTAINABLE ORGANIC CHEMISTRY

Green and sustainable organic chemistry has become a crucial field that has attempted to reduce the environmental and health effects of chemical production and ensure efficiency and innovation. Organic chemists are at the forefront of designing processes to ensure that there is less waste, less use of resources and that renewable feedstocks are used as global industries and research institutions focus on sustainable development. Paul Anastas and John Warner proposed the principles of green chemistry to underline the prevention of pollution, atom economy, energy efficiency, and safer reagents and solvents, which have radically changed the philosophy and practice of organic synthesis [19].

Among the main aims of sustainable organic chemistry is to minimize atom economy- to make sure that the biggest part of the atoms in the reactants is used in the product. Such reactions as catalytic hydrogenations, cycloadditions, and multi-component reactions are examples of such reactions in that they reduce by-products to the minimum. On the same note, substitution of toxic reagents and heavy-metal catalysts with benign reagents has come to a point of intense attention [20]. The advancement of organocatalysis and biocatalysis has offered more environment-friendly pathways to more complicated molecules utilizing non-toxic and recyclable catalysts that work in mild conditions. Solvent selection is also one of the important issues of sustainable chemistry [21]. The common organic solvents like chlorinated hydrocarbons and aromatics are very harmful to the environment. To this end, scientists are resorting to solvent free reactions, supercritical fluids, ionic liquids and aqueous phase catalysis that have a less harmful effect on the environment. Moreover, the microwave-assisted synthesis, flow chemistry, and mechanochemistry have also become energy-effective approaches by increasing the rate of reaction and reducing the wastes [22].

Another future area is the incorporation of renewable resources, including biomass, natural products, and CO 2 as organic feedstock to create products. Not only do these strategies lessen reliance on the petrochemical sources, but also allow carbon-neutral processes. Moreover, the application of life-

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

cycle assessment (LCA) software assists chemists in analyzing the environmental impact of synthetic processes of raw materials to final waste disposal [23]. Green and sustainable organic chemistry is a representation of the transformation of the efficiency-based metrics development towards the holistic approach of environmental responsibility. Through a combination of innovation and ecological consciousness, chemists are establishing a new definition of the role of organic synthesis in building a cleaner, safer, and more sustainable future of both science and society [24].

## MOLECULAR DESIGN AND FUNCTIONALIZATION.

The creative nature of organic chemistry is molecular design and functionalization, which allows the rational assembly of molecules with a desired structure, properties and functions. The power to single-atom DNA enables chemists to create compounds in various ways such as pharmaceuticals, catalysts, sensors, and advanced materials. The concept fills the gap between the synthesis and the function where the importance lies not only on the way molecules are produced but also on why they are designed in certain ways to produce the desired results [25]. The central theme of molecular design is the knowledge of structure-property relationships. Chemists can predict and control chemical reactivity, chemical stability, solubility and biological activity by systematically varying molecular frameworks, substituents, and stereochemical features. In this aspect, it is now essential to use computational methods, including molecular modeling and quantum chemical calculations, to visualize molecular orbitals, predict binding affinities, and optimize molecular geometries prior to synthesis. These predictive technologies make discovery faster and eliminate trial and error which is traditionally encouraged by organic synthesis [26].

Another principle of molecular design is functionalization which is the strategic insertion or alteration of functional groups in a molecule. The chemists can reach intricate molecular frameworks with an extraordinary degree of selectivity by utilizing all these methods of cross-coupling, selective C-H activation, and late-stage diversification. These approaches allow the physical and chemical properties to be fined to the requirements such that simple scaffolds can be converted into functional organisms with a desired performance in biological and material requirements [27]. Structural design of functional organic materials is one of the most vibrant fields of contemporary chemistry. Reconfigurable conjugation and electronic modification of organic semiconductors, light-emitting molecules and photovoltaic materials are designed to produce the best charge transport and optical characteristics. On the same note, rational molecular design has been applied in medicinal chemistry to create drugs with enhanced potency, selectivity, and metabolic stability based upon structure activity relationships (SAR) and computer aided drug design software [28].

Global Trends in Science and Technology
ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

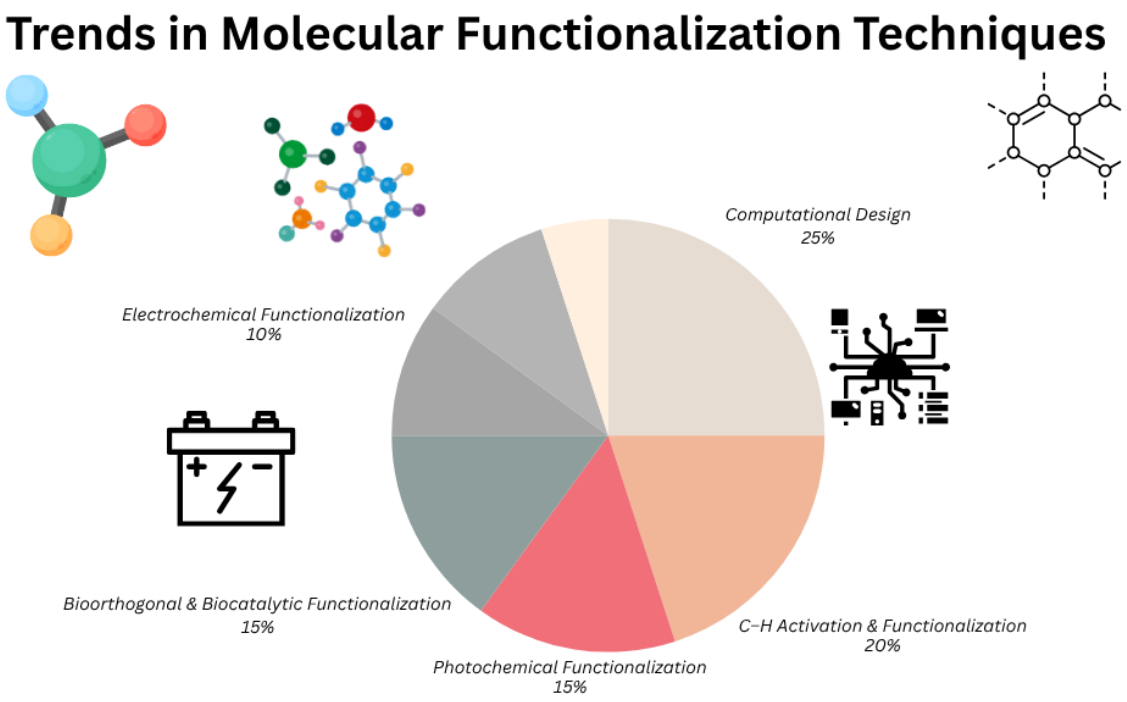


Figure: 2 showing trends in molecular functionalization techniques

Also, supramolecular and macrocyclic structures have been used to emphasize the importance of noncovalent interactions in molecular design to result in systems that can be self-assembled, recognize molecules, and be delivered where needed. In short, molecular design and functionalization represents the intellectual art of organic chemistry to be able to take mechanistic knowledge to the purposeful creativity [29]. Combining theory, synthetic invention, and practical implementation, chemists still manage to create the molecules that not only display the beauty of chemical science but also can be used to solve acute technological and biomedical problems [30].

## ORGANIC CHEMISTRY EMERGING TECHNOLOGIES

The fast changing nature of new technologies has radically altered the future of organic chemistry and altered the way reactions are designed, performed and studied. Conventional methods of laboratory use are now being supplemented with digital and automated and energy-effective techniques that increase precision, reproducibility and sustainability. Not only do these innovations have the effect of speeding up the rate of discovery, they also provide new avenues of studying chemical reactivity and molecular design on a new level of control and understanding [31]. The use of machine learning (ML) and artificial intelligence (AI) in organic chemistry is one of the most radical changes. Models based on data are also becoming popular to predict the outcome of reactions, optimize synthetic pathways and discover new catalysts. Through analysis of high-volume data of experimental and computational simulations, AI can identify complicated trends in chemical

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

reactivity that may not be intuitive to humans. The latter predictive force allows to design efficient synthetic pathways and support smarter chemistry in which computational knowledge guides an experiment [32].

Another significant improvement is automated and high-throughput synthesis. Under controlled conditions, robotic platforms and flow chemistry systems enable chemists to screen hundreds of reactions with controlled conditions to rapidly screen catalysts, solvents and substrates. Flow chemistry specifically has advantages in the form of increased safety, scalability, and reaction efficiency due to its ability to ensure accurate temperature control, pressure control, and mixing [33]. These methods have a great impact on waste reduction and enhancing reproducibility, which are in line with the philosophy of green chemistry. It has also been noted that the incorporation of mechanochemistry, which facilitates reactions with the aid of mechanical force instead of solvents is a solvent-free and energy-efficient synthetic approach. In a similar vein, electrochemical and photochemical approaches are re-established the manner in which redox reactions and radical processes are conducted, and provide cleaner and more sustainable alternatives to traditional reagents [34].

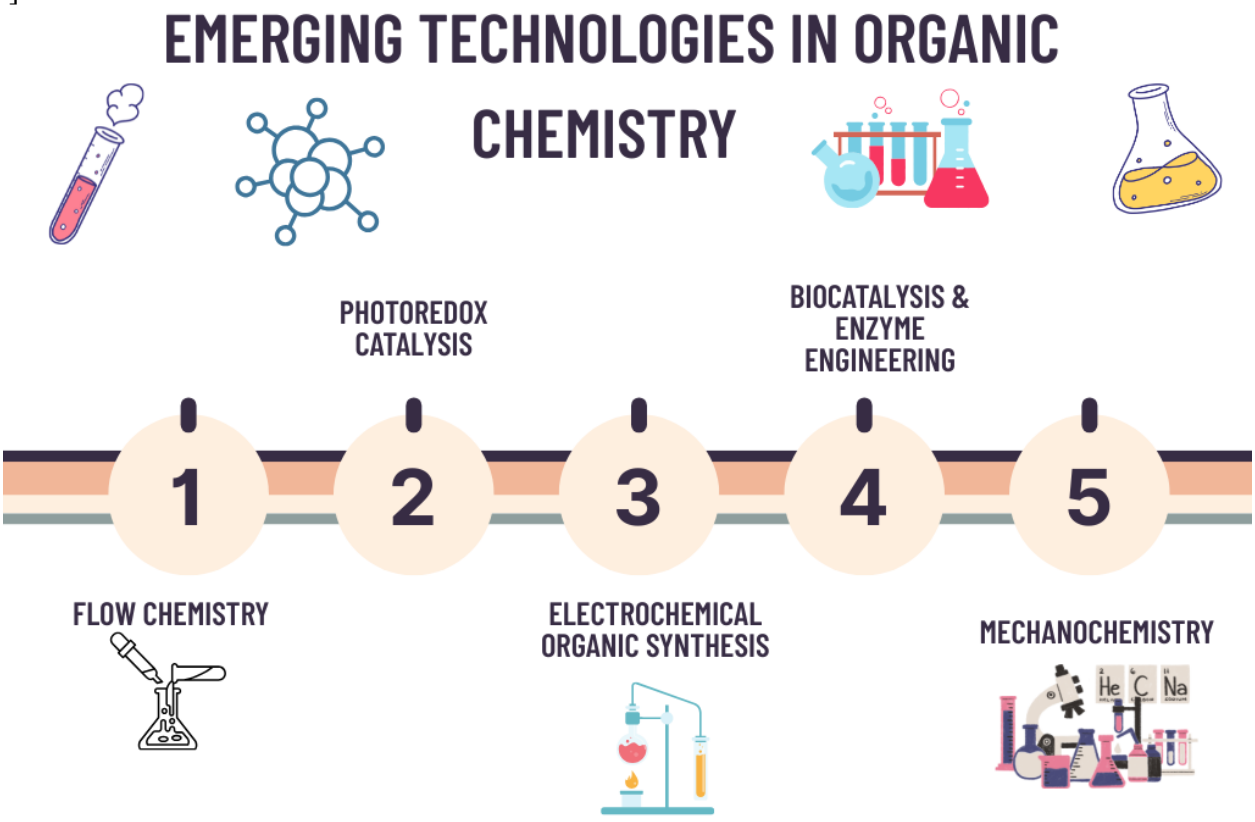


Figure: 3 showing emerging technologies of in organic chemistry

New interfaces between organic chemistry and materials science and nanotechnology have enlarged the landscape of the field, even more. Chemists are currently developing organic nanostructures,

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

hybrid materials and molecular electronics with custom functions in catalysis, sensing and energy conversion. The new technologies are leading to the paradigm shift in the field of organic chemistry that is to be directed to the intuition-based synthesis to the data-driven, automated, and sustainable science [35]. The innovations are set to change the manner in which molecular discovery is done, and will recast the future of research in organic chemistry by leveraging the combination of cutting edge instrumentation, computation, and interdisciplinary effort [36].

## DIFFICULTIES AND FUTURE HORIZONS

Nevertheless, even with the impressive advances made, the field of organic chemistry still has considerable challenges, which dictate the future of the field and opportunities in the field. Chemists are expected to meet the demands of efficiency, sustainability, and innovation to the scientific as well as the societal needs as the field becomes more complex and interdisciplinary [37]. This knowledge can help in shaping the scientific research in the new generation and ascertaining that organic chemistry continues to be a cause of modern science and technology. The enhancement of mechanistic knowledge is one of the greatest challenges. Despite the existence of strong analytical and computational methods, numerous complicated reactions, especially multistep catalytic processes, radical reactions, continue to have elusive intermediates and unpredictable selectivity [38]. The creation of more precise and available models to visualize and quantify reaction pathways is a major priority to develop. Moreover, the translation of mechanistic insight to predictive ability in the discovery of new reactions remains an unattained objective to both theoretical and experimental chemists [39].

The other significant problem is reaching universal identities to predict and design the reaction. As machine learning and artificial intelligence are becoming powerful tools, the quality of chemical data is essential and its diversity is crucial as well as its interpretability [40]. Open-access reaction databases and standardized reporting practices are necessary so as to achieve reproducibility and progress using data. The next stage of digital organic chemistry will be the implementation of these technologies integrated smoothly into the laboratory processes [41]. Sustainability is also an urgent problem. Compromising synthetic utility and environmental accountability requires the unceasing creation of more environmentally friendly reagents, recyclable catalysts, and energy-efficient procedures. One of the most pressing international agendas that chemists are supposed to achieve is carbon neutrality in chemical processes and reduced reliance on fossil-based feedstock's [42].

Future organic chemistry will have even greater horizons due to interdisciplinary nature. Such interdisciplinary work with materials science, biology and computational fields will result in new uses - smart materials and molecular machines as well as targeted therapeutics and energy solutions

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

[43]. The future of organic chemistry is in the combination of the mechanistic precision, the technological innovation, and environmental consciousness. It is not only the aim to overcome the existing challenges that will not only improve the scientific knowledge, but it is also a guarantee that organic chemistry will maintain growth to be a creative, responsible and transformative science in the 21st century [44].

## CONCLUSION

Organic chemistry has become one of the most vibrant and interdisciplinary sciences in contemporary science and keeps on forming our perception of how molecules behave and how intricate functional systems are rationally designed. Since the early theories of reaction mechanisms up to the leading edge of the molecular design, catalysis and sustainable synthesis, the field has gone through radical developments which have made it expand in scope and influence. There are several frontiers of organic chemistry that have been identified in this review and the convergence of these areas through mechanistic understanding, novel catalysis, green practices, and new technologies is a way to propel the field ahead.

The core of these developments is a thorough knowledge of reaction mechanisms. Mechanistic studies give chemists instruments to forecast and regulate chemical changes, allowing reactivity, selectivity and efficiency to be manipulated exactly. Combination of experimental methods like a sophisticated spectroscopy and kinetic analysis with computational modeling has brought a revolution to the visualization of intermediates and transition states providing unprecedented insight into reaction pathways. That mechanistic knowledge is needed not only to design new reactions, but also to optimize the existing processes in a predictable and rational way.

Catalysis and activation techniques have become an effective catalyst to the contemporary synthetic chemistry. The complex molecules can be constructed with a high level of selectivity and efficiency using transition-metal catalysis, organocatalysis, photoredox processes, and enzyme-inspired transformations. Catalysis has revolutionized synthetic approaches in the fields of pharmaceuticals, materials science and industrial chemistry by reducing activation barriers and allowing specific bond-forming processes. Also, dual and cooperative catalytic systems are extending the capabilities of what can be synthetically accessible and offer new possibilities of innovation that were not possible before.

The increased focus on green and sustainable organic chemistry is indicative of the field's concern to the environment. The integration of concepts of atom economy, minimization of solvents, and renewable feedstocks makes sure that the synthetic strategies are efficient and at the same time green. The incorporation of sustainability and innovation can be exemplified by emerging methods such as solvent-free reactions, mechanochemistry, flow chemistry, and biocatalysis, and they illustrate that

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

being environmentally friendly, in addition to being very productive in synthesis, is possible.

The art and design of molecules and their functionalization bring out the creative and intentional side of organic chemistry. Chemists can create molecules that have specified biological, electronic or optical properties by playing with structure-property relationships. Examples of these strategies include functionalization, late-stage modifications and supramolecular architectures, which are used to construct complex systems that can perform a particular task to bridge the gap between chemical synthesis and usability. This is what organic chemistry pertains to as it is important in any other field, including medicinal chemistry and materials science.

The field of study is being redefined by emerging technologies such as machine learning, artificial intelligence, automated synthesis, and computational modeling. These technologies cause more rapid reaction identification, streamline synthetic pathways, and give predictive data to allow chemists to address more complicated molecular issues with effectiveness and accuracy. Digital chemistry can be viewed as a new revolutionary period, when the data-driven theory can be used to supplement conventional intuition-based methods. In spite of these exceptional improvements there are still challenges. Complete explanation of complicated reaction mechanisms, generation of generally predictive models and attaining real sustainability in chemical reactions all remain active research topics.

To overcome these difficulties, interdisciplinary cooperation, creativity, and the desire to pursue both scientific excellence and social responsibility will be needed. Present-day organic chemistry is at the junction point of tradition and innovation. The domain keeps broadening its frontiers by merging mechanistic knowledge, catalytic innovativeness, sustainability, molecular innovativeness, and emerging technological innovation. These integrated endeavors do not only enhance our understanding of the field of molecular science but also offer real-life answers to the burning issues facing the world in the fields of medicine, materials, and energy. The future of organic chemistry is further expansion of the field as an imaginative, responsible, and transformative science, a field that will be indispensable to basic research and practicum technology in the 21st century.

## REFERENCES

[1]. Carreira EM. Introduction: Frontiers in Organic Synthesis. Chemical Reviews. 2015 Sep 9;115(17):8945-.

[2]. Carroll FA. Perspectives on structure and mechanism in organic chemistry. John Wiley & Sons; 2023 Apr 14.

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

[3]. Braga LS, Leal DH, Kuca K, Ramalho TC. Perspectives on the role of the frontier effective-for-reaction molecular orbital (FERMO) in the study of chemical reactivity: an updated review. Current Organic Chemistry. 2020 Feb 1;24(3):314-31.

[4]. Svatunek D. Computational organic chemistry: the frontier for understanding and designing bioorthogonal cycloadditions. Topics in Current Chemistry. 2024 May 10;382(2):17.

[5]. Cheng GJ, Zhang X, Chung LW, Xu L, Wu YD. Computational organic chemistry: bridging theory and experiment in establishing the mechanisms of chemical reactions. Journal of the American Chemical Society. 2015 Feb 11;137(5):1706-25.

[6]. Tan Z, Yang Q, Luo S. AI molecular catalysis: where are we now?. Organic Chemistry Frontiers. 2025;12(8):2759-76.

[7]. Yang Y, Li Q, Li Z. Advances in organic room-temperature phosphorescence: design strategies, photophysical mechanisms, and emerging applications. Materials Chemistry Frontiers. 2025;9(5):744-53.

[8]. Nakliang P, Yoon S, Choi S. Emerging computational approaches for the study of regio-and stereoselectivity in organic synthesis. Organic Chemistry Frontiers. 2021;8(18):5165-81.

[9]. Domingo LR, Acharjee N. Molecular electron density theory: a new theoretical outlook on organic chemistry. InFrontiers in Computational Chemistry: Volume 5 2020 Aug 31 (pp. 174-227). Bentham Science Publishers.

[10]. Smith MB. March's advanced organic chemistry: reactions, mechanisms, and structure. John Wiley & Sons; 2025 Aug 26.

[11]. Liao J, Yang X, Ouyang L, Lai Y, Huang J, Luo R. Recent advances in cascade radical cyclization of radical acceptors for the synthesis of carbo-and heterocycles. Organic Chemistry Frontiers. 2021;8(6):1345-63.

[12]. Khan I, Zaib S, Ibrar A. New frontiers in the transition-metal-free synthesis of heterocycles from alkynoates: an overview and current status. Organic Chemistry Frontiers. 2020;7(22):3734-91.

[13]. Li X, Xu J, Xu ZG. Precision single-atom editing: new frontiers in nitrogen insertion and substitution for the generation of N-heterocycles. Organic Chemistry Frontiers. 2024;11(14):4041-53.

[14]. Wu Z, Zhang M, Shi Y, Huang G. Mechanism and origins of stereo-and enantioselectivities of palladium-catalyzed hydroamination of racemic internal allenes via dynamic kinetic resolution: a computational study. Organic Chemistry Frontiers. 2020;7(12):1502-11.

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

[15]. Sun K, Lv QY, Lin YW, Yu B, He WM. Nitriles as radical acceptors in radical cascade reactions. Organic Chemistry Frontiers. 2021;8(3):445-65.

[16]. Han LL, Zhang QY, Li X, Qiao Y, Lan Y, Wei D. The chiral pyridoxal-catalyzed biomimetic Mannich reaction: the mechanism and origin of stereoselectivity. Organic Chemistry Frontiers. 2022;9(16):4401-10.

[17]. Guo X, Shen B, Liu C, Zhao H, Li X, Yu P, Li P. Rational design and organocatalytic enantioselective [1+ 4]-annulations of MBH carbonates with modified enones. Organic Chemistry Frontiers. 2023;10(1):150-6.

[18]. Zhang X, Cao X, Wei L, Wang Z, Wei Y, Xu L, Huang G. A pyridine-boryl radical mediated cascade reaction towards the synthesis of indolizines: a computational mechanistic analysis. Organic Chemistry Frontiers. 2024;11(15):4168-75.

[19]. Huang J, Zhang L, Meng X. Recent advances in the cyclization reactions of pyridinium 1, n-zwitterions (n= 4 and 5): scope and mechanism. Organic Chemistry Frontiers. 2023;10(11):2813-29.

[20]. Wang Y, Cobo AA, Franz AK. Recent advances in organocatalytic asymmetric multicomponent cascade reactions for enantioselective synthesis of spirooxindoles. Organic Chemistry Frontiers. 2021;8(15):4315-48.

[21]. Fu Z, Li X, Wang Z, Li Z, Liu X, Wu X, Zhao J, Ding X, Wan X, Zhong F, Wang D. Optimizing chemical reaction conditions using deep learning: a case study for the Suzuki–Miyaura cross-coupling reaction. Organic Chemistry Frontiers. 2020;7(16):2269-77.

[22]. Bianchi P, Monbaliu JC. Three decades of unveiling the complex chemistry of C-nitroso species with computational chemistry. Organic Chemistry Frontiers. 2022;9(1):223-64.

[23]. Zhang TS, Liu S, Hao WJ, Jiang B. Exploiting the reactivities of ortho-alkynyl aryl ketones: opportunities in designing catalytic annulation reactions. Organic Chemistry Frontiers. 2023;10(2):570-89.

[24]. Sun K, Wang X, Li C, Wang H, Li L. Recent advances in tandem selenocyclization and tellurocyclization with alkenes and alkynes. Organic Chemistry Frontiers. 2020;7(19):3100-19.

[25]. Wang Y, Zheng L, Wei D, Tang M. A quantum mechanical study of the mechanism and stereoselectivity of the N-heterocyclic carbene catalyzed [4+ 2] annulation reaction of enals with azodicarboxylates. Organic Chemistry Frontiers. 2015;2(8):874-84.

[26]. Melen RL. Frontiers in molecular p-block chemistry: From structure to reactivity. Science. 2019 Feb 1;363(6426):479-84.

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

[27]. Zhong F, Yang M, Ding M, Jia C. Organic electroactive molecule-based electrolytes for redox flow batteries: status and challenges of molecular design. Frontiers in Chemistry. 2020 Jun 19;8:451.

[28]. Feng F, Lai L, Pei J. Computational chemical synthesis analysis and pathway design. Frontiers in chemistry. 2018 Jun 5;6:199.

[29]. Mishra AK, Kan Y. AI Meets Chemistry: Unlocking New Frontiers in Molecular Design and Reaction Prediction. International Journal of Artificial Intelligence for Science (IJAI4S). 2025 Mar 17;1(1).

[30]. Song G, Zhang K, Wang H, Li J. Theoretical insights into the mechanism and selectivities of rhodium/amine dual catalysis in alkyne–cyclopropene reassembly reactions. Organic Chemistry Frontiers. 2025;12(22):6160-79.

[31]. Saleem F, Khan KM. Indole derivatives: unveiling new frontiers in medicinal and synthetic organic chemistry. Molecules. 2023 Jul 18;28(14):5477.

[32]. Lüder J, Manzhos S. First-principle insights into molecular design for high-voltage organic electrode materials for Mg based batteries. Frontiers in Chemistry. 2020 Feb 18;8:83.

[33]. Wang X, Zhang Z, Hu K, Yu W, Cheng Y, Song Y, Sun X, Li S, Yang T, Hu J, Jing J. Action mechanism and molecular design of indolepyrrodione inhibitors targeting IDO1. Frontiers in Molecular Biosciences. 2025 Oct 23;12:1661700.

[34]. Chaudhary D, Saunthwal RK. Cooperative iridium and organocatalysis: a new frontier in asymmetric chemistry. Organic Chemistry Frontiers. 2025;12(6).

[35]. Yang ZD, Zhang H, Zhao H, Han B. Trap mechanism based on frontier molecular orbitals of additives in polyethylene insulators: A theoretical study and molecular design strategy. International Journal of Quantum Chemistry. 2015 Oct 15;115(20):1483-9.

[36]. Sharma A, Sharma S, Sharma M, Sharma V, Sharma S, Sivanesan I. Polymeric Frontiers in Next-Generation Energy Storage: Bridging Molecular Design, Multifunctionality, and Device Applications Across Batteries, Supercapacitors, Solid-State Systems, and Beyond. Polymers. 2025 Oct 20;17(20):2800.

[37]. Xu R. Introduction-frontiers in modern inorganic synthetic chemistry. InModern Inorganic Synthetic Chemistry 2011 Jan 1 (pp. 1-7). Elsevier.

[38]. Varchi G, Brigaud T. Advances in Synthetic Organic Chemistry at the Biomedical Interface: Honoring Professor Iwao Ojima on the Occasion of his 80th Birthday. Frontiers in Chemistry. 2025;13:1721249.

ISSN : 3079-5761
Volume 1, Number 4, 2025
https://doi.org/10.70445/gtst.1.4.2025.101-115

[39]. Sasaki S, Nagatsugi F. Molecular Design for Specific Recognition and Reaction in Genome-Targeting Chemistry. Frontiers in Organic Chemistry. 2005 Mar 1;1(1):145-62.

[40]. Gat SN, Pattanaik PP, Dandela R. Recent developments in organic synthesis for constructing carbon frameworks using transposition strategies. Organic Chemistry Frontiers. 2025.

[41]. Zhang WX, Xi Z. Organometallic intermediate-based organic synthesis: organo-di-lithio reagents and beyond. Organic Chemistry Frontiers. 2014;1(9):1132-9.

[42]. Bronstein H, Nielsen CB, Schroeder BC, McCulloch I. The role of chemical design in the performance of organic semiconductors. Nature Reviews Chemistry. 2020 Feb;4(2):66-77.

[43]. Xuan F, Chu Q, Ma J, Xu K, Wang S, Zhai Y, Feng X, Zhai D, Cao L, Teng B. Frontiers in Organic Nonlinear Terahertz Crystals: Innovations in Structural Design and Optical Nonlinearity. Crystal Research and Technology. 2025 Apr;60(4):2400227.

[44]. Shaikh SA, Jain T, Sandhu G, Soni A, Jayaram B. From drug target to leads-sketching a physico-chemical pathway for lead molecule design in silico. Frontiers in Medicinal Chemistry: Volume 6. 2012 Nov 28:324-60.