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Artificial Intelligence in Green Chemistry: Optimization of Eco-Friendly Synthesis Routes

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Abstract

Green chemistry emphasizes the design of chemical products and processes that minimize environmental impact by adhering to the 12 guiding principles of sustainability. Within this framework, artificial intelligence (AI) has emerged as a transformative tool to optimize eco-friendly synthesis routes. Traditional synthetic methodologies often rely on hazardous reagents, energy-intensive conditions, and wasteful trial-and-error processes. By contrast, AI leverages machine learning models—supervised, unsupervised, and reinforcement learning—to analyze extensive chemical databases and experimental data, enabling predictive insights into reaction outcomes, catalyst selection, and retrosynthetic planning. Tools such as SynRoute and computer-assisted synthesis design (CASD) exemplify how AI can generate viable synthetic routes in seconds, offering chemists diverse options for environmentally benign transformations. Applications extend to pharmaceutical synthesis, bile acid derivatives, and green catalysis, where renewable solvents and sustainable catalysts enhance both efficiency and safety. Case studies highlight AI's role in optimizing multistep syntheses and identifying reaction conditions with high yields and minimal by-products. Despite remarkable potential, challenges persist, including poor data quality, incomplete reaction records, and algorithmic limitations in predicting reactivity and selectivity. Furthermore, ethical considerations demand transparency, fairness, and adherence to regulatory frameworks governing chemical processes. Future directions envision integration with technologies such as flow chemistry and automation, enabling real-time adaptive optimization while fulfilling sustainability standards. Multidisciplinary collaboration between chemists and data scientists is critical to harness AI's capabilities fully. Ultimately, the convergence of AI and green chemistry offers a powerful pathway to reducing chemical waste, accelerating discovery, and promoting economic, ethical, and environmental sustainability in modern chemical research.

Key-words: Green Chemistry, Artificial Intelligence, Eco-Friendly Synthesis Routes, Machine Learning, Retrosynthetic Planning, Green Catalysis, Sustainable Chemical Processes, Data-Driven Optimization

Introduction

Green chemistry seeks to transform both the use and synthesis of chemicals with ecology as the watchword. It embodies a proactive, inherent consideration of environmental impact in the design of chemicals, materials, products, and processes. Green chemistry thus offers an opportunity to bridge traditional synthetic organic chemistry practice and eco-conscious practices, thereby harmonizing scientific practice with economic and sensible regulations. Central to green chemistry is the development of eco-friendly synthesis routes, which involves employing safer starting materials and methods, minimizing hazardous by-products, and designing economical and less wasteful pathways (Liu et al., 2023).

The efficient synthesis of complex molecules mandates ample knowledge not only in chemistry but also in disparate fields. Due to the rapid growth of chemical data, however, it is impossible for any human being to amass the knowledge necessary to address and solve the problems faced in daily research. Artificial intelligence (AI) can be a useful tool in this regard. While AI has been widely applied in chemical synthesis to improve efficiency, save time and manpower, reduce errors, and enhance safety, the specific use of AI to aid physicochemical interpretation and knowledge extraction remains limited (Wang et al., 2022). The emphasis of this review, therefore, is placed on current developments of AI applications aimed at optimizing eco-friendly synthesis routes.

A comprehensive overview is provided, beginning with the fundamental set of 12 green chemistry principles, which serve as guidelines for devising more environmentally sustainable and safer products and processes. Following this, the role of AI is discussed, including an introduction to types of machine learning methods—supervised, unsupervised, and reinforcement learning—and the various chemical data sources that underpin tailored studies. Emphasis is placed on the practical significance of these methods, rooted in commercially available databases, and insights extracted from experimental data. Attention then turns to the synthesis of pharmaceutical active ingredients, bile acids, and their derivatives, which play key roles in the transition from traditional to environmentally aware processes. A discussion of a powerful catalytic approach illustrates the potential for greener routes to pharmaceuticals. Building upon this foundation, multiple case studies highlight efforts in green synthesis routes that leverage advances in AI techniques and catalytic routes; these range from replacing scarce reagents to solving longstanding docking problems. Challenges in implementing AI—including data quality, availability, and algorithmic limitations—are examined, along with future avenues of development. The review concludes with comments on ongoing trends, recognizing AI as a valuable tool for acquiring key information and forecasting complex future scenarios in sustainable chemistry (Klucznik et al., 2018).

Overview of Green Chemistry

Since the introduction of the 12 Principles in 1998, green chemistry has exerted significant influence over laboratory practice as a means of improving the environmental and economic profile of chemical processes (Liu et al., 2023). The concept sets out a series of objectives that challenge the scientific community to develop novel processes that enhance the existing approach to sustainable chemical transformation. Although the application of artificial intelligence within the field of chemistry can be traced back to the late 1960s, only in recent years has information technology become fully integrated into laboratory-based research. Through the combined efforts of experimental, theoretical, and computational modelling, the central values set out by green chemistry can be met in a sustainable manner. The principles of green chemistry, complemented by the interaction of machine learning algorithms with model- and experimental-derived datasets, open up alternative paths through the landscape of synthetic development.

The Role of Artificial Intelligence

Artificial intelligence (AI) refers to computer systems that go beyond pre-programmed tasks, learning and evolving analytically (Liu et al., 2023). AI for Chemistry (AIC) utilizes data analysis and decision-making to address complex scientific challenges such as pattern recognition, insight extraction, and relationship discovery. AI can analyze retrosynthesis data obtained from experiments and chemical databases to generate optimal synthesis steps that satisfy green-chemistry criteria.

Eco-Friendly Synthesis Routes

Eco-friendly synthesis routes are a main facet of green chemistry, involving the design of chemical pathways that minimize the use and generation of hazardous substances. A synthesis route comprises a series of chemical reactions used to obtain the target product, associated with a set of time, cost, and sustainability metrics. The ability to plan and select optimal synthesis routes is therefore an essential element of green chemistry, with artificial intelligence increasingly leveraged to identify pathways that significantly improve sustainability performance (Klucznik et al., 2018). The aim is to generate a set of candidate routes for evaluation by the chemist, highlighting a diverse range of feasible alternatives. As a representative example, SynRoute exemplifies advancements in computer-aided route design by employing

a concise set of 263 general reaction transformations to rapidly generate plausible routes for a broad range of compounds (Latendresse et al., 2023). The selected reactions emphasize well-studied chemistries supported by sufficient data to enable machine learning models to predict the feasibility of each computer-generated reaction. Experimental validations have demonstrated that viable routes can typically be identified for moderately complex, drug-like molecules, although adaptations to laboratory conditions—particularly for continuous flow chemistry platforms—may necessitate modifications to certain reaction steps. Such tools not only facilitate the efficient organization and evaluation of multiple route options through an intuitive user interface but also support the prioritization of compound libraries during early-stage drug discovery by providing synthetic feasibility assessments within approximately 30 to 60 seconds per compound. The continued integration of data-driven and in silico approaches within these frameworks underscores their pivotal role in advancing eco-friendly synthesis planning while optimizing efficiency and sustainability.

Machine Learning Techniques in Chemistry

The most common machine learning tasks supervised, unsupervised and reinforcement learning – represent different approaches to learning from data. Each technique offers distinct advantages depending on the problem in question. Besides optimizing eco-friendly chemical synthesis, these methods can address catalyst design, yield prediction and reaction condition selection. Supervised learning learns from a set of examples that link input data x with a target output y. Given a training set {(x1, y1), (x2, y2), •n, •n)} the goal is to estimate the general form of the underlying relationship y = f(x). Models use this relationship to predict y for unseen x. Most methods produce probabilistic models capable of uncertainty estimation. Examples include neural networks, Bayesian inference, and support vector machines. Unsupervised learning identifies underlying structure in a dataset x without reference to a known target y. Two main types perform either clustering into discrete groups of similar points or dimensionality reduction to reveal lower-dimensional subspaces that interpret most of the variance in data. While often applied to visualization or exploratory problems, these methods discover chemical trends and patterns. Algorithms include K018Means clustering, principal component analysis, self-organizing maps, and variants such as non-negative matrix factorization.

Reinforcement learning employs either an actor-only (policy search), critic-only (value function approximation) or an actor 6critic (both policy and value functions) method for sequential decision-making. An agent selects actions in response to an environment combined with a reward signal. The agent aims to maximize expected cumulative future reward through learning how to execute actions that transition through environment states. Models that formally balance exploration and exploitation learn optimal policies for selecting later actions that achieve long-term goals. Reinforcement techniques generate additive results through iterative improvements of policies, in desktop-to-robot workflows, and in autonomous laboratory systems. (F. Zahrt et al., 2022) (Meuwly, 2021)

5.1. Supervised Learning

Supervised learning, a machine learning technique for building predictive models from training data consisting of input-output pairs, is a prime method for optimizing eco-friendly synthesis routes. Model inputs include experimental parameters or molecular structure representations, while outputs are reaction outcomes or values such as yield or selectivity. The learning algorithm identifies a relationship that accurately maps inputs to outputs and subsequently predicts outcomes for novel inputs. Empirical records used for supervised-learning models may derive from published literature, electronic laboratory notebooks, chemical databases, or virtual screening. The capacity to optimize green synthesis routes is related to these records' scope, quantity, and fidelity (Schilter et al., 2024).

Data Sources for AI in Chemistry

Numerous databases and experimental data available for model learning and training constitute a key enabler of AI for Chemistry. Chematica is an early example, relying on a manually curated logic tree containing over 10000 reaction patterns and more than 1000 reaction conditions (Liu et al., 2023). Waller et al. extended this approach by extracting reaction data from Reaxys, generating millions of training samples for a reaction prediction model. The resulting system undergoes retrospective Monte Carlo tree search guided by neural networks, markedly outpacing Chematica in planning ability. Large data generated

in the laboratory represent a promising resource that can complement these approaches. The amount of experimental procedures published in patents and the scientific literature is also considerable. For example, high-throughput experimentation generates data on ideal reaction conditions, rendering further experimentation often inefficient. Logistic regression on a large dataset of 400 reactions is capable of identifying conditions that strongly favor or hinder a reaction (Wang et al., 2022). Nevertheless, experimental data gathered under identical conditions on the same reaction remains scarcely available. AI in Chemistry should thus complement rather than fully replace combinatorial screening.

Chemical Databases

A wide range of chemical databases provide information used to train artificial-intelligence models. One of the earliest examples of software designed to plan the synthesis of chemical compounds, ICSYNTH, employs a collection of chemical knowledge, heuristics, and rules to "build" a virtual compound from fragments to computer-predict the synthetic pathway most likely to produce the target compound (Klucznik et al., 2018). Starting with a long-known model compound, aspirin, the group discovered a pharmaceutical-input catalogue of commercially available compounds to train the platform, formulates the inverse of a computing-assisted the design successfully predicted the synthesis planning system. Similar architectures have emerged to consider the organic chemistry associated with the planning and contemporary retrosynthesis (Latendresse et al., 2023) macrocyclic (bioactive) compounds in complex natural products, most sketching and execution of using well-validated synthesis systems that is—a computational approach to digestion, preparative, and synthetic strategies for the design of molecules and prototyping of synthetic pathways. With the imminent forthcoming scarcity of new synthetic-prediction validation, pharmaceutical, and advanced chemical development is entirely driven by human consideration of chemical networks, computer-generated predictions direct the experimental approach, have proven useful in the preparation of a variety of organic compounds, readily accessible commercial biaryl precursors, and numerous (bioactive) compounds. Transitioning to programme-generated computer-predicted synthetic pathways, the target molecule from which to search the system successfully predicted the synthesis strategy, pharmaceutical-input catalogue of commercially available reaction information, and a training dataset of control compounds. Also of synthetic-chemistry importance, the platform-generated reaction pathways of organic and bioorganic laboratory and exploration of a platform can access the platform-generated the automatic generation of organic compounds.

Experimental Data

Experimental data remain a key part of the field of organic chemistry. In addition to the empirical approach, computer-assisted synthesis planning offers a third major way to predict new synthetic routes. ICSYNTH, for example, is built around a generative model that suggests collections of retrosynthetic strategies to prepare a given target. While many examples remain at the level of retrosynthesis plots, funding has limited experimental validation (Klucznik et al., 2018). Another confirmation method coupled reaction-template matching with density-functional theory energy calculations. This combination successfully identified a retro-Claisen rearrangement and proposed alternative conditions for an unreported reaction that was then experimentally verified. Further progress: reaching optimal reaction conditions is crucial for high yields, minimal by-products, and environmentally sustainable reactions. AI-driven approaches have replaced traditional trial-and-error methods, enabling data-driven and automated optimization. An integrated platform optimized four terminal alkynes and two reaction routes, achieving over 80% conversion in 23 experiments, covering around 2% of the combinatorial space. Analysis of the data identified how different reaction parameters influence outcomes, demonstrating potential for faster condition optimization and more efficient chemical processes (Schilter et al., 2024). Previous methods relied on trial-and-error techniques like one factor at a time and design of experiments, often depending on researcher expertise. Bayesian optimization has proven versatile and effective, reducing R&D costs and improving yields in flow-based reactors for reactions such as Suzuki–Miyaura coupling and C–H activation. Despite their advantages, BO methods are often seen as black boxes with limited interpretability, which impedes widespread adoption.

Synthesis of Pharmaceuticals

The synthesis of pharmaceuticals remains one of the most demanding human undertakings. Computer-assisted synthesis design (CASD) could greatly accelerate the development and production of new molecules (Klucznik et al., 2018). Vision is to supply a (medicinal) chemist with a list of pathways and the experimental conditions to complete each step. Numerous retrosynthetic analysis algorithms have been reported, many implemented in commercial software platforms. Available synthetic routes to three AZ compounds confirm route quality. Delineates a useful distinction between planning goals in a pharmaceutical, fine chemical, and bulk chemical context; prior knowledge within AZ helps identify suitable algorithms. Search speed evaluated on the CASD subset of the Reaxys database. Efficient search algorithms enable practical exploration of CASD rules but retrieval of a large number of pathways requires faster search.

Green Catalysis

Green catalysis contributes to safety by facilitating chemical transformations in aqueous media where appropriate, which is generally safer than handling typical organic solvents with low flash points. Green catalysts minimize the formation of by-products. Consequently, environmentally friendly solvents significantly impact asymmetric catalytic processes, serving as the reaction media or solvents for catalyst preparation or work-up and purification stages (Miele et al., 2022). Alternatively, catalysts derived from renewable resources are also a viable option, often demonstrating improved catalytic performance relative to their fossil-based counterparts. Various catalytic transformations may be optimized for reactions conducted in environmentally friendly solvents under laboratory conditions. Catalysts prepared from renewable sources, particularly those that can also act as chiral inducers through stereogenic centers on the catalyst structure, play a particularly important role. Beyond common hydrogenation reactions, other transformations warrant the development of innovative asymmetric catalytic protocols (G. Quesne et al., 2019). Access to novel environmentally friendly solvents widens the options available for sustainable asymmetric processes and promotes the enhanced exploitation of renewable-material-derived catalysts.

Challenges in Implementing AI

The implementation of artificial intelligence systems in green chemistry confronts notable challenges related to data quality, data availability, and the constraints of chemical reaction algorithms. Machine learning methods require not only quantity but also quality, diversity, and balance in data coverage to effectively represent candidate structures or potential actions (Gao et al., 2022). Although large chemical datasets are accessible, even leading repositories contain incomplete and low-quality reaction records, further exacerbating the data scarcity problem. Extracted chemical reaction records from published scientific articles and information related to reaction templates supplement existing data sources and should be continuously integrated to ensure up-to-date coverage (Wang et al., 2022). Furthermore, current status of AI-controlled synthesis still faces restrictive workflow procedures, hindering broad adoption. Overcoming these limitations remains an active area of work and a key focus for the advancement of AI-driven traditional chemistry laboratories.

Data Quality and Availability

Achieving optimal reaction conditions is a key component in executing chemical reactions with high conversion and yield while maintaining environmental sustainability and minimizing waste (Schilter et al., 2024). Consequently, artificial intelligence has transformed condition optimization from a trial-and-error procedure into an automated, data-driven methodology. An integrated platform that combines Bayesian optimization with automation simultaneously optimizes reaction conditions and synthetic routes for terminal alkynes. The platform conducts 23 experiments, corresponding to approximately 2% of the combinatorial search space, and attains conversions exceeding 80%, demonstrating the potential for rapid reaction optimization and enhanced process efficiency. Early methods such as trial-and-error and design of experiments depended heavily on the expertise of individual researchers. Bayesian optimization techniques have effectively reduced research and development expenditures while improving reaction yields in the optimization of flow-based transformations, including Suzuki–Miyaura coupling and C–H activation. High yields are often achieved after evaluating only a small subset of the total configuration space. Nevertheless,

the limited interpretability of such black-box Bayesian optimization models presents a barrier to their widespread adoption, particularly when addressing large search spaces.

The vast majority of publicly available reaction data is documented in an unstructured format and exhibits a strong bias towards high-yielding reactions, influencing the range of models that can be successfully developed. Several factors contributing to the success of data curation and sharing initiatives in chemistry and molecular biology provide guidance for handling reaction data; the Open Reaction Database represents a notable effort to render reaction data more findable, accessible, interoperable, and reusable (FAIR). Advances in the reporting of laboratory synthesis procedures, encompassing detailed reaction conditions, remain essential for maximizing the impact of artificial intelligence on organic synthesis. High-quality data should comprise observed products, yields, selectivities, impurities, and other relevant summary statistics obtained under a variety of experimental conditions (Mercado et al., 2023).

Algorithm Limitations

Each algorithm has a specific range of applications and limitations. Retrosynthesis software can suggest cost-effective syntheses considering only commercial reagents (Latendresse et al., 2023). These tools often generate numerous arbitrary one-step reactions, resulting in inefficient production. Postprocessing is used to identify a limited set of potential routes, which often remain impractical. Reaction predictions typically exclude crucial information regarding the quantities of reactants, solvents, and catalysts, as well as experimental conditions such as temperature and the order of reagent addition. In an analysis of 1,591 reactions from five open-access reaction databases, 696 (43.7%) provided insufficient information to generate accurate predictions, underscoring the significance of this challenge (Klucznik et al., 2018). Moreover, assessing the inherent reactivity and selectivity of reagents and reactants remains a major challenge; despite recent advances, current algorithms consider only the most common products, neglecting subtle effects critical for defining synthetic routes (Gao et al., 2022).

Future Directions

Ongoing research suggests that computer-assisted synthesis planning (CASP) represents a promising direction in the advancement of green chemistry. Despite the range of potential applications, validated experimental demonstrations of CASP-driven synthetic routes remain limited (Klucznik et al., 2018). Integration of emerging technologies is expected to advance AI-assisted modeling, formulation, and reaction-planning integration. Moreover, as regulatory frameworks evolve within the global chemical engineering sector, opportunities to incorporate advanced active-learning AI frameworks are likely to increase (Liu et al., 2023).

Technologies such as flow reactors and continuous processing can be seamlessly integrated with computer-aided synthesis planning. When the routes generated by SynRoute are applied to flow reactors, the result is an automated system for flow synthesis of organic compounds. Several works have explored the combination of flow chemistry systems and powerful computer-aided synthesis planning programs (Latendresse et al., 2023).

Inappropriate chemical synthesis significantly harms the environment. Thus, stringent regulations controlling the emission or discharge of hazardous substances are essential. Every chemical synthesis must comply with relevant laws, considering factors such as resource consumption, toxicity, and production costs. Artificial intelligence assists in designing eco-friendly synthesis routes while fulfilling regulatory requirements. Data regarding environmental laws and direct and indirect costs are vital for this approach. AI Chemistry consists of computational tools and computer programs assisting chemists in conducting chemical studies, offering expertise on specific topics, and facilitating knowledge interchange (Wang et al., 2022). Computer-aided synthesis planning (CASP) programs evaluate possible sequences for producing target molecules (Klucznik et al., 2018). Such systems learn from databases drawn from literature or commercial sources, accumulating knowledge on synthesis plans, methodologies, and reactions. Recent years have seen a proliferation of publicly available reaction databases and open-source programs implementing AS techniques.

Ethical Considerations in AI Applications

AI systems should address ethical implications of the chemical research and development process and outcomes. A comprehensive process encompasses defining desired properties, AI-based design of molecular structures, automated in-silico characterization and property evaluation, ranking of promising candidates, and AI-based reaction design for support of automated laboratory experiments. The object of development, illustrated by pesticides that are vital for food production and storage but present environmental and food chain contamination risks, demands ethically responsible conduct. Applications in sustainability consider all stakeholders involved with respect to potential tensions between collective and individual benefits and costs. Guiding principles include beneficence, non-maleficence, autonomy, justice, and explicability (Hermann et al., 2021).

Environmental sustainability represents one of the most significant challenges of the twenty-first century, demanding substantial reductions in the impact of human activities. The foundation for such advancements is Green Chemistry, a discipline devoted to both the design of environmentally friendly processes and the avoidance of wasteful procedures. Since the twentieth century, chemists have pursued research that prioritizes sustainability (Liu et al., 2023). In parallel, Artificial Intelligence (AI) introduced concepts and tools capable of accelerating the identification of new materials and exploring promising synthesis routes (Hermann et al., 2021). The intersection of these fields offers opportunities for the optimization of eco-friendly synthesis routes. By combining AI techniques with Green Chemistry systems, it is possible to accelerate the synthesis of reduced-impact pathways that adhere to the twelve principles.

Economic Implications of Green Chemistry

Green chemistry has attracted increasing attention during the past years as an attractive and attractive alternative technology in organic synthesis. Green chemistry refers to a set of principles intended to reduce or eliminate the environmental burden before the step of waste treatment and it embraces the concept of atom economy and non-hazardous substances leading to sustainable and eco-friendly technologies. Machine learning (ML) methods have proved to be promising to elucidate the complex relationship between experimental parameters and system performance and widely applied due to their high ability to discover the underlying complex mechanistic data. The demand for eco-friendly routes has attracted substantial interest in ways to determine optimal conditions and synthetic schemes for their realization. In this regard, artificial intelligence (AI) represents a new interesting and constantly developing approach to improving optimization, especially when multiple objectives and a variety of restrictive conditions must be considered. The economic implications of green chemistry are discussed in relation to the potential benefits and factors influencing sustainability.

Green chemistry has attracted considerable attention as an attractive alternative in organic synthesis. It refers to a set of principles designed to reduce or eliminate environmental burdens prior to waste treatment, embracing concepts like atom economy and non-hazardous substances to achieve sustainable and eco-friendly technologies. Machine learning (ML) methods have proven promising for elucidating the complex relationship between experimental parameters and system performance; their high capacity for uncovering underlying mechanistic data has fostered widespread application. The demand for eco-friendly routes has stimulated interest in methods to determine optimal conditions and synthetic schemes. Artificial intelligence (AI) thus emerges as a rapidly evolving approach for optimization, particularly when multiple objectives and various constraints must be addressed. (Liu et al., 2023) (Klucznik et al., 2018)

Educational Aspects of AI in Chemistry

The integration of A.I. in chemistry offers a means to accelerate the discovery and development of new materials that actively support the formation of a sustainable society, notably by optimizing eco-friendly synthesis routes (Liu et al., 2023). Beyond mere significance for a sustainable society, the application of A.I. enables the rapid development of new materials with the potential to solve a wide range of global-scale challenges. Education in A.I. supports the application of digital tools within chemistry and chemical engineering by cultivating individuals capable of interdisciplinary collaboration. Specifically, it develops professionals proficient in programming who can identify relevant research problems and communicate

effectively with data scientists and computer engineers (Wang et al., 2022). Such education thereby addresses essential prerequisites for the advancement of sustainable and efficient manufacturing processes through digital technologies, underpinning the environmentally friendly synthesis of pharmaceutical and agricultural intermediates.

Conclusion

Artificial intelligence has emerged as an invaluable tool in the pursuit of eco-friendly synthesis routes. Its applications encompass various activities vital to green chemistry, including the design of novel materials, elucidation of chemical structures, prediction of thermodynamic properties, reaction analysis, and allocation of synthetic pathways (Klucznik et al., 2018). By employing classifications such as breadth-first, depth-first, and heuristic-driven search algorithms, optimal synthetic solutions can be identified with reduced time and associated costs. Merging extensive data collections with deep learning models promises further refinement of the optimization process (Liu et al., 2023). Nevertheless, several challenges persist before artificial intelligence achieves widespread adoption across chemical research laboratories. The imperative for alternative chemicals, medicines, and fuels to replace currently employed ones—often scarce or environmentally detrimental—has intensified due to growing socio-economic and environmental concerns. Green chemistry aims to address this by exploiting catalytic systems, such as transition metal catalysts, under benign conditions to establish atom-efficient reactions with minimal by-products, thereby reducing the environmental footprint (Wang et al., 2022). However, many effective catalytic systems are discovered by chance rather than design, pointing to the need for more rational approaches. Quantum chemical simulations and molecular dynamics exemplify the computer-assisted design protocols employed to understand and design these systems more effectively. Artificial intelligence can thus play a crucial role in optimizing eco-friendly synthesis routes in line with green chemistry principles.

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