

Data Driven Organic Chemistry: Role of Artificial Intelligence in Molecular Discovery

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ABSTRACT

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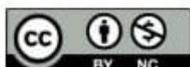
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Organic chemistry has been transformed by artificial intelligence (AI) that has facilitated the use of data in discovering molecules, predicting reactions, and optimizing syntheses. Conventional methods which depend on human intuition and trial and error tests are usually time consuming and narrow-minded. The use of AI with large chemical datasets to predict properties of molecules, create new compounds, optimize reactions, and plan synthetic pathways through machine learning, deep learning, and generative models is efficient. It is used in drug discovery, catalysis, materials science, and sustainable chemistry, which lessens the amount of work required in experiments, increases precision and efficiency. Although AI has some challenges including the quality of data, interpretation, and generalization, it supplements human knowledge, providing a breakthrough method to rapid, rational, and sustainable chemical innovation.

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INTRODUCTION

Human intuition, empirical knowledge and the step-by-step experimental exploration had long been the driving forces in organic chemistry. Over the decades, chemists were using their experience,



mechanistic knowledge, and experimentation to design molecules, make predictions of reactivity, and design synthetic paths [1]. Although this conventional method has resulted in the spectacular discoveries, it can be cumbersome, resource-demanding and restricted through the human cognitive ability in searching extensive chemical space. As the digital technologies rapidly evolve, the field of organic chemistry is also experiencing a paradigm shift to data-driven research where big data and computational chemistry are being used as the main focus of scientific decision-making [2].

The advent of artificial intelligence (AI) and machine learning (ML) has offered some potent methods in conducting the analysis of complex chemical data, reveal concealed patterns, and create valid predictions that were not achievable earlier on. The development of high-throughput experimentation, automated synthesis, cheminformatics and electronic laboratory notebooks has led to the creation of large volumes of chemical data [3]. These data, including the molecular structures, reaction conditions, yields, and physicochemical properties are the basis of data-driven organic chemistry. With the help of AI methods, it is possible to extract chemical knowledge in such data effectively, converting raw information into actionable information [4].

AI has presented great potential in the environment of molecular discovery. Molecular discovery is a traditional method of searching through an enormous chemical space, which has been estimated to contain over 10^{60} possible organic molecules. It will be impractical to experimentally explore even a fraction of this space. AI-based models are able to screen, design and prioritize molecules with desired properties in a matter of minutes and can dramatically speed up the discovery pipelines in drug development, catalysis or materials science applications [5]. Learning structure-property and reactivity relationships directly through data can augment and not supplant human knowledge, therefore AI systems can enhance it.

With these developments, there are still challenges to the use of AI in organic chemistry. There are still such pressing issues as the quality of data, bias, interpretation of models, and experimental validation. Furthermore, a large number of chemists are not formally trained in data science, developing a divide between the development and the practical use of methodology. To handle such challenges, interdisciplinary efforts will have to be made by chemists, computer scientists, and data engineers [6].

This review will present a broad summary of the use of artificial intelligence in data-driven organic chemistry and especially in molecular discovery. It explains the basic concepts, the major applications, and the recent developments and the limitations that are currently present have been critically analyzed. Throughout the article, the authors attempt to provide an understanding of the ways AI is transforming organic chemistry, as well as define future directions toward the creation of

intelligent, effective, and sustainable molecular discovery methods.

PRINCIPLES OF DATA-DRIVEN ORGANIC CHEMISTRY

Data-driven organic chemistry is based on the systematized accumulation, description and study of chemical data to reveal designs and predict molecular conduct. Data-driven strategies are based on big data, computational methods and statistics, unlike traditional methods that rely on intuition and experimental trial-and-error methods to faster discoveries and processes optimization. This method is based on the quality chemical data, which can be produced by experimental methods, computational methods, or based on literature sources [7]. Experimental results can be the results of a reaction, yield, and kinetics, thermodynamic and molecular properties, including solubility, polarity or stability. The computational datasets are generated using quantum mechanical computations, molecular dynamics simulations or cheminformatics algorithms which encode structural properties and predict properties. In the meantime, literature databases such as Reaxys, PubChem and ChEMBL have a rich source of curated chemical information, such as reactions, bioactivities and structural information [8].

Principles of Data-Driven Organic Chemistry

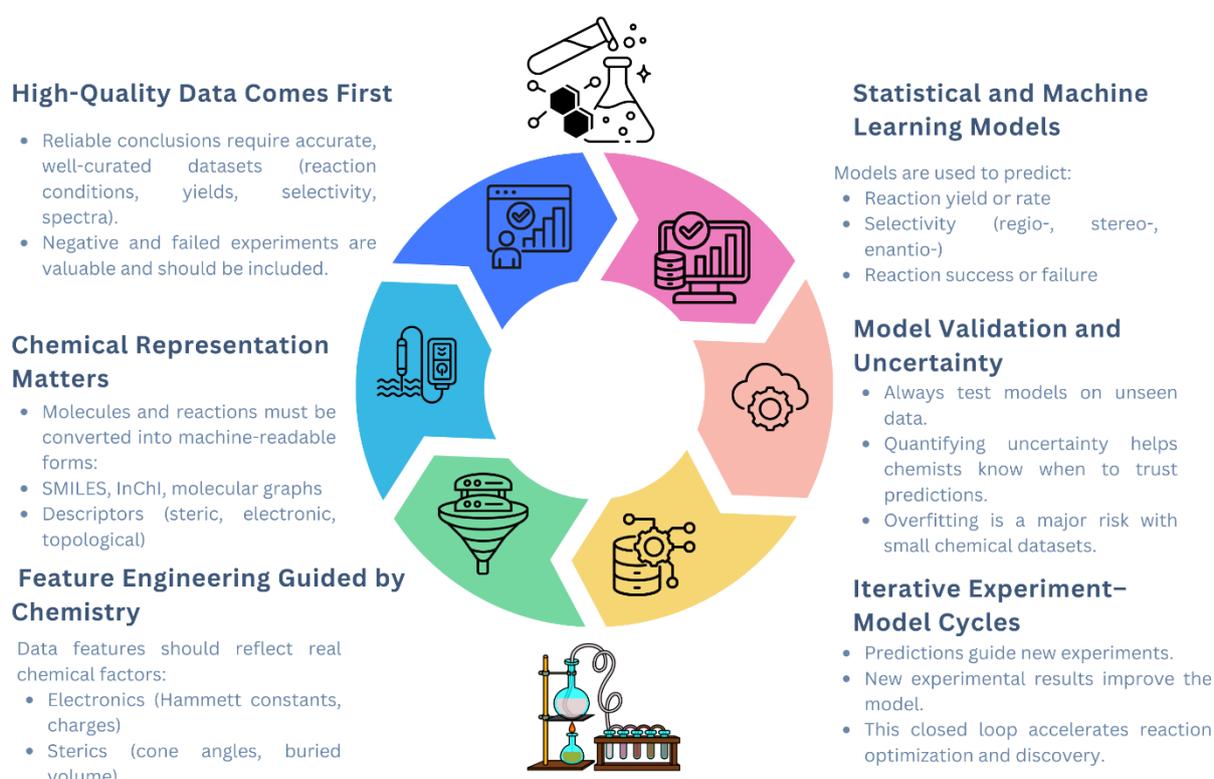


Figure 1. Principles of data driven organic chemistry

A key problem of data-driven organic chemistry is how molecular structures and chemical data can

be represented in a computational model format. There are various representations of a kind. This is because the Simplified Molecular Input Line Entry System (SMILES) represents molecules as linear sequences of characters that form a description of atoms, bonds, and connectivity and is compatible with text-based machine learning models [9]. Graph based representations regard atoms as nodes and bonds as edges, which are especially convenient in deep learning models such as graph neural networks that can be used to learn the relational structure of molecules. Molecular descriptors, fingerprints and topological indices are other representations that convert chemical structures to numerical vectors that encode physical, electronic, and geometric properties [10]. The selection of the right representation is an important issue, which can directly influence the performance and interpretability of AI models.

A quality of data and preprocessing is another important point. Raw chemical data usually has mistakes, inconsistencies or gaps of information that can have a considerable impact on the accuracy of the models. It is important to clean up, standardize and enhance datasets to construct sound predictive models. Also, dimensionality reduction methods and feature selection methods assist in concentrating on most valuable chemical properties and enhance the efficiency and interpretability of the model [11].

Lastly, data-driven organic chemistry is based not only on data and representations, but also on integrating computational instruments and AI algorithms as well as on background knowledge. Curated chemical data combined with sophisticated molecular representations and machine learning techniques have formed a potent structure to study chemical reactivity, to make predictions of properties and to design new molecules [12]. It is possible to develop these pillars to allow the successful implementation of AI in organic chemistry, where the models are not only accurate but meaningful, and preconditions the innovations in the field of molecular discovery, reaction prediction, and synthetic planning [13].

MACHINE LEARNING TECHNIQUES AND ARTIFICIAL INTELLIGENCE

Artificial intelligence (AI) has become a disruptive technology in the field of organic chemistry, offering the computer power to derive information out of highly complicated chemical data and to forecast molecular behavior with an astonishing precision. Machine learning (ML) is a subdivision of AI that allows computers to acquire patterns by data without explicit programming, and it is the fundamental component in AI in chemistry [14]. Relationships between molecular structures, reaction conditions, and chemical properties can be examined by machine learning models and can provide predictive relationships that are useful in molecular discovery, reaction optimization, and retrosynthesis planning.

There are three major categories of machine learning methods: supervised learning, unsupervised learning and reinforcement learning. With supervised learning, the models are trained on labeled data, input data (e.g. molecular structures or descriptors) are associated with known data (e.g. reaction yields, solubility, or bioactivity) [15]. The most common algorithms are the linear regression, decision trees, random forests, support committee machines, and the deep neural networks. These are the best at making predictions of properties or outcomes of new molecules, though these predictions require a diverse and representative training data [16].

Unsupervised learning, conversely, makes use of unlabeled data, and aims at the discovery of latent patterns or structures in chemical data. Clustering, dimensionality reduction, and principal component analysis are common techniques that are used to cluster molecules with similar characteristics, identify trends, or simplify high-dimensional data to be further analyzed. It is especially helpful when it comes to exploratory chemistry, where the connections between molecular features and reactivity are not so well-known [17]. Reinforcement learning is a more modern and sophisticated method of molecular design and optimization of reactions. In this case, an AI agent is trained to take sequential decisions by engaging with an environment and acting as a response to an environment (reward or penalty) [18]. Paul Reinforcement learning has been applied in organic chemistry to produce new molecules with properties of interest, to optimize syntheses, or to recommend reaction conditions that produce the highest yield at the minimum cost or wastage [19].

Machine learning, and specifically, deep learning, which is a neural network-inspired approach, has attracted specific interest due to its capability to work with complex, high-dimensional chemical data. The most common models that are used to compute molecular structures are convolutional neural networks (CNNs) and graph neural networks (GNNs), where grid-like representations of molecules are processed by CNNs, and molecular structure represented as graphs (GNNs) [20]. Generative models, including variational autoencoders (VAEs) and generative adversarial networks (GANs), have also been demonstrated to be useful in de novo molecular design in order to design entirely novel molecules with desired properties [21].

Organic chemistry involves the effective use of AI, and the quality of data, characteristics representation, and model interpretability must be taken into account. The provision of high-quality datasets, appropriate molecular descriptors, and transparent algorithms makes the predictions provided by AI reliable and chemically sensible. When these methods are united, AI presents chemists with instruments that can speed up molecular discovery, improve their reaction insight, and increase the confines of synthetic chemistry [22].

INTERFEROMETRY IN NANOTECHNOLOGY

One of the most important uses of artificial intelligence (AI) in organic chemistry is molecule property prediction. Proper prediction of molecular properties, i.e. solubility, reactivity, stability, bioactivity, and toxicity can help chemists to prioritize compounds, synthesize molecules that are of desired properties and reduce the necessity to carry out lengthy and expensive experiments. Historically, such predictions were based on empirical rules, physical models or quantum chemical calculations [23]. Although these methods can be strong when applied to small chemical spaces or with structurally homogenous molecules, they are frequently not able to scale to large chemical spaces, or molecules with diverse structures. AI, and specifically machine learning (ML), is a data-driven prediction that can be trained on large-scale data and provide fast and consistent predictions when dealing with new compounds [24].

Supervised machine learning is the most frequent in the prediction of molecular properties. The models are trained on the datasets in which the known property values are associated with the related molecular inputs. Chemical structures are represented in numbers with representations like SMILES strings, molecular fingerprint, or graph-based encodings [25]. The traditional algorithms used, including random forests, support vector machines, and gradient boosting, are used with smaller datasets and deep learning models, including convolutional neural networks (CNNs), recurrent neural networks (RNNs), and graph neural networks (GNNs), can be effectively used with larger and more complex data. GNNs and deep learning models in general are highly effective as they can explicitly learn the shape of molecules, as their atoms and bonds interact to identify overall molecular properties [26].

A major usage is in the form of quantitative structure - activity relationships (QSAR) and quantitative structure - property relationships (QSPR). The models are used to predict the molecular features in relation to chemical properties or biological activity, they are used in drug discovery, material design and catalyst optimization [27]. The use of AI-based QSAR/QSPR models can estimate activity in untested compounds, so that a researcher can concentrate on the potentials of candidate compounds, and experimental resources are not wasted on useless experiments. In the same way, solubility and partition coefficient predictive models, melting points, and stability assist chemists in the design of molecules possessing desired physicochemical properties [28].

In addition to predicting single property, AI models can be used to predict multiple properties and this allows multi-objective optimization. As an example, in medicinal chemistry, molecules may be constructed to be as potent and as possible and as non-toxic and/or with enhanced pharmacokinetic characteristics. This is obtained with multi-task learning in which one single model learns correlations

between molecular features and multiple outcomes [29]. Although the benefits are there, there are difficulties. The quality, diversity and size of training data is important in model accuracy and predictions of new chemical scaffolds can be less reliable. Interpretability is also essential because the knowledge of why a model makes and predictions allow chemists to be confident in predictions and improve them [30].

AI-based predictive molecular properties have transformed organic chemistry by accelerating the prioritization of molecules, rational design, and decreasing the amount of work needed in the laboratory. Using the combination of high-quality data, the correct molecular representations, and state-of-the-art machine learning algorithms, chemists can predict chemical behavior more efficiently, and consequently can discover molecules faster and more informatively [31].

ARTIFICIAL INTELLIGENCE IN MOLECULAR DESIGNING AND DISCOVERY

The use of artificial intelligence (AI) has radically changed the role of molecular design and discovery in organic chemistry by allowing chemists access to the tremendous chemical space more effectively than previous techniques. The search space of possible organic molecules is astronomically large, estimated to be in the excess of 10⁶⁰ potential compounds. This space is experimentally infeasible to explore, and even the traditional methods of computation are time-consuming [32]. The AI, especially machine learning and deep learning approaches, provide a data-driven approach to discovering, designing, and optimizing molecules with desirable properties, which shortens the discovery process, as well as making less reliant on trial and error discovery [33].

IMPORTANCE OF AI IN MOLECULAR DESIGN

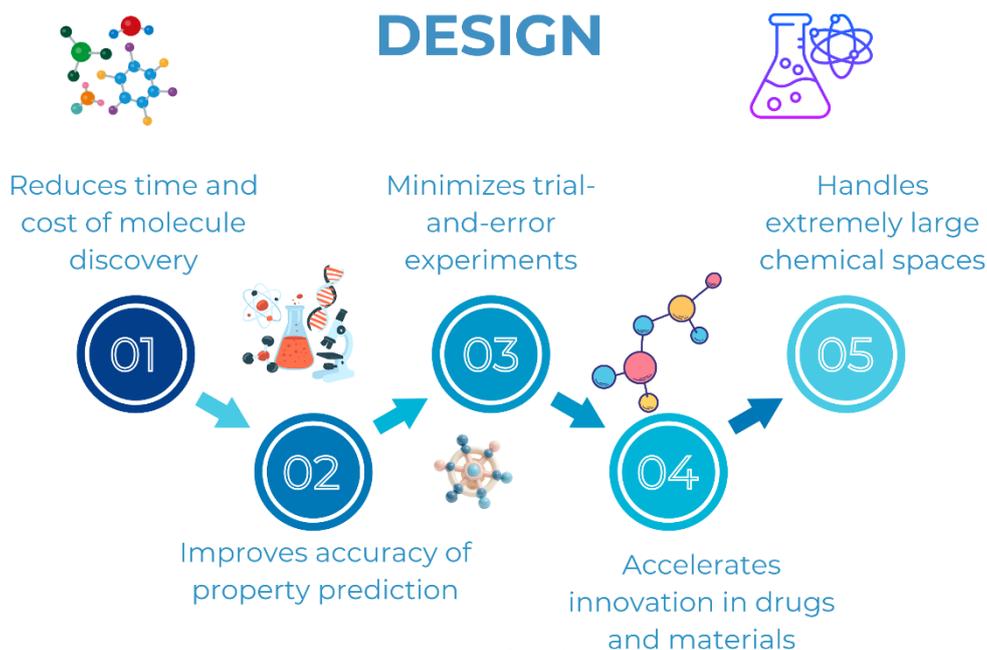


Figure 2. Importance of AI in molecular design

De novo molecular generation is one of the main ways of using AI in the field of molecular design. Generative models like variational autoencoders (VAEs), generative adversarial networks (GANs) and recurrent neural networks (RNNs) are capable of synthesizing completely novel molecular structures via learning of patterns of existing data [34]. The chemical rules and structure-property relationships are encoded in these models and thus can generate molecules with a certain design criteria, e.g., solubility, bioactivity or stability. In the context of drug discovery, it can be useful especially to suggest new drug-like molecules with improved pharmacological properties without obtaining unwanted properties such as toxicity [36].

Virtual screening and lead optimization is also another application that is critical. The AI models can be trained to quickly screen big sets of compounds on given properties and find valuable leads to be tested. Machine learning applications are used to predict binding affinity, selectivity and physicochemical properties to enable researchers to narrow their attention to high-potential molecules [37]. This ability greatly contributes to minimising time and cost involved in screening an experiment, and expedites the discovery of useful molecules to drugs, materials and catalysis [38].

AI also improves structure-activity relationship (SAR) analysis since subtle correlations between chemical structures and functional properties can be identified by the models. These understandings provide a rational way of molecular design, as they indicate the structural changes that are most likely to be beneficial or alleviate the negative impact. Moreover, AI-based platforms can combine several objectives, allowing simultaneous optimization of many molecular properties, which is necessary in diverse applications such as drug discovery, in which molecules need to meet efficacy, safety, and stability criteria [39].

Even though AI has been successful in molecular design, there are challenges. Effective predictions require good quality and variety of data, and AI models might fail in cases of extrapolating new chemical scaffolds that are not part of the training set. Moreover, it is highly important to be interpretable; chemists need to know why a model offers a specific molecule to confirm and optimize design strategies to work well [40]. AI in molecular design and discovery is a disruptive technology that supports human experience and can quickly explore chemical space, produce new molecules, and optimize molecular characteristics. Through enhanced AI, organic chemistry can be innovated more quickly, effectively, and rationally since it uses sophisticated strategies with refined chemical data at its core [41].

REACTION UNDERSTANDING AND MECHANISTIC PREDICTION

The correct prediction of chemical reactions and mechanistic pathways is one of the key problems of organic chemistry, and artificial intelligence (AI) has become a resource that can effectively be used to solve this problem. Classical methods of reaction prediction are based on the experience of chemists, their mechanistic arguments, and trial and error [42]. Although such methods have resulted in many successful syntheses, they are typically restricted in speed, scalability and capability to sample large chemical reaction space. An alternative to these methods, based on AI and especially machine learning (ML) and deep learning, can lead to more efficient and systematic prediction of the reaction outcomes, optimization of the conditions, and an understanding of the mechanism [43].

The overall process of AI-based reaction prediction is to learn reaction patterns using a large reaction dataset, e.g. a literature dataset, patent dataset, or high-throughput experiment dataset. Three-dimensional images of molecules, reactions, and intermediates are essential in terms of model accuracy. Such linear encodings as SMILES, reaction fingerprints and graph-based encodings allow algorithms to manipulate the structure of molecules and chemical transformations in a way compatible with computational models [44]. The sequence-to-sequence models, and graph neural networks (GNNs) in the domain of deep learning are especially useful as they represent the interactions and the electronic environment of atoms, which allows predicting the possible reaction products, and regioselectivity.

Among the most influential ones, there is the reaction outcome prediction, with AI models predicting the most probable products under specified reaction conditions and reactants. These models greatly minimize exhaustive experimental testing especially in complex reactions which have more than one step or delicate intermediates [45]. Likewise, yield prediction models employ AI in predicting reaction efficiency in a variety of conditions to guide chemists in optimizing such reaction parameters as temperature, solvent, catalysts, and concentration. This is not only enhancing productivity, but also aids in the sustainable and cost effective synthesis, by reducing the amount of wasted resources [46]. Mechanistic understanding is also achieved by AI. Through the analysis of large reactivity datasets (reactions), reaction models are able to find trends in reactivity and selectivity, as well as in the compatibility of functional groups, and this information can be used to give information on the underlying reaction mechanisms [47]. Other developed AI methods are a blend of prediction of reaction and understandable processes, emphasizing atoms or bonds that have the highest likelihood of transformation. This allows chemists to be able to rationalize the results of reactions, suggest alternative reactions, and plan new synthetic strategies [48].

In spite of these improvements, there are still difficulties. Probable prediction of reactions requires



extensive and high-quality datasets, and AI systems can also not deal well with infrequent reactions, or new chemistries that are not seen during training. Besides, interpretability is also of the essence; the chemists must comprehend AI recommendations so as to provide trust and applicability to experimental settings. Predicting reactions using AI and mechanism is transforming organic chemistry as it offers quick, correct and understandable forecasts [49]. When combined with massive data, molecular representations, and with the help of advanced machine learning methods, AI allows chemists to design reactions more effectively, elucidate chemical transformations better, and speed up the rate of the discovery of new molecules and synthetic pathways [50].

SYNTHETIC PLANNING AND RETROSYNTHESIS

Organic chemistry is based on the principle of retrosynthesis, which is the breakdown of a desired molecule into simpler molecules. Historically, retrosynthetic analysis has been an effort that is largely dependent on intuition and expertise of reaction mechanisms as well as being attentive to functional group compatibility. Although it has been shown to be effective, this process may be time consuming particularly in the case of complex molecules which possess many synthetic pathways [51]. Artificial intelligence (AI) has become an innovative resource in retrosynthesis and synthetic planning, which provides evidence-based techniques to automate and streamline the design of synthetic pathways.

The AI-aided retrosynthesis is based on the large reaction databases and machine-learning algorithms to compute the plausible disconnections and find possible synthetic paths. The patterns of bond formation and cleavage are learned by training models on literature, patent and experimental data curated datasets. Graph-based neural networks, sequence-to-sequence models, and transformer have been modernly applied in the process of encoding molecular structures and reaction templates [52]. Such models are able to propose any number of synthetic paths to a target molecule, prioritize them based on factors like yield, cost, or step efficiency, and even suggest alternative reagents or conditions [53].

A major benefit of AI in retrosynthesis is that it can search large chemical space, which would be unmanageable by other methods. The AI algorithms can quickly come up with thousands of existing routes, test them and pick those that are synthetically accessible and cost-effective. This is especially important with complex drug molecules, natural products, or new materials in which traditional planning might be restricted by the human cognitive abilities. Synthetic planning is also improved with the help of AI by incorporating multi-step reaction sequences [54]. Models are able to take into account reaction interdependence, and not only are the single step responses feasible, but also the success of the overall multi-step synthesis. Other more advanced systems use AI retrosynthesis with reaction prediction and property optimization, and they form a full design framework where target

molecules can be designed, optimized, and predicted, and the outcome of the design can be assessed computationally, then implemented in the lab [55].

AI-based retrosynthesis has challenges even though it promises. The quality and variety of training data have an extensive impact on model performance, and infrequent or uncommon reactions could be represented poorly. Also, it is essential that it should be interpretable, because chemists need to know why some disconnections are suggested, and determine whether given pathways are practical [56]. AI has transformed retrosynthesis and synthetic planning by automating the discovery of viable synthetic paths, allowing exploration of chemical space to be solved advantageously, and rational and data-driven decision making. Using big data, novel molecular representations, and neural networks, AI can make synthetic organic chemistry faster, more efficient, and more creative, and offers chemists with potent instruments of current molecular discovery [57].

OPTIMIZATION OF REACTIONS WITH THE USE OF AI

In organic chemistry, optimization of reactions is an important process that identifies the effectiveness, productivity, selectivity, and scalability of any chemical reaction. Historically, the optimization of reaction conditions, including temperature, solvent, catalyst, concentration and time are based on trial and error experiments and experience of the chemist. This method can be time demanding, resourceful and constrained in investigating multi-dimensional reaction space [58]. The artificial intelligence (AI) provides a data-driven approach in order to speed up the optimization of reactions by anticipating the optimal conditions, reduce effective experimental load, and enhance their reproducibility.

AI-based reaction optimization is commonly implemented by machine learning models that are trained based on the past reaction data. These models can be used to determine the effect of different conditions on the yield, selectivity, or efficiency of reactions by learning the interrelations between the parameters and the results of a reaction. The most common models are regression models, random forests, gradient boosting and deep learning networks [59]. Further methods are used to incorporate these predictive models with active learning or Bayesian optimization and promote a closed-loop workflow where AI proposes conditions, experimental results are inputted into the model and successive steps are taken to enhance precision and propinquity to optimal conditions [60].

Multi-objective optimization is one of the most robust uses of AI in this field, which balances reactions not only by their yield but also selectivity, cost, or sustainability. As an illustration, the models can be used to determine the conditions of the reactions maximizing the formation of the product with the least amount of waste, energy, or dangerous reagents, which can be considered in the context of green chemistry [61].

Applications of AI in Reaction Optimization

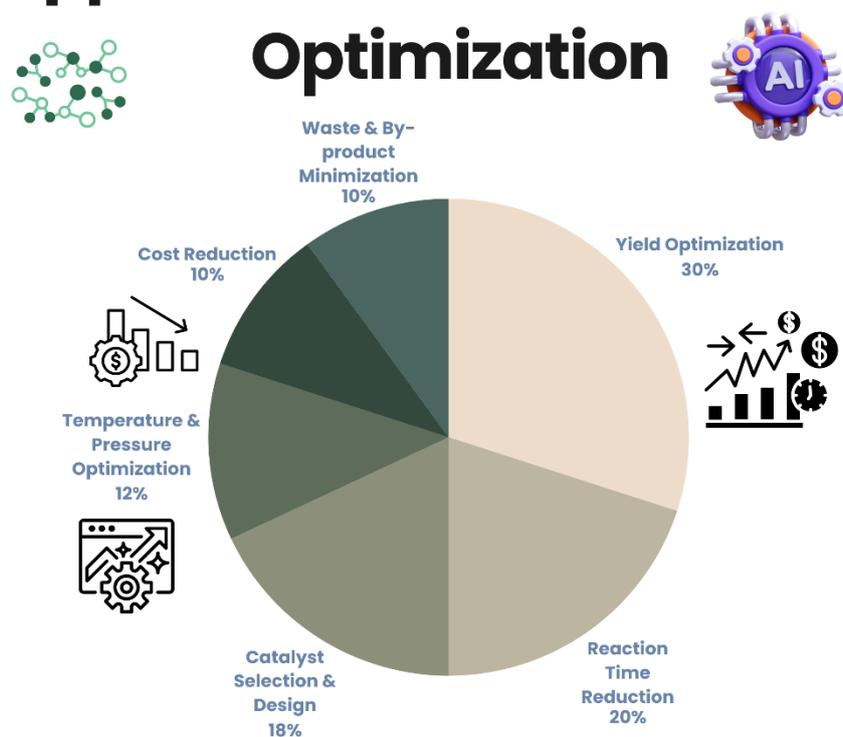


Figure 3. Applications of AI in reaction optimization

High-throughput experimentation, in which hundreds or thousands of conditionings of reaction are considered virtually and then very few actual experiments are performed, is also enabled by AI-driven optimization. This saves a lot of time, cost as well as material consumption and speeds up the discovery. Moreover, using AI it is possible to reveal non-intuitive conditions, which traditional solutions may ignore, and the reaction results can usually be improved [62].

These benefits notwithstanding, there are challenges. The pinpoint optimization requires the access to high-quality and diverse datasets and cautious selection of models. It should also be interpretable so that chemists can make sense of the reasons as to why the AI will suggest certain conditions to authenticate findings and generalize them [63]. The application of AI-based reaction optimization is changing the fields of synthetic chemistry, where the reaction parameters can be optimized fast, effectively, and intelligently. AI is able to enhance the efficiency of reactions by combining predictive models, active learning, and high-throughput experimentation as well as enabling sustainable, cost-effective, and reproducible chemical synthesis [64].

ORGANIC CHEMISTRY APPLICATIONS IN IMPORTANT AREAS

AI has been extensively applied to a variety of critical fields of organic chemistry, transforming the way chemists have undertaken evaluations of molecular design, synthesis and functional discovery. Incorporating machine learning, deep learning, and data-based solutions with experimental chemistry, AI provides more effective, rational and predictive solutions in drug discovery, catalysis, materials chemistry and sustainable synthesis [65].

AI has had a transformative effect especially in drug discovery and medicinal chemistry. The conventional drug development cycle is tedious and expensive and in most cases, it takes years of screening and optimization before it gets to the market. The AI-based models can be used to enhance this process faster by forecasting the characteristics of a molecule, including bioactivity, toxicity, solubility, and pharmacokinetics so that the chemists can focus on a promising compound to synthesize and test [66]. Generative models and reinforcement learning allow new drug-like molecules with the characteristics of activity and reduced off-target effects to be designed. Moreover, AI has the potential to optimize multi-step synthetic pathways on the complex drug scaffolds, which can save a lot of time and cost of experiment [67].

AI can assist in the discovery of the best catalysts, ligands, and reaction conditions in catalysis and reaction development. The trained machine learning models that are based on reaction datasets would be able to predict whether the reaction is reactive, selective, and could yield, informing chemists about more effective catalytic systems. AI-based optimization has also increased the rate at which homogeneous and heterogeneous catalysts are discovered and allowed the parameters of reactions to be fine-tuned to enhance their efficiency, selectivity, and sustainability [68].

AI can also be applied in materials chemistry, particularly in the design of functional materials (polymers, organic semiconductors, and molecular sensors). Predictive models are capable of estimating properties such as conductivity, stability, or mechanical strength prior to synthesis and this gives chemists an opportunity to narrow in on high-potential candidates [69]. Whole new materials designed to be useful in particular functions can be generated using generative models, and this has greatly enlarged the chemical space available to traditional experimentation.

The use of AI in green and sustainable organic synthesis is also important. AI assists in improving the environmental friendliness of chemical reactions by predicting efficient reactions, reduced waste, and minimal use of energy. The models can propose safer reagents, other solvents, and energy-saving reactions, and guide chemists to design reactions that are in line with green chemistry principles [70]. Regardless of these developments, there still are issues such as the inability to diversify datasets, apply them to new chemical scaffolds, and interpret models. These problems cannot be resolved

without constant cooperation of chemists, data scientists, and engineers [71].

AI is changing the important fields of organic chemistry by facilitating quicker, reasonable, and effective molecular discovery and development. AI-driven solutions are transforming the classic workflows and overall chemical possibilities in the fields of drug design and catalysis, materials science, and sustainable chemistry to develop innovative and environmentally responsible solutions in chemical chemistry [72].

EXISTING PROBLEMS AND SHORTCOMINGS

Although artificial intelligence (AI) has made quick leaps and is widely used in organic chemistry, the field still faces a number of challenges and limitations to its potential. The awareness of these concerns is important in successfully adopting AI in the fields of molecular discovery, prediction of reactions, and synthetic planning, as well as in making sure that AI-based strategies are dependable as well as viable. Data quality and availability is one of the major challenges [73]. The AI models are based on big and high-quality data sets to be trained, whereas chemical data is usually missing, not consistent, or biased. Experimental findings can be summarized with different degrees of specificity and negative or unsuccessful reactions are underrepresented, giving rise to models that might overestimate success rates or be unable to apply to new situations. Moreover, proprietary or other unpublished datasets do not restrict access, which narrows the variety of reactions, molecules, and conditions that AI models can be trained on [74].

The other weakness is model interpretability. Most AI and machine learning paradigms are opaque, that is, they give predictions that are not explained. Although they can predict the outcome of reactions correctly or recommend new molecules, chemists require a mechanistic knowledge in order to believe and utilize these guidelines. The inability to interpret it may hinder experimental validation and hinder the use of AI tools in research and industry [75].

The problem of generalization and extrapolations are also important. The AI models are the most effective at forecasting the outcomes in chemical spaces related to the training data. Model predictions can be invalid when faced with absolutely new molecular scaffolds, reaction types or conditions. This disadvantage is especially true in the case of innovative molecular design or exploratory synthesis when more comprehensive coverage is needed by traditional datasets [76]. Interconnection with the laboratory workflows is also a feasible problem. Predictions made by AI should be successfully converted into experimentation procedures, and the integration of computational proposals with laboratory automation, high-throughput screening, or trial-and-error analysis will need cross-functional collaborations of chemists, data scientists, and engineers [77].

Lastly, there is the issue of ethical and reproducibility. It is necessary to report the AI model



architectures, training datasets, and metrics of evaluation in a transparent way so that results can be reproduced and the discoveries made by AI can be independently verified [78].

Finally, even though AI has the potential to be transformative to organic chemistry, it is currently limited by weaknesses in data quality, interpretability, generalization, workflow integration, and reproducibility. The only way to solve these challenges is through a careful dataset curation, model transparency, collaboration between the disciplines, and further development of more methods that can combine predictive strength and chemical intuition [79]. These problems can be overcome by AI to attain dependable, expandable, and sensible applications to accelerate molecular detection and increase the efficiency and sustainability of contemporary organic chemistry [80].

CONCLUSION

The area of organic chemistry is undergoing change through artificial intelligence (AI), providing effective tools to speed up the process of discovering molecules, optimization of reactions, and novel molecules and materials. Organic chemistry has traditionally depended on intuition, experience and tedious experimentation of chemists. Although these techniques have caused some outstanding findings, time, human mental ability and resources tend to constrain them. Embracing AI in chemical science creates a concept of a data-driven approach to research to which human knowledge can be added with the help of massive data sets, computational frameworks, and machine learning to deliver more efficient and predictive results.

The ultimate case of AI in organic chemistry is built upon large-scale gathering, description, and preservation of quality chemical data. The basis of the predictive models is experimental findings, computer simulations, and literature databases that are curated. The models accuracy and interpretability is directly dependent on the molecular representation used i.e. SMILES strings, molecular fingerprints or graph-based structures. Preparation of data, feature identification, and dimensionality reduction also increase the accuracy of AI forecasting. Having strong backgrounds in place, chemists can effectively use AI tools in a variety of applications with considerable certainty.

The AI methods, such as supervised, unsupervised, reinforcement learning, and deep learning systems, such as graph neural networks and generative models, can be used by chemists to predict molecular properties, design novel molecules, and optimize reactions. The models that use AI have the capability of predicting physicochemical properties, bioactivity, and toxicity, which contribute to rational molecular prioritization during drug discovery and in materials design. De novo molecular design using generative models and reinforcement learning is much faster, and reaction optimization, retrosynthesis and synthetic planning using predictive algorithms are much faster. Such tools minimize the amount of work to be done in experiments, waste, and expose non-intuitive paths and



conditions that otherwise would be unknown.

There are numerous applications of AI to important fields of organic chemistry. AI predictive bioactivity, toxicity, and pharmacokinetics are also used in drug discovery to select promising compounds. It finds the best catalysts and reaction conditions in catalysis and reaction development, and improves efficiency and selectivity. AI-enabled prediction of material properties and new material design are useful in materials science, whereas reactions optimization to minimize waste and energy use is assisted by green and sustainable chemistry.

Nonetheless, these benefits are accompanied by such challenges as data quality and bias, interpretation of a model, generalization to new chemical spaces, adaption to laboratory processes, and reproducibility. To overcome these weaknesses, interdisciplinary efforts will be needed, models will be reported transparently and datasets will be carefully curated. With this obstacle surmounted, AI could be utilized with great reliability and efficiency to a broad range of chemical issues.

To draw a conclusion, AI is not going to replace human chemists, but a potent tool that is complementary to human intuition and experience. With the introduction of AI into the field of organic chemistry, scientists will have the ability to survey chemical space more effectively, create molecules in a more rational way, optimize reactions more effectively, and expedite the discovery of new molecules and materials. The next step of human-AI collaboration will enable the field of organic chemistry to expand its limits in discovering, producing, and creating molecules through the data and mechanistic understanding of these sciences that will transform the pharmaceutical, material, and chemical research worlds. The field of modern organic chemistry is going to be redesigned by AI that will be more intelligent, quicker, and sustainable.

REFERENCES

- [1]. Ma B, Qin N, Yan Q, Zhou W, Zhang S, Wang X, Bao L, Lu X. Advancing metal organic framework and covalent organic framework design via the digital-intelligent paradigm. *Digital Discovery*. 2026.
- [2]. Cheng M, Fu CL, Okabe R, Chotrattanapituk A, Boonkird A, Hung NT, Li M. Artificial intelligence-driven approaches for materials design and discovery. *Nature Materials*. 2026 Jan 2:1-7.
- [3]. Das B, Patrikar K, Keny AS, Mondal A. From fragments to function: data-driven design of high-performance non-fullerene acceptors for organic photovoltaics. *Molecular Systems Design & Engineering*. 2026.

- [4]. Al-Sakkari EG, Ragab A, Benali M, Ajao O, Boffito DC, Dagdougui H. Accelerated green material and solvent discovery with chemistry-and physics-guided generative AI. *Artificial Intelligence Chemistry*. 2026 Jan 2:100106.
- [5]. Lin X, Li Y, Yu X, Liu X, Lei YK, Yang YI. Harnessing Artificial Intelligence to Revolutionise Molecular Modelling and Simulations. *Applied Artificial Intelligence for Drug Discovery: From Data-Driven Insights to Therapeutic Innovation*. 2026 Jan 10:239-88.
- [6]. Yang P, Yu X, Stylianou KC, Huang L, Wang Q. Accelerating Amine-Based CO₂ Capture with Machine Learning: From Molecular Screening to Process Optimization. *Fundamental Research*. 2026 Jan 2.
- [7]. Menon RK, Hegde PS. Ai/Machine Learning–Enabled Intelligent Frameworks for NextGen Catalyst Discovery and Performance Optimization. *Journal of Research in Applied Chemistry*. 2026 Jan 2;8(2).
- [8]. Shakarami SH. Integration of Artificial Intelligence in Organic Chemistry: Recent Advances, Applications, and Challenges. *International journal of Modern Achievement in Science, Engineering and Technology*. 2025 Jun 7;2(2):130-9.
- [9]. Gangwal A, Lavecchia A. Artificial intelligence in natural product drug discovery: current applications and future perspectives. *Journal of medicinal chemistry*. 2025 Feb 7;68(4):3948-69.
- [10]. Samajdar D, Kumar M, Mishra P, Gopukumar ST. Machine Learning in Organic Chemistry: Accelerating Drug Discovery through Computational Models. *Machine Learning*.;11(2).
- [11]. Mroz AM, Basford AR, Hastedt F, Jayasekera IS, Mosquera-Lois I, Sedgwick R, Ballester PJ, Bocarsly JD, del Río Chanona EA, Evans ML, Frost JM. Cross-disciplinary perspectives on the potential for artificial intelligence across chemistry. *Chemical Society Reviews*. 2025.
- [12]. Siddiqui B, Yadav CS, Akil M, Faiyyaz M, Khan AR, Ahmad N, Hassan F, Azad MI, Owais M, Nasibullah M, Azad I. Artificial intelligence in computer-aided drug design (cadd) tools for the finding of potent biologically active small molecules: Traditional to modern approach. *Combinatorial Chemistry & High Throughput Screening*. 2025 Jan 15.
- [13]. Nsouli R, Galiyan G, Ackerman-Biegasiewicz LK. Advancing Organic Chemistry Using High-Throughput Experimentation. *Angewandte Chemie International Edition*. 2025 Sep 26;64(40):e202506588.
- [14]. Wong F, Omori S, Li A, Krishnan A, Lach RS, Rufo J, Wilson MZ, Collins JJ. An explainable deep learning platform for molecular discovery. *Nature Protocols*. 2025 Apr;20(4):1020-56.

- [15]. Uceda RG, Gijón A, Míguez-Lago S, Cruz CM, Álvarez de Cienfuegos L, Mota AJ, Miguel D, Cuerva JM. Chiral Intelligence: The Artificial Intelligence-Driven Future of Chiroptical Properties. *ChemPhotoChem*. 2025 May 1:2500079.
- [16]. Ozcan A, Coudert FX, Rogge SM, Heydenrych G, Fan D, Sarikas AP, Keskin S, Maurin G, Froudakis GE, Wuttke S, Erucar I. Artificial Intelligence Paradigms for Next-Generation Metal–Organic Framework Research. *Journal of the American Chemical Society*. 2025 Jun 24;147(27):23367-80.
- [17]. Kathawate LG, Shelke RN, Pansare DN, Sarkate AP. Computational Tools and Techniques in Planning Organic Synthesis. In *Artificial Intelligence for Chemical Sciences* 2025 May 9 (pp. 57-72). Apple Academic Press.
- [18]. Cannavacciuolo FD, Falivene L, Zhang Z, Takasao G, De Canditiis D, Khoshsefat M, Chammingkwan P, Antinucci G, Taniike T, Cipullo R, Cavallo L. Data Driven Modeling of Ziegler–Natta Polypropylene Catalysts: Revisiting the Role of the Internal Donor. *ACS Catalysis*. 2025 Mar 24;15(7):5770-80.
- [19]. Phul, S.; Kuenze, G.; Vanoye, C. G.; Sanders, C. R.; George, A. L., Jr.; Meiler, J. Predicting the functional impact of KCNQ1 variants with artificial neural networks. *PLOS Computational Biology* 2022, 18 (4), No. e1010038.
- [20]. Van Breugel, M.; Rosa e Silva, I.; Andreeva, A. Structural validation and assessment of AlphaFold2 predictions for centrosomal and centriolar proteins and their complexes. *Communications Biology* 2022, 5 (1), 312.
- [21]. Lin, M. H.; Tu, Z.; Coley, C. W. Improving the performance of models for one-step retrosynthesis through re-ranking. *Journal of Cheminformatics* 2022, 14 (1), 15.
- [22]. Rani M. Role of Machine Learning in Inorganic and Coordination Chemistry: Applications and Challenges. *IJSAT-International Journal on Science and Technology*. 2025 Jun 25;16(2).
- [23]. Ishida, S.; Terayama, K.; Kojima, R.; Takasu, K.; Okuno, Y. AIDriven Synthetic Route Design Incorporated with Retrosynthesis Knowledge. *Journal of Chemical Information and Modeling* 2022, 62 (6), 1357–1367.
- [24]. Barnard, A. S.; Fox, B. L. Importance of Structural Features and the Influence of Individual Structures of Graphene Oxide Using Shapley Value Analysis. *Chem. Mater.* 2023, 35 (21), 8840–8856.
- [25]. Arsalan MH, Mubin O, Al Mahmud A, Khan IA, Hassan AJ. Mapping Data-Driven Research Impact Science: The Role of Machine Learning and Artificial Intelligence. In *Metrics* 2025 Apr 2 (Vol. 2, No. 2, p. 5). MDPI.

- [26]. Thanh HV, Dai Z, Rahimi M. Data-driven explainable machine learning approaches for predicting hydrogen adsorption in porous crystalline materials. *Journal of Alloys and Compounds*. 2025 May 3:180709.
- [27]. Berber S, Brückner M, Maurer N, Huwer J. Artificial intelligence in chemistry research—Implications for teaching and learning. *Journal of Chemical Education*. 2025 Mar 6;102(4):1445-56.
- [28]. Ackermann, M.; Haase, C. Machine learning-based identification of interpretable process-structure linkages in metal additive manufacturing. *Additive Manufacturing* 2023, 71, No. 103585.
- [29]. Graille, M.; Sacquin-Mora, S.; Taly, A. Best Practices of Using AI-Based Models in Crystallography and Their Impact in Structural Biology. *Journal of Chemical Information and Modeling* 2023, 63 (12), 3637–3646.
- [30]. Thanh HV, Dai Z, Rahimi M. Data-driven explainable machine learning approaches for predicting hydrogen adsorption in porous crystalline materials. *Journal of Alloys and Compounds*. 2025 May 3:180709.
- [31]. Kleinert, F.; Leufen, L. H.; Lupascu, A.; Butler, T.; Schultz, M. G. Representing chemical history in ozone time-series predictions – a model experiment study building on the MLair (v1.5) deep learning framework. *Geosci. Model Dev.* 2022, 15 (23), 8913–8930.
- [32]. Carvalho, R. P.; Brandell, D.; Araujo, C. M. An evolutionary driven AI model discovering redox-stable organic electrode materials for alkali-ion batteries. *Energy Storage Materials* 2023, 61, No. 102865.
- [33]. Kopac T. Leveraging Artificial Intelligence and Machine Learning for Characterizing Protein Corona, Nanobiological Interactions, and Advancing Drug Discovery. *Bioengineering*. 2025 Mar 18;12(3):312.
- [34]. Chen J, Gao Q, Huang M, Yu K. Application of modern artificial intelligence techniques in the development of organic molecular force fields. *Physical Chemistry Chemical Physics*. 2025.
- [35]. Wu Y, Li X, Guo R, Xu R, Ju MG, Wang J. How to accelerate the inorganic materials synthesis: from computational guidelines to data-driven method?. *National Science Review*. 2025 Apr;12(4):nwaf081.
- [36]. Parveen F, Slater AG. Digitalisation of catalytic processes for sustainable production of biobased chemicals and exploration of wider chemical space. *Catalysis Science & Technology*. 2025;15(6):1689-701.

- [37]. Song T, Luo M, Zhang X, Chen L, Huang Y, Cao J, Zhu Q, Liu D, Zhang B, Zou G, Zhang G. A multiagent-driven robotic ai chemist enabling autonomous chemical research on demand. *Journal of the American Chemical Society*. 2025 Mar 8;147(15):12534-45.
- [38]. Luo S, Deng J, Jia G. Physical information neural network combined with the symbolic regression: A machine learning method for prediction of dielectric constants in organic liquids and water mixtures. *Journal of Molecular Liquids*. 2025 Jan 1;417:126544.
- [39]. Wang Z. *Data-Driven ComputerAided Molecular, Material and Process Design for Efficient Separation Systems* (Doctoral dissertation, Otto-von-Guericke-Universität Magdeburg).
- [40]. Bonciolini S, Pulcinella A, Noël T. Tech-enhanced synthesis: exploring the synergy between organic chemistry and technology. *Journal of the American Chemical Society*. 2025 Aug 5;147(32):28523-45.
- [41]. Badrinarayanan S, Magar R, Antony A, Meda RS, Barati Farimani A. MOFGPT: Generative design of metal–organic frameworks using language models. *Journal of Chemical Information and Modeling*. 2025 Aug 28;65(17):9049-60.
- [42]. Zhang M, Deng Y, Zhou Q, Gao J, Zhang D, Pan X. Advancing micro-nano supramolecular assembly mechanisms of natural organic matter by machine learning for unveiling environmental geochemical processes. *Environmental Science: Processes & Impacts*. 2025;27(1):24-45.
- [43]. He Z, Bi H, Liang B, Li Z, Zhang H, Wang Y. Frontier molecular orbital weighted model based networks for revealing organic delayed fluorescence efficiency. *Light: Science & Applications*. 2025 Feb 10;14(1):75.
- [44]. Hong Y, Hou B, Jiang H, Zhang J. Machine learning and artificial neural network accelerated computational discoveries in materials science. *Wiley Interdisciplinary Reviews: Computational Molecular Science*. 2020 May;10(3):e1450.
- [45]. Tan EX, Nguyen LB, Jin Y, Lv Y, Phang IY, Ling XY. SERS cheminformatics: opportunities for data-driven discovery and applications. *ACS Central Science*. 2025 Aug 5;11(11):2034-52.
- [46]. Jain M, Deleu T, Hartford J, Liu CH, Hernandez-Garcia A, Bengio Y. Gflownets for ai-driven scientific discovery. *Digital Discovery*. 2023;2(3):557-77.
- [47]. Choudhary N, Bharti R, Sharma R. Role of artificial intelligence in chemistry. *Materials Today: Proceedings*. 2022 Jan 1;48:1527-33.

- [48]. Strieth-Kalthoff F, Szymkuc S, Molga K, Aspuru-Guzik A, Glorius F, Grzybowski BA. Artificial intelligence for retrosynthetic planning needs both data and expert knowledge. *Journal of the American Chemical Society*. 2024 Apr 10;146(16):11005-17.
- [49]. Jiang X, Luo S, Liao K, Jiang S, Ma J, Jiang J, Shuai Z. Artificial intelligence and automation to power the future of chemistry. *Cell Reports Physical Science*. 2024 Jul 17;5(7).
- [50]. Zhu Y, Li S, Chen J, Zhao D, Wang X, Li Y, Liu Y, Kong Y, Zhang B, Liu C, Hou T. SynGFN: learning across chemical space with generative flow-based molecular discovery. *Nature Computational Science*. 2025 Nov 13:1-0.
- [51]. Thakkar A, Johansson S, Jorner K, Buttar D, Reymond JL, Engkvist O. Artificial intelligence and automation in computer aided synthesis planning. *Reaction chemistry & engineering*. 2021;6(1):27-51.
- [52]. Zhuo Y, Brgoch J. Opportunities for next-generation luminescent materials through artificial intelligence. *The Journal of Physical Chemistry Letters*. 2021 Jan 10;12(2):764-72.
- [53]. Abranches JD. *Thermodynamics-Informed Machine Learning for the Design of Sustainable Materials: The Dawn of Digital Molecular Discovery*. University of Notre Dame; 2024.
- [54]. Coley CW, Thomas III DA, Lummiss JA, Jaworski JN, Breen CP, Schultz V, Hart T, Fishman JS, Rogers L, Gao H, Hicklin RW. A robotic platform for flow synthesis of organic compounds informed by AI planning. *Science*. 2019 Aug 9;365(6453):eaax1566.
- [55]. Greenman KP. *Optical Property Prediction and Molecular Discovery through Multi-Fidelity Deep Learning and Computational Chemistry*. Massachusetts Institute of Technology; 2024.
- [56]. Liang J, Xu S, Hu L, Zhao Y, Zhu X. Machine-learning-assisted low dielectric constant polymer discovery. *Materials Chemistry Frontiers*. 2021;5(10):3823-9.
- [57]. Blakemore DC, Castro L, Churcher I, Rees DC, Thomas AW, Wilson DM, Wood A. Organic synthesis provides opportunities to transform drug discovery. *Nature chemistry*. 2018 Apr;10(4):383-94.
- [58]. Singh SK, Sose AT, Wang F, Bejagam KK, Deshmukh SA. Data driven discovery of MOFs for hydrogen gas adsorption. *Journal of Chemical Theory and Computation*. 2023 Sep 27;19(19):6686-703.
- [59]. Zheng P, Yang W, Wu W, Isayev O, Dral PO. Toward chemical accuracy in predicting enthalpies of formation with general-purpose data-driven methods. *The journal of physical chemistry letters*. 2022 Apr 13;13(15):3479-91.
- [60]. Nising CF, von Nussbaum F. Industrial Organic Synthesis in Life Sciences—Today and Tomorrow. *European Journal of Organic Chemistry*. 2022 May 6;2022(17).

- [61]. Ferraz-Caetano J. The artificial intelligence explanatory trade-Off on the logic of discovery in chemistry. *Philosophies*. 2023 Feb 23;8(2):17.
- [62]. Li X, Vaghefinazari B, Würger T, Lamaka SV, Zheludkevich ML, Feiler C. Predicting corrosion inhibition efficiencies of small organic molecules using data-driven techniques. *npj Materials degradation*. 2023 Aug 9;7(1):64.
- [63]. Sanchez-Lengeling B, Outeiral C, Guimaraes GL, Aspuru-Guzik A. Optimizing distributions over molecular space. An objective-reinforced generative adversarial network for inverse-design chemistry (ORGANIC).
- [64]. Thakkar A, Schwaller P. How AI for synthesis can help tackle challenges in molecular discovery: Medicinal chemistry and chemical biology highlights. *Chimia*. 2021 Aug 17;75(7-8):677-.
- [65]. Baum ZJ, Yu X, Ayala PY, Zhao Y, Watkins SP, Zhou Q. Artificial intelligence in chemistry: current trends and future directions. *Journal of Chemical Information and Modeling*. 2021 Jul 15;61(7):3197-212.
- [66]. Baró EL, Nadal Rodríguez P, Juárez-Jiménez J, Ghashghaei O, Lavilla R. Reaction space charting as a tool in organic chemistry research and development. *Advanced Synthesis & Catalysis*. 2024 Feb 20;366(4):551-73.
- [67]. Nandy A, Duan C, Taylor MG, Liu F, Steeves AH, Kulik HJ. Computational discovery of transition-metal complexes: from high-throughput screening to machine learning. *Chemical reviews*. 2021 Jul 14;121(16):9927-10000.
- [68]. Singh S, Hernández-Lobato JM. Data-driven insights into the transition-metal-catalyzed asymmetric hydrogenation of olefins. *The Journal of Organic Chemistry*. 2024 Aug 16;89(17):12467-78.
- [69]. Djoumbou-Feunang Y, Wilmot J, Kinney J, Chanda P, Yu P, Sader A, Sharifi M, Smith S, Ou J, Hu J, Shipp E. Cheminformatics and artificial intelligence for accelerating agrochemical discovery. *Frontiers in Chemistry*. 2023 Nov 29;11:1292027.
- [70]. Marom N. Collaborative Research: Data Driven Discovery of Singlet Fission Materials. NSF Award Number 2021803. Directorate for Mathematical and Physical Sciences. 2021 Feb;20(2021803):21803.
- [71]. Runqiu S, Guihua L, Su A. Bayesian optimization for chemical synthesis in the era of artificial intelligence: Advances and applications. *Processes*. 2025;13(9):2687.
- [72]. Gómez-Bombarelli R, Aguilera-Iparraguirre J, Hirzel TD, Duvenaud D, Maclaurin D, Blood-Forsythe MA, Chae HS, Einzinger M, Ha DG, Wu T, Markopoulos G. Design of efficient

- molecular organic light-emitting diodes by a high-throughput virtual screening and experimental approach. *Nature materials*. 2016 Oct;15(10):1120-7.
- [73]. Tharwani KK, Kumar R, Ahmed N, Tang Y. Large language models transform organic synthesis from reaction prediction to automation. *arXiv preprint arXiv:2508.05427*. 2025 Aug 7.
- [74]. He C, Zhang C, Bian T, Jiao K, Su W, Wu KJ, Su A. A review on artificial intelligence enabled design, synthesis, and process optimization of chemical products for industry 4.0. *Processes*. 2023 Jan 19;11(2):330.
- [75]. Ess DH, Jelfs KE, Kulik HJ. Chemical design by artificial intelligence. *The Journal of Chemical Physics*. 2022 Sep 28;157(12).
- [76]. Yoshikawa I, Aghababaei Tafreshi O, Sun YC, Matsuura N, Sotowa KI, Naguib HE. Data-Driven Discovery of Multifunctional Organic Polymer Aerogels by Machine Learning-Assisted Large-Scale Property Screening. *Industrial & Engineering Chemistry Research*. 2025 May 23.
- [77]. Ricci E, De Angelis MG. A perspective on data-driven screening and discovery of polymer membranes for gas separation, from the molecular structure to the industrial performance. *Reviews in Chemical Engineering*. 2024 Jul 26;40(5):567-600.
- [78]. Tripathi A, Misra K, Dhanuka R, Singh JP. Artificial intelligence in accelerating drug discovery and development. *Recent Patents on Biotechnology*. 2023 Mar 1;17(1):9-23.
- [79]. Visan AI, Negut I. Integrating artificial intelligence for drug discovery in the context of revolutionizing drug delivery. *Life*. 2024 Feb 7;14(2):233.
- [80]. Zacharov I, Arslanov R, Gunin M, Stefonishin D, Bykov A, Pavlov S, Panarin O, Maliutin A, Rykovanov S, Fedorov M. “Zhores”—Petaflops supercomputer for data-driven modeling, machine learning and artificial intelligence installed in Skolkovo Institute of Science and Technology. *Open Engineering*. 2019 Oct 26;9(1):512-20.