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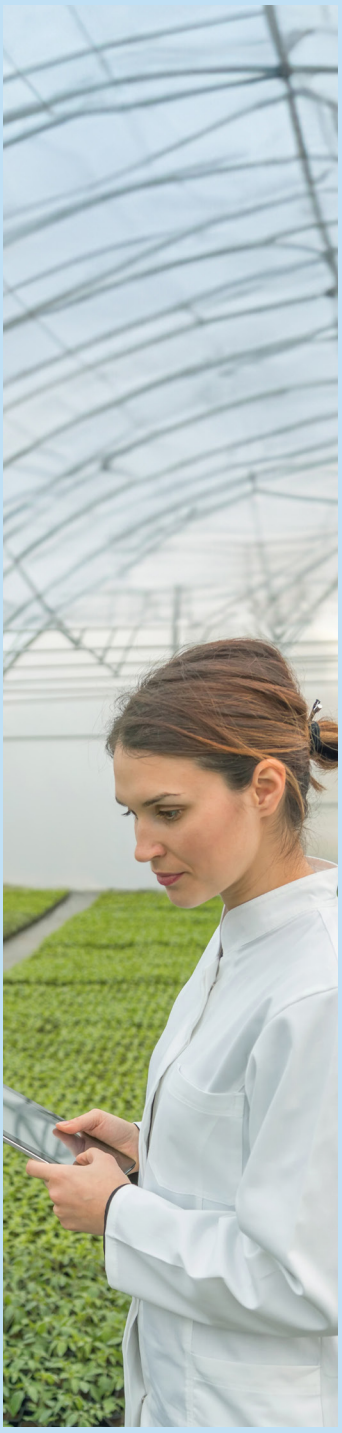

AI: THE CATALYST IN AGROCHEMICAL DISCOVERY

Abstract

Artificial Intelligence (AI) is a new paradigm in agrochemical innovation to overcome pest resistance and deliver sustainable crop protection products with superior environmental and toxicological profiles. This white paper discusses the transformative potential of AI in agrochemical R&D. It highlights the opportunity for IT to contribute while minimizing the cost and time to introduce a new agrochemical product.

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Introduction

The integration of AI into multifaceted datasets enables researchers to uncover the interplay between agrochemicals, target pests, crop species, and their ecosystems. This holistic approach of amalgamating chemical, biological-driven research has the potential to develop 'smart' agrochemicals with enhanced activity, sustainability and an improved toxicity profile. A comprehensive analysis drives the discovery of next-generation crop protection products that are superior in terms of efficacy and agricultural sustainability. By leveraging this knowledge ecosystem, scientists can create targeted solutions in a shorter R&D timeline and at reduced costs.

Challenges in Agrochemical Discovery

In conventional agrochemical discovery, enterprises need to navigate several challenges for the discovery of effective and sustainable agrochemicals[1].

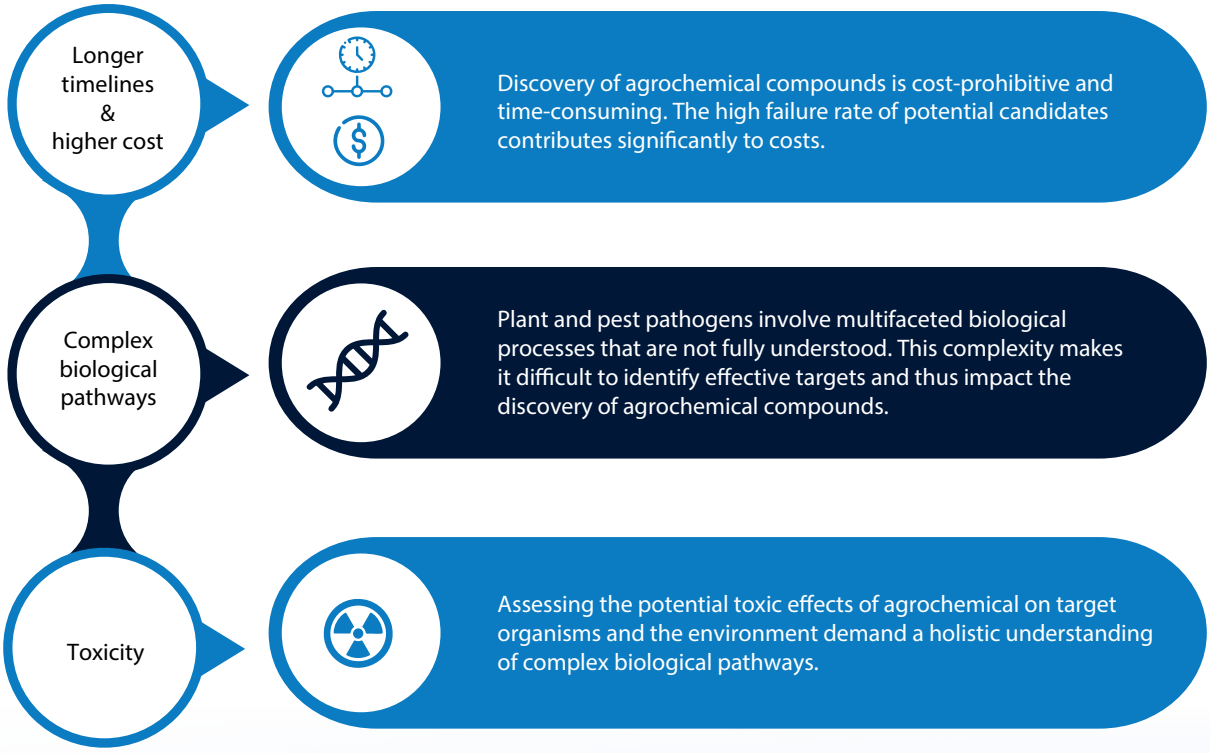


Figure 1: Agrochemical discovery challenges

IT companies are developing technology-based solutions to address challenges across the agrochemical discovery process.

Pathway for AI Integration into Agrochemical Discovery

The pathway begins with the analysis of historical data by taking into consideration several parameters related to the identification of the target, designing of the molecule, and finally, predicting toxicity. This process involves multiple iterations to identify and deliver novel agrochemical compounds. Figure 2 illustrates how AI supports the discovery process for agrochemicals.

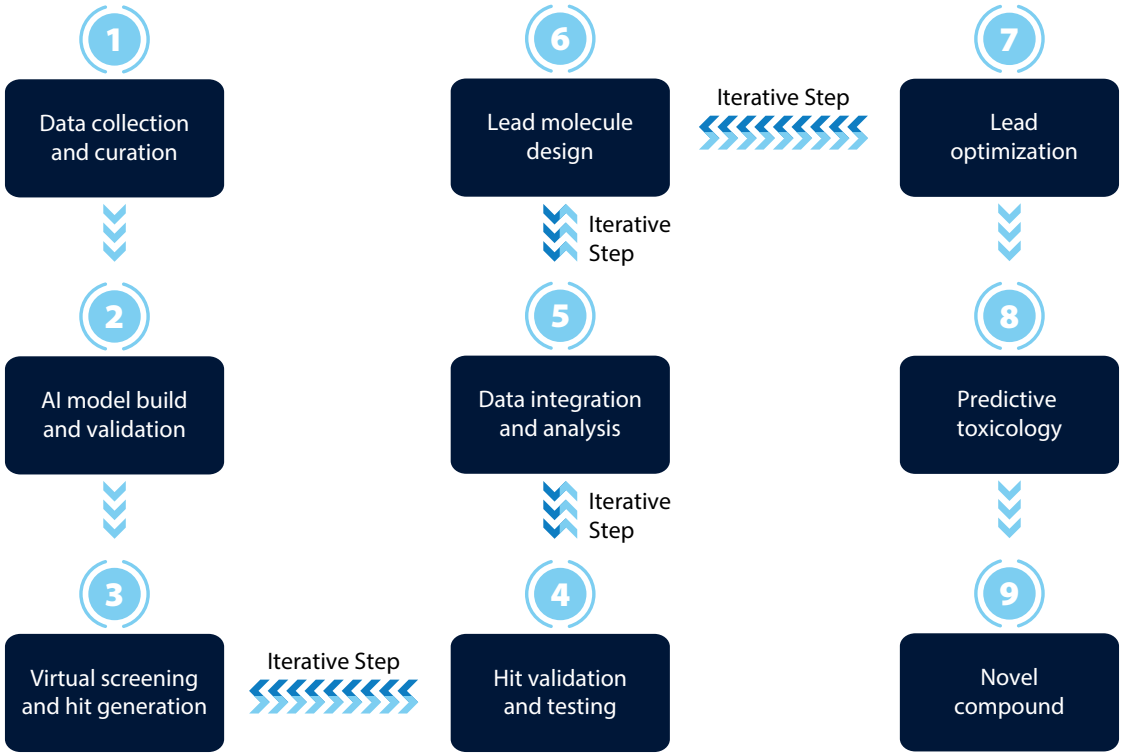


Figure 2: Artificial intelligence assisted discovery process for agrochemicals

Data Collection and Curation

By combining different types of data (like chemical, biological, genomic, and environmental), scientists can better understand how agrochemicals (like pesticides) interact with pests, crops, and the environment. This helps them discover new and more effective agrochemicals.

AI Model Development and Validation

For identification of molecules with the desired profile, a multi-layered AI/ML model is developed that combines the concepts of chemistry, biology, and crop protection products. This model assesses a database of millions of compounds with relevant positive and negative profiles (positive compounds exhibit desired activity while negative compounds lack activity). Typically, a robust predictive module requires multiple training iterations. Thereafter, the build model is tested and validated with different datasets. The validated model can be used to find mechanism of action (MOA), hit identification, lead generation, lead optimization, and prediction of toxicity.

Virtual Screening and Hit Generation

Virtual screening has been successfully adopted to identify potential drug-like molecules in the pharma industry. Similarly, agrochemical companies are implementing virtual screening to identify hits for novel pesticides. In this process, a molecule shows an activity threshold in the preliminary test. Virtual screening algorithms and molecular docking simulations are being used to select hit molecules from a large dataset of chemical libraries. During this process, researchers prioritize the best binding or robust interactions between the target and the compound. This technology intervention guides researchers to select candidate molecules (hit molecule) for lab testing.

Hit Validation and Testing

Hit validation and testing is a crucial stage in agrochemicals discovery. It is used to filter the 'false positive' hits and mitigate risks at a later stage. Hit molecules are synthesized and tested against the target to validate the identified hits. Validated hits are then used as a base for further exploration.

Data Integration and Analysis

Experimental and computational hits are run concurrently to distil more knowledge on hit compounds. AI uncovers structure-activity relationships and optimization directions. This stage focuses on activity as well as desired agrochemical properties.

Lead Molecule Design: Chemical Space Exploration

Once validated hits are identified, the next stage involves a broad exploration of the chemical landscape, Structure-Activity Relationship (SAR), and structure modulation with activity and testing, to define the general areas of activity. The structures of the hit molecules are researched to identify the molecule with the desired activity profile of an agrochemical, which can be a potential lead molecule. AI-led technologies can identify potential active ingredients promptly, expedite the validation of target sites in pests or pathogens, and optimize the molecular structure of agrochemical compounds. By leveraging Machine Learning (ML) algorithms and big data analytics, researchers can potentially uncover innovative agrochemicals with improved specificity, reduced environmental footprint, and enhanced crop protection capabilities.

Lead Optimization

In the R&D process, during lead optimization, a molecule that exhibits agrochemical activity is fine tuned for the desired physicochemical, Absorption, Distribution, Metabolism, and Excretion (ADME) and toxicity profile. AI models incorporate physical, chemical and toxicological profiles to select a candidate. In quantitative structure-activity relationship (QSAR) modelling, AI and ML models scan large datasets for chemical structures, biology interaction and toxicity to support designing of agrochemical molecules[2,3]. QSAR models based on Artificial intellgence, correlate chemical structures with their biological activities, which provides direction on how compounds can be modified to enhance the profile further. The lead optimization stage propels the candidate to move forward if it meets the criteria[3].

Predictive Toxicology

Forecasting the toxicity of any agrochemical is imperative to avoid failure at a later stage. An extensively trained AI model with a large dataset can predict the pattern and toxicity. Such a system accounts for properties such as agrochemical likeness, molecular features, and target-based information, and protein targets' characteristics in formulating a 'score' that measures whether a candidate fails due to its high level of toxicity[3].

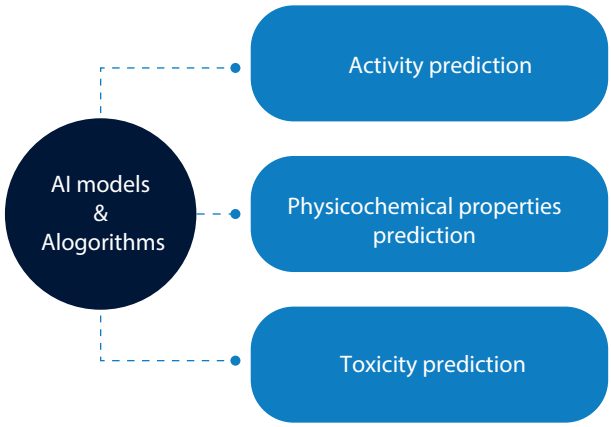


Figure 3: Potential of AI in designing of agrochemicals

Benefits of AI in Agrochemical R&D

Conventional crop protection R&D demands a significant investment in time, effort, and cost. Typically, it takes more than a decade to develop a crop protection product[4,5]. AI-driven methodologies leverage data-driven insights to streamline the R&D process, which significantly reduces the need for extensive experimental iterations. Integration of AI into the agrochemical discovery process is pivotal to the growth of this industry (Figure 4).

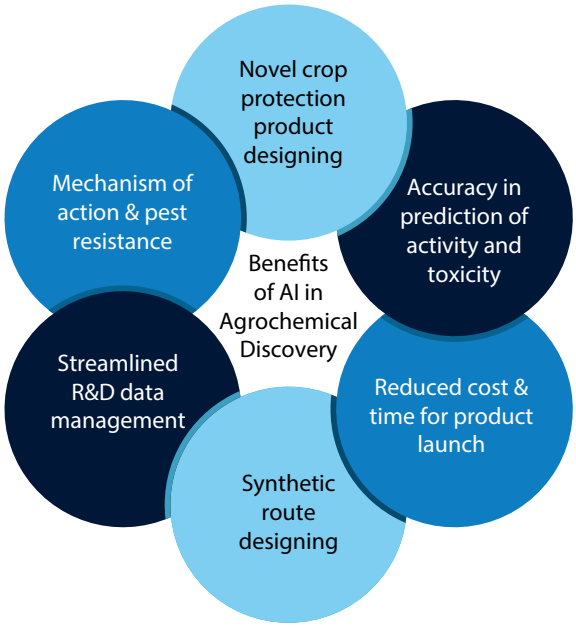


Figure 4: Benefits of AI in agrochemical discovery

AI has a multiplier effect on the agrochemical discovery process:

- Virtual screening expedites the screening of a huge compound library. The positive rate can reach up to 5-20%, which is significantly higher than 0.01% in conventional random screening[2].
- AI models can predict the activity, pest resistance, physico-chemical and toxicity profile of a molecule, and expedite the designing of a novel compound with desired agrochemical properties[1].
- AI helps analyse and design the best synthetic route design. AI-led technologies are used extensively in the pharmaceutical industry for designing the synthetic route for chemicals, thereby saving cost by 30-50%[6].
- AI helps streamline R&D data management in experimental planning, sample generation, testing, and data analysis.

Leveraging AI for Agrochemical Discovery

AI-led technologies accelerate the discovery of novel crop protection solutions while reducing the time and cost of development. Leading agrochemical companies have recognized the potential of AI and are either integrating it into their research processes or collaborating with AI companies.

- Bayer is utilizing AI for crop protection research to accelerate the R&D process, improve accuracy, and enhance sustainability. CropKey, Bayer's AI platform transforms crop protection R&D by identifying target proteins with AI. Unlike the conventional process of screening thousands of molecules, CropKey focuses on designing molecules with specific properties and safety profiles, minimizing off-target activity, and rationalizing production costs. This approach has delivered 3x more mechanism-of-action in early research[7] compared to similar exercises a decade ago.
- Syngenta is collaborating with Insilico Medicine, a leader in AI and deep learning, to expedite the discovery of more effective crop protection solutions and advance food security while protecting the ecosystem. This collaboration is focused on AI-led technologies to design novel and active molecules in an accelerated timeframe and rationalized cost structure.[8] Syngenta has partnered with IBM for AI and NLP-based IBM's RXN to design more sustainable and efficient routes for chemical synthesis[9], thereby enhancing crop protection research by accelerating synthesis of chemicals.
- BASF is integrating AI techniques to enhance efficiency and rationalize cost of agrochemical research. BASF collaborated with Dotmatics to enhance its R&D IT infrastructure through the 'Data to Value' project. This partnership helps streamline R&D data management in experimental planning, sample generation, testing, and data analysis[10].

Strategy for AI-driven Agrochemical Discovery

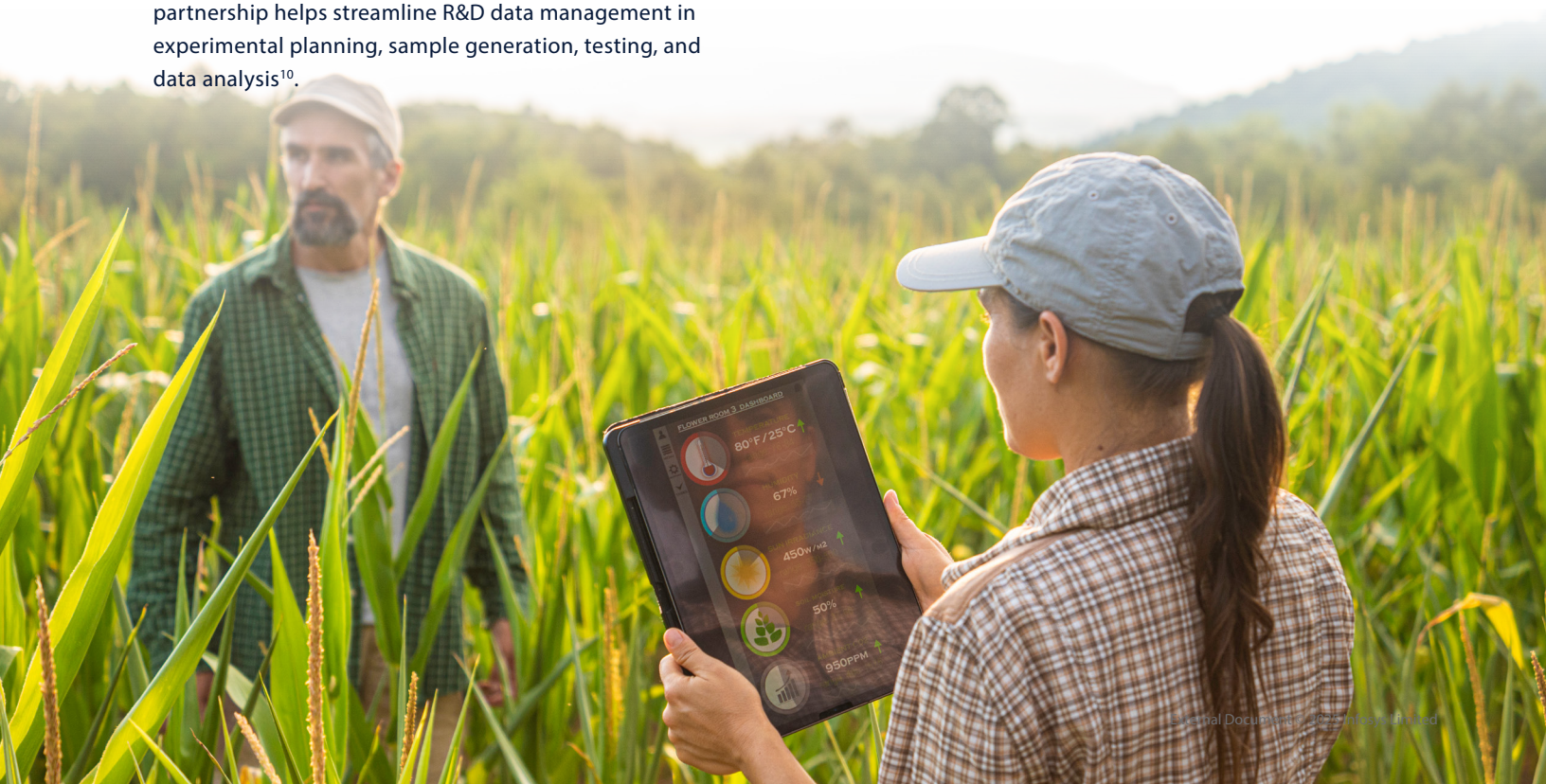
The trifecta of agility, collaboration and predictive systems enabled by AI is the catalyst for next-generation agrochemicals. The success of AI-driven agrochemical discovery depends on how enterprises respond to shifts in business and technology. The combination of researchers' knowledge and AI-led discoveries can significantly reduce the time-to-market and cost to deliver effective novel agrochemicals with a safe toxicity profile. A report from Agrematch, an AI-led agri-tech company, states that their build models have the potential for discovery of herbicidal compounds in less than a year with huge saving[5].

Infosys Case Study

The traditional method for developing agrochemical compounds is resource-intensive, time consuming and results in delayed timelines. The primary challenges -

- Requires manual design, efficacy and toxicity screening, and repeat experiments to validate results.
- Delays overall R&D timeline, which slows down the introduction of new agrochemicals to the market.
- Existing agrochemicals often lose efficacy over time due to resistance development and pose toxicity (environmental and off target) concerns.

PoC: An AI/ML-assisted model is developed to design agrochemicals for superior efficacy, minimal toxicity, and a lower risk of resistance development. This innovative model is precisely tailored to target specific diseases and pathogens.



POC Workflow

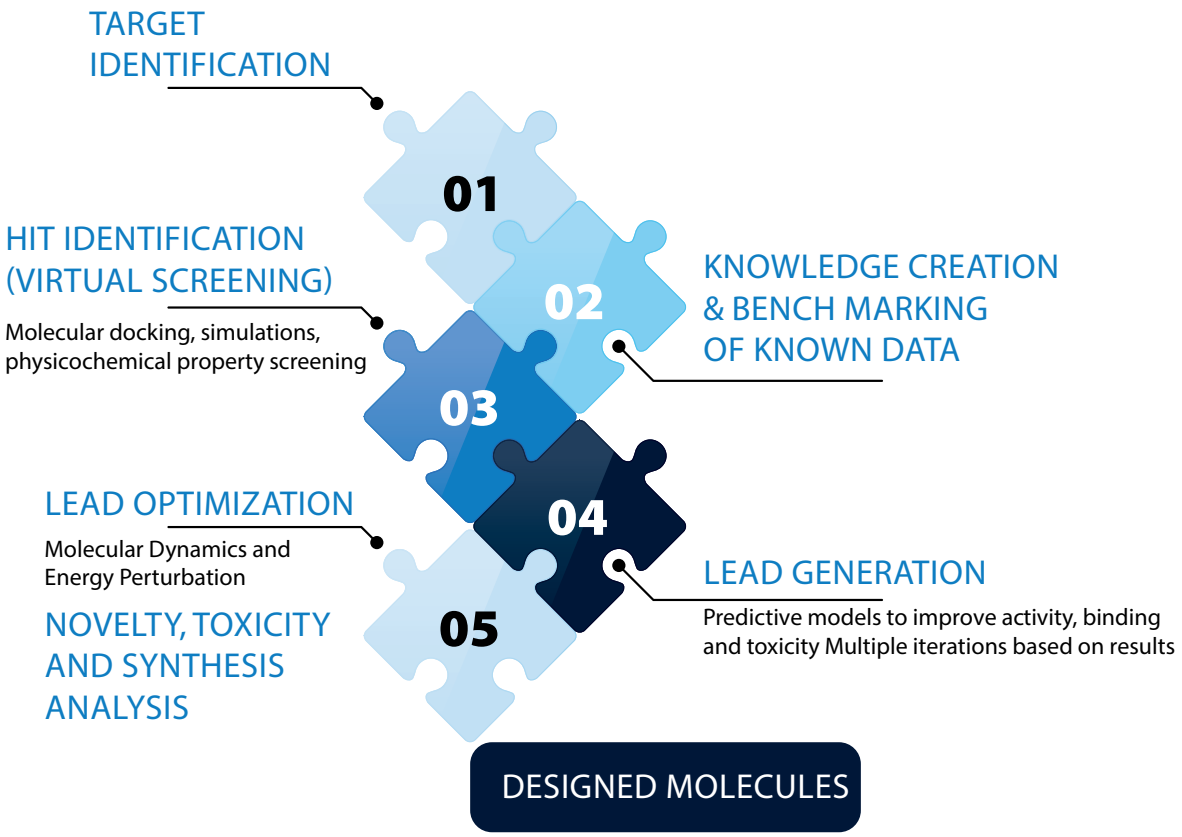


Figure 5: Workflow for AI-based agrochemicals design

These models are ready to design new agrochemicals for desired activity and minimal toxicity for different targets.

Conclusion

Integration of AI into agrochemical research and development has the potential to transform the agrochemical discovery process. In molecular docking, drug design, predictive toxicology modelling, and computational chemistry, AI accelerates compound discovery, optimizes structures, and enhances efficacy and safety. It streamlines discovery processes, reduces costs, and promotes environment-friendly solutions. AI is modernizing agriculture, boosting food security, minimizing the environmental impact, and developing safer agrochemicals. This AI-driven transformation is making the agrochemical sector adopt sustainable practices by innovating and optimizing every aspect of agrochemical R&D.

Infosys Agrochemical R&D Centre of Excellence (CoE)

Infosys has established an Agrochemical R&D CoE to address challenges in the discovery of novel crop protection chemicals. Our CoE seeks to transform the crop protection industry by leveraging an AI suite of cutting-edge technologies. We are collaborating with universities and AI start-ups to offer deep technology solutions for -

- Novel target identification: AI-driven target discovery to reduce physical experiments
- Virtual screening: In-silico compound screening to reduce physical testing of compounds
- Predictive modeling: Efficacy and toxicity models for compounds
- Data analytics: Analysis of large datasets to identify patterns and correlations
- Compound design: AI-optimized novel compound design
- Synthetic route design: AI-driven design of synthetic route for compounds

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