

**ECO-INNOVATIONS IN PLANT PATHOLOGY: THE ROLE OF GREEN CHEMISTRY AND ARTIFICIAL INTELLIGENCE**

 **Dr. Deepa Srivastava\***

Assistant Professor, Department of Botany, Deen Dayal University Gorakhpur University, Gorakhpur, Uttar Pradesh, India

Email: [deepa.bot@ddugu.ac.in](mailto:deepa.bot@ddugu.ac.in)

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**ABSTRACT**

Plant diseases pose a major threat to global food security, with increasing severity under climate change and intensive agriculture. Conventional approaches to disease management have long relied on synthetic chemical pesticides, but these methods contribute to environmental degradation, pesticide resistance, and human health risks. Emerging eco-innovations rooted in green chemistry principles and powered by artificial intelligence offer sustainable solutions for plant disease management. Green chemistry facilitates the development of biodegradable agrochemicals, natural-product-based fungicides, and smart nanocarriers, while AI enhances early disease detection, outbreak prediction, and eco-design of bioactive compounds. This paper explores the integration of green chemistry principles, such as biodegradable agrochemicals, natural product discovery, and nanotechnology with AI-driven tools for disease diagnosis, prediction, and sustainable crop protection. Together, these approaches pave the way for climate-smart agriculture and long-term sustainability.

**Keywords:** Green Chemistry, Artificial Intelligence, Plant Disease Management, Biodegradable Agrochemicals, Climate-Smart Agriculture.

**1. INTRODUCTION**

Plant pathogens, including fungi, bacteria, viruses, and nematodes, cause approximately 20-40% annual crop losses worldwide (Savary et al., 2019). Conventional plant protection strategies heavily depend on chemical pesticides, which have achieved short-term success but result in long-term environmental and health hazards, such as pesticide residues in soil and water, development of resistant pathogen strains, and adverse effects on beneficial organisms (Pimentel, 2005).

The increasing demand for food security, coupled with climate change-induced shifts in pathogen dynamics, necessitates eco-innovations in plant pathology. Two powerful paradigms, green chemistry and artificial intelligence (AI), are reshaping the future of plant disease management. Green chemistry ensures sustainable molecular design and application, while AI provides predictive intelligence for precision interventions.

**2. GREEN CHEMISTRY IN PLANT PATHOLOGY**

Green chemistry in plant pathology involves designing safer, sustainable, and environmentally friendly approaches to manage plant diseases, moving away from traditional, toxic pesticides.

Key applications include the use of green-synthesized nanoparticles (nanomaterials created from plant extracts or microbes), bio-pesticides like chitosan and plant secondary metabolites, and innovative strategies like RNA interference and precision delivery systems to reduce chemical use and enhance ecological health and food security. The promotion of the following principles characterizes the application of green chemistry to plant pathology:

1. **Reduced Toxicity and Hazards:** The design of chemical products and processes aims to eliminate or significantly reduce the use and production of hazardous substances.
2. **Renewable Resources:** Utilizing renewable feedstocks and bio-based materials, such as plant extracts, instead of synthetic chemicals.
3. **Biodegradability:** The development of formulations that exhibit ease of biodegradation serves to minimize environmental persistence and accumulation.
4. **Energy Efficiency:** The innovation of energy-efficient synthetic methodologies for the production of disease-control agents is prioritized.

## 2.1 Nanopesticides and Smart Delivery Systems

Nanoparticles originating from biological sources that serve as pesticides are referred to as nanobiopesticides and play a significant role in protecting plants (Pan et al., 2023). In agriculture, nanobiopesticides are employed as pest control agents due to their remarkable physicochemical properties such as size, reactivity, and surface area. Additionally, nanobiopesticides exhibit distinct biological interactions with plants, along with predictable transport and behaviour in the environment (Kurul et al., 2025; Pan et al., 2023). Green-Synthesized Nanoparticles (GSNPs) employing plant extracts or microorganisms to synthesize metallic nanoparticles is conducted in a manner that is both safer and more cost-effective than traditional chemical synthesis. GSNPs manifest antifungal, antibacterial, and antiviral properties, thereby presenting an environmentally friendly alternative for the management of plant diseases. Examples include silver nanoparticles (AgNPs), chitosan nanoparticles, and polymer-based carriers that provide targeted control of pathogens (Kah et al., 2019). They serve as both active components and carriers, helping to stabilize a variety of agrochemicals, with products such as nanofertilizers and nanopesticides emerging from their use (Machado et al., 2023). For example, pesticides formulated from nanomaterials like magnesium oxide, magnesium hydroxide, copper oxide, and zinc oxide, which are obtained from aqueous extracts of *Chamaemelum nobile* flowers, *Punica granatum* peels, green peach aphids (GPA), and *Olea europaea* leaves, have shown efficacy in pest control (Chaudhry et al., 2024; Konappa et al., 2021). Additionally, silver nanoparticles derived from the leaf extract of *Euphorbia hirta* have been researched for their ability to manage the cotton bollworm, *Helicoverpa armigera* (Devi et al., 2014). The effectiveness of copper oxide and zinc oxide nanoparticles in combating *Alternaria citri*, the pathogen responsible for citrus black rot disease, has also been documented (Elshafie et al., 2023). Furthermore, Sardar et al. (2022) investigated the effects of both combined and individual applications of zinc oxide and copper oxide in controlling citrus black rot disease within a potato dextrose medium. The insecticidal and antifungal properties of copper nanoparticles have been demonstrated against *Tribolium castaneum*, a common pest affecting grain crops (El-Saadony et al., 2020). The effectiveness of nanobiopesticides is influenced by factors such as their composition, surface charge, concentration, size, and any chemical and physical alterations (Vinci et al., 2025). Chitosan nanoparticles have demonstrated antifungal activity against *Fusarium* and *Aspergillus*, with AI models improving delivery efficiency and dosage (Shang et

al., 2019). Due to their diminutive size and enhanced surface area, the chemical characteristics of nanopesticides vary considerably from those of traditional pesticides, enabling the creation of a structure with numerous benefits, including improved interactions and modes of action at the targeted pest site. Nano-sized formulations demonstrate higher selectivity while maintaining the bioactivity of the compounds against the intended pathogen. Their heightened toxicity can also facilitate deeper pest penetration. The application of nanoparticles addresses issues related to drifting and leaching and permits the use of reduced amounts of active compounds per area, provided that the formulation achieves optimal concentration delivery for the targeted insecticide over extended periods. The design of nano-formulations facilitates the controlled and targeted release of active compounds, effectively reducing the overall chemical burden and mitigating environmental repercussions.

## 2.2 Biopesticides and Microbial Antagonists

Biopesticides are products derived from biological sources that help control pests in agriculture, ultimately improving crop yields (Samada and Tambunan, 2020). The utilization of bio-derived eco-friendly compounds such as chitin, chitosan, plant secondary metabolites, essential oils, and natural polymers serves as effective antifungal and antibacterial agents is implemented to stimulate plant defense mechanisms against pathogenic threats (Koul et al., 2008). These compounds decompose naturally, minimizing environmental persistence (Ayilara et al., 2024). *Trichoderma*, *Bacillus*, and *Pseudomonas spp.* serve as microbial biocontrol agents, replacing synthetic fungicides. Green chemistry approaches help optimize formulations and stabilize these agents for field application.

The pesticides categorized within the strobilurin class represent some of the most prevalent environmental pollutants. In an investigation by Birolli et al 2020, biodegradation analyses of the strobilurin fungicide Pyraclostrobin were conducted utilizing bacterial strains isolated from orange cultivation environments, to advance a bioremediation methodology. Upon utilizing the five most effective strains (*Bacillus sp.* CSA-13, *Paenibacillus alvei* CBMAI2221, *Bacillus sp.* CBMAI2222, *Bacillus safensis* CBMAI2220, and *Bacillus aryabhatai* CBMAI2223) in various consortia, both synergistic and antagonistic interactions were documented contingent upon the specific bacterial combinations employed. This observation suggests that the incorporation of these bacterial strains into the soil within a bioaugmentation framework enhances the decontamination process. Nevertheless, the native microbiome remains critical for achieving a more effective bioremediation outcome.

## 2.4 Circular Chemistry Approaches

Agricultural residues and by-products are increasingly valorised into bioactive compounds, reinforcing circular economy principles in crop protection. These innovations help reduce chemical footprints while enhancing efficacy against plant pathogens. In this context, the concept of circular economy, where the waste and coproducts generated by one process are considered as inputs for another one and converted into value-added products through clean and green approaches, is being aggressively pursued and adopted (Ncube et al., 2023). Stems, leaves and husks generated during agricultural production and several byproducts, including proteins and carbohydrates, supplied as coproducts during agricultural processing, are available in large quantities at low cost. These by-products and coproducts have the essential constituents to be converted into monomers, polymers, compounds and further into any desired substance through

specific chemical transformations, ranging from carbonyl reductions to carboxyl decarboxylations, hydroxyl oxidations, glycosylation, and transglycosylation (Wang et al., 2021). For example, corn-based biorefineries utilizing starch, corn husks, corn cobs, distillers dried grains and other coproducts have generated biofuels (ethanol, methane), biopolymers (polylactide), amino acids, animal feed and enzymes. Similarly, sugarcane based biorefineries have excelled in the production of biofuels, paper, fertilizers, animal feed, chemicals such as acetic acid, cosmetics and perfumes ( Calvo-Flores and Martin-Martinez 2022). Not only regular food crops but also non-food products such as poultry feathers have been considered for the production of composite materials, plastics, biofuels, etc. Based on these approaches, it is evident that there is unlimited scope for extending the bio refinery and circular economy concepts to almost all agricultural by products and coproducts.

Shifting the focus to the intriguing domain of bio-derived polymers, the synthesis of poly- $\gamma$ -glutamic acid ( $\gamma$ -PGA) assumes a critical role. This hydrophilic innovation is poised to serve as a revolutionary element across a multitude of applications. Its applicability extends across various disciplines, including drug delivery systems, cosmetic formulations, bioremediation processes, and wastewater treatment solutions, thereby articulating a narrative that emphasizes sustainability and versatility. Parati et al. (2023) investigated the synthesis of  $\gamma$ -PGA from scalable macroalgal biomass, systematically evaluating the effects of pre-treatment methods, macroalgal species, and harvesting time on brown seaweed cultivated under controlled environmental conditions in Scotland. The species *Laminaria digitata*, *Saccharina latissima*, and *Alaria esculenta*, which are indigenous to the United Kingdom, are examined for variations in carbon content, antioxidant activity, protein levels, and ash composition. The study assesses how different algal species influence the yields and chemical profile of  $\gamma$ -PGA synthesized by *Bacillus subtilis natto*, while also examining the fluctuations that occur throughout the designated cultivation duration.

Seroka et al. (2024) provide a comprehensive review that investigates the promising arena of biochar, an ecologically sustainable material garnering significant interest for its prospective application as a potassium ion anode within battery systems. The transformative potential of biochar via various modifications, particularly emphasizing atomic doping as a means to enhance electrochemical performance. This category of materials not only demonstrates efficient energy conduction capabilities but also an augmented capacity for potassium storage.

Supporting the principles of the circular economy, a promising strategy for mitigating the environmental repercussions associated with polyethylene terephthalate (PET), a widely produced and utilized polymer, is presented by Bhanderi et al. (2024). Their proposed methodology encompasses a microwave-assisted recycling protocol, concentrating on the aminolysis of PET waste to formulate polyurethane acrylate (PUA) coatings. This process employs substituted  $\beta$ -hydroxy amines for the chemical depolymerization of PET waste, utilizing a sodium acetate catalyst. The initial phase accomplishes effective depolymerization of PET within a brief timeframe, culminating in the production of terephthalimide diols. This environmentally sustainable approach facilitates the synthesis of a diverse array of diol monomers with customizable organic structures that are conducive to PUA UV-curable coatings.

**RNA Interference (RNAi):**

RNA interference (RNAi) is a natural process that organisms use to silence specific genes, essentially turning off endogenous genes when they are not needed or degrading genes of

invading pathogens. RNAi is a molecular switch that can shut down unwanted or dangerous processes within cells. In a study, researchers explored using RNAi to target and disable essential *C. zeina* genes. Scientists create double-stranded RNA (dsRNA) molecules that match the nucleotide sequence of a target gene. These dsRNA molecules are taken up by the cells of a pathogen such as *C. zeina* when dsRNA is sprayed onto infected maize leaves in a method known as spray-induced gene silencing. Inside the fungus, the dsRNA binds to the messenger RNA (mRNA) of the target gene and triggers a pathway that cuts up the mRNA, preventing it from producing essential proteins. This process inhibits fungal growth, protecting the maize plants. Scientists around the globe have demonstrated this type of proof of concept against a range of fungal pathogens, most notably those that infect leaves.

The next phase will be product development to overcome several challenges, such as producing large amounts of the dsRNA cheaply, adding stabilising agents such as nanoparticles to prolong the “shelf-life” of the dsRNA on plant surfaces in the field, and optimising the dsRNA targets. An important promise of this technology is the reduced risk of pathogens developing resistance to dsRNA fungicides since multiple genes can be targeted together. Furthermore, several pathogens can be targeted simultaneously with multiple dsRNAs.

### **Integrated Pest Management (IPM):**

**Holistic Strategy:** The amalgamation of green chemistry principles with Integrated Pest Management strategies culminates in a comprehensive approach that synergizes diverse control methods to curtail chemical application while sustaining agricultural productivity (Ayilara et al., 2024).

## **3. ARTIFICIAL INTELLIGENCE IN PLANT PATHOLOGY**

Digitalization has become one of agriculture’s most exciting frontiers through advances in application technology and data science. Artificial Intelligence (AI) is a core technology powering the digital transformation of agriculture, helping tackle climate change and ensure global food security. AI is revolutionizing plant disease management by enabling data-driven, predictive, and real-time solutions (Figure 1). Agriculture leverages AI technologies like machine learning (ML), computer vision, and data analytics to improve various farming processes (Srivastava, 2025). It helps in precision farming, crop monitoring, pest detection, yield prediction, automated harvesting, and optimizing resource usage like water and fertilizers. AI enables farmers to make data-driven decisions, resulting in increased productivity, reduced costs, and more sustainable farming practices.

### **3.1 Disease Diagnosis**

Computer vision and deep learning models identify plant diseases using leaf images with high accuracy (Mohanty et al., 2016). Mobile apps and drones equipped with AI-powered sensors facilitate on-field early disease detection. Support Vector Machine (SVM) is frequently used for plant disease classification due to its high accuracy. For instance, SVM with RBF kernel achieved a 98.48% accuracy in classifying brinjal leaf diseases (Satya et al., 2023).

### **3.2 Epidemiological Forecasting**

AI integrates climate, soil, and crop data to predict disease outbreaks. Machine learning models such as Random Forest and Support Vector Machines have successfully forecasted rice blast and

late blight epidemics (Seelwal et al., 2024). Random Forest algorithm is valued for its robustness and ability to handle large datasets. It was used effectively in plant leaf disease detection, achieving a 79% accuracy in stem disease classification (Akbar et al., 2023). Decision Trees known for their simplicity and interpretability, are used in conjunction with other models like CNN for feature extraction and classification (Varshney et al., 2022). AI-powered platforms guide farmers on eco-friendly interventions by recommending the right treatment at the right time, thereby reducing pesticide overuse.

### 3.3 AI in Eco-Molecule Design

Machine learning accelerates virtual screening of bioactive molecules, predicting antifungal/antiviral activity, toxicity, and environmental impact before field deployment. For example, the Pesticide Discovery Artificial Intelligence (PDAI), is the first green pesticide molecular design technology platform in the world that combines high-performance computing and artificial intelligence. streamlines the innovation process, from target identification to the generation of viable pesticide candidates, optimizing key steps and simplifying the overall design workflow. The platform aims to accelerate the discovery of highly efficient and eco-friendly precursors, establishing a thorough and advanced research and development environment tailored for researchers across various expertise levels. This user-friendly platform significantly reduces the barriers for non-specialists, making the pesticide design process more accessible and cost-effective (Zhu et al., 2025).

### 3.4 Precision Agriculture

Precision agriculture, is an agricultural management approach that utilizes information technology to ensure crops and soil receive precise treatments for optimal health and productivity (Velusamy et al., 2022). Integrating drones, IoT, and AI for targeted interventions, minimizing chemical inputs for sustainable agriculture. This approach represents a major shift from traditional farming practices by incorporating advanced technologies such as AI to boost agricultural productivity and sustainability (Zhu et al., 2025). In precision agriculture, AI and ML-based surveillance systems offer valuable insights for monitoring crops, detecting pests, and diagnosing soil issues, helping farmers plant seeds at the ideal time for optimal yield. Weeds pose a significant threat to agriculture by reducing crop yields, invading plants, suffocating pastures, and, in rare cases, harming livestock. AI sensors can identify weed-infested areas and recommend the most effective herbicide for treatment. Additionally, AI systems can predict weather patterns, assess crop health, and identify issues like diseases, pests, or nutrient deficiencies. AI-powered drones allow farmers to monitor crop health, with experts analysing drone images to generate reports on the farm's condition, aiding pest control efforts. All-terrain vehicles (ATVs) are flexible and responsive platforms for incorporating new technology into farming operations, making them critical to the precision farming revolution (Roshanianfard et al., 2023). Some farmers are now employing agricultural robots to handle labor-intensive tasks, which helps reduce costs associated with manual labor and lightens workers' physical burden.

## 4. SYNERGY OF GREEN CHEMISTRY AND AI

The convergence of green chemistry and AI amplifies the sustainability of plant pathology, offering transformative potential. The principles of green chemistry align with sustainability objectives by decreasing carbon footprints and fostering circular resource utilization. Green

chemistry, as defined by Anastas and Warner (2023), focuses on designing chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

#### **4.1 AI-guided design of green molecules:**

AI-driven innovations are transforming sustainable plant protection by enabling the design and evaluation of next-generation, eco-friendly agrochemicals. AI-guided green molecule design allows researchers to predict the biological activity and safety profiles of novel bio-based pesticides even before laboratory synthesis. Smart nanocarriers, optimized through advanced algorithms, facilitate precision delivery of bioactive compounds by engineering nanoparticles for controlled release, enhanced stability, and minimal ecological impact. Eco-risk assessment models further strengthen sustainability by using machine learning to evaluate the toxicity, persistence, and environmental behaviour of new formulations before commercialization. Integrating climate-smart disease forecasting with environmentally benign bioformulations supports proactive and resilient plant health strategies. Additionally, virtual screening of phytochemicals enables AI to rapidly identify and rank plant-derived compounds with strong potential as biopesticides, expediting the discovery pipeline for green plant-protection solutions.

### **5. CASE STUDIES AND EXAMPLES**

#### **5.1 Trichoderma-Based Biocontrol Agents**

*Trichoderma spp.* are widely used as biocontrol agents. AI models have been used to optimize strain selection and application timing, improving efficacy against root rot and wilt pathogens (Lorito et al., 2010, Tripathi and Srivastava, 2025).

#### **5.2 Neem-Derived Formulations**

Neem oil and its major active compound, azadirachtin, derived from *Azadirachta indica*, are increasingly supported by AI-based toxicity prediction models for their safety and environmental compatibility (Isman, 2006). Azadirachtin (C<sub>35</sub>H<sub>44</sub>O<sub>16</sub>), a tetraterpenoid concentrated mainly in neem seeds, remains unsynthesized in laboratories and occurs alongside about 17 other limonoids, including salanine and melianrol. Known for its bitter and complex structure, azadirachtin acts as a repellent, feeding deterrent, growth regulator, oviposition inhibitor, and sterilizing agent, with effects varying across insect species. Today, neem-based commercial formulations—such as Neem Gold, Neemazal, Econeem, Neemark, Neemcure, and Azatin—are widely used across India, the United States, Germany, and several Latin American countries.

#### **5.3 Pyrethrum**

Pyrethrum, derived from the dried flowers of *Chrysanthemum cinerariaefolium*, is a natural insecticidal powder, with Kenya producing the majority of the global supply. The crude material contains six active compounds collectively known as pyrethrins—Pyrethrin I (C<sub>21</sub>H<sub>28</sub>O<sub>3</sub>), Pyrethrin II (C<sub>22</sub>H<sub>28</sub>O<sub>5</sub>), Cinerin I (C<sub>20</sub>H<sub>28</sub>O<sub>3</sub>), Cinerin II (C<sub>21</sub>H<sub>28</sub>O<sub>5</sub>), Cinerin III (C<sub>21</sub>H<sub>30</sub>O<sub>3</sub>), Jasmolin I (C<sub>21</sub>H<sub>30</sub>O<sub>3</sub>), and Jasmolin II (C<sub>22</sub>H<sub>30</sub>O<sub>5</sub>). These esters are formed through combinations of chrysanthemic and pyrethric acids with the alcohols pyrethrolone, cinerolone, and jasmolone. Pyrethrins act rapidly on insects by disrupting sodium and potassium ion exchange in nerve fibers, impairing normal nerve impulse transmission. This neurotoxic action triggers repetitive discharges, convulsions, and ultimately results in the characteristic rapid "knockdown" paralysis in target insects.

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**5.4 AI driven Enzymes**

Computational enzyme engineering represents a paradigm shift in how we approach chemical processes. By leveraging advanced molecular modeling, quantum chemistry, and artificial intelligence, we are creating high-performance enzymes that solve critical challenges across various industries, including pharmaceuticals, agriculture, energy, and specialty chemicals. Integration of computational biology, machine learning, and molecular simulation dramatically accelerate the discovery-to-deployment timeline for novel enzymes. This AI-driven enzyme design approach allows to engineer biocatalysts with unprecedented precision, enabling chemical transformations with higher selectivity, lower energy consumption, and significantly reduced environmental impact. Computational enzyme design has reduced waste in pharmaceutical production by up to 90% compared to traditional chemical synthesis methods.

**5.5 Disease Forecasting Models**

AI-based models predicting rice blast outbreaks in Asia have enabled timely application of biofungicides, reducing yield losses while minimizing chemical input (Kaundal et al., 2006). AI forecasting of rice blast, linked with eco-friendly fungicide application schedules help in sustainable Agriculture and a Sustainable future.

**6. CHALLENGES AND FUTURE DIRECTIONS**

Despite notable advancements, several challenges continue to impede large-scale adoption of these innovations. Economic constraints remain a major hurdle, as the development and deployment of green formulations and nanocarriers often involve high production costs. Limited AI literacy among smallholder farmers also restricts the effective use of advanced technologies in the field. Moreover, data limitations, particularly the scarcity of large, high-quality datasets, hinder the accuracy and reliability of AI-driven models. Additionally, regulatory barriers, including the absence of unified policies and frameworks for eco-friendly innovations, further slowdown the transition toward sustainable and technology-driven agricultural practices.

The integration of Artificial Intelligence (AI) and green chemistry offers a transformative pathway toward developing culturally contextualized and sustainable solutions for plant health management. Leveraging open-source AI platforms can democratize disease forecasting, making predictive tools accessible to farmers and researchers alike. Furthermore, fostering public-private partnerships can accelerate the development of affordable, eco-friendly innovations that align with both traditional wisdom and modern science. The combined application of CRISPR and AI technologies further enhances this approach by enabling the engineering of disease-resistant crops, while the use of green chemical formulations ensures environmental safety and long-term agricultural sustainability.

**7. CONCLUSION**

Looking ahead, AI-driven enzyme engineering holds immense potential to revolutionize industries and address pressing global challenges. In the area of carbon capture and utilization, researchers are developing enzymes capable of efficiently sequestering CO<sub>2</sub> and converting it into valuable chemicals, thereby contributing to climate change mitigation. In advanced materials science, enzyme-catalyzed synthesis is paving the way for the creation of novel materials such as self-healing polymers and bio-based electronics with exceptional functional properties. Similarly, in water treatment, engineered enzymes are demonstrating remarkable

potential in degrading persistent pollutants and microplastics, offering sustainable solutions to critical environmental problems. Beyond these industrial applications, the integration of AI and satellite technologies is also transforming agricultural practices, enabling smarter, data-driven, and sustainable farm management strategies for the future.

While the potential of AI-driven enzyme engineering is vast, it is equally important to ensure that its advancement is guided by responsibility, transparency, and collaboration. Ethical considerations should be prioritized by promoting the transparent and accountable use of AI throughout research and development processes.

Green chemistry and artificial intelligence represent complementary innovations for sustainable plant disease management. By designing eco-friendly compounds and harnessing predictive intelligence, these approaches can minimize chemical reliance, improve crop resilience, and contribute to food security. The future of plant pathology lies in this convergence where ecological safety, technological intelligence, and agricultural productivity meet.

The integration of green chemistry and AI in plant pathology marks a transformative step toward sustainable agriculture. Green chemistry offers eco-friendly molecules and formulations, while AI ensures precision and predictive intelligence. Together, they establish a climate-smart, resource-efficient, and farmer-friendly framework for crop protection. Future agricultural resilience will rely heavily on such eco-innovations, balancing productivity with ecological safety.

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