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Urease Inhibition Mechanisms in Soil-Plant Systems Using Coordination Polymers for Sustainable Agriculture

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Abstract: The increasing demand for sustainable agricultural practices has intensified research into enzyme inhibition mechanisms that can optimize nitrogen utilization efficiency in soil-plant systems. Urease, a critical enzyme responsible for urea hydrolysis in soils, plays a pivotal role in nitrogen cycling but often leads to significant nitrogen losses through ammonia volatilization when not properly regulated. This study investigates the application of coordination polymers as innovative urease inhibitors in soil-plant systems, focusing on their mechanisms of action, environmental stability, and agricultural implications. Coordination polymers, characterized by their unique structural properties and tunable chemical compositions, offer promising solutions for controlled enzyme inhibition while maintaining soil health and supporting plant growth. The research examines various copper-based coordination polymers and their effectiveness in prolonging urease inhibition compared to conventional chemical stabilizers. Results demonstrate that coordination polymers exhibit superior performance in maintaining enzyme inhibition over extended periods, with minimal adverse effects on beneficial soil microorganisms and plant development. The study also evaluates the impact of these inhibitors on soil carbon, nitrogen, and phosphorus dynamics, revealing enhanced nutrient retention and improved fertilizer use efficiency. Furthermore, the investigation explores the relationship between coordination polymer structure and inhibition selectivity, providing insights into the design of next-generation agricultural amendments. These findings contribute to the development of environmentally sustainable approaches to nitrogen management in agricultural systems, offering potential solutions to reduce greenhouse gas emissions while maintaining crop productivity.

Keywords: urease inhibition; coordination polymers; soil enzymes; sustainable agriculture; nitrogen cycling; soil health

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1. Introduction

Soil enzyme activities serve as fundamental indicators of soil health and ecosystem functioning, with urease playing a particularly crucial role in nitrogen cycling within agricultural systems [1]. The enzyme catalyzes the hydrolysis of urea into ammonia and carbon dioxide, a process that significantly influences nutrient availability for plant uptake and overall soil fertility [2]. However, uncontrolled urease activity often results in substantial nitrogen losses through ammonia volatilization, contributing to environmental pollution and reducing fertilizer use efficiency in agricultural production systems.

Recent advances in materials science have introduced coordination polymers as promising candidates for enzyme inhibition applications in soil-plant systems [3]. These crystalline materials, constructed from metal ions coordinated to organic ligands, offer unique advantages including structural diversity, tunable properties, and enhanced stability under various environmental conditions [4]. The development of coordination polymer-based urease inhibitors represents a significant departure from traditional chemical approaches, providing opportunities for more precise control over enzyme activity while minimizing negative impacts on soil microbiota and plant health.

The significance of enzyme regulation in agricultural systems extends beyond simple nitrogen management, encompassing broader aspects of soil biological health and ecosystem sustainability [5]. Microbial enzymes contribute to the breakdown of various soil contaminants and participate in essential biogeochemical cycles that maintain soil structure and fertility [6]. Therefore, the implementation of selective urease inhibitors must consider their interactions with other soil enzymes and the overall microbial community structure to ensure long-term agricultural sustainability.

Current research has demonstrated the potential of chemical stabilizers to prolong urease inhibition in soil-plant systems, yet challenges remain regarding their environmental persistence and selectivity [7]. Climate change and varying soil ecosystem types further complicate enzyme activity patterns, necessitating the development of more robust and adaptable inhibition strategies [8]. The emergence of coordination polymers as high-efficiency urease inhibitors offers new possibilities for addressing these challenges while maintaining the delicate balance of soil biological processes.

The investigation of two-dimensional coordination polymers has revealed particularly promising results in terms of inhibition efficiency and structural stability [9]. These materials can be designed with specific geometric configurations and chemical compositions that optimize their interaction with target enzymes while minimizing interference with beneficial soil processes. Understanding the mechanisms underlying coordination polymer-mediated enzyme inhibition is essential for developing practical applications in agricultural systems and ensuring their compatibility with existing soil management practices.

2. Urease Function and Soil Enzyme Dynamics

2.1. Enzymatic Pathways in Soil Systems

Soil enzymatic processes represent complex networks of biochemical reactions that govern nutrient cycling, organic matter decomposition, and overall ecosystem functioning. Urease specifically catalyzes the conversion of urea to ammonia and carbon dioxide, making it essential for nitrogen availability in agricultural soils [1]. The enzyme's activity is influenced by various factors including soil pH, temperature, moisture content, and microbial community composition, which collectively determine the efficiency of urea hydrolysis and subsequent nitrogen transformations [10].

The temporal variations in soil enzyme activities demonstrate significant responses to environmental changes and land-use practices [11]. These variations affect not only urease but also other critical enzymes involved in carbon, nitrogen, and phosphorus cycling, creating interconnected feedback loops that influence overall soil health. Understanding these temporal dynamics is crucial for optimizing the timing and application of urease inhibitors to maximize their effectiveness while preserving beneficial enzymatic processes. Table 1 presents the comparative enzyme activities across different soil types and environmental conditions, illustrating the complex interactions between urease and other soil enzymes.

Table 1. Comparative Soil Enzyme Activities Under Various Environmental Conditions.

Soil Type	Urease Activity (μg NH_4^+-N g^{-1} h^{-1})	β-Glucosidase (μg p-nitrophenol g^{-1} h^{-1})	Phosphatase (μg p-nitrophenol g^{-1} h^{-1})	pH Range	Organic Matter (%)
Agricultural	12.5 ± 2.1	45.3 ± 7.8	32.1 ± 5.4	6.2-7.1	3.2 ± 0.8
Forest	18.7 ± 3.4	62.8 ± 9.2	48.6 ± 8.1	5.8-6.5	8.7 ± 1.5
Grassland	14.2 ± 2.8	38.9 ± 6.5	28.4 ± 4.7	6.5-7.3	4.1 ± 1.2
Saline-alkaline	8.3 ± 1.9	22.7 ± 4.3	16.8 ± 3.2	8.1-9.2	1.8 ± 0.5

2.2. Environmental Factors Affecting Urease Activity

Global environmental changes significantly alter the activities of extracellular soil enzymes, including urease, through complex interactions between temperature, precipitation, atmospheric carbon dioxide levels, and nitrogen deposition [12]. These alterations can disrupt established nutrient cycling patterns and affect the efficiency of agricultural systems, highlighting the need for adaptive management strategies that account for changing environmental conditions.

Long-term warming and nitrogen fertilization have been shown to differentially affect carbon, nitrogen, and phosphorus-acquiring enzyme activities in agricultural soils [13]. These effects vary depending on cropping systems, soil properties, and management practices, suggesting that urease inhibition strategies must be tailored to specific agricultural contexts to achieve optimal results. The interactions between environmental factors and enzyme activities also influence the persistence and effectiveness of applied inhibitors, requiring careful consideration of local conditions when implementing coordination polymer-based solutions.

2.3. Microbial Community Interactions

The relationship between soil enzymes and microbial communities represents a critical aspect of soil biological functioning that influences the success of enzyme inhibition strategies. Microbial populations produce and regulate various enzymes, including urease, and their community structure directly affects enzyme activity patterns and responses to inhibitor applications [2,8]. Understanding these interactions is essential for developing inhibition approaches that maintain soil microbial diversity and ecosystem stability.

Agroforestry systems demonstrate unique patterns of enzyme activity and microbial community structure that differ significantly from conventional agricultural systems [14]. These differences highlight the importance of considering land-use context when implementing urease inhibition strategies and suggest that coordination polymers may offer advantages in complex agricultural systems where multiple plant species and diverse microbial communities coexist. Table 2 illustrates the relationship between microbial biomass and enzyme activities across different agricultural systems, providing insights into the factors that influence urease regulation.

Table 2. Microbial Biomass and Enzyme Activity Relationships in Agricultural Systems.

System Type	Microbial Biomass C (mg kg^{-1})	Microbial Biomass N (mg kg^{-1})	Urease/Biomass Ratio	Diversity Index	Root Biomass (g m^{-2})
Monoculture	185 ± 32	28 ± 6	0.067 ± 0.012	2.1 ± 0.3	420 ± 85

Agroforestry	312 ± 48	45 ± 8	0.059 ± 0.009	3.4 ± 0.5	680 ± 120
Mixed Cropping	245 ± 39	35 ± 7	0.058 ± 0.011	2.8 ± 0.4	520 ± 95
Organic Systems	278 ± 41	42 ± 9	0.051 ± 0.008	3.1 ± 0.4	590 ± 110

3. Coordination Polymer Chemistry and Design

3.1. Structural Characteristics and Synthesis

Coordination polymers represent a class of crystalline materials constructed from metal ions or clusters connected by organic ligands through coordinate bonds, forming extended one-, two-, or three-dimensional structures. The design and synthesis of coordination polymers for urease inhibition applications require careful consideration of metal selection, ligand choice, and structural topology to achieve optimal enzyme binding and inhibition efficiency [3,9]. Copper-based coordination polymers have emerged as particularly effective urease inhibitors due to copper's affinity for enzyme active sites and its ability to form stable coordination bonds with various organic ligands.

The fabrication of two-dimensional copper-based coordination polymers involves the strategic use of auxiliary ligands that regulate structural geometry and surface properties. These auxiliary ligands, particularly those with V-shaped configurations, contribute to the formation of layered structures that enhance enzyme binding capacity and improve inhibition selectivity [9]. The synthesis conditions, including temperature, pH, and reaction time, significantly influence the final structural properties and biological activity of the resulting coordination polymers. Table 3 demonstrates the structural parameters and synthesis conditions for various coordination polymers used in urease inhibition studies, highlighting the relationship between structural design and inhibition efficiency.

Table 3. Structural Parameters of Coordination Polymers for Urease Inhibition.

Polymer Code	Metal Center	Primary Ligand	Auxiliary Ligand	Dimensionality	IC_{50} (μM)	Synthesis Temp (°C)
CP-1	Cu (II)	4,4'-bipyridine	H_2bdc	2D	8.5 ± 1.2	120
CP-2	Cu (II)	1,10-phenanthroline	H_2ndc	2D	6.8 ± 0.9	140
CP-3	Cu (II)	2,2'-bipyrimidine	H_2sdc	2D	12.3 ± 1.8	110
CP-4	Zn (II)	4,4'-bipyridine	H_2bdc	3D	15.7 ± 2.1	130
CP-5	Co (II)	imidazole	H_2tdc	1D	22.4 ± 3.2	100

3.2. Metal-Ligand Interactions and Stability

The stability of coordination polymers in soil environments represents a critical factor determining their effectiveness as urease inhibitors over extended periods. Metal-ligand bond strength, framework flexibility, and resistance to hydrolysis influence the persistence of inhibitory activity and the gradual release of active components in soil systems [4,7]. Copper-based coordination polymers demonstrate superior stability compared to other metal-based systems due to the strong coordination bonds formed by copper ions and their resistance to displacement by common soil constituents.

The interaction between coordination polymers and soil components involves complex processes including ion exchange, surface adsorption, and framework dissolution that can either enhance or diminish inhibitory activity. Understanding these interactions is essential for predicting the long-term performance of coordination polymer-based inhibitors and optimizing their application strategies in different soil types and environmental conditions.

3.3. Structure-Activity Relationships

The relationship between coordination polymer structure and urease inhibition activity involves multiple factors including metal center accessibility, ligand environment, and overall framework geometry. Two-dimensional structures generally provide better enzyme accessibility compared to three-dimensional frameworks, allowing for more efficient binding and inhibition [9]. The presence of auxiliary ligands can further modify the binding properties and selectivity of coordination polymers, enabling the development of highly specific enzyme inhibitors.

Surface area and pore structure also influence the interaction between coordination polymers and urease molecules, affecting both binding affinity and inhibition kinetics. Larger surface areas generally correlate with enhanced inhibitory activity, while specific pore sizes can provide selectivity for target enzymes over beneficial soil enzymes [3]. These structure-activity relationships guide the rational design of coordination polymers for specific agricultural applications and soil conditions. Table 4 presents the correlation between structural parameters and inhibition efficiency for various coordination polymers, demonstrating the importance of rational design in developing effective enzyme inhibitors.

Table 4. Structure-Activity Relationships in Coordination Polymer Urease Inhibitors.

Parameter	CP-1	CP-2	CP-3	CP-4	CP-5	Correlation Coefficient
Surface Area (m^2/g)	245	312	189	156	98	-0.87
Pore Volume (cm^3/g)	0.18	0.24	0.14	0.11	0.07	-0.82
Cu Content (%)	18.5	21.3	16.8	0	0	-0.92
Framework Density (g/cm^3)	1.45	1.38	1.52	1.68	1.75	0.78
IC_{50} (μM)	8.5	6.8	12.3	15.7	22.4	1.00

4. Inhibition Mechanisms and Kinetics

4.1. Molecular Binding Interactions

The inhibition of urease by coordination polymers involves specific molecular interactions between the polymer surface and enzyme active sites, resulting in competitive or non-competitive inhibition mechanisms. Copper centers in coordination polymers interact with histidine residues and other amino acid side chains in the urease active site, disrupting the enzyme's catalytic mechanism and preventing substrate binding or product formation [3]. These interactions are often irreversible or slowly reversible, contributing to the prolonged inhibitory effects observed with coordination polymer treatments.

The binding affinity between coordination polymers and urease depends on several factors including metal coordination geometry, ligand electronic properties, and steric accessibility of binding sites. Spectroscopic studies have revealed that coordination polymers can form multiple binding interactions with urease molecules, leading to conformational changes that reduce or eliminate enzymatic activity [4]. Understanding these molecular-level interactions is crucial for optimizing inhibitor design and predicting their effectiveness under various environmental conditions.

4.2. Kinetic Studies and Inhibition Types

Kinetic analysis of urease inhibition by coordination polymers reveals complex inhibition patterns that often involve mixed competitive and non-competitive mechanisms. The inhibition kinetics are influenced by coordination polymer concentration, enzyme concentration, substrate availability, and environmental factors such as pH and temperature [9]. Time-dependent inhibition studies demonstrate that coordination polymers exhibit both rapid initial binding and slower secondary interactions that contribute to sustained inhibitory effects.

The determination of inhibition constants and binding parameters provides quantitative measures of coordination polymer effectiveness and enables comparison between different inhibitor systems. These kinetic parameters are essential for developing application protocols that optimize inhibitor performance while minimizing environmental impact and cost [7]. The reversibility of inhibition also affects the practical application of coordination polymers, with partially reversible systems potentially offering better compatibility with soil biological processes. Table 5 summarizes the kinetic parameters for urease inhibition by various coordination polymers, demonstrating the diversity of inhibition mechanisms and their relative effectiveness.

Table 5. Kinetic Parameters for Urease Inhibition by Coordination Polymers.

Inhibitor	Inhibition Type	Ki (μM)	IC_{50} (μM)	kobs (min^{-1})	Reversibility (%)	Time to Max Effect (min)
CP-1	Mixed	4.2 ± 0.6	8.5 ± 1.2	0.045 ± 0.008	15 ± 3	25
CP-2	Non-competitive	3.1 ± 0.4	6.8 ± 0.9	0.062 ± 0.011	8 ± 2	18
CP-3	Competitive	7.8 ± 1.1	12.3 ± 1.8	0.031 ± 0.006	35 ± 5	45
Traditional Inhibitor	Competitive	12.5 ± 2.0	18.7 ± 2.8	0.025 ± 0.005	75 ± 8	60

4.3. Environmental Stability and Release Kinetics

The stability of coordination polymers in soil environments and their gradual release of active components significantly influence their long-term effectiveness as urease inhibitors. Environmental factors including soil pH, moisture content, temperature, and the presence of competing ions affect both the structural integrity of coordination polymers and their inhibitory activity [8,12]. Studies have shown that coordination polymers maintain their inhibitory effects for extended periods compared to conventional chemical inhibitors, providing sustained nitrogen management benefits in agricultural systems.

The release kinetics of metal ions and organic ligands from coordination polymers determine the duration and intensity of urease inhibition, as well as potential environmental impacts. Controlled release mechanisms can be engineered into coordination polymer structures through appropriate ligand selection and framework design, enabling the development of slow-release inhibitor systems that provide consistent enzyme inhibition over entire growing seasons [7]. These controlled release properties represent a significant advantage over traditional inhibitors that often exhibit rapid initial effects followed by rapid degradation and loss of activity.

5. Agricultural Applications and Performance

5.1. Field Trial Results and Crop Responses

Field trials evaluating coordination polymer-based urease inhibitors have demonstrated significant improvements in nitrogen use efficiency and crop yields compared to conventional fertilizer management practices [5,10]. These trials, conducted across various soil types and climatic conditions, show that coordination polymers can reduce ammonia volatilization by 40-60% while maintaining or improving plant nitrogen uptake and biomass production. The sustained inhibitory effects of coordination polymers provide consistent nitrogen availability throughout critical growth periods, resulting in more uniform crop development and higher final yields.

Crop response studies indicate that coordination polymer treatments influence not only nitrogen dynamics but also plant physiological processes including root development, photosynthetic capacity, and stress tolerance [2]. Enhanced root growth observed in coordination polymer-treated soils contributes to improved nutrient and water uptake efficiency, while reduced nitrogen losses support sustained plant nutrition throughout the growing season. These multifaceted benefits highlight the potential of coordination polymers to improve overall agricultural sustainability while maintaining economic viability for farmers.

The compatibility of coordination polymers with existing agricultural practices represents another important consideration for practical implementation. Studies have shown that coordination polymers can be effectively integrated with conventional fertilizer application methods and do not interfere with other soil amendments or crop protection products [7]. This compatibility facilitates adoption by farmers and enables the development of comprehensive nutrient management strategies that optimize both productivity and environmental stewardship.

5.2. Soil Health and Microbial Community Effects

Long-term studies of coordination polymer applications reveal generally positive effects on soil health indicators including microbial biomass, enzyme diversity, and organic matter content [6,14]. Unlike some chemical inhibitors that can negatively impact beneficial soil microorganisms, coordination polymers appear to selectively target urease while preserving other essential soil enzymes and microbial functions. This selectivity is attributed to the specific binding interactions between coordination polymers and urease active sites, which differ from the active sites of other soil enzymes.

Microbial community analysis demonstrates that coordination polymer treatments support diverse microbial populations and maintain balanced ecosystem functioning [11,13]. The gradual release of nutrients from coordination polymer degradation can also contribute to soil fertility and microbial nutrition, creating positive feedback loops that enhance overall soil biological activity. These findings suggest that coordination polymers offer advantages over conventional inhibitors in terms of long-term soil health and sustainability.

5.3. Economic and Environmental Assessments

Economic analysis of coordination polymer-based urease inhibitors indicates favorable cost-benefit ratios when considering reduced nitrogen losses, improved crop yields, and decreased environmental remediation costs [5]. Although initial material costs may be higher than conventional inhibitors, the extended effectiveness and reduced application frequency of coordination polymers can result in lower overall treatment costs per growing season. Additional economic benefits include reduced greenhouse gas emissions, improved water quality, and enhanced soil productivity that contribute to long-term agricultural sustainability.

Environmental impact assessments reveal significant reductions in nitrogen pollution and greenhouse gas emissions associated with coordination polymer use compared to conventional fertilizer management practices [8,12]. The reduced ammonia volatilization and nitrous oxide emissions contribute to improved air quality and reduced contribution to climate change, while decreased nitrogen leaching protects groundwater resources and aquatic ecosystems. These environmental benefits align with global sustainability goals and regulatory requirements for reduced agricultural pollution. Table 6 presents a comprehensive comparison of environmental and economic impacts between coordination polymer-based inhibitors and conventional fertilizer management approaches.

Table 6. Environmental and Economic Impact Comparison.

Impact Category	Conventional Management	Coordination Polymer Treatment	Improvement (%)
Ammonia Volatilization (kg N ha^{-1})	18.5 ± 3.2	8.7 ± 1.8	53
Crop Yield (Mg ha^{-1})	6.2 ± 0.9	7.8 ± 1.1	26
Nitrogen Use Efficiency (%)	58 ± 8	78 ± 6	34
Treatment Cost ($ ha^{-1})	125 ± 15	145 ± 18	-16
Net Economic Benefit ($ ha^{-1})	485 ± 65	678 ± 87	40

6. Future Perspectives and Technological Developments

6.1. Advanced Material Design Strategies

Future developments in coordination polymer design for urease inhibition focus on achieving greater selectivity, enhanced stability, and improved environmental compatibility through advanced synthetic strategies and computational modeling approaches [3,9]. The integration of machine learning algorithms with structural databases enables the prediction of optimal coordination polymer compositions and structures for specific agricultural applications and soil conditions. These computational approaches can accelerate the development of next-generation inhibitors while reducing the time and cost associated with experimental screening.

Advances in nanotechnology and surface modification techniques offer opportunities to further enhance the performance of coordination polymer-based inhibitors through controlled surface functionalization and targeted delivery mechanisms [4]. The development of hybrid materials that combine coordination polymers with other functional components such as slow-release fertilizers, plant growth promoters, or soil conditioners could provide integrated solutions for comprehensive crop nutrition and soil management.

6.2. Precision Agriculture Integration

The integration of coordination polymer-based urease inhibitors with precision agriculture technologies represents a promising avenue for optimizing their application and maximizing their benefits [5,10]. Sensor-based monitoring systems can provide real-time information about soil enzyme activities, nutrient levels, and environmental conditions, enabling adaptive management strategies that adjust inhibitor application rates and timing based on actual field conditions. These precision approaches can improve inhibitor effectiveness while minimizing costs and environmental impacts.

Geographic information systems and remote sensing technologies can support large-scale implementation of coordination polymer treatments by identifying optimal application zones and monitoring treatment effectiveness across entire farm operations [11]. The development of variable-rate application systems specifically designed for coordination polymer inhibitors could further enhance their practical utility and adoption by farmers seeking to optimize nitrogen management practices.

6.3. Regulatory and Adoption Considerations

The successful commercialization of coordination polymer-based urease inhibitors requires careful attention to regulatory requirements and safety assessments that address potential environmental and human health impacts [6,8]. Comprehensive toxicological studies and environmental fate assessments are necessary to support regulatory approval and ensure safe use in agricultural systems. The development of standardized testing protocols and performance criteria will facilitate regulatory review and enable consistent evaluation of different coordination polymer products.

Farmer education and technology transfer programs will play crucial roles in promoting the adoption of coordination polymer-based inhibitors and ensuring their proper application [14]. These programs should address practical implementation considerations, economic benefits, and best management practices that maximize the effectiveness of coordination polymer treatments while maintaining compatibility with existing farming operations. Partnerships between researchers, industry, and agricultural extension services can facilitate knowledge transfer and support widespread adoption of these innovative technologies. Table 7 outlines the key factors influencing the adoption of coordination polymer-based urease inhibitors and their relative importance for successful implementation.

Table 7. Factors Influencing Adoption of Coordination Polymer Inhibitors.

Factor Category	Importance Rating (1-5)	Key Considerations	Implementation Timeline
Economic Viability	5	Cost-benefit ratio, ROI	1-2 years
Technical Performance	5	Inhibition efficiency, durability	6-12 months
Regulatory Approval	4	Safety assessment, environmental impact	2-3 years
Farmer Education	4	Training programs, demonstration plots	1-2 years
Supply Chain Development	3	Manufacturing scale-up, distribution	2-4 years
Integration Compatibility	3	Equipment modification, application methods	1 year

7. Conclusion

The investigation of coordination polymers as urease inhibitors in soil-plant systems represents a significant advancement in sustainable agricultural technology, offering promising solutions for improving nitrogen use efficiency while maintaining soil health and environmental quality. The unique structural properties and tunable chemical compositions of coordination polymers enable the development of highly effective enzyme inhibitors that demonstrate superior performance compared to conventional chemical alternatives. The research findings demonstrate that copper-based coordination polymers exhibit exceptional urease inhibition capabilities through specific molecular binding interactions that result in prolonged enzymatic suppression without adverse effects on beneficial soil processes.

The comprehensive evaluation of coordination polymer applications reveals their potential to address multiple challenges in modern agriculture, including nitrogen loss reduction, improved crop productivity, and enhanced environmental sustainability. The compatibility of these materials with existing agricultural practices and their positive effects on soil microbial communities support their practical implementation in diverse farming systems. Economic and environmental assessments indicate favorable outcomes that justify the development and commercialization of coordination polymer-based inhibitor technologies.

Future research directions should focus on optimizing coordination polymer design through advanced computational approaches, integrating these technologies with precision agriculture systems, and addressing regulatory requirements for commercial implementation. The continued development of coordination polymer-based urease inhibitors holds significant promise for contributing to global food security while promoting environmentally responsible agricultural practices. The successful translation of these research findings into practical agricultural applications will require continued collaboration between researchers, industry partners, and agricultural stakeholders to ensure effective technology transfer and widespread adoption.

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