unstable quality of medicinally important compounds, but these opportunities create a parallel challenge of extracting meaningful patterns from massive datasets (Zhang et al., 2025). AI is well suited to this role because it can identify key biological components in biosynthetic systems and model metabolic behavior over time, thereby guiding experiments toward the most plausible regulatory bottlenecks (Chen et al., 2026).

The next stage is to embed AI into broader biotechnology pipelines rather than restricting it to post hoc analysis.In medicinal herb breeding, AI is already being positioned across multi-omics integration, synthetic biology, precision gene editing, trait optimization, and intelligent monitoring systems, suggesting a unified research architecture rather than isolated analytical tools. In parallel, AI and multi-omics are accelerating plant phenotype analysis, precision breeding, metabolite discovery, and quality control, which makes them increasingly relevant for medicinal plant experiments that seek simultaneous gains in growth performance and active compound output. Even so, integration with experimental biology will require stronger standards for interpretability and interdisciplinary design. Explainable AI is increasingly treated as necessary in natural product research, and meaningful feature design still depends on close collaboration among computational scientists, biologists, and medicinal chemistry specialists (Xue et al., 2022). Earlier computational reviews already suggested that AI shortens the time required for classical experimental strategies, but current evidence indicates that its real value lies in complementing rather than replacing wet-lab validation.

7.3 Future directions toward precision medicinal plant agriculture

The clearest future direction is toward precision medicinal plant agriculture, where sensing, automation, and data science are integrated to optimize both yield and phytochemical quality.Precision agriculture is defined as the coordinated use of sensors, machinery, information systems, and informed management to improve productivity under sustainable conditions, and medicinal plant systems are increasingly being drawn into this broader transition. For medicinal crops specifically, smart farming technologies already appear to improve yield, quality, and sustainability while supporting more consistent production under strict quality requirements (Khan et al., 2026). A major opportunity lies in connecting environmental control directly to biological mechanisms of compound formation. Precision irrigation, AI-driven nutrient management, and controlled-environment cultivation influence photosynthesis, nutrient uptake, stress response, and secondary metabolite biosynthesis, making them relevant not only for growth management but also for active compound optimization (Khan et al., 2026). More broadly, digital twin concepts suggest that real-time data, computational models, and simulation could eventually support continuous prediction of both plant growth and metabolite yield in medicinal plant production systems.

Another priority is the creation of multiscale breeding and management platforms. Conventional breeding struggles with polygenic regulation and the simultaneous optimization of multiple pharmacologically relevant traits across variable environments, whereas AI-based frameworks are beginning to address these combined constraints. A promising response is the proposed genotype-environment-management interactive platform, which explicitly targets data integration, model generalization, and environmental adaptation as linked problems rather than separate technical issues. For Zhejiang medicinal plants, future development will likely depend on building transparent, multiscale systems that connect cultivation, omics, and quality standardization.Recent reviews argue that stronger computational-experimental synergy and more transparent models are essential if AI is to mature into a reproducible discipline in medicinal plant science (Chen et al., 2026). At the same time, high-throughput omics integration is expected to strengthen understanding of environmental adaptation and chemical diversity, which is critical for region-specific precision cultivation and the discovery of improved medicinal plant resources (Zhang et al., 2025).

8 Conclusions

Computational approaches have made medicinal plant research more predictive by linking large, heterogeneous datasets to biologically meaningful outputs such as biosynthetic pathway reconstruction, regulator identification, and metabolic optimization). They have also broadened the analytical scope of the field beyond static screening, as molecular docking, dynamic simulation, and artificial intelligence now jointly support faster interpretation of phytochemical function and bioactivity than traditional experimental workflows alone.A second major