contribution is the integration of multi-source evidence across chemistry, plant organs, and environmental context, which improves medicinal plant quality evaluation and better reflects the ecological regulation of active compounds. At the molecular level, newer sequencing and transcriptome-based approaches have further enabled identification of genes, miRNAs, and biosynthetic pathways underlying medicinal compound formation, giving computational medicinal botany a stronger mechanistic basi. Computational methods have also contributed directly to phytochemical discovery and optimization. Machine learning combined with in vitro culture has been used to identify the major factors controlling phenolic compound biosynthesis and extraction, showing that computational models can guide bioactive compound production rather than only describe it.In parallel, AI-assisted metabolomics has expanded quality assessment, metabolite variation analysis, and early detection tasks, indicating that computational tools are becoming central to the full analytical pipeline of phytochemical research.

These contributions are not limited to medicinal plant cultivation but extend to drug discovery translation.In silico network analysis, screening, and pharmacokinetic prediction can prioritize active phytochemicals and clarify likely mechanisms before wet-lab validation, which reduces experimental burden and accelerates downstream pharmacological studies.More broadly, computational approaches are now treated as an initial key step in natural-product-based drug discovery, especially when integrated with experimental validation and modern AI methods. For sustainable cultivation, computational modeling enables site-specific decision making by connecting medicinal plant performance to soil, climate, and ecological conditions.Machine learning with GIS and soil analysis can rapidly map suitable planting areas and optimize cultivation practices, which is particularly useful for vulnerable or region-specific medicinal herbs. Spatial prediction studies further show that environmental variables can be ranked by their influence on secondary metabolite yield, allowing cultivation zones to be selected not only for survival or biomass, but also for high-value compound accumulation (Dastres et al., 2025). This has direct implications for resource conservation and regional quality management.In geo-authentic medicinal materials, ecological conditions strongly affect active ingredient accumulation, and machine learning models can forecast the geographic distribution of high-quality compounds more systematically than scattered field sampling alone. Cultivation verification studies confirm that combining field sampling, predictive simulation, and regional validation can identify optimal production areas while supporting sustainable utilization and industrial development.

Computational methods also strengthen quality control by shifting evaluation from single indicators toward integrated chemical and biological signatures. AI can correlate chemical fingerprints with documented efficacy, helping build a data-driven framework for standardization, clarification of material basis, and analysis of synergistic effects in complex medicinal systems. This is important because medicinal plant safety and efficacy depend on multi-component quality, while current quality evaluation still often overlooks variation across different medicinal parts. Sustainability also depends on the ability to adapt cultivation systems to climate change and anthropogenic disturbance.Ensemble modeling has shown that future suitable habitats for medicinal species can shift substantially under different emission scenarios, and species-specific barcoding can complement these predictions by improving germplasm identification for cultivation planning. At the production-system level, smart hydroponic and automated monitoring approaches suggest that data-driven cultivation can improve performance while enhancing sustainability, offering useful models for controlled medicinal plant production. The next stage of computational medicinal botany will likely be defined by multiscale integration.Systems biology frameworks increasingly combine co-expression analysis, regulatory network inference, graph-based learning, and explainable AI to generate interpretable predictions for complex traits and environmental responses. This trajectory is especially important for medicinal plants because future progress depends on bridging molecular networks with field-scale phenotypes across species and environments rather than analyzing each data layer in isolation.

A parallel frontier is the development of digital twin frameworks for medicinal plant agriculture. Digital twins can create real-time virtual replicas of crops or farms to support prediction and decision-making, with clear potential for optimizing irrigation, fertilization, pest management, and individualized cultivation strategies. Early agricultural digital twin work already shows that interactive, data-linked platforms can integrate multi-scale