4 Computational Analysis of Active Compound Accumulation Mechanisms

4.1 Biosynthetic pathways and regulatory networks of bioactive compounds

Computational analysis of active compound accumulation in Zhejiang medicinal plants begins with reconstructing biosynthetic pathways and the regulatory networks that control them.Recent reviews show that omics platforms now enable comprehensive mapping of biosynthetic pathways, regulatory circuits, and spatial chemical distributions, which has made pathway discovery in medicinal plants far more systematic than earlier gene-by-gene approaches (Latif and Nawaz, 2025). This is important because medicinal metabolites are produced through complex pathways whose full elucidation is necessary for predicting metabolic switches and building sustainable production strategies (Chen et al., 2026). A central advance has been the move from simple correlation to network-based inference of regulatory control. Multi-omics studies can link transcripts, metabolites, proteins, and chromatin features into layered networks that identify co-regulated genes and likely regulatory nodes, while newer AI-enabled approaches aim to infer missing links and pathway bottlenecks more directly. Evidence from medicinal plants supports this framework: transcriptomic analysis in *Cibotium barometz* identified tissue-specific key enzymes and transcription-factor correlations for lignin and flavonoid pathways, while integrated profiling in *Trichosanthes kirilowii* highlighted Tk_ERF4 and related regulators as coordinators of tissue- and stage-specific bioactive compound biosynthesis (Zhang et al., 2025; Gao et al., 2026).

4.2 Metabolomics and multi-omics integration for compound prediction

For compound prediction, metabolomics serves as the most direct layer because metabolites are the executors of gene function and the final products of pathway activity. Metabolomics combined with other omics can reveal metabolite-gene associations at the whole-genome level, identify enzymes that control production or transformation, and provide a systems-level basis for predicting which compounds accumulate in specific tissues or developmental stages. In medicinal plants, this integrated strategy is increasingly viewed as the most effective route to uncover complex specialized-metabolite pathways that cannot be resolved by single-omics data alone.

Prediction becomes more powerful when integration is spatiotemporal rather than static.Transcriptomics and metabolomics provide complementary information by associating temporal and spatial gene-expression patterns with metabolite abundance, and time-series regulatory analysis is especially useful for resolving dynamic pathway components (Singh et al., 2022). Recent medicinal-plant work confirms this value: integrated multiomics in *Trichosanthes kirilowii* resolved tissue-specific accumulation of cucurbitacin B, terpenoids, and flavonoids and identified the color-changing fruit stage as a critical window for secondary metabolism, while spatial multi-omics in other systems is expected to clarify synthesis, transport, and accumulation at cell-level resolution (Wu et al., 2025; Gao et al., 2026).

4.3 Environmental and agronomic regulation of active compound accumulation

Active compound accumulation is also shaped by environmental and agronomic regulation, so computational models must account for external drivers rather than treating metabolism as genetically fixed. Broad reviews show that secondary-metabolite accumulation responds strongly to light, temperature, soil water, fertility, salinity, and other environmental factors, and even a change in one factor can alter metabolite content under otherwise similar conditions (Pant et al., 2021). This sensitivity explains why prediction models for Zhejiang medicinal plants should incorporate field microclimate, soil status, and developmental context when estimating active compound accumulation.

Mechanistically, environmental regulation acts through stress and signaling networks that alter biosynthetic gene expression and metabolite flux. Stress conditions elevate reactive oxygen species, activate MAPK cascades, and trigger hormonal pathways involving salicylic acid, jasmonic acid, ethylene, and abscisic acid, which then regulate transcription factors and biosynthetic modules linked to specialized-metabolite accumulation. Light is one of the clearest examples: different light qualities, intensities, and photoperiods modulate pathway activity through photoreceptor-mediated signaling and circadian regulation, making light management a plausible lever for directed enhancement of medicinal compounds under controlled or precision cultivation systems (Wu et al., 2025).