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DockingDB, a powerful computational tool, is being launched to speed up research into plant hormones

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A research team has successfully created the 'DockingDB' online database, which is designed for the large-scale reverse virtual screening of plant hormones. It integrates over 5,700 experimentally elucidated plant-protein structures and can swiftly predict hormone–protein interactions. This achievement provides a powerful computational tool for the systematic analysis of the action network of plant hormones and the design of new plant growth regulators.

A retrospective on traditional approaches

The journey to understand plant hormone biosynthesis, transport, action, and degradation has been a story of painstaking discovery. The fundamental limitation of this 'one gene at a time' research paradigm is its high degree of dependence on chance. Researchers start from phenotype, locate mutations, and then identify genes; the entire process is akin to a process of elimination, and only in the most fortuitous cases can the gene be discovered by chance to be related to hormone signals. The randomness and uncertainty inherent in this method invariably result in a gradual progression. For this obvious reason, the path to discovering plant hormone signaling has been notoriously slow: over 60 years for auxin and 30 years to piece together brassinosteroid signaling[1].

From prediction to validation

The newly released DockingDB (https://cbi.gxu.edu.cn/DockingDB) enables a hypothesis-driven research approach by systematically predicting protein–hormone interactions[2]. Its value lies in integrating computational predictions with experimental validation. Researchers can query the database to rapidly identify potential hormone receptors or binding proteins, and then prioritize candidates by combining predicted binding affinity with empirical knowledge.

Following this, researchers can verify the limited number of high-priority candidates using established genetic and biochemical methods. This workflow can reduce the timeline for identifying novel hormone-binding proteins from years to months.

As a case in point, upon releasing DockingDB, the research team used it to predict the binding of AtPMT1 to cytokinin. Molecular dynamics simulations and subsequent microscale thermophoresis were then employed to confirm the interaction. This end-to-end process demonstrates a significantly higher screening efficiency compared to conventional, non-guided discovery efforts.

Potential impact on understudied hormones and crops

Almost every key agronomic trait in crops is associated with plant hormones, including their biosynthesis, transport, signaling, and degradation[3]. However, research on plant hormones in crops remains considerably behind that in the model plant Arabidopsis. Relying solely on knowledge transferred from Arabidopsis to crops is risky, given their differences in genome architecture and trait formation. Moreover, hormone studies in Arabidopsis itself still await further discovery.

While DockingDB can support prior research by highlighting previously overlooked factors, its greatest potential lies in advancing studies on under-explored non-model crops and newly identified bioactive molecules. The database offers a way forward by predicting interactions across diverse plant species and identifying conserved signaling modules that can be validated in tractable experimental systems.

For crop improvement, this approach can accelerate the identification of farmer-relevant traits. Rather than depending solely on mutation screening or extensive laboratory work, breeders can use the database to pinpoint genes that regulate stress responses, flowering time, plant architecture, and other important characteristics.

Conclusions and future perspectives

DockingDB builds on the rich legacy of plant hormone research, shifting the discovery paradigm from serendipity to systematic prediction. It leverages structural data—and future integration of the growing AlphaFold repository—to efficiently map hormone-protein interactions, a step beyond structure prediction alone. Future integration of predicted proteomes will greatly expand its utility for non-model species.

While computational predictions require experimental validation and have inherent limitations, the open-access platform is designed to evolve. It aims to augment, not replace, traditional biology by making validation more targeted and efficient. In facing global agricultural challenges, DockingDB bridges rigorous classical research with modern computational scale, offering a new path to decode plant signaling.

Conflict of interest

The authors declare that they have no conflict of interest

Dates

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