Molecular Determinants Elucidate the Selectivity in Abscisic acid Receptor and HAB1 Protein Interactions

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Jing-Fang Yang
Central China Normal University
ORCID: <https://orcid.org/0000-0002-3507-1664>

Chun-Yan Yin
Central China Normal University
ORCID: <https://orcid.org/0000-0002-1918-3367>

Di Wang
Central China Normal University
ORCID: <https://orcid.org/0000-0002-2080-0625>

Chen-Yang Jia
Central China Normal University
ORCID: <https://orcid.org/0000-0003-3731-3919>

Ge-Fei Hao
Central China Normal University

✉ gehao@mail.ccnu.edu.cn Corresponding Author

Guang-Fu Yang
Central China Normal University
ORCID: <https://orcid.org/0000-0003-4384-2593>

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Abstract

The abscisic acid (ABA), as a pivotal plant hormone, plays a key role in controlling the life cycle and adapting to the environmental stresses. The receptors of ABA are the Pyrabactin Resistance /Pyrabactin Resistance -Like/Regulatory Component of ABA Receptors (PYR/PYL/RCAR, PYLs for simplicity), which regulate the Protein Phosphatase 2Cs (PP2Cs) in the signal pathway. As an important ABA mimicking ligand, Pyrabactin shows the activation function to parts of members of PYLs, such as PYR1 and PYL1. Due to the antagonism of Pyrabactin to PYL2, it was used as a probe to discover a part of ABA receptors. Since then, many researchers have been trying to find out the determinants of the selective regulation of PYLs and PP2Cs interaction. However, the roles of residues on the selective regulation of PYR1/PYL2 and PP2Cs interaction induced by Pyrabactin are still ambiguous. This research investigated the selective activation mechanism of Pyrabactin through the sequence alignment, molecular docking, molecular dynamics simulation, and binding free energy calculation. Furthermore, the electrostatic and hydrophobic interaction differences induced by Pyrabactin and agonists were compared. The results indicate that Leu137/Val114, Ser85/Ser89, and Gly86/Gly90 from the pocket and gate of PYR1/PYL2 are the vital residues for the selective activation of Pyrabactin. Meanwhile, the electrostatic interaction between PP2Cs and PYLs complexed with agonists was improved. This mechanism provides strong support for the design of selective agonists and antagonists.

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