

Arvenin I の合成および機能解析に関する研究

Synthetic and Functional Investigation of Arvenin I

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研究成果概要

Arvenin I is a natural product belonging to the cucurbitacin family and is structurally defined as cucurbitacin B 2-O- β -D-glucoside. Recent work demonstrated that arvenin I activates T cells by covalently modifying the kinase MKK3 and activating the p38 MAPK signaling pathway, thereby improving mitochondrial function in exhausted T cells and enhancing antitumor immune responses.

In my project, cucurbitacin B, the aglycone of arvenin I, is used as a starting scaffold to design and synthesize arvenin-based derivatives in order to investigate the structure–activity relationships of this compound class.

The supercomputer resources were used for molecular docking simulations to evaluate potential interactions between these compounds and candidate protein targets. Docking studies were performed to predict possible binding modes and guide the design of derivatives.

Additionally, computational modeling was used to explore the possible cellular uptake mechanism of arvenin I derivatives. Because arvenin I contains a glucose moiety, it was hypothesized that the compound may enter cells through glucose transporters. To investigate this possibility, a homology model of a GLUT glucose transporter was generated using the supercomputer system.

Overall, the supercomputer resources were essential for supporting the computational analysis of ligand–protein interactions and transporter recognition, complementing the synthetic chemistry and biological evaluation.