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Paper Title: Design and Molecular Dynamics Simulation of Thieno-pyrimidine Derivative JAK3 Inhibitor

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## Abstract

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Protein kinase is a major class of intracellular signaling enzyme, described as important drug targets. Janus Kinase 3 (JAK3) is involved in immune signaling pathways that affect immune cell functions and have been considered as potential targets for cancer therapy. In this study, the effect of linker stereoisomer of newly designed JAK3 inhibitors was elucidated using the 10-ns molecular dynamics (MD) simulation. The obtained results revealed that (R)-stereoisomer had a better binding activity than (S)-stereoisomer.

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