

Usage Report for Fiscal Year 2023

**Project Title: Molecular dynamics simulations and structure modeling of biological macromolecules**

**Name:**

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1 . If no job was executed, specify the reason.

Our primary goal for this project is to develop and apply integrative approaches that combine molecular dynamics simulations with experimental data to gain a deeper understanding of the structure and dynamics of protein molecules. During the fiscal year, we gained access to external HPC resources and prioritized their use instead of dedicated infrastructure.