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Molecular dynamic simulation of space and earth-grown crystal structures of thermostable T1 lipase geobacillus zalihae revealed a better structure (Article)

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Abstract

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Less sedimentation and convection in a microgravity environment has become a well-suited condition for growing high quality protein crystals. Thermostable T1 lipase derived from bacterium Geobacillus zalihae has been crystallized using the counter diffusion method under space and earth conditions. Preliminary study using YASARA molecular modeling structure program for both structures showed differences in number of hydrogen bond, ionic interaction, and conformation. The space-grown crystal structure contains more hydrogen bonds as compared with the earth-grown crystal structure. A molecular dynamics simulation study was used to provide insight on the fluctuations and conformational changes of both T1 lipase structures. The analysis of root mean square deviation (RMSD), radius of gyration, and root mean square fluctuation (RMSF) showed that space-grown structure is more stable than the earth-grown structure. Space-structure also showed more hydrogen bonds and ion interactions compared to the earth-grown structure. Further analysis also revealed that the space-grown structure has long-lived interactions, hence it is considered as the more stable structure. This study provides the conformational dynamics of T1 lipase crystal structure grown in space and earth condition. © 2017 by the authors.

Author keywords

Geobacillus zalihae | Hydrogen bond | Ion interaction | Microgravity | Molecular dynamic simulation | T1 lipase

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