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Journal of Molecular Modeling
Volume 26, Issue 6, 1 June 2020, Article number 142

Comparative modelling studies of fruit bromelain using molecular dynamics simulation

(Article)

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Abstract

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Fruit bromelain is a cysteine protease accumulated in pineapple fruits. This proteolytic enzyme has received high demand for industrial and therapeutic applications. In this study, fruit bromelain sequences QIM61759, QIM61760 and QIM61761 were retrieved from the National Center for Biotechnology Information (NCBI) Genbank Database. The tertiary structure of fruit bromelain QIM61759, QIM61760 and QIM61761 was generated by using MODELLER. The result revealed that the local stereochemical quality of the generated models was improved by using multiple templates during modelling process. Moreover, by comparing with the available papain model, structural analysis provides an insight on how pro-peptide functions as a scaffold in fruit bromelain folding and contributing to inactivation of mature protein. The structural analysis also disclosed the similarities and differences between these models. Lastly, thermal stability of fruit bromelain was studied. Molecular dynamics simulation of fruit bromelain structures at several selected temperatures demonstrated how fruit bromelain responds to elevation of temperature.

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Prominence percentile: 96.166 ⓘ

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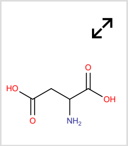

Author keywords

Comparative modelling | Cysteine protease | Fruit bromelain | MD simulation | Thermostability

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Chemicals and CAS Registry Numbers:

bromelain, 37189-34-7, 9001-00-7; papain, 9001-73-4

Funding details

Funding sponsor	Funding number	Acronym
Universiti Malaysia Pahang	RDU180345,PGRS180362	

Funding text

This research was supported by the Universiti Malaysia Pahang through research grants RDU180345 and PGRS180362.

ISSN: 16102940
CODEN: JMMOF
Source Type: Journal
Original language: English

DOI: 10.1007/s00894-020-04398-1
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< Back to results | 1 of 1

^ Top of page