FACULTY OF SCIENCE
CHIANG MAI UNIVERSITY

Title :   Molecular dynamics simulations on SARS-CoV-2 main protease enzyme catalysis

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Major :   Chemistry

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ABSTRACT

Currently, the virus responsible for causing COVID-19 (coronavirus disease starting in 2019) or SARS-CoV-2 enzyme remains a significant global health threat and has caused massive population deaths. SARS-CoV-2 M^{pro} (Main Protease) plays a crucial role in the viral replication process by cleaving polypeptides synthesized from the viral RNA to generate essential proteins for viral proliferation. Therefore, inhibiting the activity of SARS-CoV-2 M^{pro} is a key target in this study. As a result, the activity of SARS-CoV-2 M^{pro} is considered the most important target in this study. Thus, it is important to identify the factors affecting the activity of the enzyme to design effective enzyme inhibitors. First, This study began with the utilization of 3D structure of SARS-CoV-2 M^{pro} enzyme from the PDB code 2Q6G as the initial data NAMD program was employed in performing molecular dynamics simulations to investigate the dynamics of SARS-CoV-2 M^{pro} at different temperatures (300, 350, 400 and 450 K). The analyzed amino acid distances, RMSD, RMSF, hydrogen bonding analysis and solvent accessible

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surface area (SASA) that are important in the understanding of enzyme activity and the effects of conformational flexibility on enzyme catalysis. The results of the study showed that the mutant structure had a greater distance between the active site atoms and the substrate at all the simulation steps as compared to the wild type structure where at some simulation steps the active site atoms were closer to the substrate. Additionally, the wild type enzyme showed increased atomic movements with temperature. The RMSD values of the mutant structure supported the fact that it is able to retain the stability of structure at high temperatures. The hydrogen bond analysis also showed that there was a big difference in the hydrogen transfer efficiency between His41 and Ala41, which showed different bonding patterns. Across all temperature conditions, the mutant enzyme exhibited notable differences from the wild type, suggesting a potential reduction in its ability to break polypeptides. This finding implies that the mutant could hinder the viral replication process by limiting active-site reactivity, providing insights for the design of effective enzyme inhibitors or antiviral drugs targeting SARS-CoV-2 in future applications.
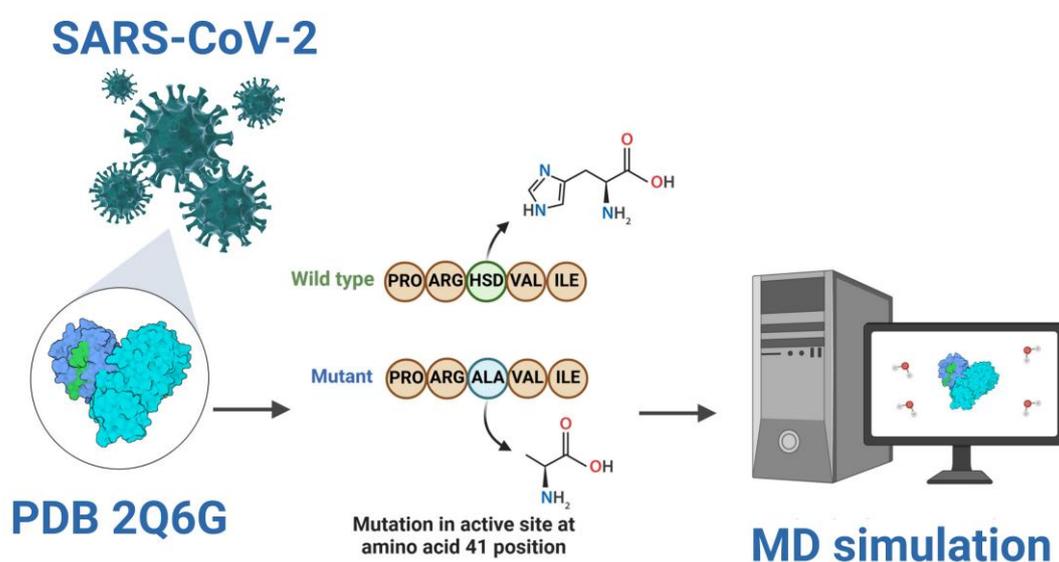
Title name guide.

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Microbiology	จุลชีววิทยา
Zoology	สัตววิทยา
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Physics	ฟิสิกส์
Computer Science	วิทยาการคอมพิวเตอร์
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