

พลวัตเชิงโมเลกุลของไดไฮโดรฟอสเฟตในมนุษย์

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**MOLECULAR DYNAMICS OF  
HUMAN DIHYDROFOLATE REDUCTASE**

**MISS ATCHARA WIJTKOSOOM**

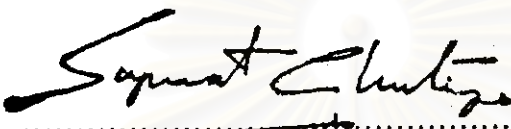
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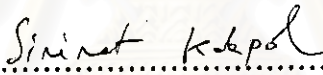
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พิมพ์ต้นฉบับบทความวิจัยนี้พร้อมกันในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว

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ในการศึกษานี้ ได้สร้างโครงสร้างทางพลศาสตร์ของเอนไซม์ในสารละลาย ณ อุณหภูมิ 300 เคลวิน และ 310.5 เคลวิน ผลของการศึกษาชี้ให้เห็นว่าโครงสร้างเฉลี่ยของเอนไซม์จากมนุษย์เปรียบเทียบกับได้กับโครงสร้างของคอมเพล็กซ์แบบไบนารีที่ได้จากการศึกษาด้วยเทคนิครังสีเอ็กซ์และเทคนิคนิวเคลียร์แมกเนติกส์เรโซแนนซ์ ณ อุณหภูมิ 298 เคลวิน สามารถสังเกตพบการขยายเพียงเล็กน้อยของโปรตีน การเปลี่ยนแปลงของโครงสร้างทุติยภูมิ การขาดของพันธะไฮโดรเจน และการเกิดพันธะไฮโดรเจนขึ้นมาใหม่ของบางส่วนโดยการนำเอาข้อมูลการศึกษาของรังสีเอ็กซ์และนิวเคลียร์แมกเนติกส์เรโซแนนซ์ของคอมเพล็กซ์แบบไบนารีระหว่างเอนไซม์-ลิแกนด์ เช่น โฟเลต และเมโททริเซทมาพิจารณา นอกจากนี้ การเปรียบเทียบของแบบจำลองโครงสร้างทางพลวัตระหว่างอุณหภูมิทั้งสองที่แตกต่างกันแสดงถึงความคล้ายในลักษณะของโครงสร้างทุติยภูมิแบบปกติและการม้วนงอของโปรตีน

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In this study, the dynamics structures of the enzyme in aqueous solution at 300 Kelvin and 310.5 Kelvin were obtained. The results indicate that the average structure of the human apo-enzyme from this study is comparable to the binary complex obtained from X-ray and nuclear magnetic resonance techniques studied at 298 Kelvin. Slight expansion of the protein, the changes of the secondary structure element, the disruption of hydrogen bonds and the formation of the new ones for some segments could be observed by taking the X-ray and the nuclear magnetic resonance studies of the binary enzyme-ligands, folate and methotrexate, complexes into consideration together with this study. Furthermore, comparisons of the simulated dynamics structures between the two different temperatures show their structural similarity in terms of the regular secondary structure and overall folding of the protein.

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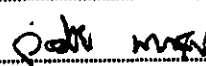
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