

สมบัติเชิงโครงสร้างและเชิงอิเล็กทรอนิกส์ของสารเชิงซ้อนดีเอ็นเอ-เอโรแมติกโครโมฟอร์แบบอินเตอร์คาเลต
: การศึกษาโดยวิธีกลศาสตร์ควอนตัมร่วมกับพลวัตโมเลกุล



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STRUCTURAL AND ELECTRONIC PROPERTIES OF DNA-INTERCALATED AROMATIC
CHROMOPHORE COMPLEXES: A COMBINED QUANTUM MECHANICS AND
MOLECULAR DYNAMICS STUDY

Miss Parawan Chuichay

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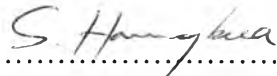
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Thesis Co-advisor Professor Dr. Notker Rösch


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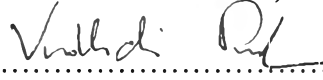
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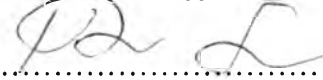
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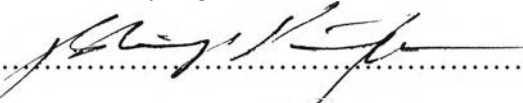
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ภาควิชา ๖๖๖ : สมบัติเชิงโครงสร้างและเชิงอิเล็กทรอนิกส์ของสารเชิงซ้อนดีเอ็นเอ-เอโรแมติกโครโมฟอร์แบบอินเตอร์คาลาต: การศึกษาโดยวิธีกลศาสตร์ควอนตัมกับพลวัตโมเลกุล. (STRUCTURAL AND ELECTRONIC PROPERTIES OF DNA-INTERCALATED AROMATIC CHROMOPHORE COMPLEXES: A COMBINED QUANTUM MECHANICS AND MOLECULAR DYNAMICS STUDY) อ.ที่ปรึกษา : ศ. ดร. สุพจน์ หารหนองบัว, อ.ที่ปรึกษาร่วม PROF DR. NOTKER RÖSCH , 156 หน้า. ISBN 974-53-2496-5

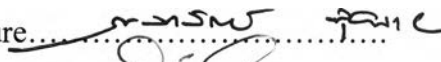


การคำนวณทางกลศาสตร์ควอนตัม และแบบจำลองพลวัตเชิงโมเลกุลถูกนำมาใช้ในศึกษาสมบัติทางโครงสร้าง และทางอิเล็กทรอนิกส์ของสารเชิงซ้อนดีเอ็นเอ อินเตอร์คาลาตเอโรแมติกโครโมฟอร์ ในขั้นแรกได้ศึกษาสเปกตรัมเชิงอิเล็กทรอนิกส์ของโครโมฟอร์ซึ่งได้แก่ สารอะครีดิน และอนุพันธ์ของอะมิโนอะครีดิน ไพโรนีน 6จี และโรดามีน 6จี ในสถานะแก๊ส และในสารละลาย โดยใช้ระเบียบวิธีเคมีเอ็มพีริกัลแบบ เอ็นดีดีโอ-จี และเอเอ็ม1 และระเบียบวิธีทางกลศาสตร์ควอนตัมแบบ ทีดี ดีเอฟที ผลจากการคำนวณพบว่าพลังงานการดูดกลืนของอะครีดิน และอนุพันธ์อะมิโนอะครีดิน มีค่าสอดคล้องกับผลการทดลองและผลการคำนวณที่มีความแม่นยำสูง ในขณะที่พลังงานของโรดามีน 6จี ค่าจากการคำนวณสูงกว่าจากการทดลอง พบว่าสเปกตรัมการดูดกลืนจะเปลี่ยนแปลงเมื่อทำการศึกษาในสารละลาย นอกจากนี้ได้ศึกษาแบบจำลองพลวัตเชิงโมเลกุลของไพโรนีน 6จี แคตไอออนไดเมอร์ และ โรดามีน 6จี แคตไอออนไดเมอร์ ในสารละลาย ผลจากการศึกษาพบว่าโครงรูปของไพโรนีน 6จี และโรดามีน 6จี มีการหมุนไปมาได้ง่าย นอกจากนั้นยังพบว่าแรงไฟฟ้าสถิตระหว่างตัวทำละลาย และสารละลาย มีส่วนสำคัญอย่างยิ่งที่ทำให้โครโมฟอร์เสถียรอยู่ได้ งานวิจัยในส่วนสุดท้ายได้จำลองพลวัตโมเลกุลเพื่อศึกษาสมบัติทางโครงสร้าง และพลวัตของสารเชิงซ้อนอนุพันธ์โรดามีน 6จี กับดีเอ็นเอ สามระบบ ซึ่งการวางตัวของโครโมฟอร์สัมพันธ์กับเบสคู่กันของดีเอ็นเอมีความยืดหยุ่นมาก นอกจากนี้ยังพบว่าการมีอันตรกิริยาแบบสแตกกิ้ง กับโครโมฟอร์ มีผลกระทบน้อยมากบนเบสลำดับที่สองและสาม

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KEY WORD: CHROMOPHORE / DNA / RHODAMINE / MD / SIMULATION
 PARAWAN CHUICHAY: STRUCTURAL AND ELECTRONIC
 PROPERTIES OF DNA- INTERCALATED AROMATIC CHROMOPHORE
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The quantum mechanical calculations and molecular dynamic simulations were used to investigate the structural and electronic properties of DNA-Intercalated aromatic chromophore complexes. In the first step, electronic spectra of chromophores, acridine, aminoacridine derivatives, pyronine 6G and rhodamine 6G, were studied in gas phase and in aqueous solution using semiempirical, NDDO-G and AM1 and quantum mechanical methods, TDDFT. The calculated absorption energies of the acridine and aminoacridine derivatives agree well with the experiment and the high level of theory, while overestimates that of the rhodamine 6G the experimental value. Changes of the absorption spectra were observed when solvent effects were included. Then, molecular dynamics simulations on the dimers of the positively charged pyronine 6G and rhodamine 6G in aqueous solutions were carried out using newly generated force field parameters. It was found that monomers of pyronine 6G and rhodamine 6G easily undergo relative rotations. Moreover, stability of the dimer was observed to be obviously dominated by the electrostatic interaction between the solute and its aqueous environment. Finally, MD simulations were performed to study conformational features and dynamics of three complexes of rhodamine-6G derivative with DNA. Highly flexible of the chromophore orientations relative to guanine base of DNA was observed. Additionally, the stacking interaction with chromophore effects only slightly on the second and the third base pairs.

Department.....Chemistry.....Student's signature.....
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