

ชอลเวชันของบีตา-ดี-กลูโคซามีนในน้ำโดยวิธีมอนติคาร์โล

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SOLVATION OF β -D-GLUCOSAMINE IN WATER
BY MONTE CARLO METHOD

Mr. Khatcharin Siriwong

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science in Chemistry

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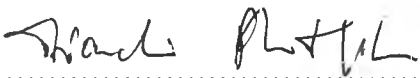
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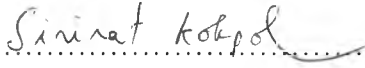
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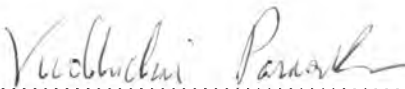
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คัชรินทร์ ศิริวงศ์ : ซอลเวชันของบีตา-ดี-กลูโคซามีนในน้ำโดยวิธีมอนติคาร์โล (SOLVATION OF β -D-GLUCOSAMINE IN WATER BY MONTE CARLO METHOD) อาจารย์ที่ปรึกษา : รศ. ดร. สุพจน์ ทารหนองบัว, 121 หน้า. ISBN 974-346-119-1.

ได้ทำการศึกษาหาโครงสร้างของสารละลายกลูโคซามีนที่อุณหภูมิ 25 องศาเซลเซียสโดยวิธีมอนติคาร์โลตามแบบของเมโทรโปลิส ระบบที่ศึกษาประกอบด้วยอนุภาคทั้งหมด 202 อนุภาค ได้แก่ กลูโคซามีน 1 โมเลกุลซึ่งวางอยู่ตรงกลางของกล่องลูกบาศก์ และน้ำ 201 โมเลกุล ค่าความหนาแน่นของน้ำจากการทดลองที่นำมาใช้มีค่า 1 กรัมต่อลูกบาศก์เซนติเมตร ความยาวของกล่องลูกบาศก์ซึ่งมีคุณสมบัติพีริออดิกมีค่าเท่ากับ 18.26 อังสตรอม ในการศึกษานี้ได้พัฒนาฟังก์ชันศักย์เพื่อแทนแรงกระทำระหว่างกลูโคซามีน-น้ำจากการคำนวณโดยวิธีดีเซดพีแอบ อินซิโอ ส่วนฟังก์ชันศักย์ที่แทนแรงกระทำระหว่างน้ำ-น้ำได้เลือกใช้ฟังก์ชันเอ็มซีวาย ผลการศึกษาพบว่าชั้นซอลเวชันแรกปรากฏที่ระยะ 4.6 อังสตรอม ห่างจากจุดศูนย์กลางของกลูโคซามีนซึ่งประกอบด้วยน้ำ 7 โมเลกุล ซึ่งพบว่าน้ำ 1 โมเลกุลอยู่ที่ระนาบของลิแกนด์ ในขณะที่อีก 2 และ 4 โมเลกุลอยู่ที่ระยะ 2 - 4 อังสตรอม เหนือและใต้ระนาบของลิแกนด์ตามลำดับ ในจำนวนน้ำทั้ง 7 โมเลกุล พบว่ามีเพียง 1 โมเลกุล ที่เกิดพันธะไฮโดรเจนแบบตรงกับอะตอมออกซิเจนที่อยู่ในวงของกลูโคซามีน นอกจากนี้ยังพบชั้นซอลเวชันที่สองซึ่งประกอบด้วยน้ำ 19 โมเลกุล อย่างชัดเจน

ภาควิชาเคมี.....
สาขาวิชาเคมี.....
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ลายมือชื่อนิสิต
ลายมือชื่ออาจารย์ที่ปรึกษา
ลายมือชื่ออาจารย์ที่ปรึกษาร่วม

4172237523 : MAJOR CHEMISTRY

KHATCHARIN SIRIWONG : SOLVATION OF β -D-GLUCOSAMINE IN WATER BY MONTE CARLO METHOD. THESIS ADVISOR : ASSOC. PROF. SUPOT HANNONGBUA, Ph.D. 121 pp. ISBN 974-346-119-1.

The solvation structure of glucosamine in aqueous solution at 25 °C has been investigated using the Metropolis Monte Carlo scheme. The system contains 202 rigid particles, including one glucosamine molecule, which fixed at the center of the cube, and 201 water molecules. An experiment density of 1 g.cm⁻³ of water was used, a periodic side length of 18.26 Å was yielded. A glucosamine-water potential function has been newly developed based on DZP *ab initio* calculations, while the MCY potential function was employed to describe water-water interactions. The first solvation shell appears at 4.6 Å from the center of glucosamine with the coordination numbers of 7 water molecules. The results indicate clearly that 1 water molecule lies in the ligand's plane while 2 and 4 water molecules are about 2 – 4 Å above and below the plane, respectively. Among the 7 water molecules, only that binding to ring oxygen atom displays linear H – bond. In addition, second solvation shell with contains 19 water molecules has been also clearly detected.

ภาควิชา เคมี
สาขาวิชา เคมี
ปีการศึกษา 2543

ลายมือชื่อนิสิต
ลายมือชื่ออาจารย์ที่ปรึกษา
ลายมือชื่ออาจารย์ที่ปรึกษาร่วม

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