

Biological macromolecular chemistry

2 units (selection)

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Target) The goal is to understand the structure and function of biological macromolecules from the perspective of molecular recognition and interaction.

Outline) How do biological macromolecules recognize the target molecule and function? An introduction to the basic structural biology and stereochemistry of biological macromolecules. Topics include protein and nucleic acid structure. Students should make presentations focusing the molecular recognition and interaction of biological macromolecules based on the PDB data and their recent scientific papers with molecular modeling software "MacroModel".

Style) Lecture

Keyword) *intermolecular interactions, molecular recognition, protein data bank, molecular modeling*

Fundamental Lecture) "Biomolecular Design"(0.5)

Relational Lecture) "Advanced Cell Physiology"(0.5), "Advanced enzyme engineering"(0.5)

Requirement) To understand the organic chemistry, medicinal chemistry, and the enzyme engineering

Notice) None

Goal)

1. To understand the principle of structure and function of biological macromolecule.
2. To understand the mechanisms of molecular recognition of biological macromolecule through PDB database search and molecular modeling software.

Schedule)

1. Orientation
2. Lecture 1: force interactions involved in the drug-protein complex
3. Exercise 1: search for a protein target for drug
4. Lecture 2: stereochemical interactions involved in the drug-protein complex
5. Exercise 2: search for 3D structures of targeting protein from the PDB
6. Lecture 3: mechanisms of enzyme catalysis
7. Exercise 3: conformational analysis of targeting protein
8. Lecture 4: drug design and drug action
9. Exercise 4: conformational analysis of drug

10. Lecture 5: Drug design with computational chemistry

11. Exercise 5: molecular modeling of drug

12. Lecture 6: Molecular modeling with MacroModel

13. Exercise 6: molecular modeling of protein

14. Exercise 7: molecular modeling of drug-protein complex

15. Exercise 8: evaluation of molecular modeling

16. Report

Evaluation Criteria) Only the student of the attendance rate 80% or more is evaluated by report(100%).

Textbook) R. B. Silverman; The ORGANIC CHEMISTRY of DRUG DESIGN and DRUG ACTION, ELSEVIER

Reference) T. L. Lemke, D. A. Williams, V. F. Roche, S. W. Zito; FOYE'S PRINCIPLES OF MEDICINAL CHEMISTRY, Lippincott Williams & Wilkins

Contents) <http://cms.db.tokushima-u.ac.jp/cgi-bin/toURL?EID=216730>

Student) Able to be taken by student of other department

Contact)

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Note) 授業を受ける際には、2時間の授業時間毎に2時間の予習と2時間の復習をしたうえで授業を受けることが、授業の理解と単位取得のために必要である。