

Biomolecular Design

2 units (selection)

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Target) 生体機能修飾物質 (特に生理活性物質や医薬品) の設計, 合成, 生物活性の基礎となる分子機能工学的概念としての “医薬品エレクトロニクス medicinal electronics” について講述する.

Outline) 分子機能工学に関する重要な基礎的な概念としての分子軌道論による生体機能修飾物質 (特に生理活性物質や医薬品) の生体機能分子設計について解説し, “医薬品エレクトロニクス medicinal electronics” 的思考力を向上させる.

Style) Lecture

Keyword) *biomolecular functional design, molecular orbital theory*

Relational Lecture) “**Biological macromolecular chemistry**”(0.5)

Goal)

1. 分子機能工学手法としての分子軌道論を理解し, 実際, Hückel 法を使ってエチレンからベンゼンまでの分子軌道を手計算で求める.
2. medicinal electronics 的思考力の向上のため, 簡単な生体機能修飾作用物質の分子軌道計算を実践し, それらの物性や生物活性を定量的に論じることにより, 分子軌道論の果実を味わう.

Schedule)

- 1.) Biomolecular (functional) design and the concept of molecular orbital
2. Enzymatic reaction and molecular orbital
3. Quantum theory-based atomic structure and molecular bonds
4. Molecular structures and the concept of hybridized orbitals. Subject review report-1
5. Heteroatom containing structures. Discussion on subject review report-1
6. Structures of intermediates. Subject review report-2
7. Molecular orbital calculation-1: localized π -bond. Discussion on subject review report-2
8. Molecular orbital calculation-2: localized π -bond. Subject review report-3
- 9.) Molecular orbital calculation-3: localized π -bond. Discussion on subject review report-3
10. Molecular orbital calculation-4: delocalized π -bond (butadiene)
11. Round-table discussion on subject review report-4
12. Molecular orbital calculation-5: delocalized π -bond (cyclobutadiene). Subject review report-5

13. Round table discussion on subject review report-5

14. Another biomolecular design concepts: scaffold or “Ken-zan”, pharmacophores, isosteres

15. Round table discussion on subject review report-6

16. Round-table discussion on this class “biomolecular design”

Evaluation Criteria) 課した全課題レポート (100%) で評価する. レポートはそれぞれ 100 点満点で評価し, すべてのレポートが 60 点以上の場合をもって合格とする.

Textbook) Katsuhiko Saito “KozoYukikagaku(in Japanese)(Structural Organic Chemistry)”(Sankyo-Syuppan) and CD-ROM “ WinMopac Version 3.0.3 (Trial) In Noriaki Hirayama, “Jissen Ryoshi-Kagaku (in Japanese: Practical Quantum Chemistry)”

Contents) <http://cms.db.tokushima-u.ac.jp/cgi-bin/toURL?EID=216878>

Student) Able to be taken by student of other department

Contact)

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Note) When you take this class, it is necessary to do preparation for 2h and review for 2h every 2h class for your understanding and taking credit.