UNIVERSITY of MISKOLC
Faculty of Materials and Chemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Molecular Design and Docking

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COURSE DESCRIPTION

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Molecular Design and Docking

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Lecturer

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Recommendation

The couse is proposed for all students of the Antal Kerpely Doctoral School, with a special focus on students interested in chemistry and computer simulations.

Language

English.

Scope

The main goal of the course is to provide students with an overview of molecular docking and to teach them how to utilize this technique in various applications, complementing experimental methods.

Methodology

The course is conducted through in-person lectures and practical sessions. The lectures and practices are structured to provide a comprehensive understanding of various molecular docking approaches. Students are then trained to apply these using various software packages, enabling them to apply their knowledge practically to systems of interest.

Topics

1. Molecular Docking.
2. Molecular Docking software packages.
3. Target identification and preparation.
4. Ligand preparation.
5. Applications in drug design.

References

Review papers in the topic such as:

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3151162/pdf/nihms-308746.pdf
https://www.nature.com/articles/s41598-023-40160-2
https://link.springer.com/article/10.1007/s00706-023-03076-1

Book in the topic:

Mohane S. Coumar (ed.): *Molecular Docking for Computer-Aided Drug Design Fundamentals, Techniques, Resources and Applications.* **2021** Academic Press (Elsevier) (ISBN: 978-0-12-822312-3)
https://www.sciencedirect.com/book/9780128223123/molecular-docking-for-computer-aided-drug-design.

Exam

Project work.

Complex exam questions

1. Define molecular docking!
2. Describe the two main steps of molecular docking, posing and scoring.
3. Explain the rigid-rigid, rigid-flexible, and flexible-flexible docking scenarios and point out their potential applicability.
4. What is „blind docking” and how does it work?
5. How to apply molecular docking in drug design? Notable examples!