| General Information | | | |
|---|---|---|---|
| **Course name** | Basics of Molecular Simulations | **ECTS Credits** | 4 |
| | | **Semester** | S |

## Aims

Introduction to the principles of computational simulations of biomolecular objects from point of view of complex IT application in practice.

## Content

Essential structural characteristics of biomolecules. Foldamers - the definition and its importance. Computational predictions of folding as optimization problem. Propagators - algorithms for the time evolution and their use in molecular dynamics. Monte Carlo methods - algorithms and parallelization. Computational challenges of biomolecular simulations - description of chemical reactions, free energy evaluation, protein folding. Simulations of rare events. Computational complexity, less traditional optimization techniques and heuristics.

## Assessment Methods and Criteria

Written test and elaboration of referate. Exam.

**Grading Scale (in %):**
A: 91% - 100%
B: 81% - 90%
C: 71% - 80%
D: 61% - 70%
E: 51% - 60%
F: 0% - 50%

**Grading System:**

The University recognises the following six degrees for the evaluation of the study results:

a) A – excellent (excellent results) (numerical value 1)

b) B – very good (above average results) (1.5)

c) C – good (average results) (2)

d) D – satisfactory (acceptable results) (2.5)

e) E – sufficient (results meet the minimum criteria) (3)

f) FX –failed (requires further work) (4)

## Bibliography


- Schlick, Tamar. Molecular Modeling and Simulation. 1st ed. Springer, 2002.

- Allen, M. P., and D. J. Tildesley. Computer Simulation of Liquids. Oxford University Press, USA, 1989.