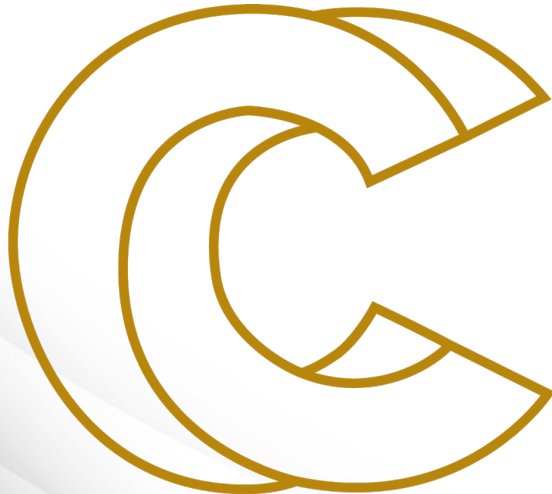




EURO^{4SEE}

Generating Mutant Protein Structures Using Advanced Techniques

Tandac Furkan Guclu

Sabancı University

Welcome to the Course



Meet the Instructor – Tandac Furkan Guclu

- BSc from Hacettepe University Biology Department
- MSc from Marmara University Bioengineering Department
- PhD from Sabancı University Molecular Biology, Genetics and Bioengineering Department
- Currently, works on biophysical basis of mutational effects in proteins

Preknowledge/Prerequisite(s)

- Experience with the terminal/command line
- Programming skills in Python
- Intermediate knowledge of protein structures and molecular dynamics simulations

*Molecular Dynamics Simulations of Small Molecules
course*

- Prologue – Why We Need to Understand Mutant Proteins
- Lecture 1 – Mutation and Minimization (MuMi) for Mutant Protein Design
- Lecture 2 – Free Energy Perturbation (FEP) for Mutant Structures and Relative Binding Energies
- Lecture 3 – Deep Learning Approaches for Mutant Structures

What this course is

In this course you will learn

- Structural basis of mutational changes
- Analysis of single-mutation landscapes
- Thermodynamic cycles and energetic costs of mutations
- High-throughput generation of mutant structures

What this course isn't

In this course you will NOT learn about

- Application of methods rather than their development
- Algorithm implementation and hard coding
- Quantum mechanical basis of free energy changes

Set Up/Configure/Install



Attendees are expected to use VMD, NAMD, Python, and the terminal.
All prerequisites were covered in the *Molecular Dynamics Simulations of Small Molecules* course.

Thanks!



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