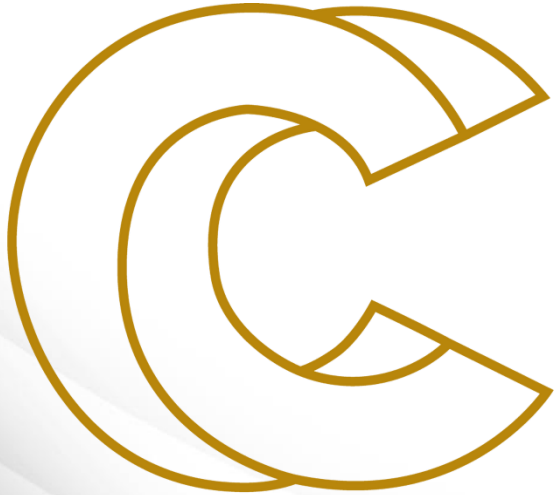
Sabancı Üniversitesi

TÜBİTAK



EURO 4SEE

Residue Networks: Understanding the Time Evolution and Mutations of Proteins from a Graph Theoretical Perspective

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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 terminal/command line
- General understanding of molecular dynamics simulations and protein structures
- Programming skills in Python.
- ‘Molecular Dynamics Simulations of Small Molecules’ course

Course Overview

- Lesson 1: Introduction to graphs and measures
- Lesson 2: Proteins as graphs and residue networks
- Lesson 3: Time evolution of residue networks and communities

What this course is

In this course you will learn

- Brief introduction to graph theory and its measures
- Construction of residue networks
- Relationship between graph theoretical measures and protein dynamics

What this course isn’t

In this course you will NOT learn about

- Principles of molecular dynamics simulations covered in the *Molecular Dynamics Simulations of Small Molecules* course
- Focus restricted to graph measures
- Implementation exclusively in Python

Set Up/Configure/Install

Attendees expected to install and configure

- Nanoscale Molecular Dynamics (NAMD) and Visual Molecular Dynamics (VMD) software
- A favorite text editor such as Sublime text, Notepad++…
- Anaconda package manager with networkx, jupyter lab, prody, matplotlib and numpy packages

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Thanks!

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