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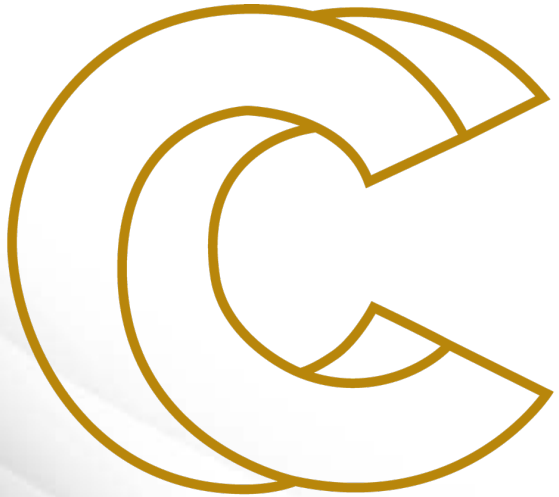

EURO^2

Molecular Dynamics Simulations of Small Molecules

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 organic chemistry
- Basic programming skills in Python.

What you will learn

- Performing and analysis of Molecular Dynamics simulations of butane, pentane and multiple-ethane molecules
- The basics of Molecular Simulation software — NAMD (Nanoscale Molecular Dynamics) —
- Conducting analyses such as torsion angle, potential of mean force, pairwise distance and diffusion coefficient calculation by using python programming language in jupyter lab

Course Overview

The course will be conducted in an applied manner

- Lesson 1 – Molecular Dynamics simulation of butane and analysis of torsion angle
- Lesson 2 – Molecular Dynamics simulation of pentane and calculation Potential of Mean Force
- Lesson 3 – Molecular Dynamics simulations of multiple ethane molecules in water box and calculation of diffusion coefficient

What this course is

In this course you will learn

- Basics of Molecular Dynamics simulation and its analyses
- An in-depth information of force-fields
- Computing energy surface of a small molecule
- Bonded and non-bonded interactions that govern dynamics

What this course isn’t

In this course you will NOT learn about

- Quantum Mechanics/Molecular Mechanics calculations
- Comparison of different force-fields and Molecular Dynamics software
- Only python programming language will be used
- Complex molecules (proteins, large polymers)

Introduction and 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 jupyter lab, prody, matplotlib and numpy packages

Thanks

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