EURO²

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İTÜ Faculty of Computer and Informatics Engineering

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Welcome to the Course

Asst.Prof Sefer BADAY

- İTÜ Faculty of Computer and Informatics Engineering
- Artificial Intelligence and Data Engineering

Preknowledge/Prerequisite(s)

- Basic knowledge in molecular docking

- Familiarity with Linux/Unix operating systems

- Basic programming skills in Python

- Basic Knowledge in slurm job submission etc on a HPC

What you will learn

How to perform high troughput virtual screening of a large molecule library using AutoDock Vina program on a HPC center.

Course Overview

- Molecular docking is one of the very standart way of finding a candidate molecule for a target of interest

- Huge chemical libraries or databases available

- For example ZINC20 database contains 230 million ready-to-dock molecules

- With this course you will be able to screen large molecule libraries.

What this course is

- Preparing input files for AutoDock Vina program to be executed simulataneously on multiple computing nodes

- Analysis and merge the docking results
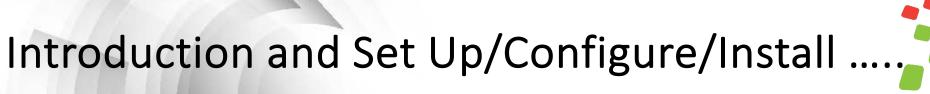
What this course isn't

- About teaching the basics of molecular docking

Lessons

- Lesson1: Preparing PDBQT file for protein
- Lesson2: Preparing PDBQT files for a libray of molecules
- Lesson3: Distributing docking calculations to multiple jobs
- Lesson4: Analyzing and cleaning the output files

Introduction and Set Up/Configure/Install …..

- Obtaining Vina executable file from https://vina.scripps.edu/downloads/

- An access to a HPC

Thanks