

İTÜ



# C EURO<sup>2</sup>

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# Welcome to the Course



***Asst.Prof Sefer BADAY***

- ITÜ 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 throughput virtual screening of a large molecule library using AutoDock Vina program on a HPC center.***

# Course Overview



- Molecular docking is one of the very standard 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 simultaneously on multiple computing nodes
- Analysis and merge the docking results

# What this course isn't



- About teaching the basics of molecular docking

- 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



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