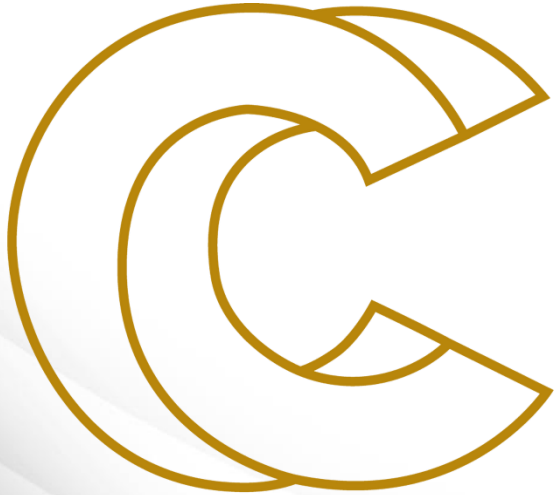

EURO 4SEE

MM/GB(P)SA free energy calculations using various programs

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Welcome to the Course

Assoc.Prof Sefer BADAY

- İTÜ Informatics Institute Applied Informatics Department
- Research focus is discovering novel drug molecules using molecular modeling, molecular dynamics simulations and artificial intelligence tools

Preknowledge/Prerequisite(s)

- Basic knowledge in Molecular Dynamics simulations
- Familiarity with Linux/Unix operating systems
- Basic Knowledge in slurm job submission etc on a HPC
- General knowledge in MM/GB(P)SA calculations

Course Overview

- MM/PBSA: Molecular mechanics/Poisson−Boltzmann surface area
- MM/GBSA Molecular mechanics/Generalized-Born surface area

very popular binding free energy calculations

gmx_MMPBSA: a new tool to perform end-state free energy calculations with GROMACS

MS Valdés-Tresanco, ME Valdés-Tresanco, PA Valiente, E Moreno

Journal of chemical theory and computation, 2021 · ACS Publications

> Molecular mechanics/Poisson–Boltzmann (Generalized-Born) surface area is one of the most popular methods to estimate binding free energies. This method has been proven to balance accuracy and computational efficiency, especially when dealing with large systems. As a result of its popularity, several programs have been developed for performing MM/PB(GB)SA calculations within the GROMACS community. These programs, however, present several limitations. Here we present gmx_MMPBSA, a new

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MMPBSA.py: An Efficient Program for End-State Free Energy Calculations

BR Miller III, TD McGee Jr, JM Swails… - Journal of chemical …, 2012 - ACS Publications

… Before describing the capabilities of **MMPBSA.py**, we will briefly review the theory and … that **MMPBSA.py** can perform. First, we will describe the general workflow for using **MMPBSA.py** …

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The **MM/PBSA** and MM/GBSA methods to estimate ligand-binding affinities

S Genheden, U Ryde - Expert opinion on drug discovery, 2015 - Taylor & Francis

… The **MM/PBSA** approach Here, we will describe the **MM/PBSA** approach as it was originally defined by Kollman et al. Citation[7,8]. Since then, the method has been developed and …

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Course Overview

- Lesson1: MM/PBSA calculation using CaFE (NAMD)
- Lesson2: MM/GB(P)SA Using AmberTools (Amber)
- Lesson3: MM/PBSA calculation using gmx_MMPSA (Gromacs)

What this course is

- About how to perform MM/GB(P)SA calculations on HPC

What this course isn’t

- About details of theory behind MM/GB(P)SA calculations
- Which one should preferred? MM/GBSA or MM/PBSA

Introduction and Set Up/Configure/Install .....

- VMD
- CaFE
- AmberTools
- MMPBSA.py
- Gmx_MMPBSA

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Thanks!

Co-funded by
the European Union

EuroHPC
Joint Undertaking

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101191697. The JU receives support from the Digital Europe Programme and Germany, Türkiye, Republic of North Macedonia, Montenegro, Serbia, Bosnia and Herzegovina.