GraphPro

MD ANALYSIS
UGM 2023

A python framework for protein deep geometrical learning

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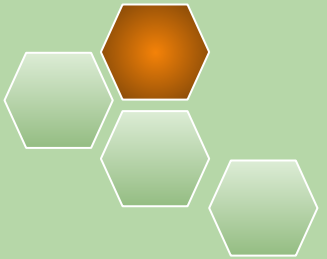


Allostery pocket detection

Our ongoing work

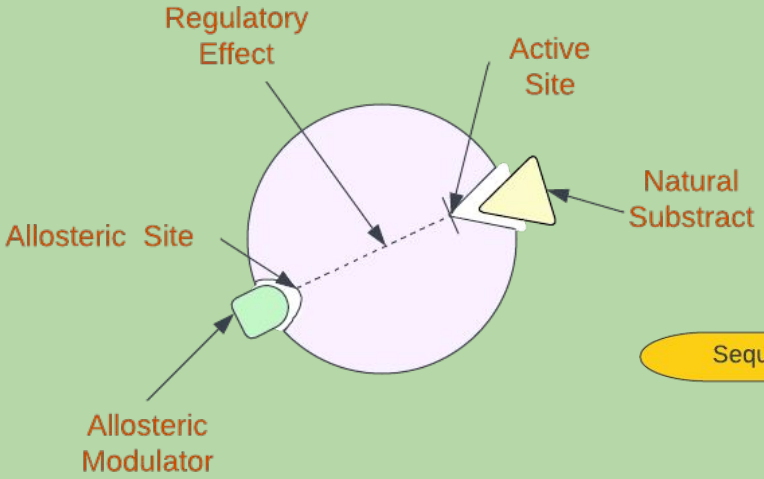
Graph representation

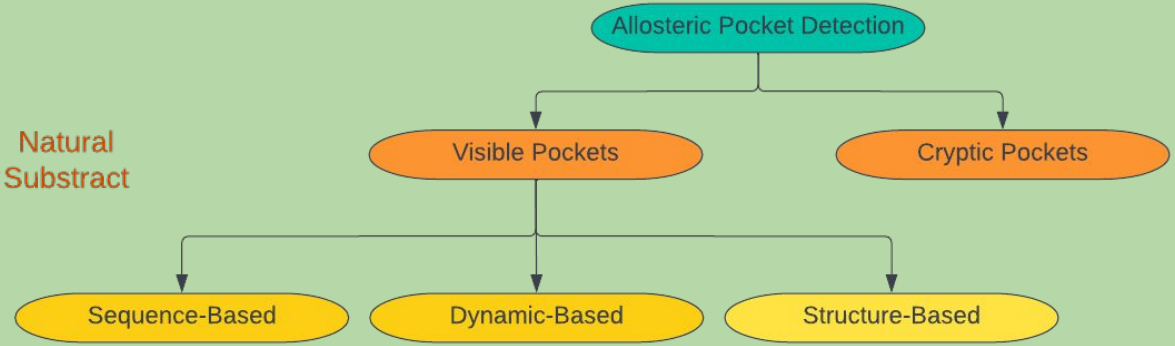
Our machine learning approach

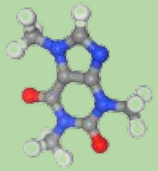
GraphPro Framework

Our solution for complex representational learning component

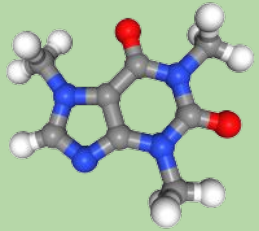
Allostery pocket detection

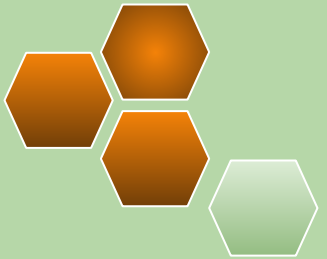






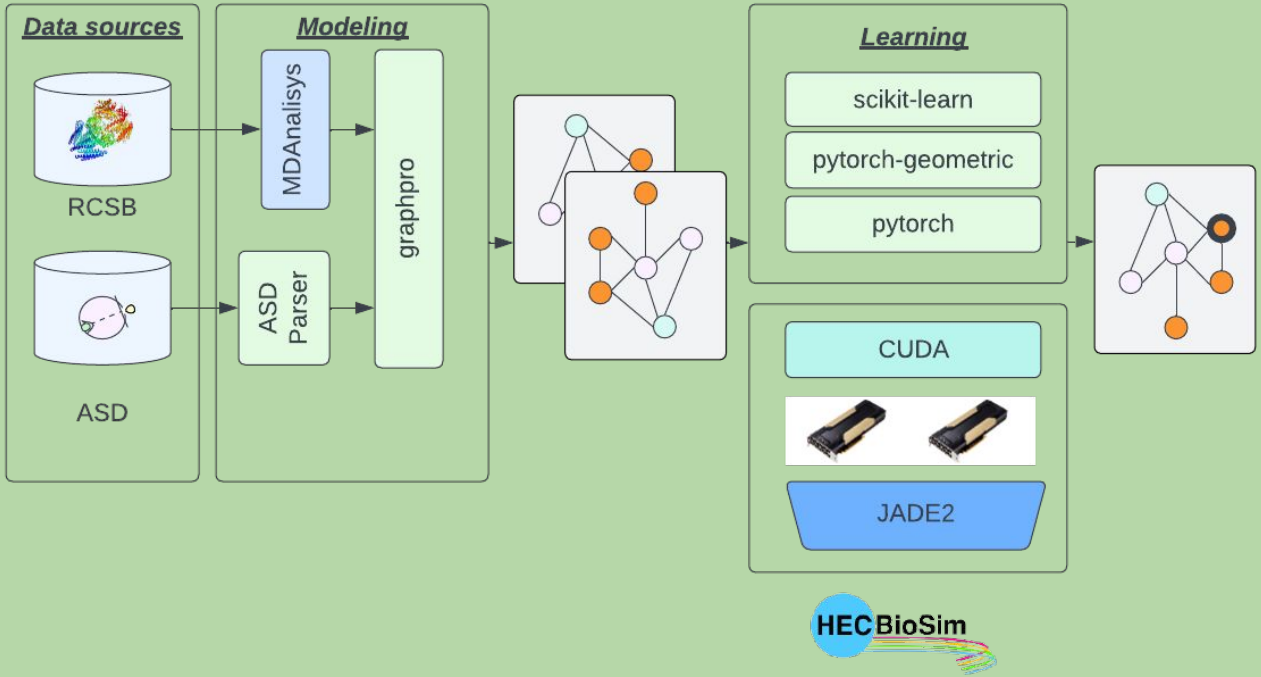
Graph Representation



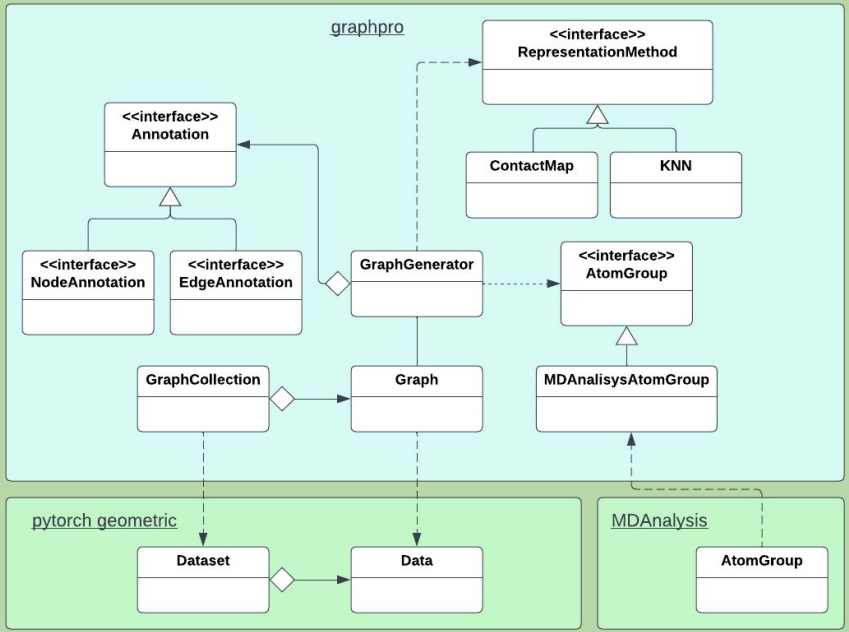


The Protein Data Bank (2000) Nucleic Acids Research. http://rcsb.org

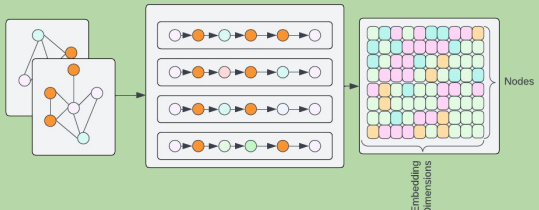
ASD: a comprehensive database of allosteric proteins and modulators. Nucleic Acids Res. 2011 Jan;39

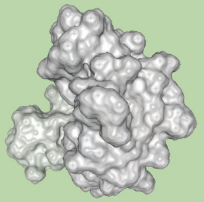


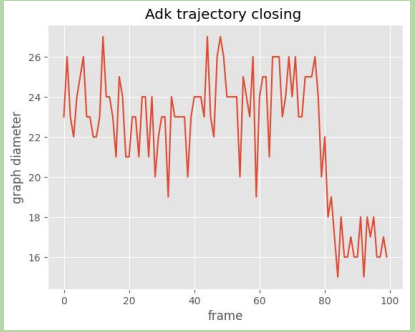
GraphPro Framework




```python
# pip or conda install
pip install graphpro
conda install -c conda-forge graphpro

import graphpro as gp
from graphpro.graphgen import ContactMap

# Transform trajectory to a collection of graphs
graph_gen = gp.md_analisys(u)
trajectory_graphs = graph_gen.generate_trajectory(ContactMap(cutoff=6))

# Diameter calculation
diameter_in_frame = [approximation.diameter(graph.to_networkx())
 for graph in trajectory_graphs]
```







Demo

https://tinyurl.com/grahprodemo

Project

https://github.com/pegerto/grahpro

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