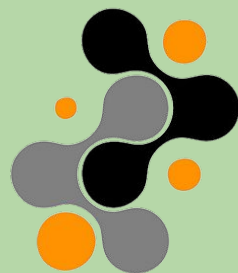
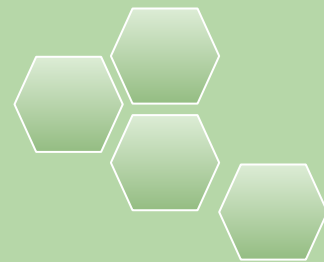


GraphPro



MD
ANALYSIS
UGM 2023



A python framework for protein deep geometrical learning

Fernández P, Dantu, S.C, Pandini. A.
Brunel University London



Brunel
University
London



Allosteric pocket detection

Our ongoing work



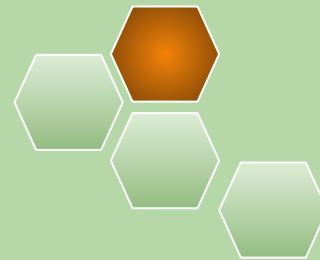
Graph representation

Our machine learning
approach



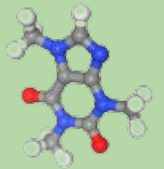
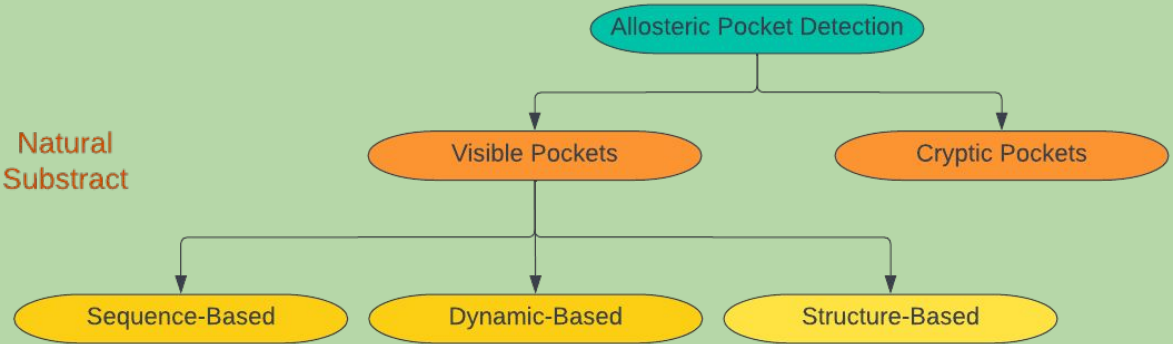
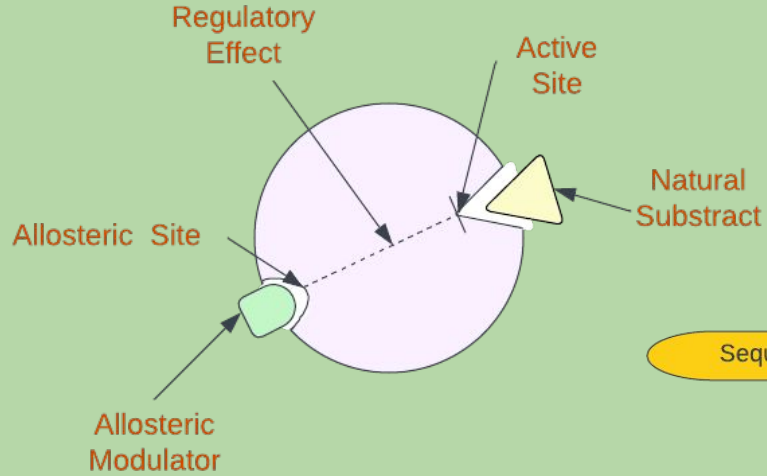
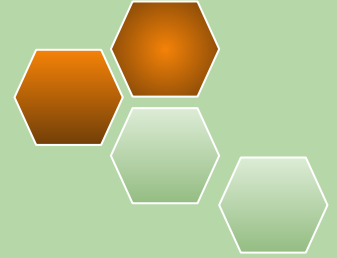
GraphPro Framework

Our solution for complex
representational learning
component



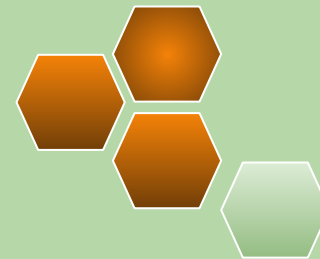
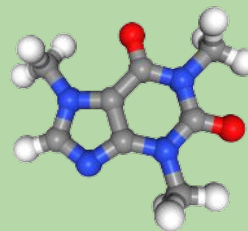


Allosteric pocket detection



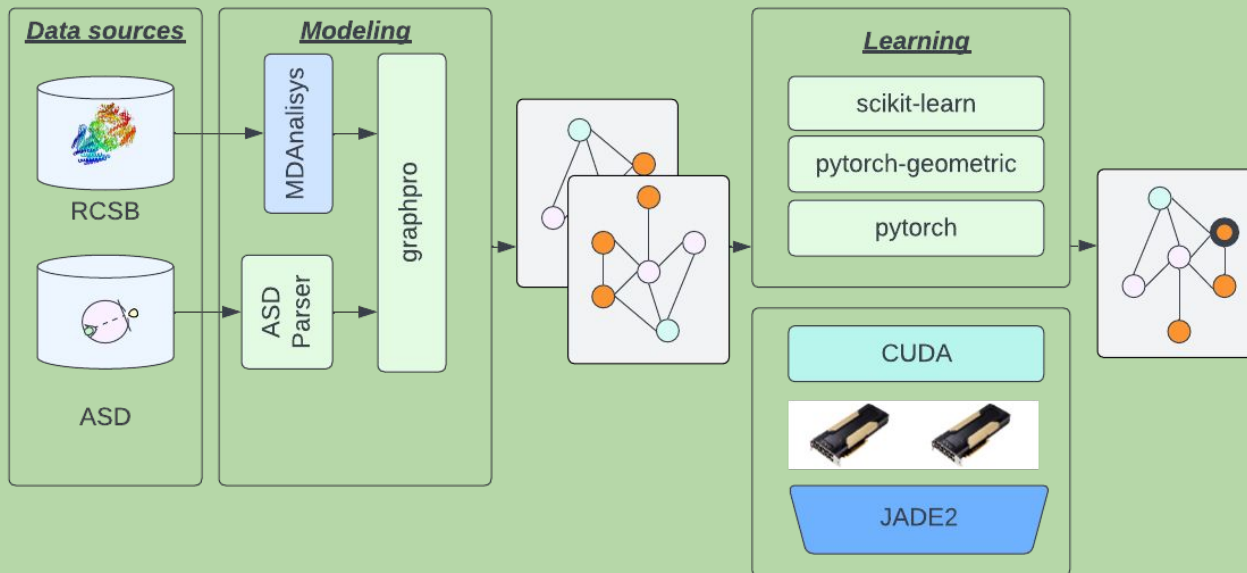


Graph Representation



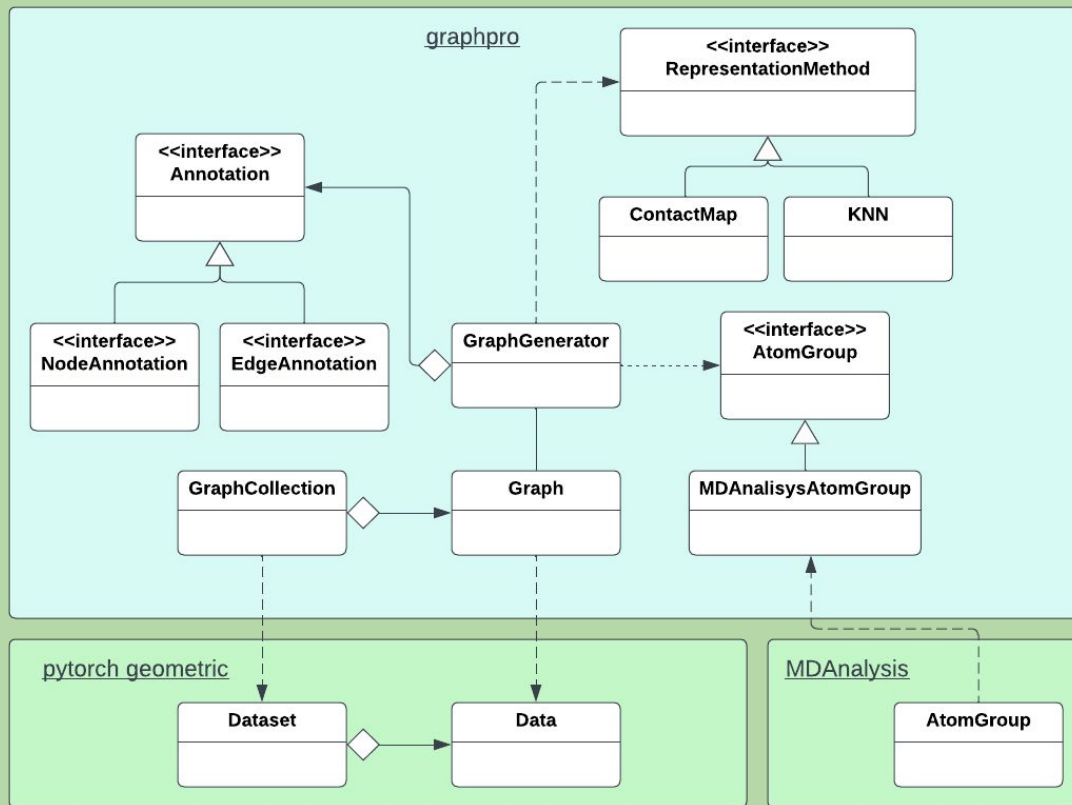
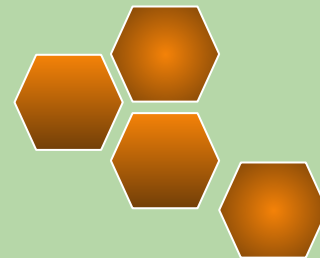
The Protein Data Bank
(2000) Nucleic Acids
Research.
<http://rcsb.org>

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





GraphPro Framework



```
import graphpro as gp
from graphpro.graphgen import ContactMap
```

```
graph_gen = gp.md_analisis(u)
graph = graph_gen.generate(ContactMap(cutoff=8))
graph.plot()
```

Demo



<https://tinyurl.com/grahprodemo>

Project



<https://github.com/pegerto/grahpro>

Pegerto Fernandez
Computational Biology Group
pegerto.fernandez@brunel.ac.uk

