DockNmine, a web portal to assemble and analyse virtual and experimental interaction data

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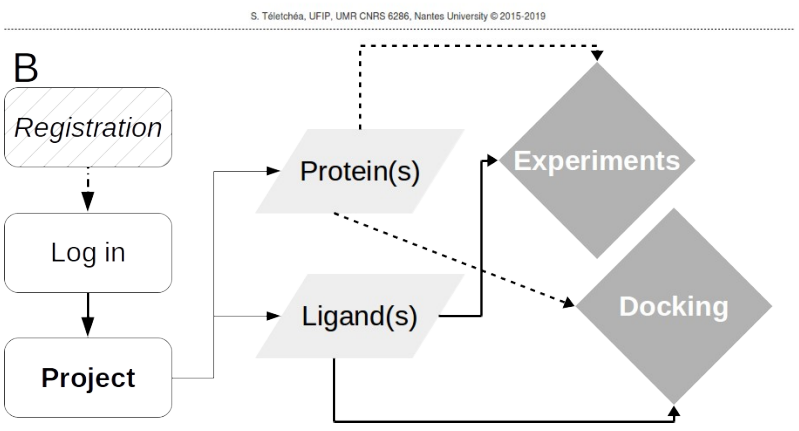
Rdkit UGM 2022

Screening data **management**

- Lack of formal quantitative data
- Need for a shared description of ligands and targets for different users (biologists, chemists, modellers, …)
- Need for controlling data visibility (publication, patent)
  - By user
  - By project
- Need to compare experiments and predictions
- Automated analysis (ROC, MCC, ...)
- Each analysis and data must be **easily** available
- Data transformation, *i.e.* for (deep) machine learning

dockNmine

A



1) **Do** your experiments
2) **Do** your docking calculations
3) **Assemble** them in dockNmine
4) **Analyse** them automatically: raw data, ROC, Screening Explorer, …

→ Automatic extractions and analysis:

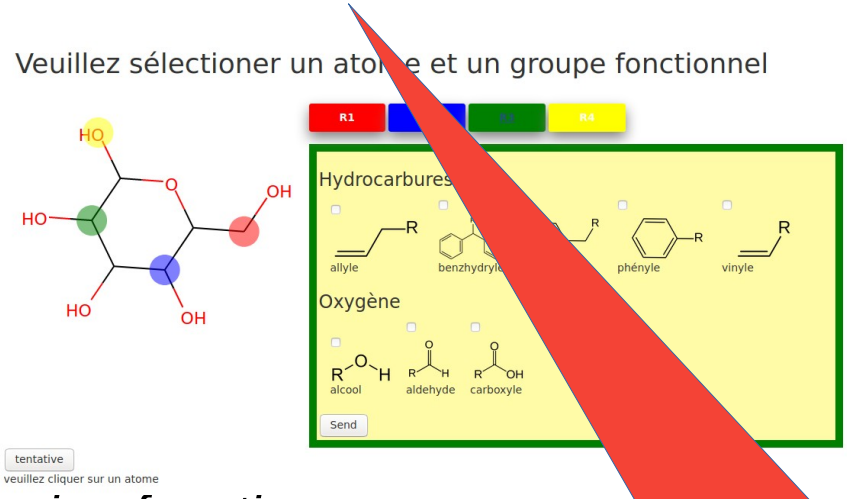
- Uniprot
- ChEMBL (web client, may time out)
- PubChem
- PubMed
- PDB (RCSB), …

Django, rdkit, biopython, biojs, bootstrap, Screening Explorer (http://stats.drugdesign.fr/)

https://docknmine.ufip.univ-nantes.fr/ (v2)
https://www.mdpi.com/1422-0067/20/20/5062/htm

What's next?

- ✔ Advanced job management (celery + rabbitMQ)
- ✔ Rdkit-JS integration (WIP)
- ✔ Interactive docking (*low throughput < 100 mol*) on designed library

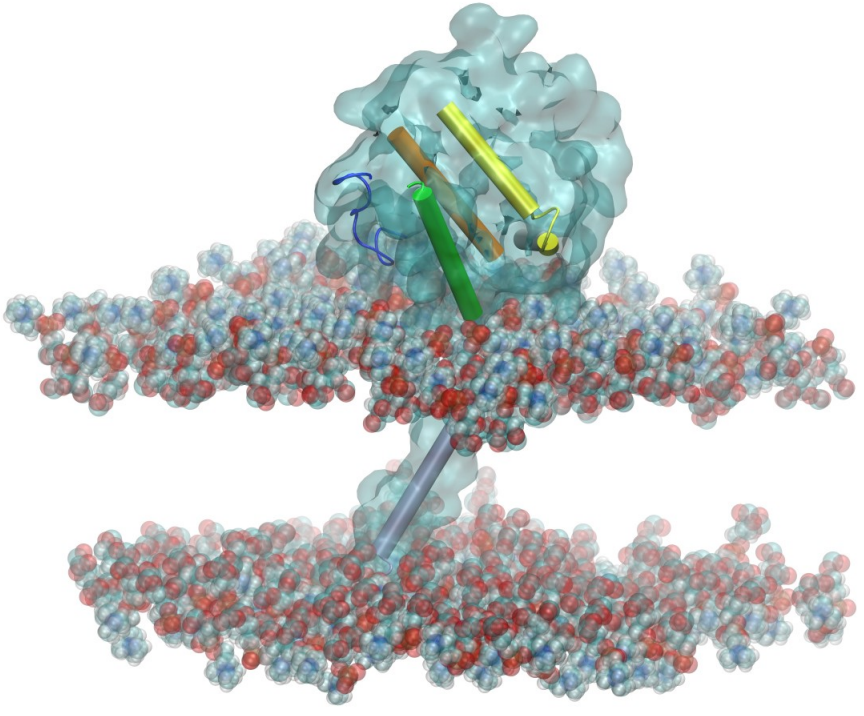


- – *More control on scoring functions*
- – *Data import / export (dataframe)*
- – *Advanced analysis and/or integration*
  - http://chemmine.ucr.edu/
  - https://chembench.mml.unc.edu/
  - http://rxnmapper.ai/
  - https://aws.amazon.com/fr/about-aws/whats-new/2020/09/amazon-aurora-postgresql-supports-rdkit-extension/

HACKATHON!

Thank you for your attention

Post-doc !!!



Exploration of Bak-Bcl-xL Binding Modes

http://piramid-research.fr/
ANR-16-IDEX-0007