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

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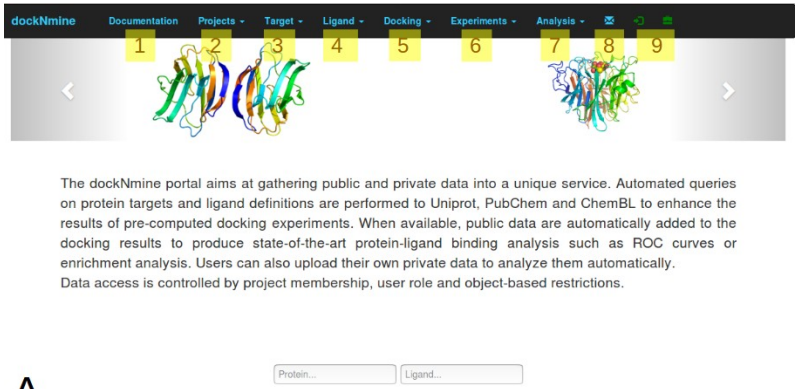
Rdkit Virtual UGM 2020

http://ufip.univ-nantes.fr/tools/docknmine/

Screening data management

- Lack of formal quantitative data
- Need for a common definition (ligand names, molecules)
- Need for controling data visibility (publication, patent)
  - By user
  - By project
- Need to compare experiments and predictions
- Automatic established analysis (ROC, MCC, ...)
- Each analysis and data must be **easily** available

dockNmine



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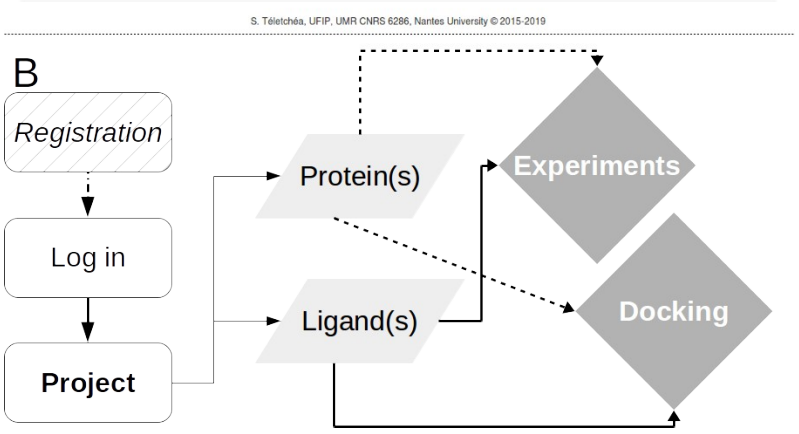


1) **Do** your experiments
2) **Do** your docking calculations
3) **Assemble** them in dockNmine
4) **Analyse** them automatically: raw data, ROC, Screening Explorer, …

→ Automatic extractions and analysis:

- Uniprot
- ChEMBL
- PubChem
- PubMed
- PDB (RCSB), …

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

Data transformation, *and scores*

Difficult to compare values between 2 experiments

A transformation must be applied

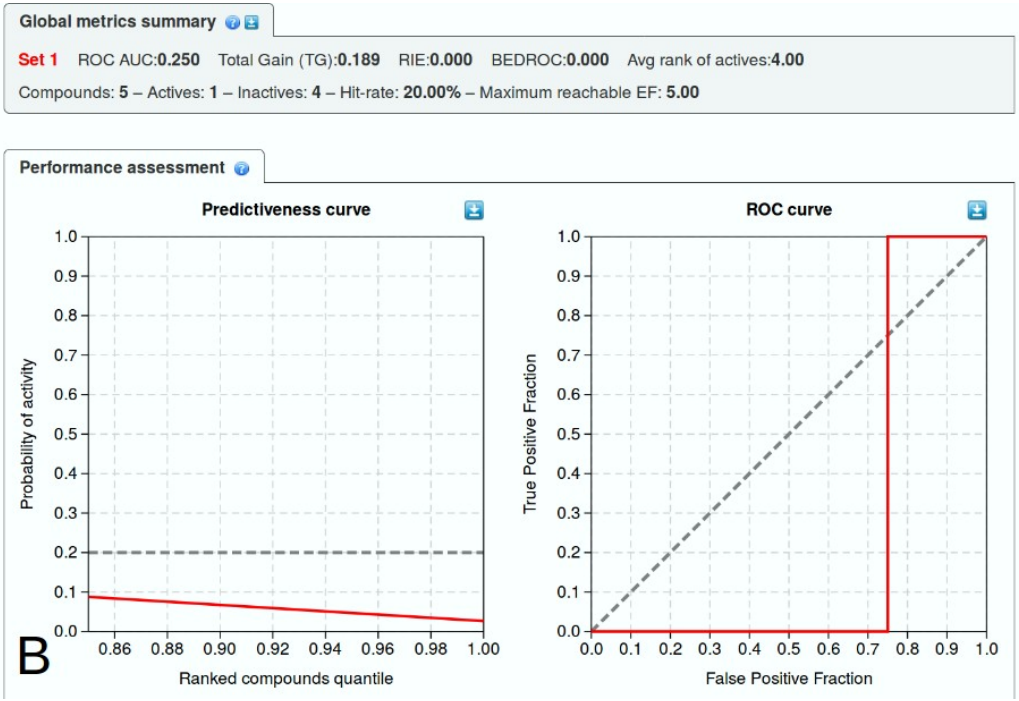
→ a scoring procedure must be applied, for now, as simple as:

3 : Good binder (ITC =< 100 nM)

2 : Medium binder (ITC >100 nM and =< 1 µM)

1 : Low binder (ITC > 1µM)

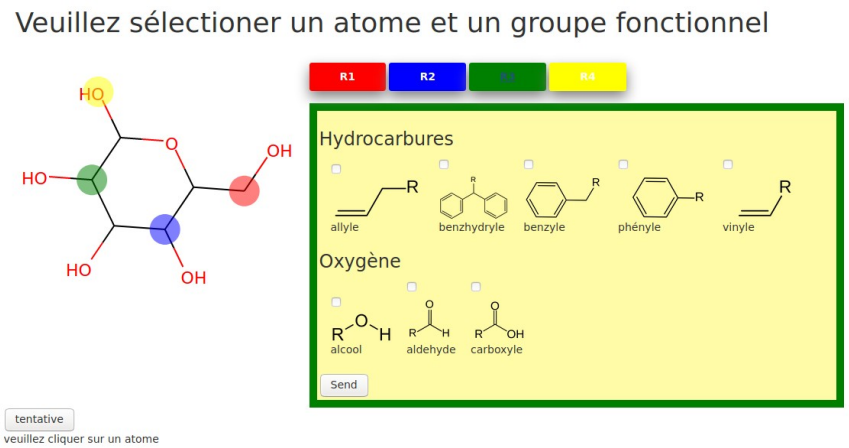
A dedicated work is needed for each method...



Wang, Y. *et al.* PubChem's BioAssay Database. *Nucleic Acids Res.* **40,** D400–D412 (2012).

What's next?

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



- – *More control on scoring functions*
- – *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/

Thank you for your attention

http://piramid-research.fr/