

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

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# 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

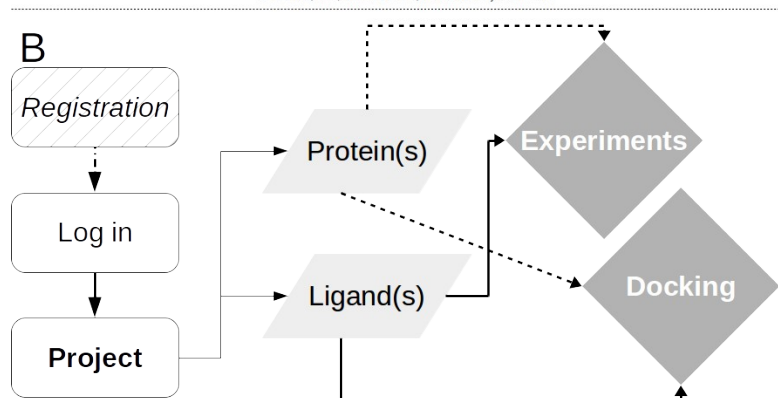


The dockNmine portal aims at gathering public and private data into a unique service. Automated queries on protein targets and ligand definitions are performed to Uniprot, PubChem and ChemBL to enhance the results of pre-computed docking experiments. When available, public data are automatically added to the docking results to produce state-of-the-art protein-ligand binding analysis such as ROC curves or enrichment analysis. Users can also upload their own private data to analyze them automatically. Data access is controlled by project membership, user role and object-based restrictions.

A

B



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:

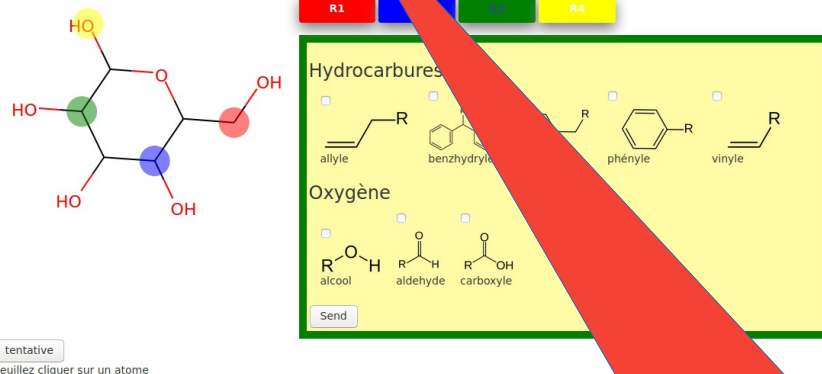
- Uniprot
- ChEMBL (web client, may time out)
- PubChem
- PubMed
- PDB (RCSB), ...

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

# What's next?

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

Veuillez sélectionner un atome et un groupe fonctionnel



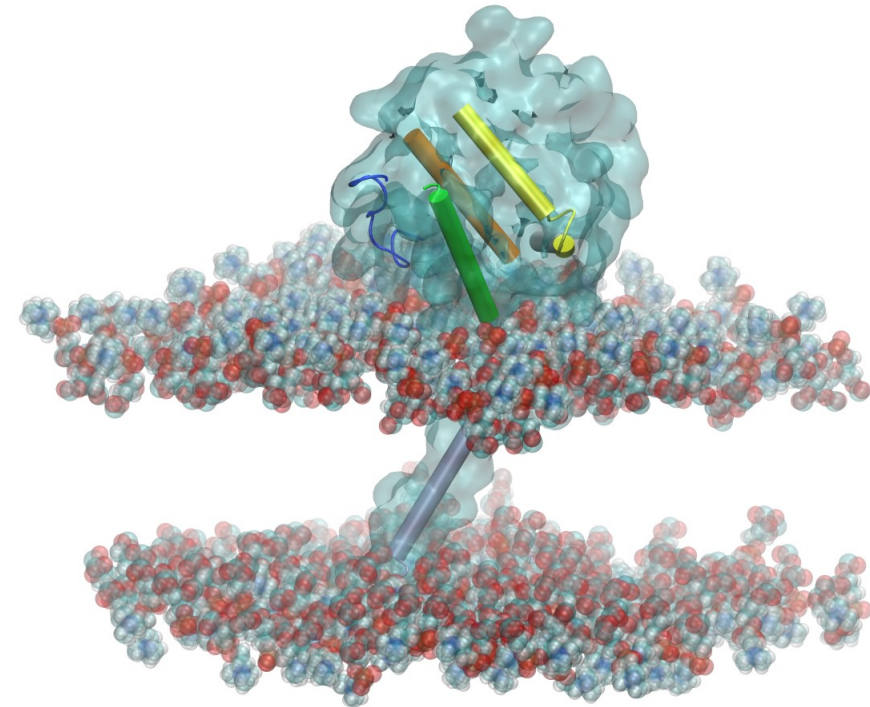
- *More control on scoring functions*
- *Data import / export (dataframe)*
- *Advanced analysis and/or integration*

- <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