

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

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Rdkit Virtual UGM 2020

- Lack of formal quantitative data
- Need for a common definition (ligand names, molecules)
- Need for controlling 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

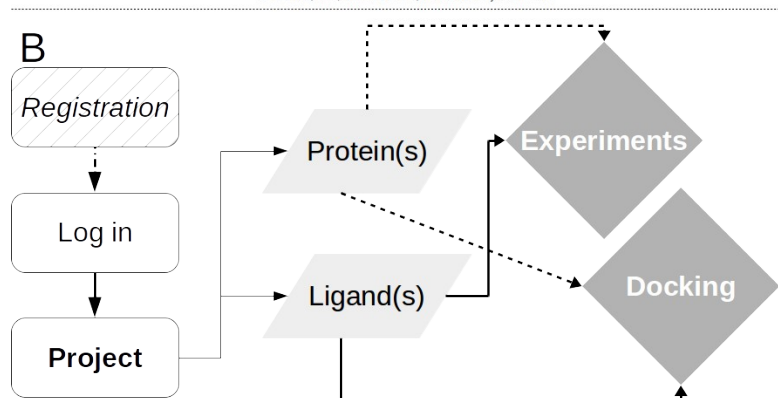


The dockNmine portal aims at gathering public and private data into a unique service. Automated queries on protein targets and ligand definitions are performed to Uniprot, PubChem and ChemBL to enhance the results of pre-computed docking experiments. When available, public data are automatically added 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

Protein... Ligand...

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
- PubChem
- PubMed
- PDB (RCSB), ...

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

Difficult to compare values between 2 experiments

A transformation must be applied

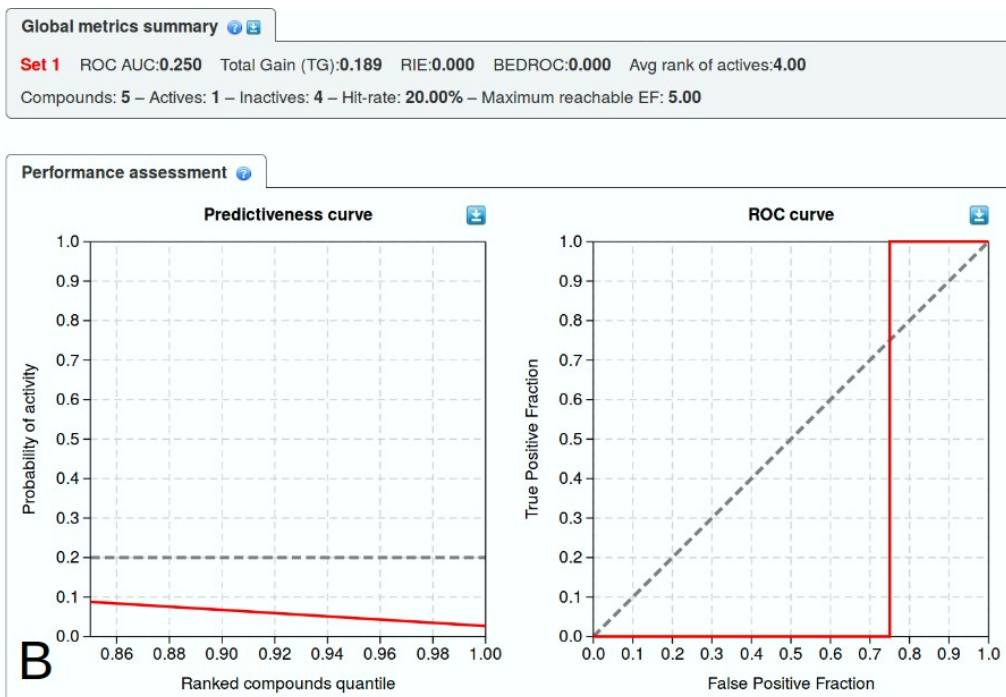
→ a scoring procedure must be applied, for now, as simple as:

3 : Good binder (ITC \leq 100 nM)

2 : Medium binder (ITC > 100 nM and ≤ 1 μ M)

1 : Low binder (ITC > 1 μ M)

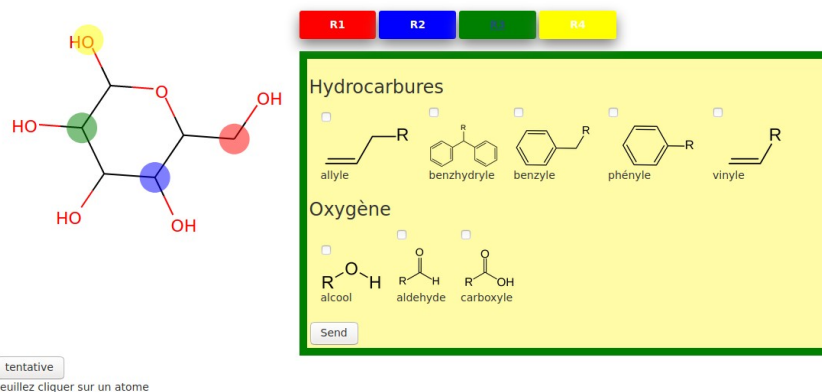
A dedicated work is needed for each method...



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

- ✓ Proper 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*
- *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

