

Mobyle @ RPBS

A web portal for structural bioinformatics and chemoinformatics.

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2009/11/13



- 1 Portal overview
 - Introduction
 - Architecture

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2 Portal features

- 3D bioinformatics resource
- Programs XML
 - Datatypes
 - Java Applets
- Usage

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Introduction

RPBS Project

- Collaborative research in the field of structural bioinformatics
- Services related to protein structure

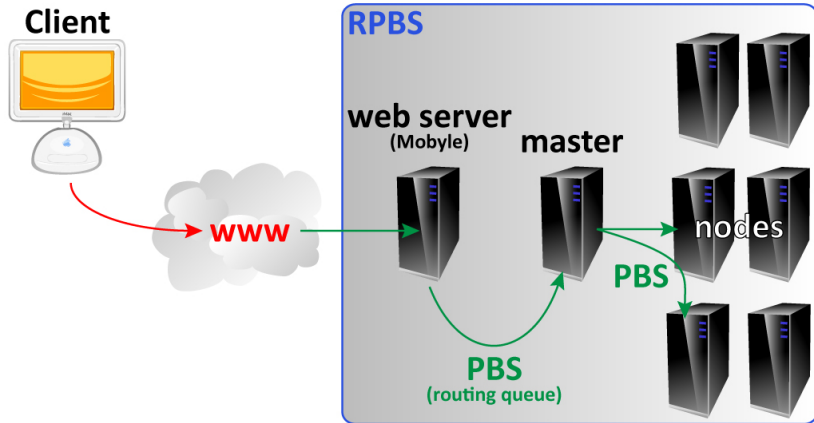
P-Server

- The first framework used at RPBS
- Mobyly inherited from some of its features
- All P-Server services moved to Mobyly@RPBS

Mobyly RPBS server

`http://mobyly.rpbs.univ-paris-diderot.fr`

Architecture



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- **Structure**
 - Relevant and RPBS-specific tools for protein structure **analysis** (*Stride, ASA, H-Bonds, PCE-pKa, PCE-pot, TEF, ...*), **edition** (*side-chains substitution, add hydrogens, ...*), **prediction** (*HCA, PSIPRED, SSpro, PEP-FOLD, MIR*), **quality assessment** (*QMean*) ...

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MobyleNet

→ homology modeling pipeline

Datatypes

- Parameters datatype is the core of MobyNet (MobyNet) pipelining capability
- MobyNet common scheme for typing arguments.
See : <http://mobynet.rpbs.univ-paris-diderot.fr/doc/types.html>

Class	SuperClass	DataFormat
Sequence	-	FASTA, CLUSTAL, PIR, GDE, EMBL, GENBANK, SWISSPROT, PIR_3D
Alignment	-	
Structure	AbstractText	PDB, xyz, Mol2, smiles, sdf
...		

- There is no relevant converter for structural data, each parameter needs an accurate <DataFormat>

Java Applets

JME editor

Draw compound using JME, get its description in the smiles format. Load compound description, graphical JME.

Reset

SMILES/MOL data

Use this applet to edit your SMILES

CLRNWDEL 123 D-R | +A | UDC

C

N

O

S

F

Cl

Br

I

P

X

R

JME Molecular Editor, NoVerto Pharma AG

You can draw a molecule using the and Get its smiles (1D) or mol (3D). Or, you can Draw the drug description in MOL format.

An online file format conversion tool

* : mandatory parameter

Mobyle@RPBS

Contact us

Programs

Search

- Drugs
- Microarray
- Sequence
- Structure
- Tests
 - jalview_example
 - jmol_example
 - king_example
 - webmol_example
- genouest
- lipm
- pasteur

Data Bookmarks

PDB: parameter_1.data refresh

Jobs

jmol_example - 11/12/09 22:11:21 refresh

Tutorials

- How to use Mobyle? A step by step tutorial
- Registration information
- Sequence formats
- Alignment formats

(guest) set email | sign-in | sign-out

Welcome Programs Data Bookmarks Jobs Tutorials

jmol_example 11/12/09 22:11:21 x

✓ http://mobyle.rpbs.univ-paris-diderot.fr/data/jobs/jmol_example/N26943542812109

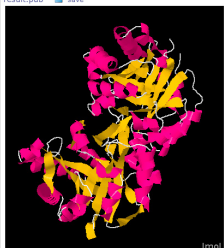
update job status ask for help back to program form remove this job

results

Results Paragraph

-Jmol structure viewer (PDB)

result.pdb save



Jmol

full screen view bookmark as: result.pdb or <-> further analysis

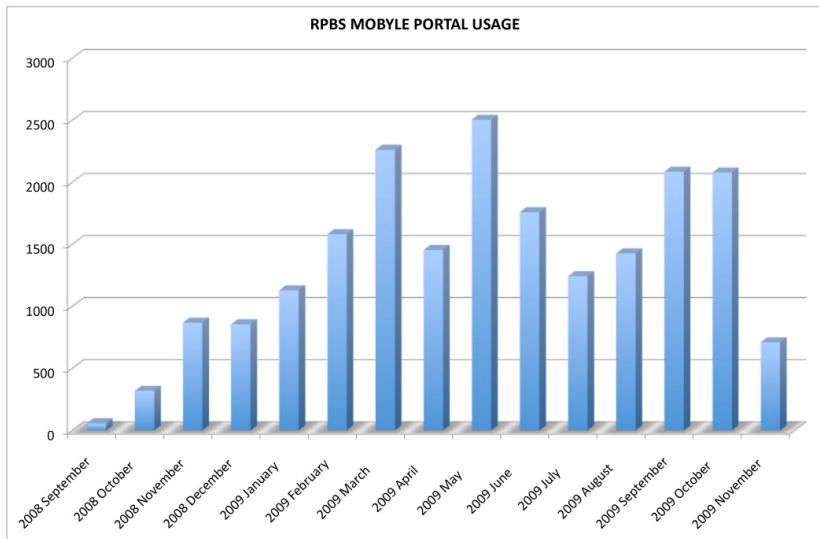
HEADER	ISOMERASE (INTRAMOLECULAR OXIDOREDUCTASE)
TITLE	STRUCTURE OF TRIOSE PHOSPHATE ISOMERASE
COMPND	MOL_ID: 1;
COMPND	2 MOLECULE: TRIOSEPHOSPHATE ISOMERASE;
COMPND	3 CHAIN: A, B;
COMPND	4 EC: 5.3.1.11;
COMPND	5 ENGINEERED: YES
SOURCE	MOL_ID: 1;
SOURCE	2 ORGANISM_SCIENTIFIC: GALLUS GALLUS;

Java Applets

JMol applet example :

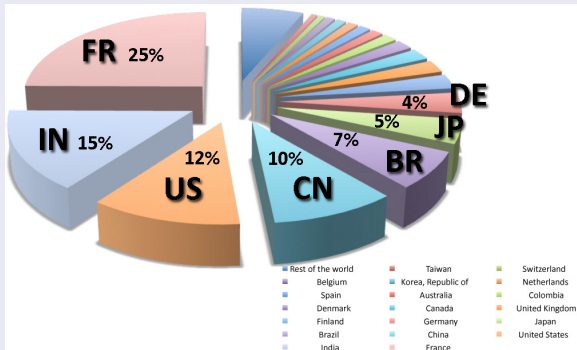
```
<interface>  
  <table xmlns="http://www.w3.org/1999/xhtml" width="100%">  
    <tr>  
      <td width="50%">  
        <applet code="JmolApplet" archive="/portal/applets/jmol/JmolApplet.jar"  
          width="100%" height="450px">  
          <param name="progressBar" value="true"/>  
          <param name="load" value="$resultfile"/>  
        </applet>  
      </td>  
      <td width="50%">  
        <object xmlns="http://www.w3.org/1999/xhtml" type="text/plain" data="$  
          resultfile" height="250px"/>  
      </td>  
    </tr>  
  </table>  
</interface>
```

Usage



Usage

Jobs location (2009/09 to 2009/11)



Stats

- Around **20000 jobs** launched since september 2008 from more than **5000 different locations**
- More than **5000 jobs** since **september 2009**
- **France** represents only **25%** of the jobs



B. Néron, H. Ménager, C. Maufrais, N. Joly, J. Maupetit, S. Letort, S. Carrere, P. Tuffery, and C. Letondal.

Mobyle : a new full web bioinformatics framework.
Bioinformatics, 25 :3005–3011, Nov 2009.



J. Maupetit, P. Derreumaux, and P. Tuffery.

PEP-FOLD : an online resource for de novo peptide structure prediction.
Nucleic Acids Res., 37 :498–503, Jul 2009.



O. Sperandio, M. Petitjean, and P. Tuffery.

wwLigCSRre : a 3D ligand-based server for hit identification and optimization.
Nucleic Acids Res., 37 :W504–509, Jul 2009.