

Mobyle @ RPBS

A web portal for structural bioinformatics and chemoinformatics.

Julien Maupetit¹, Bertrand Néron², Hervé Ménager²,
Corinne Maufrais², Nicolas Joly², Catherine Letondal²,
Pierre Tufféry¹.

¹**RPBS**
Université Paris Diderot Paris 7
Bâtiment Lamarck
36, rue Hélène Brion
75013 Paris, France

²**Groupe Lociciels
et banques de données**
Institut Pasteur
28, Rue du Docteur Roux
75724 PARIS Cedex, France

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Mobylye project

What is Mobylye ?

- a new scientific analysis web portal
- provides an access to command line tools via a web interface
- emphasis on :
 - usability for users,
 - extensibility for developers,
 - maintainability for server administrators.



Outline

1 Mobyle project

Outline

- 1 Mobylye project
- 2 RPBS Mobylye portal

Outline

- 1 Mobylye project
- 2 RPBS Mobylye portal
- 3 What's next ?

- 1 Mobylye project
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 - Participative design
 - Functionalities
 - Architecture overview
 - XML program description
 - XML program description
 - Quick tour : workspace
 - Quick tour : form submission
 - Quick tour : results
 - In test : the "grid" mode

2 RPBS Mobylye portal

3 What's next ?

Motivation

Key problem

ease the access to bio/chemo-informatics tools, for scientists.

- bioinformatics tools are often command-line tools
- command line-tools → steep learning curve
- providing a web interface, which biologists are more familiar with
- developing custom cgis is both a time consuming and error-prone approach.

Based on former projects

→ **PISE** system (1999, C. Letondal) and **P-Serveur** (2004, P. Tufféry et al.)

Participative design

User interviews, participatory workshops

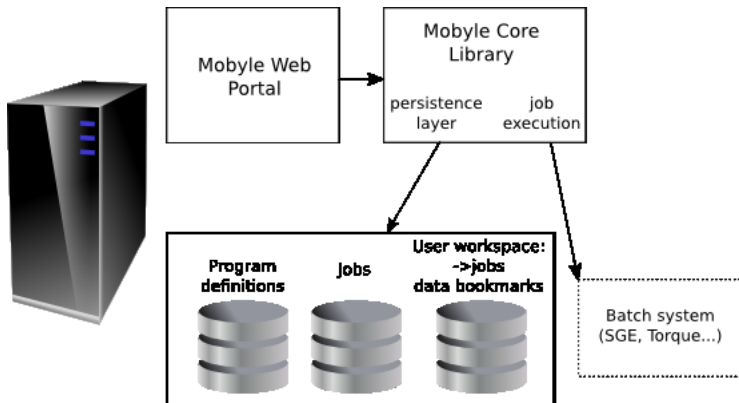
- need for a stable and integrated set of tools
- synthetic view of results and analysis
- re-usability features
- user-defined and ready-to-use "pipelines"

→ skepticism towards complex products

Functionalities

- Users :
 - service search/discovery
 - service usage and documentation
 - data and services integration
 - workspace navigation
- Admins :
 - users assistance
 - job management, tracability
- Developers :
 - easy integration for new tools

Architecture overview



XML program description

- information in Mobylye : stored in XML format (program definition, job status)

- what is a mobyle program description ?
 - a network service definition
 - a program wrapper
 - a UI (User Interface) definition
 - a "semantic" description

XML program description

```

<?xml version="1.0" encoding="ISO-8859-1"?>
...
<program>
  <head>
    <name>blast2</name>
    <version>2.2.17</version>

    <doc>
      <title>BLAST2</title>
      <description>
        <text lang="en">NCBI BLAST, with gaps</text>
      </description>
      <authors>Altschul, Madden, Schaeffer, Zhang, Miller, Lipman</authors>
      <reference>Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaeffer,
        Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997),
        Gapped BLAST and PSI-BLAST: a new generation of protein database
        search programs, Nucleic Acids Res. 25:3389-3402.</reference>

      <doclink>http://www.ncbi.nlm.nih.gov/books/bv.fcgi?rid=handbook.chapter.
        ch16</doclink>
      <doclink>http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/tut1.html</
        doclink>
    </doc>
    <category>database:search:homology</category>
    <env name="BLASTDB">/path/to/db</env>
    <env name="BLASTMAT">/path/to/mat</env>
  </head>

```

XML program description

```

, ,
<paragraph>
  <name>query</name>
  <prompt lang="en">Query Sequence</prompt>
  <argpos>4</argpos>

  <parameters>
    <parameter ismandatory="1" issimple="1" ismaininput="1">
      <name>query_seq</name>
      <prompt lang="en">Query (-i)</prompt>
      <type>
        <datatype>
          <class>Sequence</class>
        </datatype>
        <acceptedDataFormats>
          <dataFormat>FASTA</dataFormat>
        </acceptedDataFormats>
        <card>1,n</card>
      </type>

      <format>
        <code proglang="perl">"_i_$query"</code>
        <code proglang="python">"_i"+ str(query_seq)</code>
      </format>
      <comment>
        <text lang="en">Read (first, query) sequence or set from file</text>
      </comment>
    </parameter>

```

Quick tour : workspace

Mobylye@RPBS

Note: This is still a beta version (0.5).

You

e-mail [login](#) [register](#)

e-mail

Programs

- > Drugs
- > Sequence
- > Structure
- > Analysis
- > Edition
- > H-MSA
- > Homology
- > Mutations
- > Pockets
- > Prediction
- > Superposition
 - ProfFiv2_5
 - iSuperpose

Data Bookmarks

Jobs

Tutorials

- [How to use Mobylye? A step by step tutorial](#)
- [Registration information](#)
- [Sequence formats](#)
- [Alignment formats](#)

Welcome Programs **Data Bookmarks** Jobs Tutorials

iSuperpose

iSuperpose

Programs keywords search

Tab-based organisation

Programs classification

Input data

* Reference Structure : (PDB) ?

Paste

* Mobile Structure : (PDB) ?

Paste

Sequence alignment (optional): (Sequence) ?

Paste

* : mandatory parameter

Reference:

Author(s): J. Mautpetit, P. Tuffery

Quick tour : form submission

Mobylye@RPBS

Note: This is still a beta version (0.9).

You

← mail [login to register](#)

← mail

Programs

- ▷ Drugs
- ▷ Sequence
- ▷ Structure
- ▷ Analysis
- ▷ Edition
- ▷ Homology
- ▷ Mutations
- ▷ Pockets
- ▷ Prediction
- ▷ Superposition
- ▷ ProfIiv2_8
- iSuperpose

Data Bookmarks

Jobs

Tutorials

- [How to use Mobylye? A step by step tutorial](#)
- [Registration information](#)
- [Sequence formats](#)
- [Alignment formats](#)

authentication

Welcome Programs Data Bookmarks Jobs Tutorials

iSuperpose

A comprehensive tool to superpose protein structures.

Reset

Run

Launch

Input data

Reference Structure : (PDB) 2 **Bank**

Paste DB File

PDB

HEADER	DE NOVO DESIGN	31-JAN-97
1ABZ	ALPHA-T-ALPHA, A DE NOVO DESIGNED PEPTIDE, NMR,	
23		
TITLE	2	
STRUCTURES		
COMPND	POL_ID:	

Mobile Structure : (PDB) 2

Paste DB File

PDB

HEADER	DE NOVO DESIGN	31-JAN-97
1ABZ	ALPHA-T-ALPHA, A DE NOVO DESIGNED PEPTIDE, NMR,	
23		
TITLE	2	
STRUCTURES		
COMPND	POL_ID:	

Sequence alignment (optional): (Sequence) 2

Paste DB File

*: mandatory parameter

Quick tour : results

Mobylye@RPBS

Note: This is still a beta version (0.9).

Job status

Welcome Programs **Data Bookmarks** Jobs Tutorials

iSuperpose
11:05:08 00:34:01

✓ <http://mobylye.rpbs.univ-paris-diderot.fr/tmp/iSuperpose/525690472122921>

update job status ask for help << go back to program remove this job

results

Superposed PDB: (PDB)

iSuperpose.pdb **ssvs**

HEADER	1	C1	SIN	A	0	15.254	-0.007	3.211	1.00	0.00	
HETATM	2	O1	SIN	A	0	16.425	-0.874	3.019	1.00	0.00	O
HETATM	3	O2	SIN	A	0	14.337	-1.894	2.539	1.00	0.00	O
HETATM	4	C2	SIN	A	0	14.909	0.287	4.404	1.00	0.00	C
HETATM	5	C3	SIN	A	0	13.772	1.237	4.018	1.00	0.00	C
HETATM	6	C4	SIN	A	0	12.591	1.037	4.971	1.00	0.00	C
HETATM	7	O3	SIN	A	0	11.729	0.213	4.737	1.00	0.00	O
HETATM	8	H21	SIN	A	0	15.778	0.862	4.685	1.00	0.00	H
LINKAGE	9	14.856	-0.706	6.557	1.00	0.00	...

moving_data-iSuperpose.pdb

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

Alignment: (Text)

moving_data-ssvs

parameters

Mobylye Structure: (PDB)

file format detection program re-formatted file

moving_data

Reference Structure: (PDB)

file format detection program re-formatted file

reference_data

Command line

```
iSuperposev2.py -r reference_data -m moving_data -o iSuperpose.pdb -g iSuperpose.fasta -M iSuperpose.TMScores -a CA
```

job archive

download this job as an archive

Data type

Results

Bookmark for later use

Chain directly

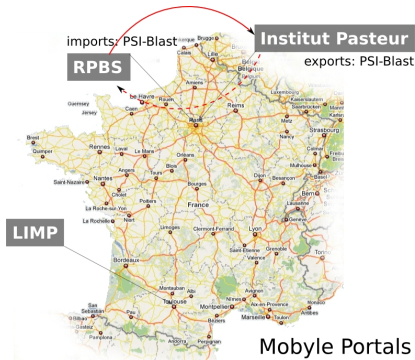
Job archive

Command line

In test : the "grid" mode

Principle

Each portal can import/export a specific service to/from a specific Mobyle portal.



Advantages

- The user-invoqued service is remotely executed to the single portal.
- Service maintainers are service deployers.
- Portal specificity is kept, but not restrictive.

→ Smart way to deploy services.

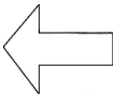
In test : the "grid" mode

Mobyle@RPBS

Note: This is still a beta version (0.9).

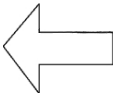
The screenshot shows the Mobyle@RPBS interface. At the top, there is a navigation menu with 'Welcome', 'Programs', 'Data Bookmarks', 'Jobs', and 'Tutorials'. Below this, there is a 'You' section containing an 'e-mail' field and links for 'sign in' and 'register'. A search bar is located under the 'Programs' section. The 'Programs' menu is expanded, displaying a list of categories: 'Drugs', 'Sequence', 'Structure', 'pasteur', 'database', 'search', 'homology', 'psiblast', 'pattern', 'sequence', and 'structure'. At the bottom of the interface, there are sections for 'Data Bookmarks' and 'Jobs'.

Welcome to Mobyle, a portal for bioinf



Optional: you can [register](#) or [sign-in](#) to **save** your work

register [here](#)).



Select an analysis in the **Programs** [menu](#).

In test : the "grid" mode

Mobyale portal

http://mobyale.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py

GaladalSites ▾ Mail ▾ Protein Structure ▾ Journaux ▾ Databases ▾ Web Servers ▾ Mobyale ▾ RPBS ▾ Admin System ▾ MTI ▾ Congres ▾ Utils ▾

biograle 200... LYON-BUSIN... Transilien S... ABCDTrains... Gmail - BIO... Mobyale portal NCBI Sequen...

Note: This is still a beta version (0.9).

You

e-mail [sign in](#) [register](#)

e-mail [petit@univ-paris-diderot.fr]

Programs

Drugs
 Sequence
 Structure

pasteur
 database
 search
 homology
 psiblast
 pattern
 sequence
 structure

Data Bookmarks

Jobs

Tutorials

- [How to use Mobyale? A step by step tutorial](#)
- [Registration information](#)
- [Sequence formats](#)
- [Alignment formats](#)

Welcome Programs Data Bookmarks Jobs Tutorials

PSI-Blast@pasteur x

PSI-Blast@pasteur

Position Specific Iterative Blast

* Sequence File (-i) (Sequence)

Paste : DB : File

```

121 kaadavseal lavatpvagk daitqvats srdeqigaly gegmnkvgtd gvsveesst
181 ldtelefteg vgfdkgflsa yfvtdfdseq avlddpvlvl hqekissipe llpmlkvte
241 sgkplliuae dlegealatl vvnssirktk avavkspffg drrkafledl aivtggqvvv
301 petglvlrev gtdvlgsarr vvvskddtii vdgggsndav akrvnlrae ievdsaedwr
361 eklgervakl aggvavikvg avtetalkkr keavedavaa akasieegil aggggalvqc
421 gaalkqrts ltgdealgid vffealkkpr ywiatnagld gavvvdksvg lpaghqlnas
481 tlygydivad gvvdpvkvtv savinaaava rmlttetav vdkpakteeh dhhqhah
//
  
```

Start of required region in query (-S)

End of required region in query (-H)

* Protein database (-d)

Scoring option

Terminé

In test : the "grid" mode

The screenshot shows a web browser window with the URL `http://mobylye.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py`. The page title is "Mobylye portal". A yellow box highlights a message: "Your job is being submitted. Loading".

The page content includes:

- Navigation:** GaladalSites, Mail, Protein Structure, Journaux, Databases, Web Servers, Mobylye, RPBS, Admin System, MTI, Congres, Utils.
- Left Sidebar:**
 - e-mail: julien.maupetit@univ-paris
 - Programs: Search
 - Drugs, Sequence, Structure
 - pasteur
 - database
 - search
 - homology
 - psiblast
 - pattern
 - sequence
 - structure
 - Data Bookmarks
 - Jobs refresh
 - Tutorials refresh
 - How to use Mobylye? A step by step tutorial
 - Registration information
 - Sequence formats
 - Alignment formats

Main Content:

- PSI-Blast@pasteur
- Position Specific It
- Reset
- ask for help
- * Sequence File (-i) (Sequence)
- Paste : DB : File clear data
- Sequence file content:


```
121 kaadavseal lavatpvagk daitqvavts srdeqigalv gegmknvgtd gvvsvveesst
181 ldtelefteg vgfdkgflsa yfvtdfdaqg avlddpvlvl hqekisslpe llpmlekvtv
241 sgkpllivae dlegealatl vvnsirktilk avavkspffg drrkafledl aivtggqvvn
301 petglvlrev gtdvlgsarr vvvskddtii vdgggsandav akrvnlrae ievsdsewdr
361 ekqlervakl aggvavikvg avtetalkkr kesvodavaa akasieegii agggsalvqc
421 gaalkqrts ltgdealgid vffealkapl ywiatnagld gavvvdksvj lpaghglnas
481 tlgugdlyad gvvdpvkvtv savlnaasva rmmlettetav vdkpakteeh dhghgh
```
- Start of required region in query (-S)
- End of required region in query (-H)
- * Protein database (-d) ? uniprot: Universal Protein Resource
- Scoring option
 - Cost to open a gap (-G)
 - Cost to extend a gap (-E)
 - Similarity matrix (-M) BLOSUM62
- Filtering and masking options ?

Transfert des données depuis mobylye.rpbs.univ-paris-diderot.fr...

In test : the "grid" mode

The screenshot shows a web browser window with the URL `http://mobyble.rpbs.univ-paris-diderot.fr/cgi-bin/portal.py`. The page title is "Mobyble@RPBS". A navigation menu includes "Welcome", "Programs", "Data Bookmarks", "Jobs", and "Tutorials".

Note: This is still a beta version (0.9).

User Information:
 You: e-mail [sign in](#) [register](#)
 e-mail: `julien.maupetit@univ-paris`

Programs: Search

Data Bookmarks:
 Sequence: `query.data` [refresh](#)

Jobs:
 ✓ `psiblast - 11/05/08 22:30:44` [refresh](#)

Tutorials:
 • [How to use Mobyble? A step by step tutorial](#)

Job Details:
 Welcome Programs Data Bookmarks Jobs Tutorials
 psiblast 11/05/08 22:30:44
 ✓ <http://mobyble.pasteur.fr/Mobyble/Results/psiblast/A14920970576048>
 update job status ask for help << go back to program remove this job

results

Blast text report (BlastTextOutput)

psiblast.txt [save](#)

BLASTP 2.2.18 [Mar-02-2008]

Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaffer, Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997), "Gapped BLAST and PSI-BLAST: a new generation of protein database search programs", *Nucleic Acids Res.* 25:3389-3402.

Reference for compositional score matrix adjustment: Altschul, Stephen F.,

[full screen view](#) [bookmark](#) as: psiblast.txt

Blast html report (BlastHtmlOutput)

psiblast.html [save](#)

Terminé

- 1 Mobyle project
- 2 **RPBS Mobyle portal**
 - Portal overview
 - Usage @ RPBS
- 3 What's next ?

Further improvements

- 1 Mobyle project
- 2 RPBS Mobyle portal
- 3 What's next ?
 - Further improvements
 - Near futur

Near futur

Mobyle next release v0.95

- Coming in early november
- Freely distributed
- Mobyle grids supported

→ Interested in being a Mobyle portal ? **Contact us!**

`mobyle-project@rpbs.univ-paris-diderot.fr`