Docking
Principes et méthodes

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Docking entre molécules

Définition

Le docking est une méthode qui prédit l'orientation d'une molécule par rapport à une autre pour avoir le complexe le plus stable.

Il est fréquemment utilisé sur l'étude de la cible moléculaire des médicaments et réduire les essais expérimentaux.

Deux approches

- Basée sur la complémentarité des surfaces
- Basée sur le calcul de l'énergie du complexe

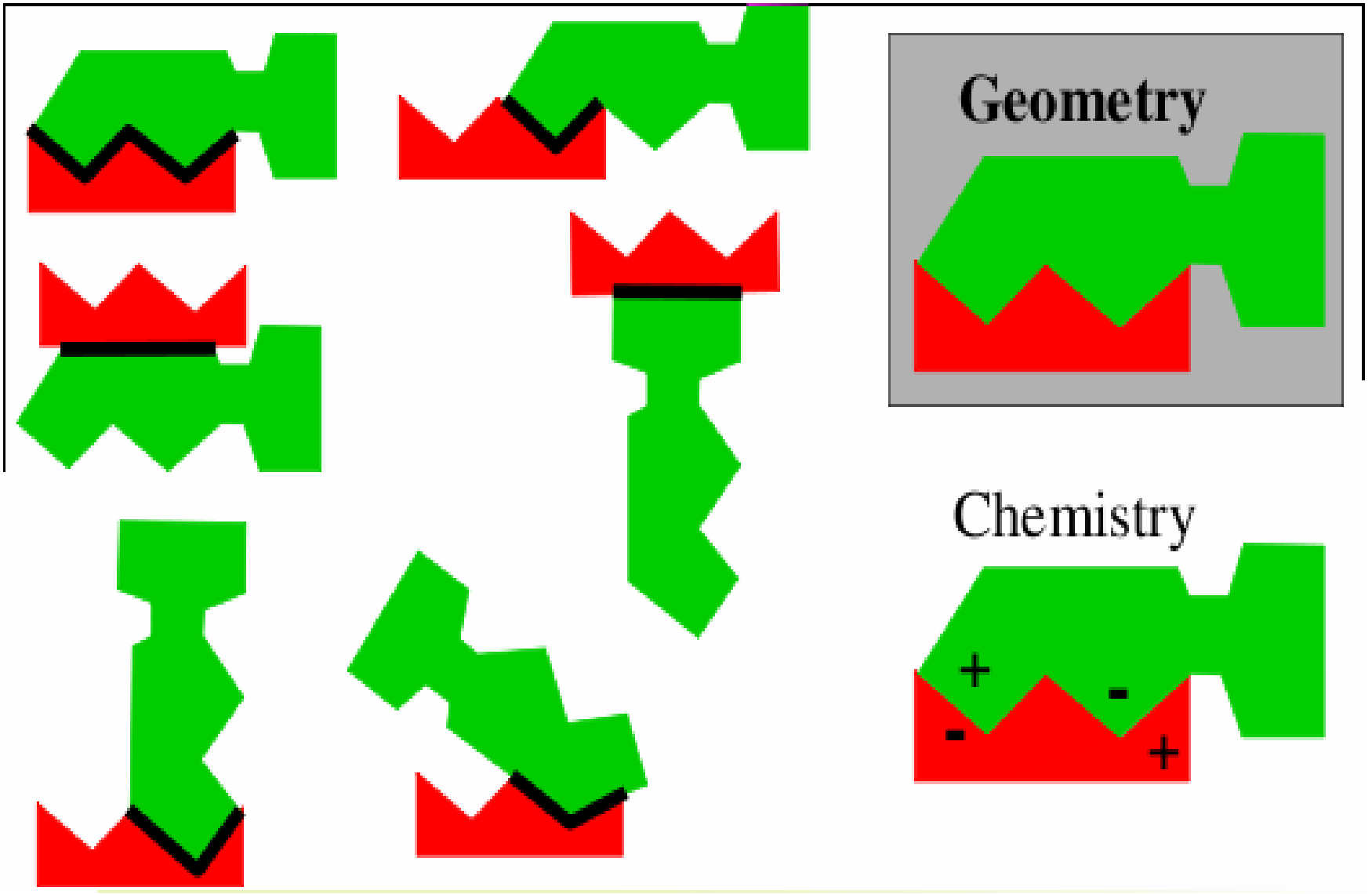
Docking entre protéines et molécules

Le concept du Docking:
Input: une paire de molécules représentée en 3D (pdb)

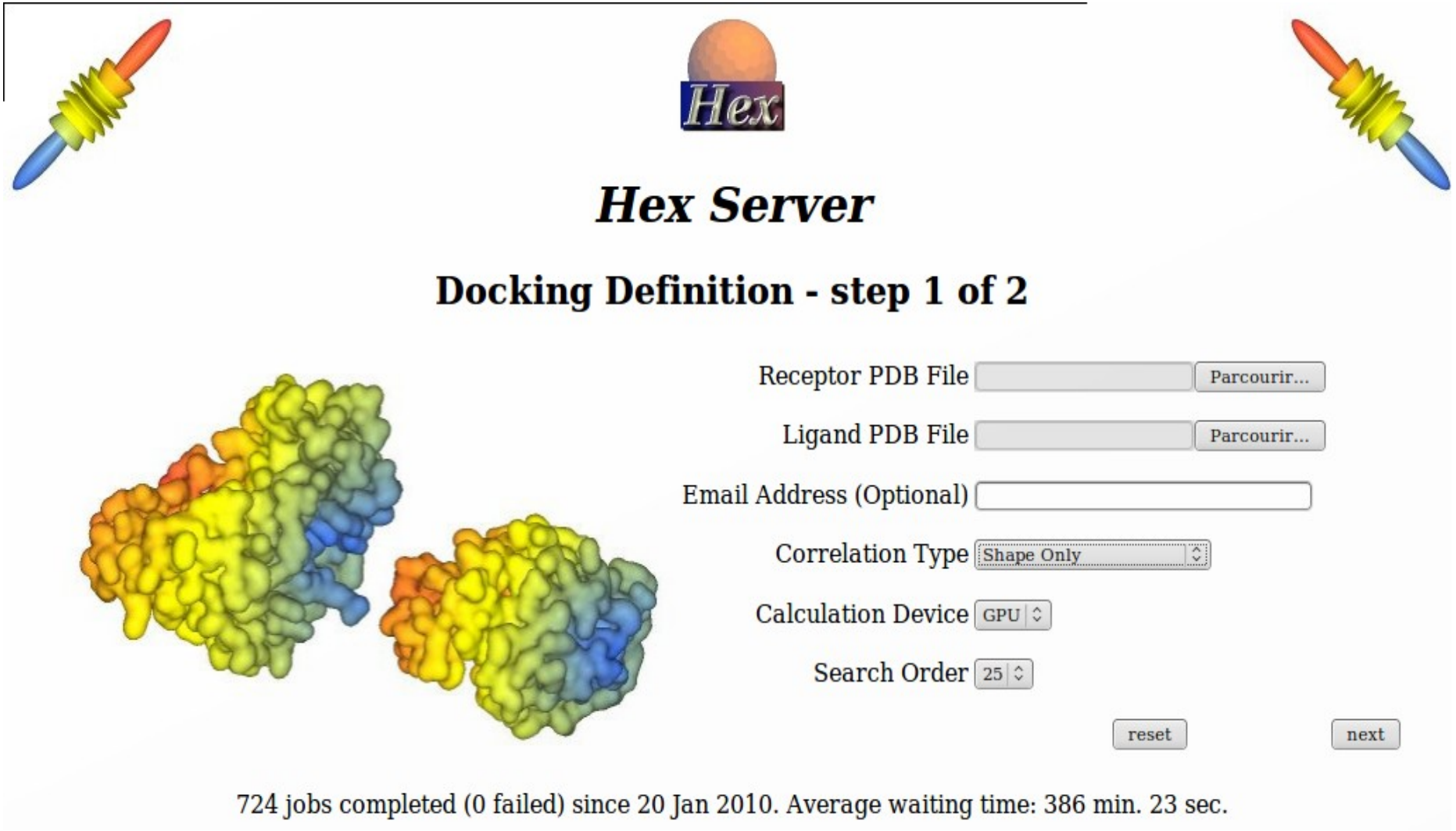
Ce qui est recherché:
•Décider si les molécules forment un complexes (interaction/liaison)
•Prédire la structure 3D du compplexe
•En déduire la fonction

Signification / Application / Motivation
•La conception des médicaments assistée par ordinateur

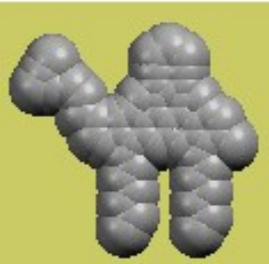
Les forces régissant la reconnaissance biomoléculaire
•Van der Waals, Électrostatique, contacts hydrophobes, liaisons hydrogène, pont de sels
•La forme et la surface de contact


Geometry
Chemistry
+
-
-
+

Hex: logiciel de docking



PerlMol: convertisseur de format de fichier en chimie



Introduction

Features

Quick Tutorial

Reference Manual

Examples

Download & Installation

Mailing List

Bugs and Requests

Support this project

SOURCEFORGE.NET

PerlMol - Download and Installation

The PerlMol modules are being developed for perl 5.8.x and are known to work under Windows, Linux, FreeBSD, Solaris, and OS X. They are backward-compatible with perl 5.6.x, but you are strongly encouraged to upgrade to 5.8.x because support for older versions may be removed in the future. PerlMol depends on other modules available on CPAN, such as Math::VectorReal. See the README files for details.

There are three main ways of installing the PerlMol modules:

1. Automated installation using the CPAN.pm module - recommended way for UNIX-compatible systems.
2. Manual install of the PerlMol bundle - alternative way if CPAN.pm is not an option for some reason.
3. PPM package for Windows ActivePerl 5.8 - easiest way of installing under Windows.
4. CVS Repository - for developers that know what they are doing and are interested in trying the latest unreleased development versions.

Automated installation via CPAN.pm

If you have the CPAN module configured properly, you can install each module separately by using `perl -MCPAN -e 'install Chemistry::Mol'` (to give an example). To install the latest bundle do `perl -MCPAN -e 'install PerlMol'`. **But note that some of the most recent modules may not be included in the bundle yet.**

Install de PerMol

Automated installation via CPAN.pm

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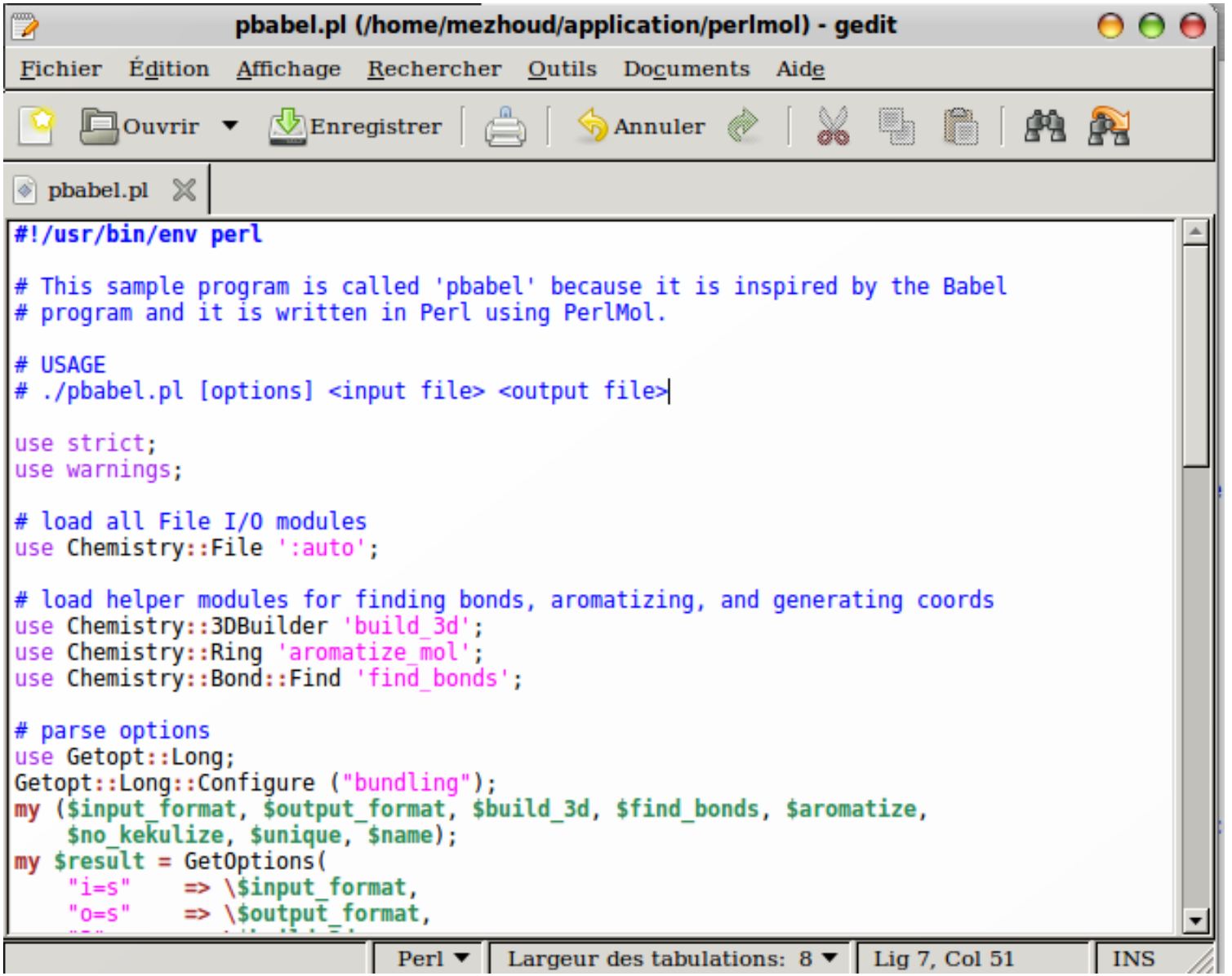
You can also download the tarballs for individual modules and install them yourself by following the instructions on the README files, either from CPAN or from SourceForge.net.

Configurer le packet .pl



Télécharger le packet nécessaire pour la conversion

PerlMol - Example: File conversion

File conversion example

Added by Ivan Tubert-Brohman (itub@cpan.org)

This sample program is called 'pbabel' because it is inspired by the Babel program and it is written in Perl using PerlMol.

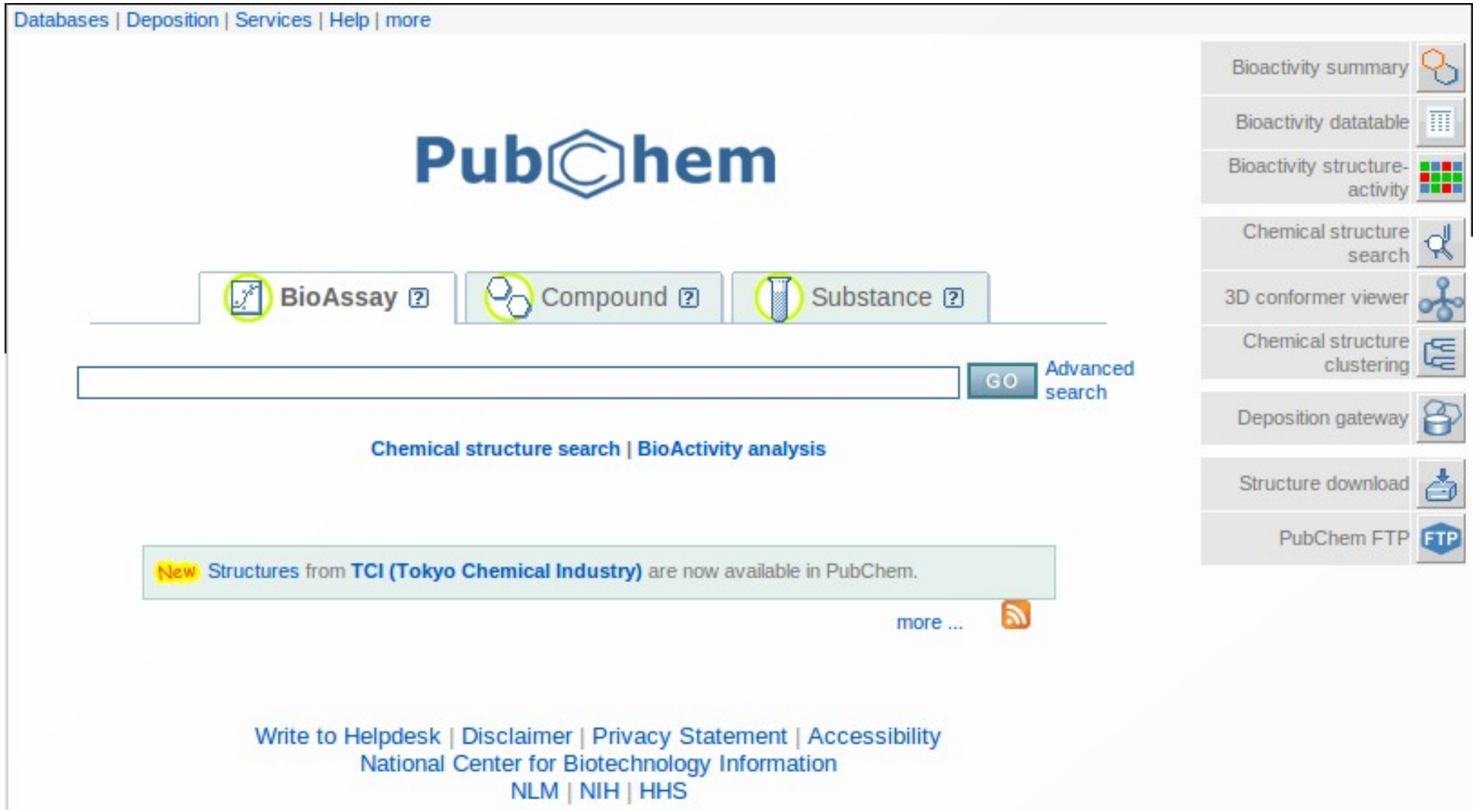
Usage

```
./pbabel.pl [options] <input file> <output file>

Options:
    -i <input format>
    -o <output format>
    -3      build 3d coordinates
    -b      find bonds
    -a      aromatize
    -K      don't kekulize (only for reading SMILES)
    -u      unique (only for writing SMILES)
    -n      include name (only for writing SMILES)

Available file formats:
    dumper
    formula
    formula_pattern
    mdl
    midas
    mop
    pdb
    sdf
    sln
    smarts
    smiles
    xyz
```

Files

- pbabel.pl - the program
- amines.sdf - sample sdf file
- amines.smi - sample sdf file, generated with ./pbabel.pl -nu

http://pubchem.ncbi.nlm.nih.gov/



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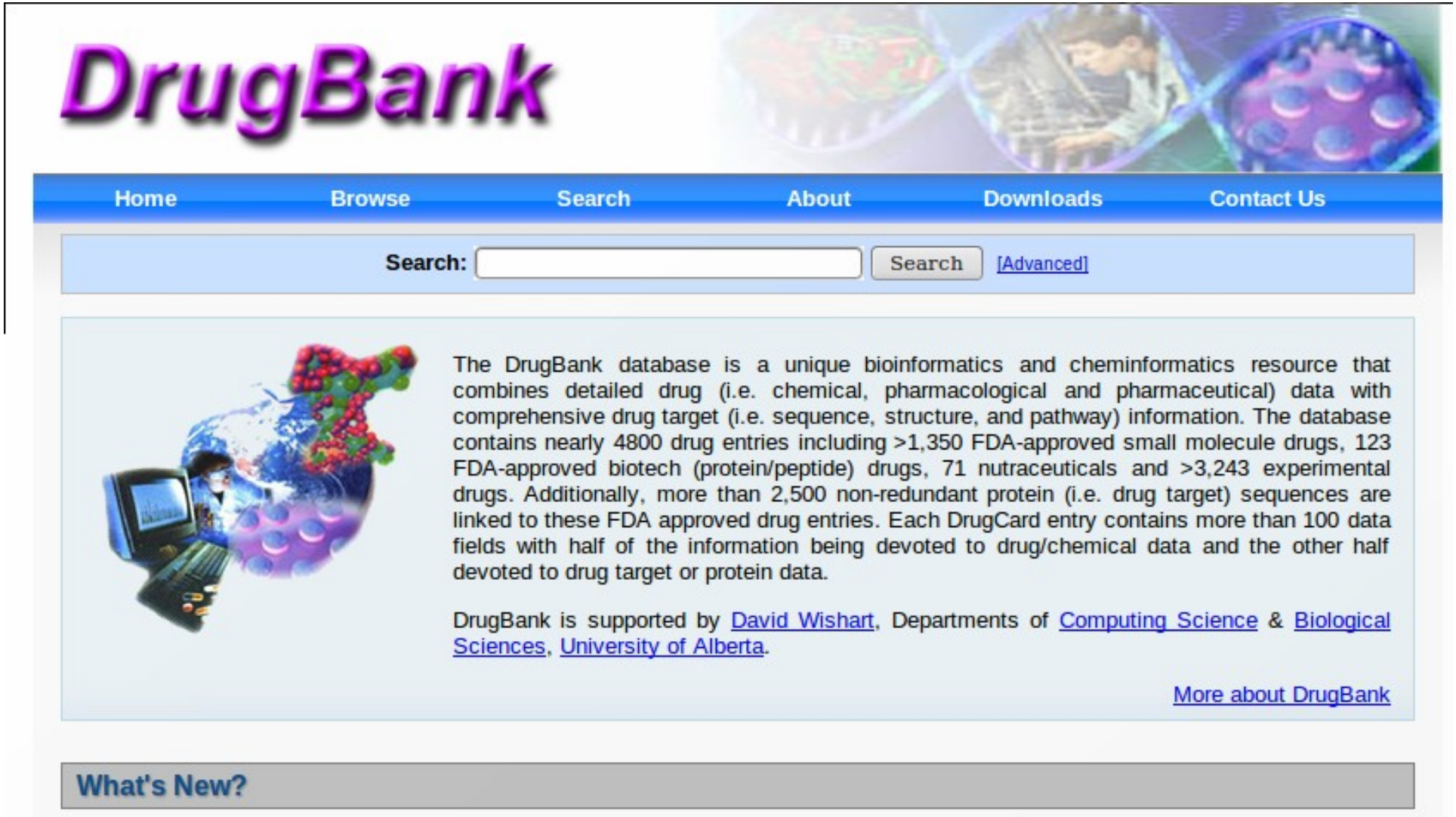

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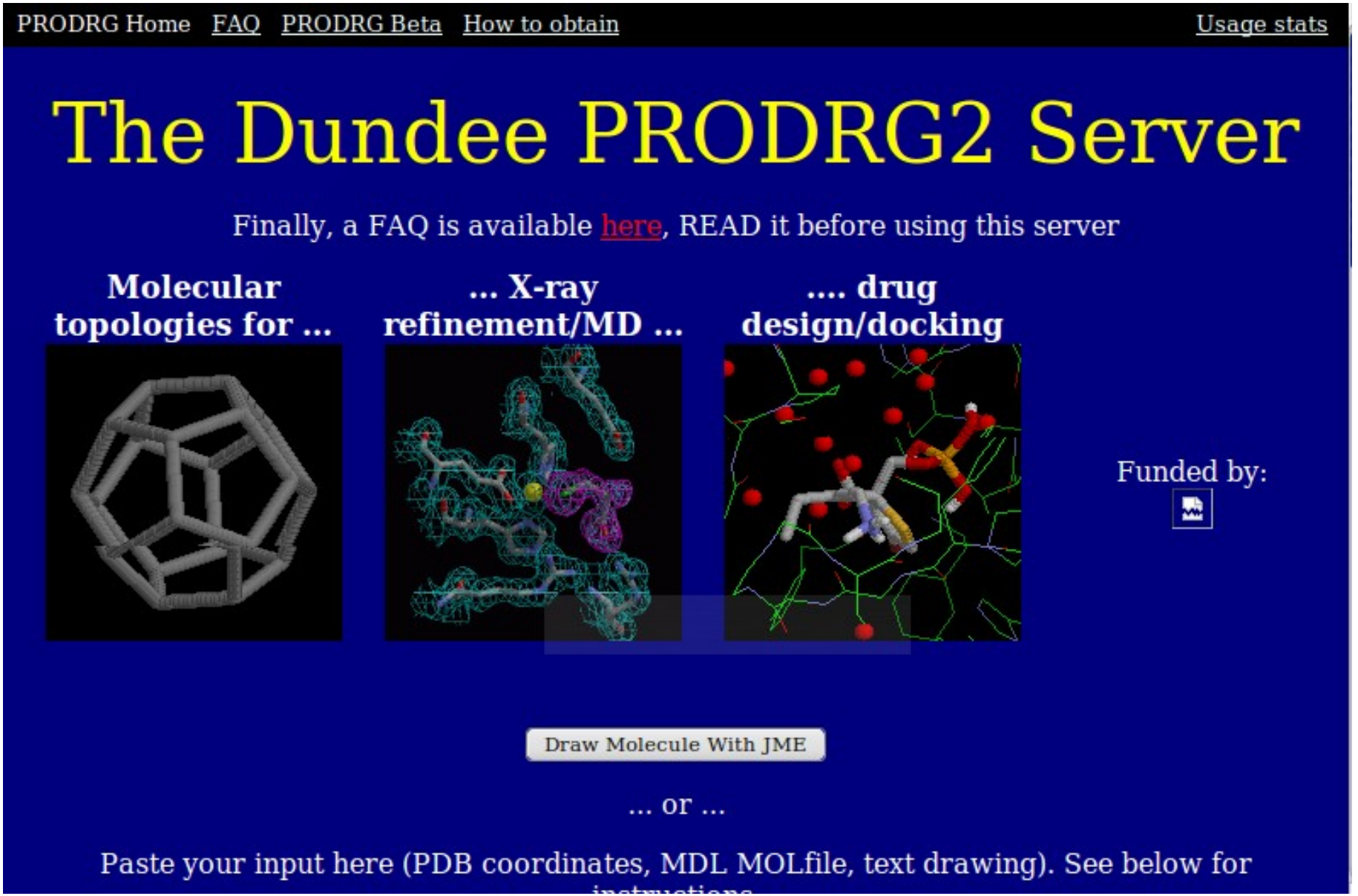
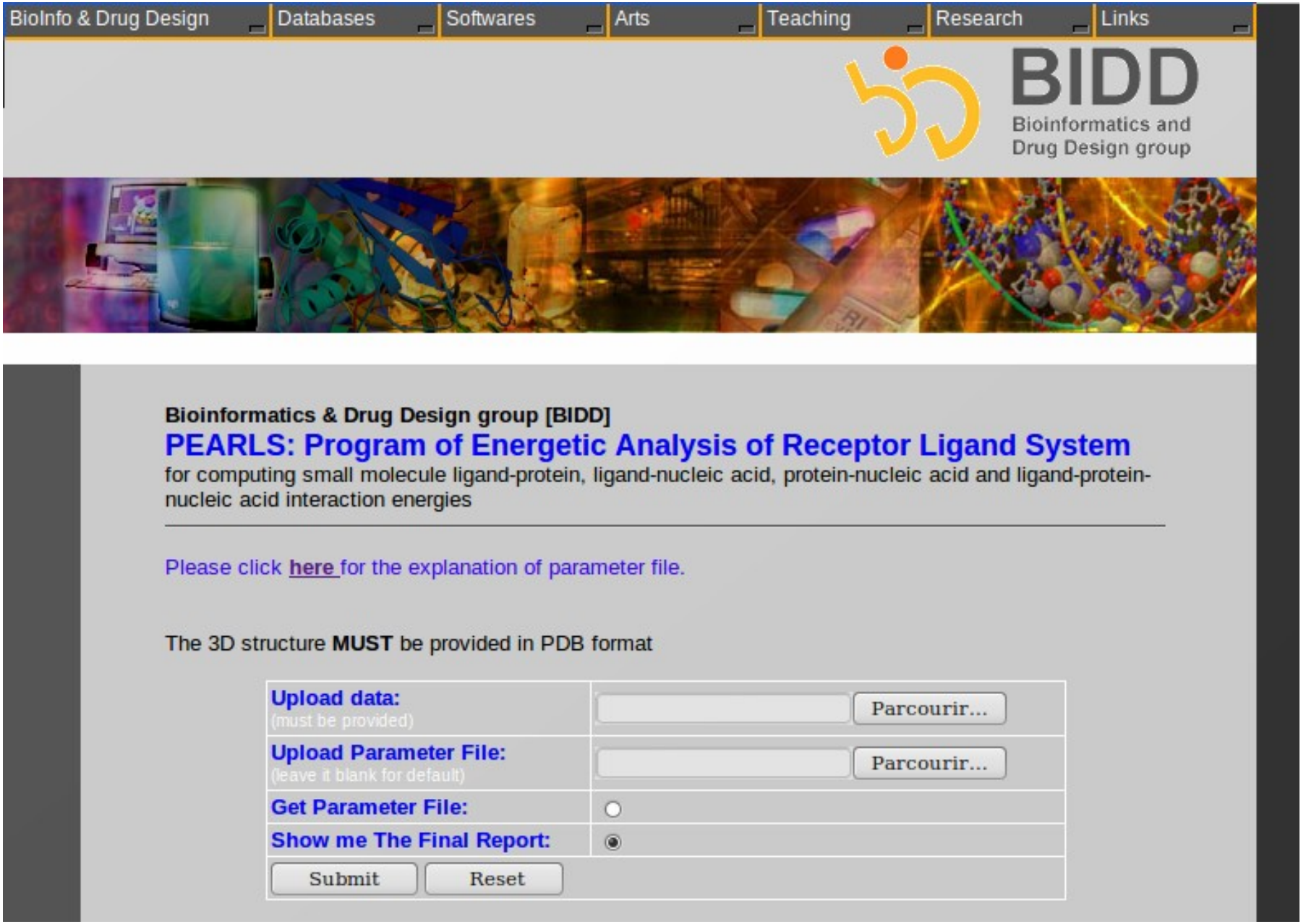


http://ang.cz3.nus.edu.sg/cgi-bin/prog/rune.pl?adv=true



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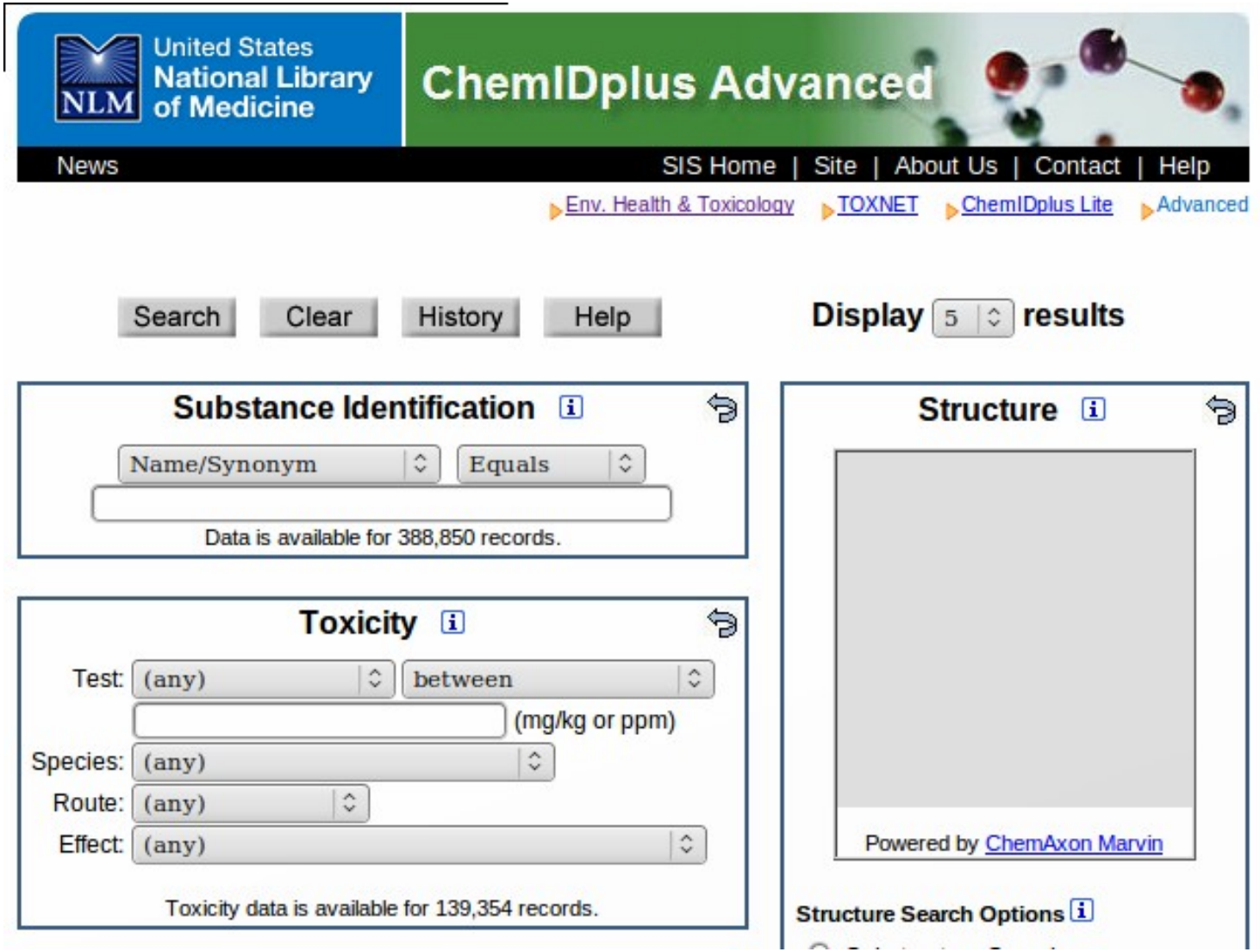
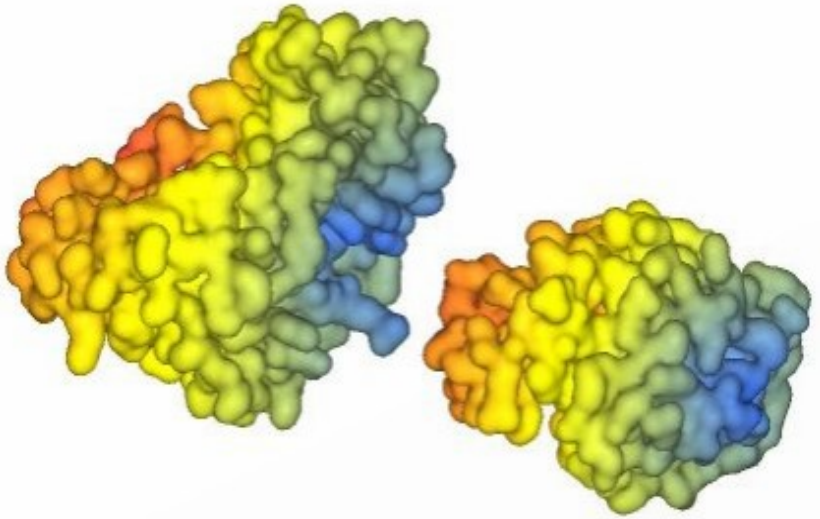


http://www.loria.fr/~ritchied/hex/

Hex Server

Docking Definition - step 1 of 2



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Email Address (Optional) [ ]

Correlation Type [Shape Only]

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