

Docking

Principes et méthodes

Karim Mezhoud
CNSTN

kmezhoud@gmail.com

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:

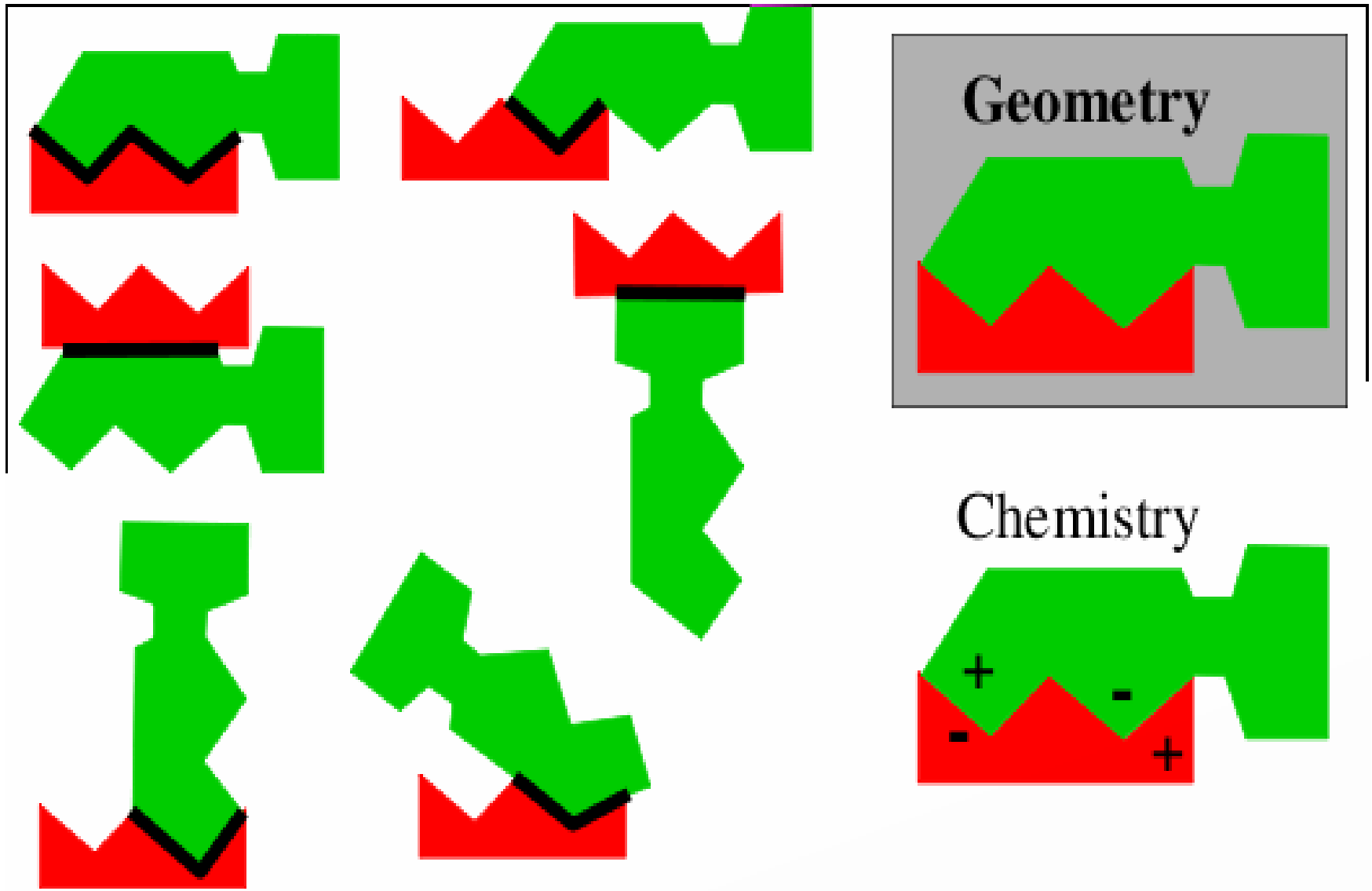
- Décider si les molécules forment un complexe (interaction/liaison)
- Prédire la structure 3D du complexe
- En déduire la fonction

Signification / Application / Motivation

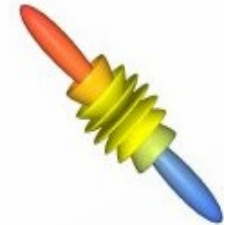
- La conception des médicaments assistée par ordinateur

Les forces régissant la reconnaissance biomoléculaire

- Van der Waals, Électrostatique, contacts hydrophobes, liaisons hydrogène, pont de sels
- La forme et la surface de contact

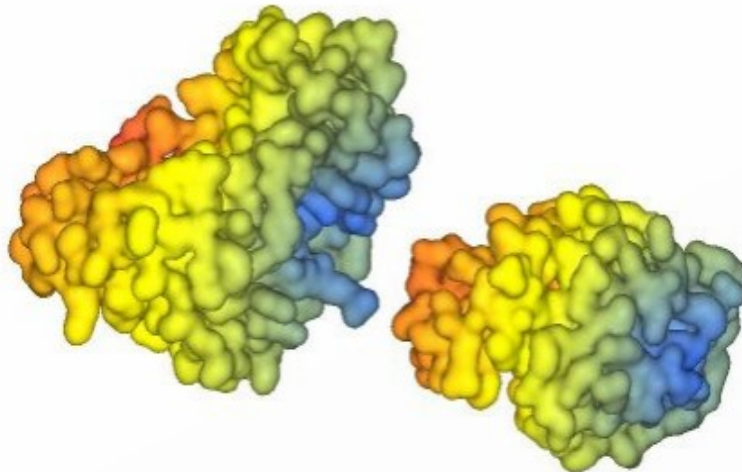


Hex: logiciel de docking



Hex Server

Docking Definition - step 1 of 2



Receptor PDB File

Ligand PDB File

Email Address (Optional)

Correlation Type

Calculation Device

Search Order

724 jobs completed (0 failed) since 20 Jan 2010. Average waiting time: 386 min. 23 sec.

PerlMol: convertisseur de format de fichier en chimie



[Introduction](#)

[Features](#)

[Quick Tutorial](#)

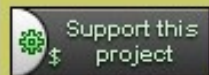
[Reference Manual](#)

[Examples](#)

[Download & Installation](#)

[Mailing List](#)

[Bugs and Requests](#)



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.**

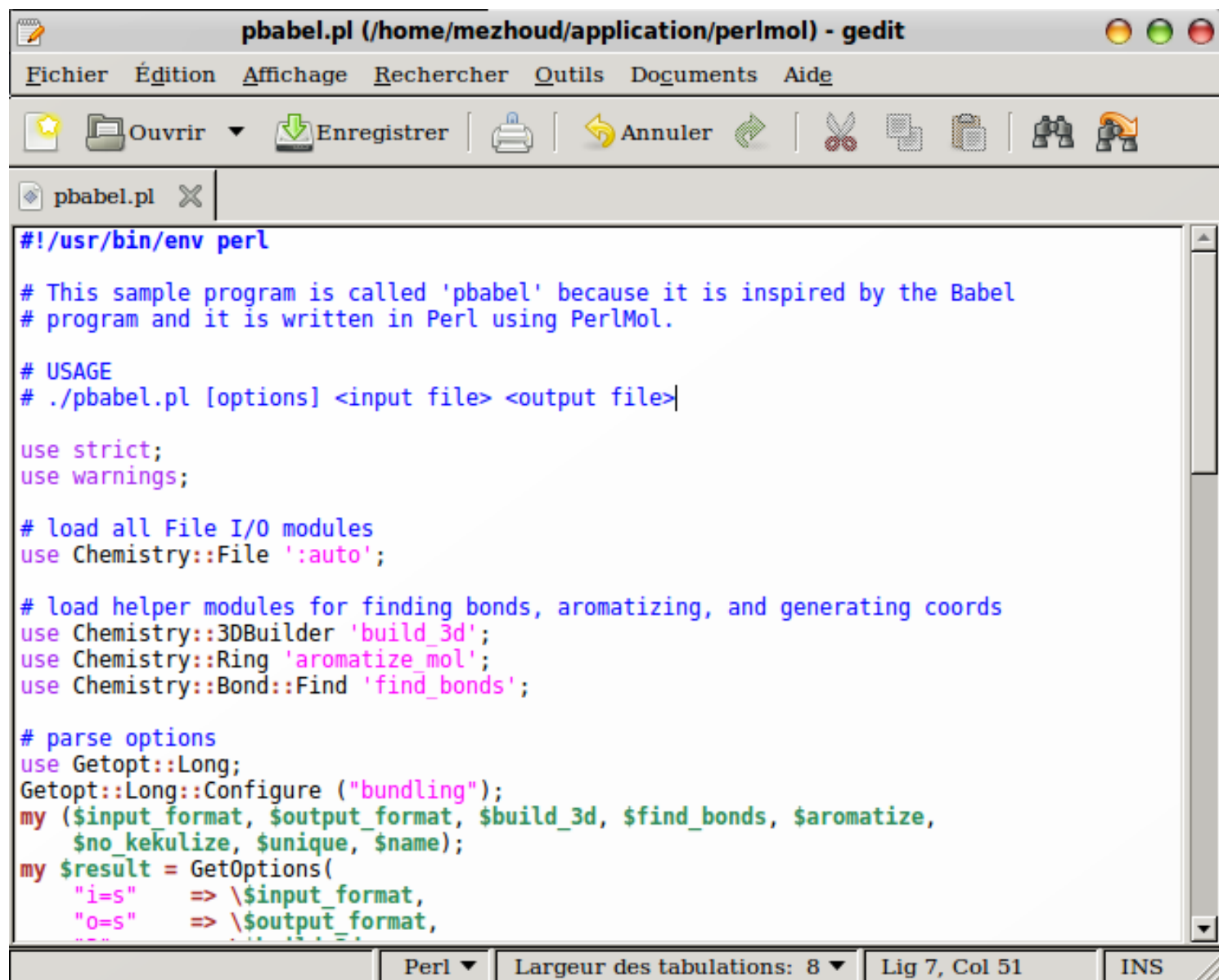
Install de PerMol

Automated installation via CPAN.pm

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.**

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



```
#!/usr/bin/env perl

# 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>

use strict;
use warnings;

# load all File I/O modules
use Chemistry::File ':auto';

# load helper modules for finding bonds, aromatizing, and generating coords
use Chemistry::3DBuilder 'build_3d';
use Chemistry::Ring 'aromatize_mol';
use Chemistry::Bond::Find 'find_bonds';

# parse options
use Getopt::Long;
Getopt::Long::Configure ("bundling");
my ($input_format, $output_format, $build_3d, $find_bonds, $aromatize,
    $no_kekulize, $unique, $name);
my $result = GetOptions(
    "i=s"    => \$input_format,
    "o=s"    => \$output_format,
```


Télécharger le packet nécessaire pour la conversion



[Introduction](#)

[Features](#)

[Quick Tutorial](#)

[Reference Manual](#)

[Examples](#)

[Download & Installation](#)

[Mailing List](#)

[Bugs and Requests](#)



SOURCEFORGE.NET

PerIMol - 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 PerIMol.

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 amines.sdf > amines.smi`

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

[Databases](#) | [Deposition](#) | [Services](#) | [Help](#) | [more](#)

PubChem



[BioAssay](#) ?



[Compound](#) ?



[Substance](#) ?

GO

[Advanced search](#)

[Chemical structure search](#) | [BioActivity analysis](#)

New Structures from **TCI (Tokyo Chemical Industry)** are now available in PubChem.

[more ...](#)



[Write to Helpdesk](#) | [Disclaimer](#) | [Privacy Statement](#) | [Accessibility](#)
National Center for Biotechnology Information
[NLM](#) | [NIH](#) | [HHS](#)

[Bioactivity summary](#)



[Bioactivity datatable](#)



[Bioactivity structure-activity](#)



[Chemical structure search](#)



[3D conformer viewer](#)



[Chemical structure clustering](#)



[Deposition gateway](#)



[Structure download](#)



[PubChem FTP](#)



<http://www.drugbank.ca/>

DrugBank



[Home](#)

[Browse](#)

[Search](#)

[About](#)

[Downloads](#)

[Contact Us](#)

Search:

[\[Advanced\]](#)



The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information. The database contains nearly 4800 drug entries including >1,350 FDA-approved small molecule drugs, 123 FDA-approved biotech (protein/peptide) drugs, 71 nutraceuticals and >3,243 experimental drugs. Additionally, more than 2,500 non-redundant protein (i.e. drug target) sequences are linked to these FDA approved drug entries. Each DrugCard entry contains more than 100 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

DrugBank is supported by [David Wishart](#), Departments of [Computing Science](#) & [Biological Sciences](#), [University of Alberta](#).

[More about DrugBank](#)

What's New?

<http://davapc1.bioch.dundee.ac.uk/prodrng/index.html>

[PRODRG Home](#) [FAQ](#) [PRODRG Beta](#) [How to obtain](#)

[Usage stats](#)

The Dundee PRODRG2 Server

Finally, a FAQ is available [here](#), READ it before using this server

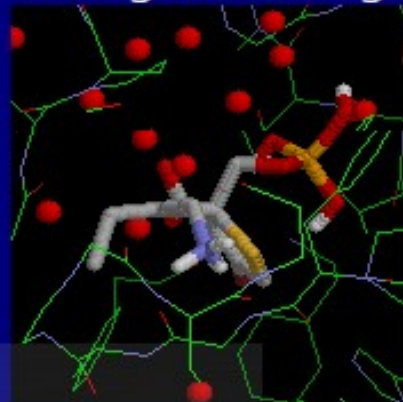
**Molecular
topologies for ...**



**... X-ray
refinement/MD ...**



**.... drug
design/docking**



Funded by:




Draw Molecule With JME

... OR ...


Paste your input here (PDB coordinates, MDL MOLfile, text drawing). See below for instructions

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

BioInfo & Drug Design | Databases | Softwares | Arts | Teaching | Research | Links



BIDD
Bioinformatics and
Drug Design group



Bioinformatics & Drug Design group [BIDD]

PEARLS: Program of Energetic Analysis of Receptor Ligand System


for computing small molecule ligand-protein, ligand-nucleic acid, protein-nucleic acid and ligand-protein-nucleic acid interaction energies

Please click [here](#) for the explanation of parameter file.

The 3D structure **MUST** be provided in PDB format

Upload data: (must be provided)	<input type="text"/>	Parcourir...
Upload Parameter File: (leave it blank for default)	<input type="text"/>	Parcourir...
Get Parameter File:	<input type="radio"/>	
Show me The Final Report:	<input checked="" type="radio"/>	
<input type="button" value="Submit"/>		<input type="button" value="Reset"/>

http://chem.sis.nlm.nih.gov/chemidplus/

 United States National Library of Medicine

ChemIDplus Advanced

News SIS Home | Site | About Us | Contact | Help

[▶ Env. Health & Toxicology](#) [▶ TOXNET](#) [▶ ChemIDplus Lite](#) [▶ Advanced](#)

Search Clear History Help

Display results

Substance Identification [i](#)

Name/Synonym Equals

Data is available for 388,850 records.

Toxicity [i](#)

Test: between

(mg/kg or ppm)

Species:

Route:

Effect:

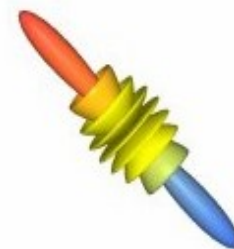
Toxicity data is available for 139,354 records.

Structure [i](#)

Powered by [ChemAxon Marvin](#)

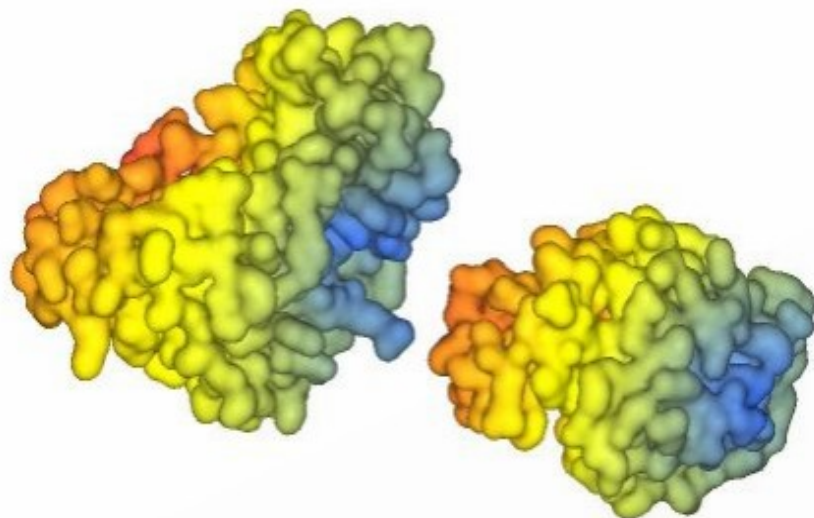
Structure Search Options [i](#)

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



Hex Server

Docking Definition - step 1 of 2



Receptor PDB File

Ligand PDB File

Email Address (Optional)

Correlation Type

Calculation Device

Search Order

756 jobs completed (0 failed) since 20 Jan 2010. Average waiting time: 0 min. 10 sec.