# FittingWizard v0.8.0 : software prerequisites and installation procedure

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## 1 Java version

Oracle's Java proprietary implementation is required for running this software under Linux : this can be downloaded at :
http://www.oracle.com/technetwork/java/javase/downloads/index.html

Download the `JRE` if you just plan to use the software, or the `JDK` if you plan some Java software development.

### 1.1 Fedora / RedHat Entreprise Linux / CentOS

Check this page for instructions if you are using either Fedora 12 to 20 or RedHat/CentOS 5.10 to 6.5 :
http://www.if-not-true-then-false.com/2010/install-sun-oracle-java-jdk-jre-7-on-fedora-centos-red-hat-rhel/
Please follow all the steps of the procedure, and do not forget the step `alternatives -config java` for enabling the use of the Oracle implementation.

### 1.2 Ubuntu

Check this page for instructions if you are using Ubuntu :
http://www.wikihow.com/Install-Oracle-Java-on-Ubuntu-Linux

## 2 Babel/Open Babel

Open Babel is a toolkit for manipulating chemical data : in this toolkit it is mainly used for chemical coordinates file conversion. Some Linux distributions provide binary compiled versions.

Otherwise check http://openbabel.org/wiki/Main_Page for instructions and manual download and compiling.

## 3 VMD compatibility

This software allows you to visualize the resulting multipoles within VMD.
First you need to install VMD : Download here and see here for installation instructions.

Then you need to compile a small fortran software provided in the `./scripts` subdirectory with the following command : `gfortran fieldcomp_dyna.f90 -o fieldcomp`.

If `gfortran` is not installed, use `"yum install gcc-gfortran"` for Fedora/CentOS/RedHat or `"apt-get install gfortran"` for Ubuntu.

# 4 Python 2.7

You need to have a Python 2.7 scripting environment installed : this is already the case for most of the Linux distributions, if not please check the documentation pages of your distribution for more instructions.

Alternatively, you can download and compile Python 2.7 by yourself :
http://www.python.org/download/releases/2.7/

## 4.1 NumPy and SciPy

NumPy and SciPy are two Python modules used for scientific and mathematics computations. Most of the Linux distributions will provide a way of directly installing binary versions of those libraries.

Otherwise, check http://www.numpy.org/ and http://www.scipy.org/ for more instructions or for a manual install.

## 4.2 RDKit

RDKit is an open source toolkit for cheminformatics. See http://sourceforge.net/projects/rdkit/files/ for downloading the sources and http://rdkit.org/docs/index.html for installation instructions.

A few remarks:

If you need to compile RDKit by yourself, you will require several packages:

- Python development libraries : under Ubuntu, install `"apt-get install python-dev"`, under Fedora or CentOS/RHEL install `"yum install python-devel"`, if you compiled Python by yourself you should have it.
- Flex and Bison and Cmake, 3 packages used for building the software suite: `"yum install flex bison cmake"` or `"apt-get install flex bison cmake"`. If you need to install the doftware manually, check:
  - http://www.gnu.org/software/bison/
  - http://flex.sourceforge.net/
  - http://www.cmake.org/cmake/resources/software.html
- The boost library, a collection of tools commonly used in modern programming: install with `"yum install boost boost-devel"` or `"apt-get install libboost-all-dev"`. Alternatively for a manual install, see http://www.boost.org/users/download/

Before running the `"make"` command and after using `"cmake"` (see RDKit docs), run `"cmake -D RDK_INSTALL_INTREE=OFF ."` for choosing as installation path the default `/usr/local/`

Once the software is installed you need to define the two following environment variables : `export PYTHONPATH=/usr/local/lib64/python2.7/site-packages/`

```
export LD_LIBRARY_PATH=/usr/local/lib/
```

Then open a `python2.7` intepreter and try the following two commands to test the installation:

```
import rdkit
from rdkit import Chem
```

If no error message is displayed `RDKit` can be properly used by `FittingWizard`