# Steps to install Chemical Development Kit (CDK)

## CDK – Python wrapper

For linux on the server

**Install CDK python wrapper**

Source: <https://github.com/sebotic/cdk_pywrapper>

1. Create CDK wrapper directory
2. In CDK wrapper directory:~$ git clone https://github.com/sebotic/cdk\_pywrapper.git
3. In CDK wrapper directory:~$ pip3 install py4j –user
4. In CDK wrapper directory:~$ pip3 install . –user

**Run a script in python**

1. In CDK wrapper directory:~/cdk\_pywrapper/cdk$ python3

Example script which generates the InChIKey of a SMILE:

>>> from cdk\_pywrapper.cdk\_pywrapper import Compound

>>> smiles = 'CCN1C2=CC=CC=C2SC1=CC=CC=CC3=[N+](C4=CC=CC=C4S3)CC.[I-]'

>>> cmpnd = Compound(compound\_string=smiles, identifier\_type='smiles')

>>> ikey = cmpnd.get\_inchi\_key()

>>> print(ikey)

MNQDKWZEUULFPX-UHFFFAOYSA-M

## CDK – Java

For linux on the server

**Install Apache Maven**

1. Go to https://maven.apache.org/download.cgi and download apache-maven-3.5.3-bin.tar.gz (or a newer version).
2. Upload apache-maven-3.5.3-bin.tar.gz to a new CDK directory in your workspace.
3. In CDK directory:~$ tar xvf apache-maven-3.5.3-bin.tar.gz
4. Add apache-maven-3.5.3 to .bashrc or .profile:
   1. In home directory:~$ nano .bashrc
   2. Add: export PATH=”~/path/to/apache-maven-3.5.3/bin:$PATH”
   3. Close and save file
   4. In home directory:~$ source .bashrc

**Install CDK**

Source: <https://github.com/cdk/cdk> and <https://github.com/cdk/cdk-build-util>

Compiling the CDK library

1. In CDK directory:~$ git clone <https://github.com/cdk/cdk.git>
2. In CDK directory:~$ cd cdk/
3. In CDK directory:~/cdk$ mvn package –DskipTests #check if the tests pass

This will produce a 'jar' file for each module located in each modules 'target/' directory. The uber jar with everything included is located in cdk/bundle/target/cdk-<version>.jar.

Creating the JavaDoc documentation for the API

1. In CDK directory:~/apache-maven-3.5.3$ git clone https://github.com/cdk/cdk-build-util
2. In CDK directory:~/apache-maven-3.5.3$ cd cdk-build-util
3. In CDK directory:~/apache-maven-3.5.3/cdk-build-util$ mvn install

Building a large bundled jar with all dependencies

1. In CDK directory:~/cdk$ mvn install -DskipTests=true
2. In CDK directory:~/cdk$ cd bundle
3. In CDK directory:~/cdk/bundle$ mvn package

**Install JDK and NetBeans**

1. Go to http://www.oracle.com/technetwork/java/javase/downloads/jdk-netbeans-jsp-142931.html and download jdk-8u171-nb-8\_2-linux-x64.sh (or a newer version).
2. Upload jdk-8u171-nb-8\_2-linux-x64.sh to the CDK directory in your workspace.
3. In CDK directory:~$ chmod +x jdk-8u171-nb-8\_2-linux-x64.sh
4. In CDK directory:~$ ./ jdk-8u171-nb-8\_2-linux-x64.sh
5. Then a GUI opens, and JDK and NetBeans can be installed. Store JDK and NetBeans in the CDK directory.
6. Add, export PATH="~/path/to/netbeans-8.2/bin:$PATH", to .bashrc (see Install Apache Maven, step 4)
7. In CDK directory:~/netbeans-8.2/bin$ netbeans $
8. The NetBeans GUI will open. You can look into and test the CDK code if you like (see https://github.com/cdk/cdk/wiki/Building-CDK).

**Run a script in Java**

1. Make a new project.
2. Right click on Libraries and then add JAR/folder.
3. Select and add all jar files shown.
4. Example script to depict a compound as an image (source: http://ctr.wikia.com/wiki/ Depict\_a\_compound\_as\_an\_image#CDK.2FJava).

package testcdk;

import org.openscience.cdk.CDKConstants;

import org.openscience.cdk.interfaces.\*;

import org.openscience.cdk.silent.SilentChemObjectBuilder;

import org.openscience.cdk.smiles.SmilesParser;

import java.awt.Color;

import org.openscience.cdk.depict.DepictionGenerator;

/\*\*

\*

\* @author stokm006

\*/

public class TestCDK {

public static void main(String[] args) throws Exception {

IChemObjectBuilder bldr = SilentChemObjectBuilder.getInstance();

SmilesParser smipar = new SmilesParser(bldr);

IAtomContainer mol = smipar.parseSmiles("CN1C=NC2=C1C(=O)N(C(=O)N2C)C");

mol.setProperty(CDKConstants.TITLE, "caffeine");

DepictionGenerator dptgen = new DepictionGenerator();

// size in px (raster) or mm (vector)

// annotations are red by default

dptgen.withSize(200, 250)

.withMolTitle()

.withTitleColor(Color.DARK\_GRAY);

dptgen.depict(mol)

.writeTo("~/path/to/CDK/caffeine.png");

}

}

1. Run the script in NetBeans
2. The result (caffeine.png) is stored in the CDK directory:

