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Manual

Image Comparator

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Step 1: Source code

git clone https://github.com/ontochem/ImageComparator.git

Step 2: Compile, build and execute the source code using maven

```
// compile on linux
git clone git@git.ontochem.intra:sbarnabas/imagecomparator.git
cd imagecomparator
mvn clean
mvn package
java -jar target/*-jar-with-dependencies.jar
```

```
// compile on mac
brew install maven
git clone git@git.ontochem.intra:sbarnabas/imagecomparator.git
cd imagecomparator
mvn clean
mvn package
java -jar target/*-jar-with-dependencies.jar
```

Step 3: Creating an input file

Format: <column 1: complete path of the image file with its name> comma <column 2: structure (structure can be either smiles or reaction smiles)>. A sample file is placed in the "src/main/resources/sample.txt"

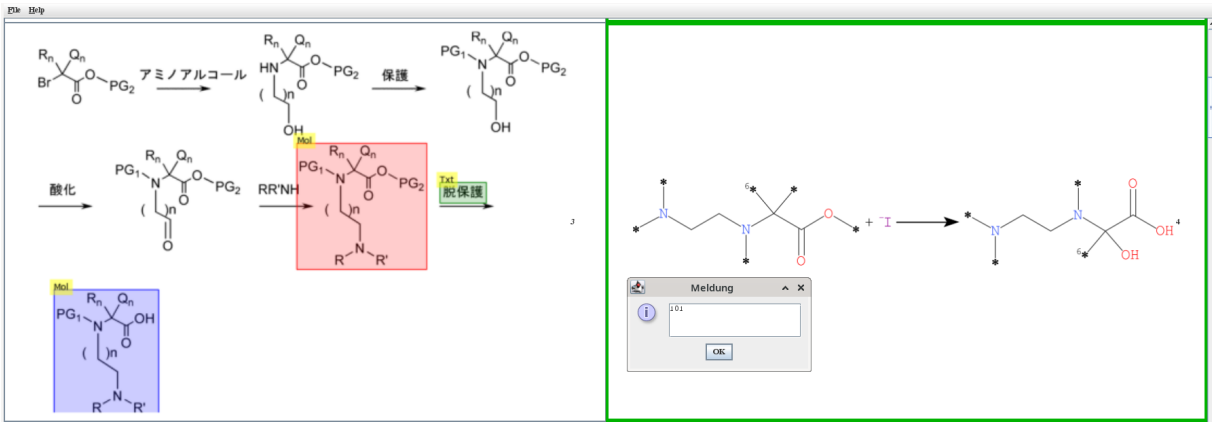
Step 4: Load input file or a restart file

After executing the source code (step 2), a graphical user interface will appear. Press the "File" button and load the input file (.txt) created in step 3. A restart file is generated when the "saveAs" button is clicked using image comparator software. This file has an additional third column with user comments. This restart file can also be loaded directly into the image comparator software without any modifications.

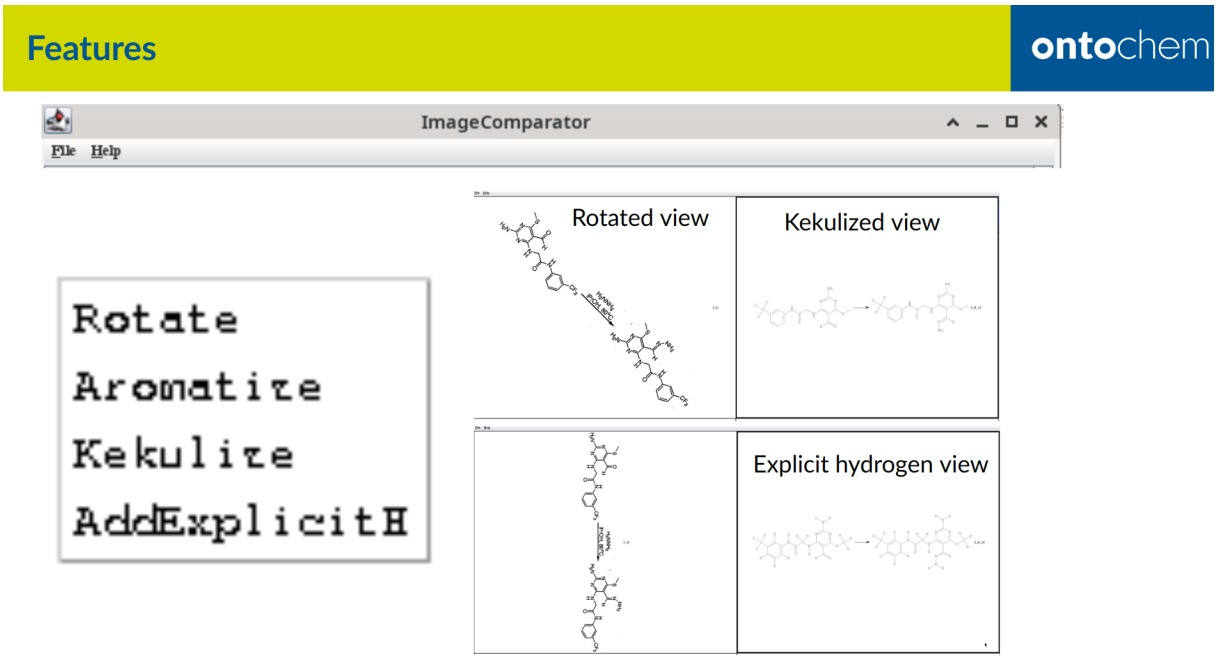
Step 5: Mouse clicks

left click: prints information about the image on screen

right click: message icon appears and the user can enter his/her comments in it, which will be saved and the image icon is highlighted in green



middle click: changes the display of the smiles or reaction smiles based on user choice (kekulization, aromatization, explicit hydrogen, rotation)



Step 6: Save output file

For each image, right click on the image and add a comment in the widget. Once you have finished adding comments to all the images, press the “saveAs” button in the menubar and save it. The response will be saved in the output file.
Format: Image file, structure, comments