



Manual

Image Comparator

AUTHOR(S)

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Halle (Saale), 20 June, 2023

Step 1: Source code

```
git clone git@git.ontochem.intra:sbarnabas/imagecomparator.git
```

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

```
cd imagecomparator
mvn clean compile exec:java
```

Step 3: Creating input file

Format: imageFile structure (structure can be either smiles or reaction smiles)

Extension: create a file in this format and save it as ".txt"

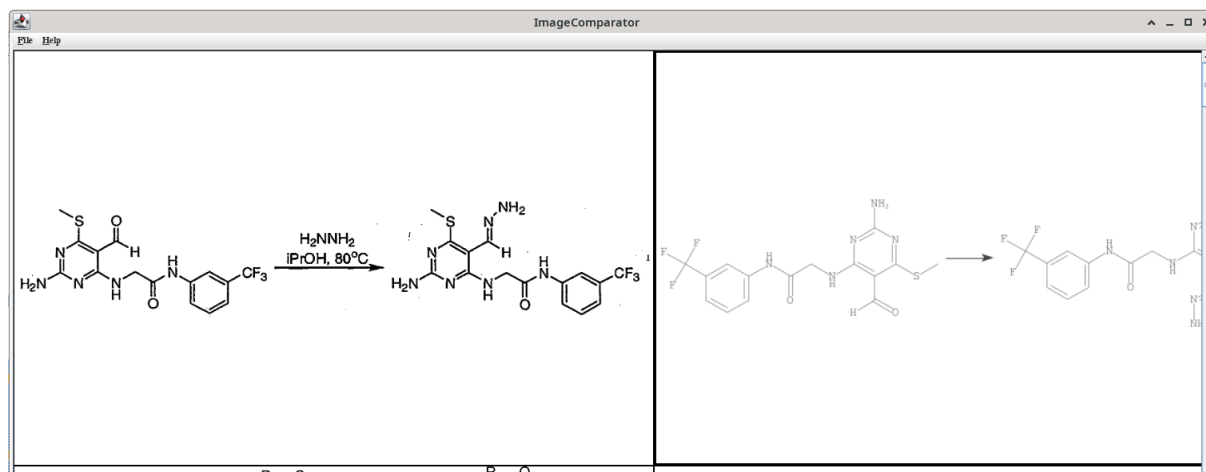
Example: <image file.tif>space<reaction smiles or smiles>

Step 4: Load input file

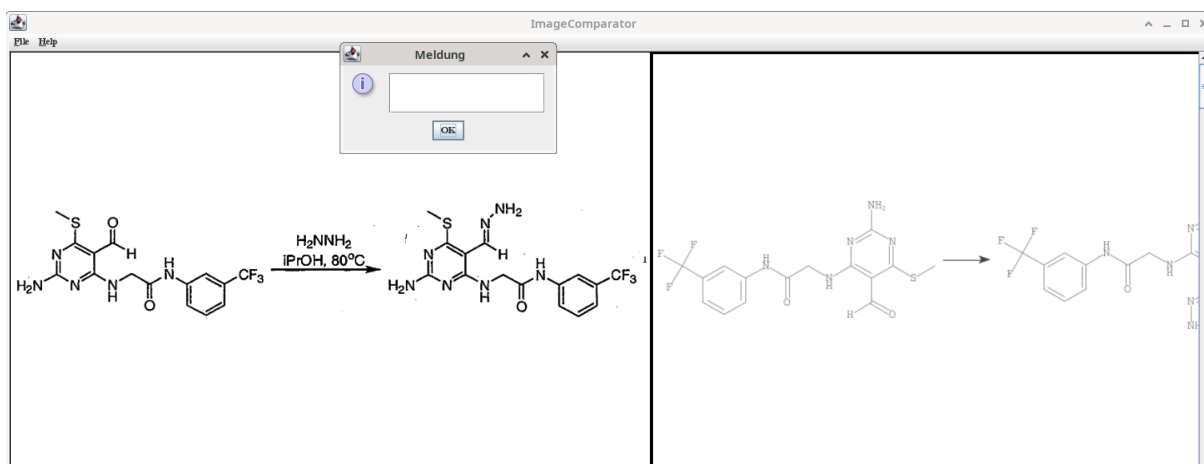
After executing the source code (step 2), a graphical user interface will appear. Press the "File" button and load the input file (.txt) created in step 3.

Step 5: Mouse clicks

left click: prints information about the image on screen

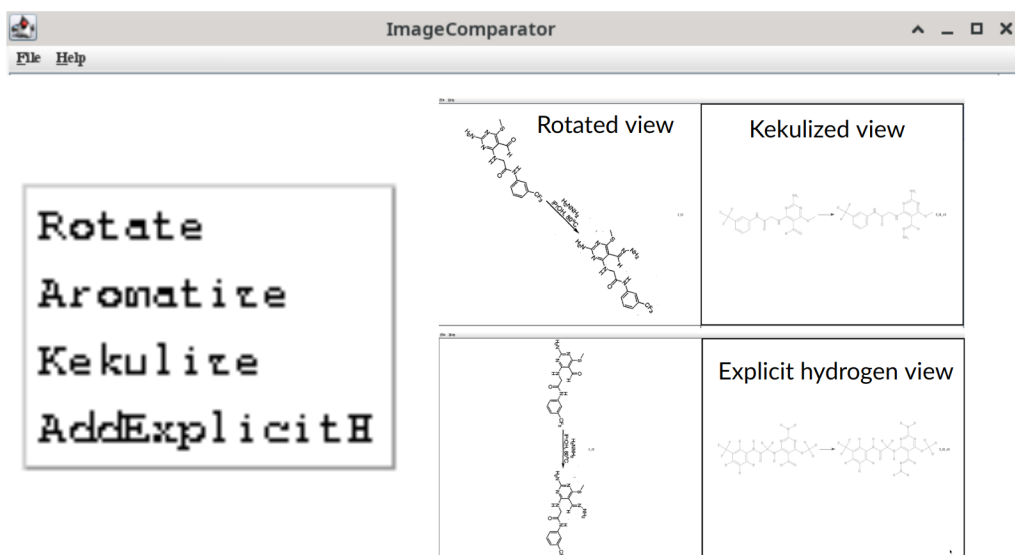


right click: message icon appears and the user can enter his/her comments in it, which will be saved



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

Features



Step 6: Save output file

On each image, right click and add a user comment to the respective image. 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 Id, Image file, structure, comments

Example:<serial No>,<image file.tif>,<reactions miles>,<user comments>