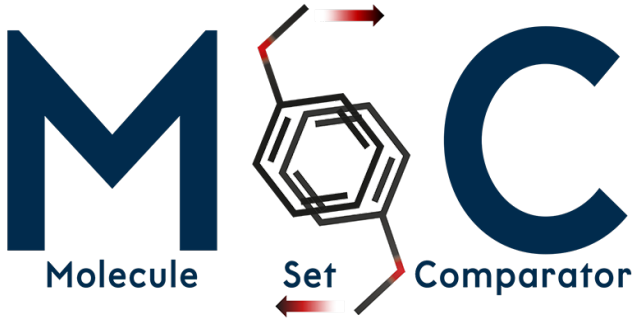


# Molecule Set Comparator (MSC)
## - A short introduction -

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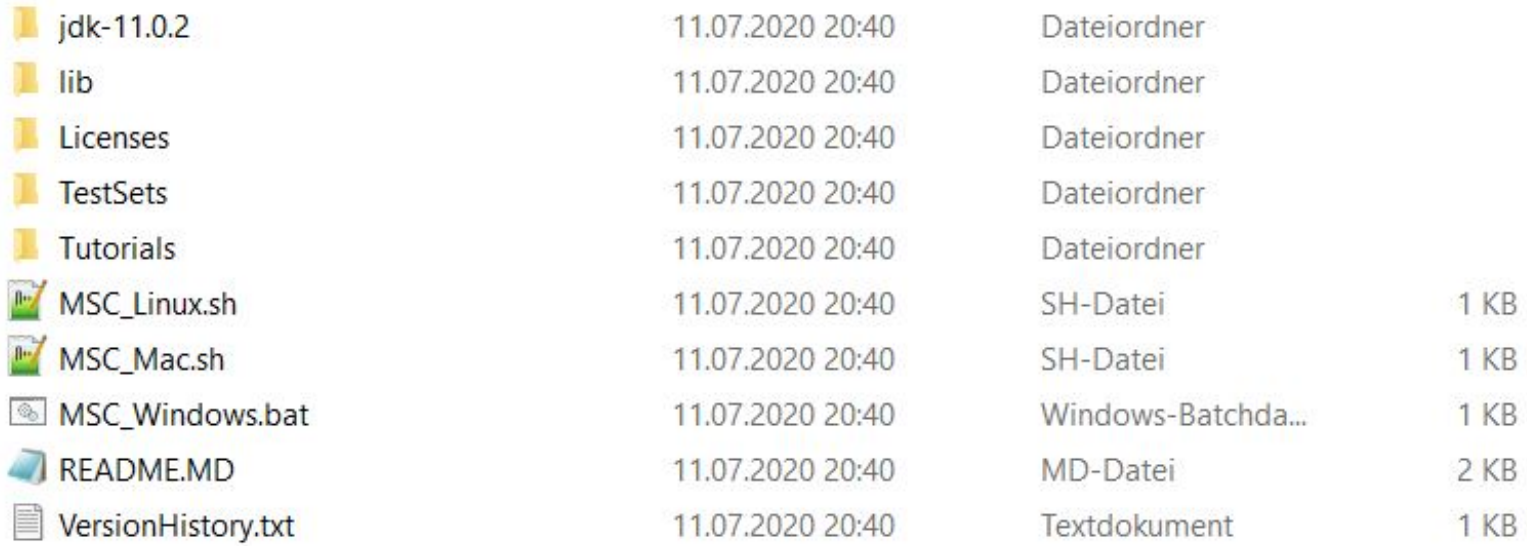
# Starting the application

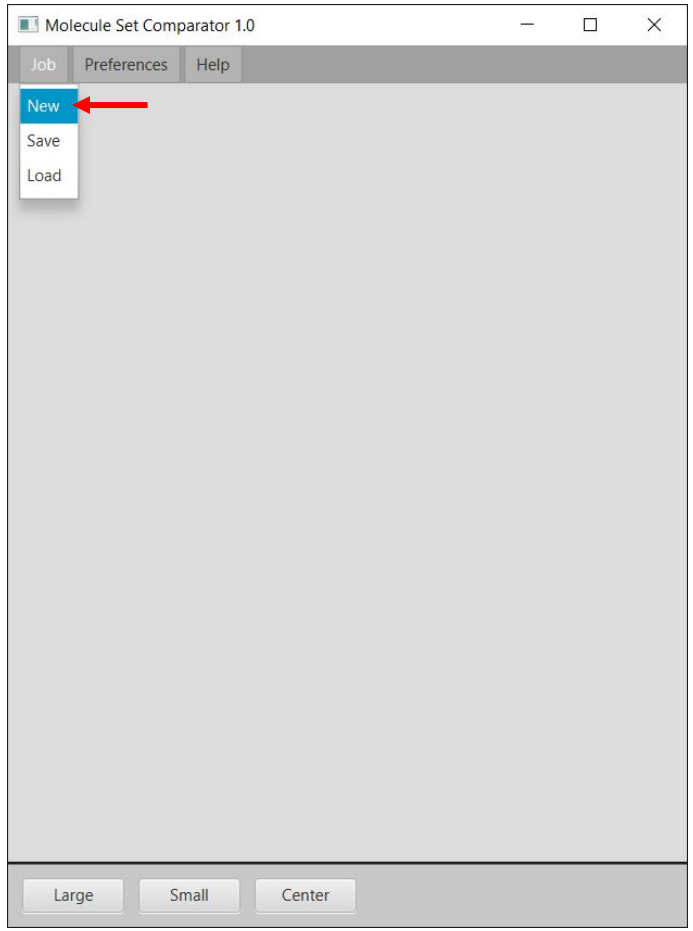
- Open the “MSC_1.0” folder
- Select and execute one of the “MSC_<OS>” files where <OS> should be your operating system.
- To have a smooth performance, the RAM allocation to the JVM is set to 4GB as a default.
- If you want to start the MSC with a different RAM specification, you must edit one of the existing “MSC_<OS>” files by changing the “-Xmx?g” option in the third row. ? specifies the amount of RAM (in gigabytes) that will be allocated to the JVM

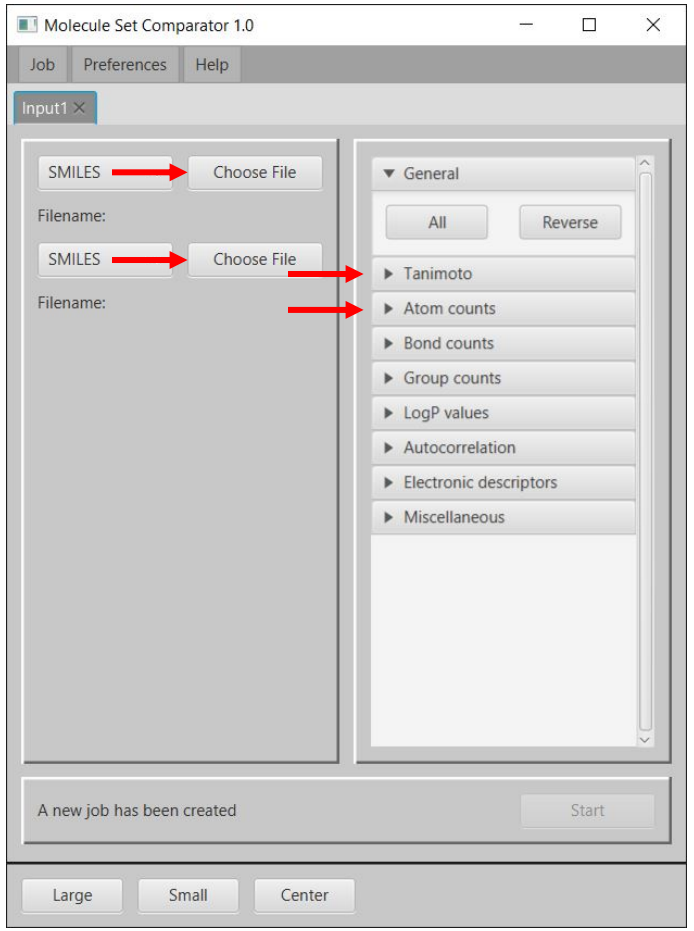


| | | | |
|---|---|---|---|
| jdk-11.0.2 | 11.07.2020 20:40 | Dateiordner | |
| lib | 11.07.2020 20:40 | Dateiordner | |
| Licenses | 11.07.2020 20:40 | Dateiordner | |
| TestSets | 11.07.2020 20:40 | Dateiordner | |
| Tutorials | 11.07.2020 20:40 | Dateiordner | |
| MSC_Linux.sh | 11.07.2020 20:40 | SH-Datei | 1 KB |
| MSC_Mac.sh | 11.07.2020 20:40 | SH-Datei | 1 KB |
| MSC_Windows.bat | 11.07.2020 20:40 | Windows-Batchda... | 1 KB |
| README.MD | 11.07.2020 20:40 | MD-Datei | 2 KB |
| VersionHistory.txt | 11.07.2020 20:40 | Textdokument | 1 KB |

# Initializing a new job

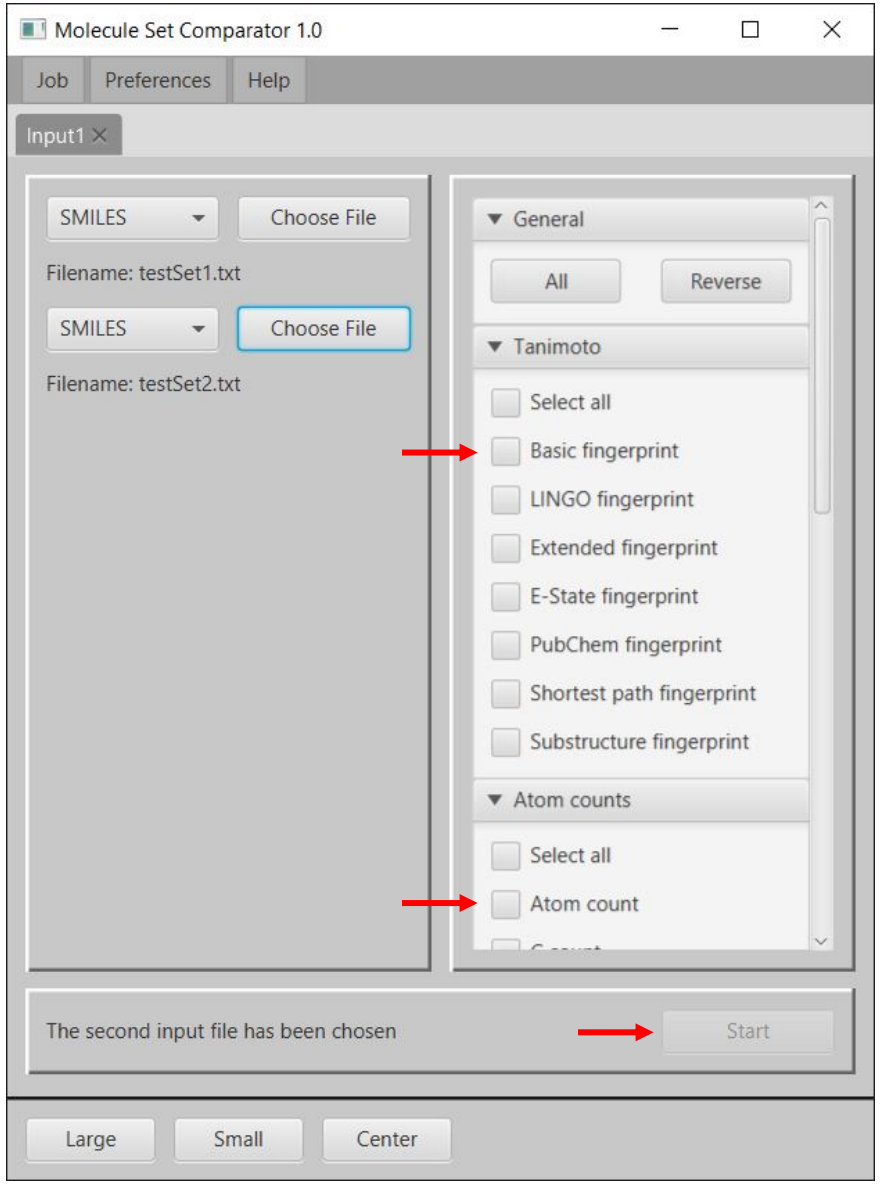
- Create a new job by choosing **Job -> New** in the menu bar.
- Then click on the **Choose File** button.
- Navigate to the *"TestSets"* folder in the MSC folder and select the *"testSet1.txt"* file.
- Repeat the same steps to select the *"testSet2.txt"* file.
- Finally, click the **Tanimoto** and **Atom counts** drop-down menus (marked with red arrows) to expand them.



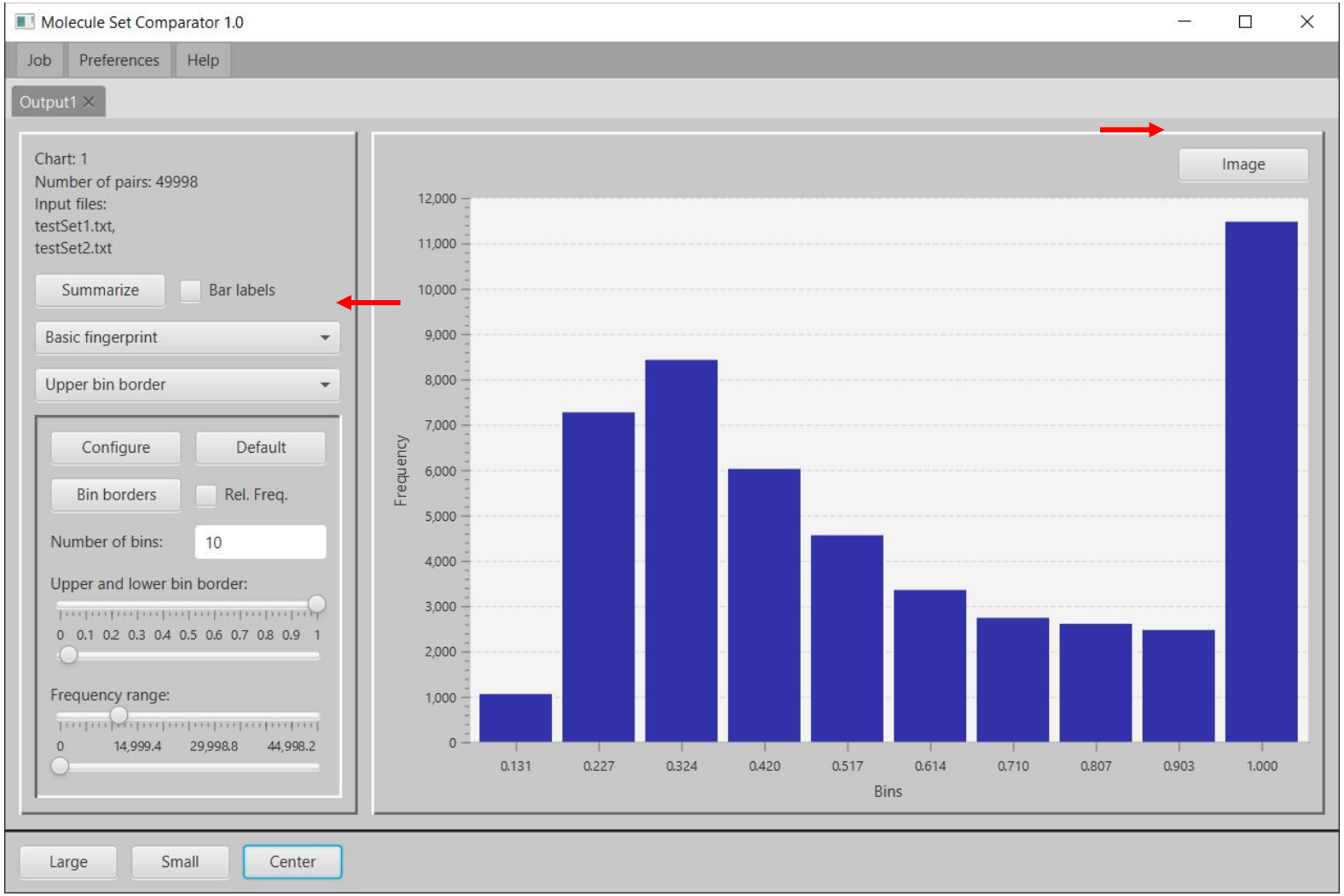
# Initializing a new job

- Select the **Basic fingerprint** and **Atom count** checkboxes.
- Then start the job by pressing the **Start** button and wait until the job finished.



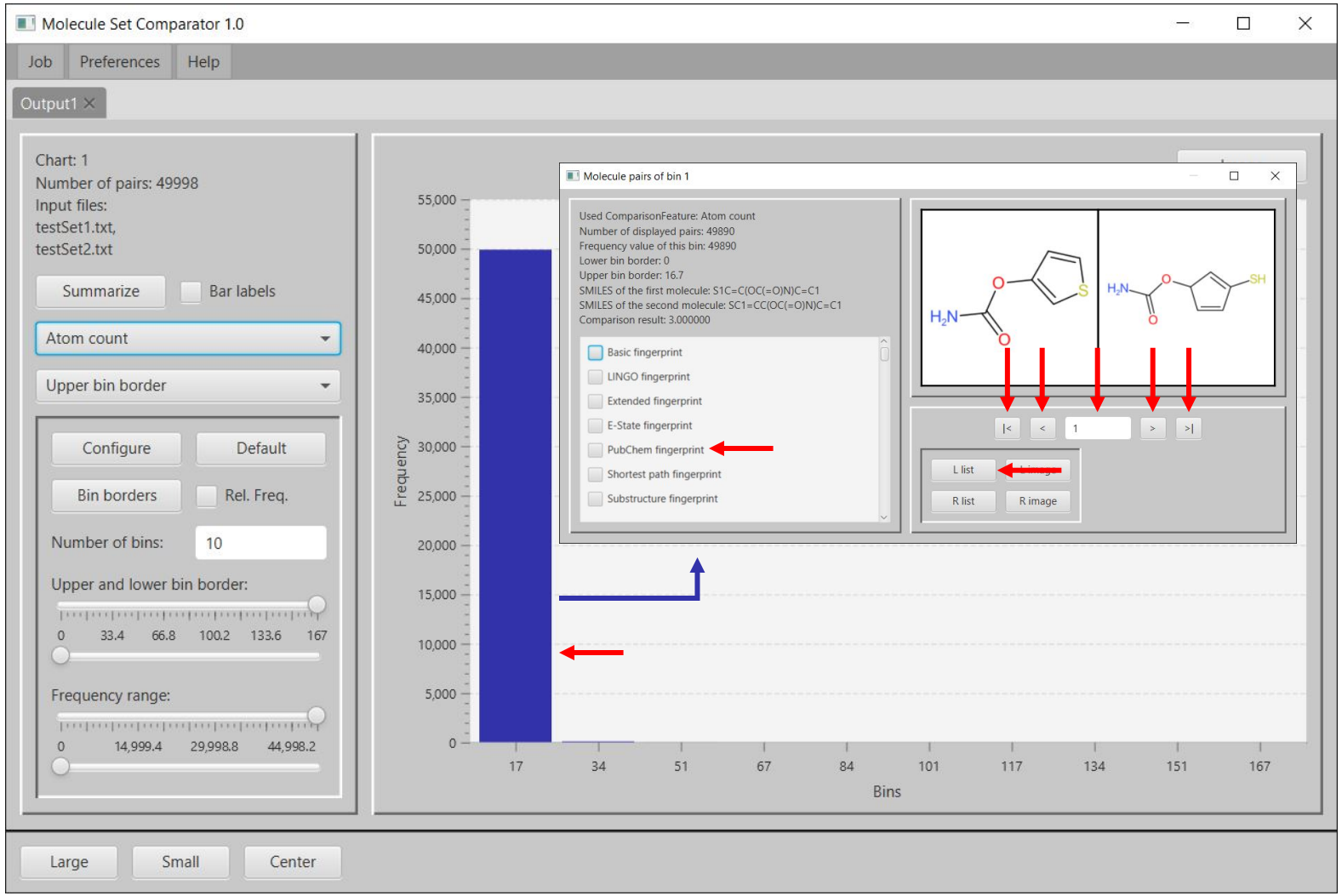
# The output tab

- Once the execution completes, a separate tab with the results will pop up.
- You can save the chart as a PDF file by clicking on the **Image** button.
- Switch to the chart of the “Atom count” descriptor by pressing the upper choice box and choosing “Atom count”



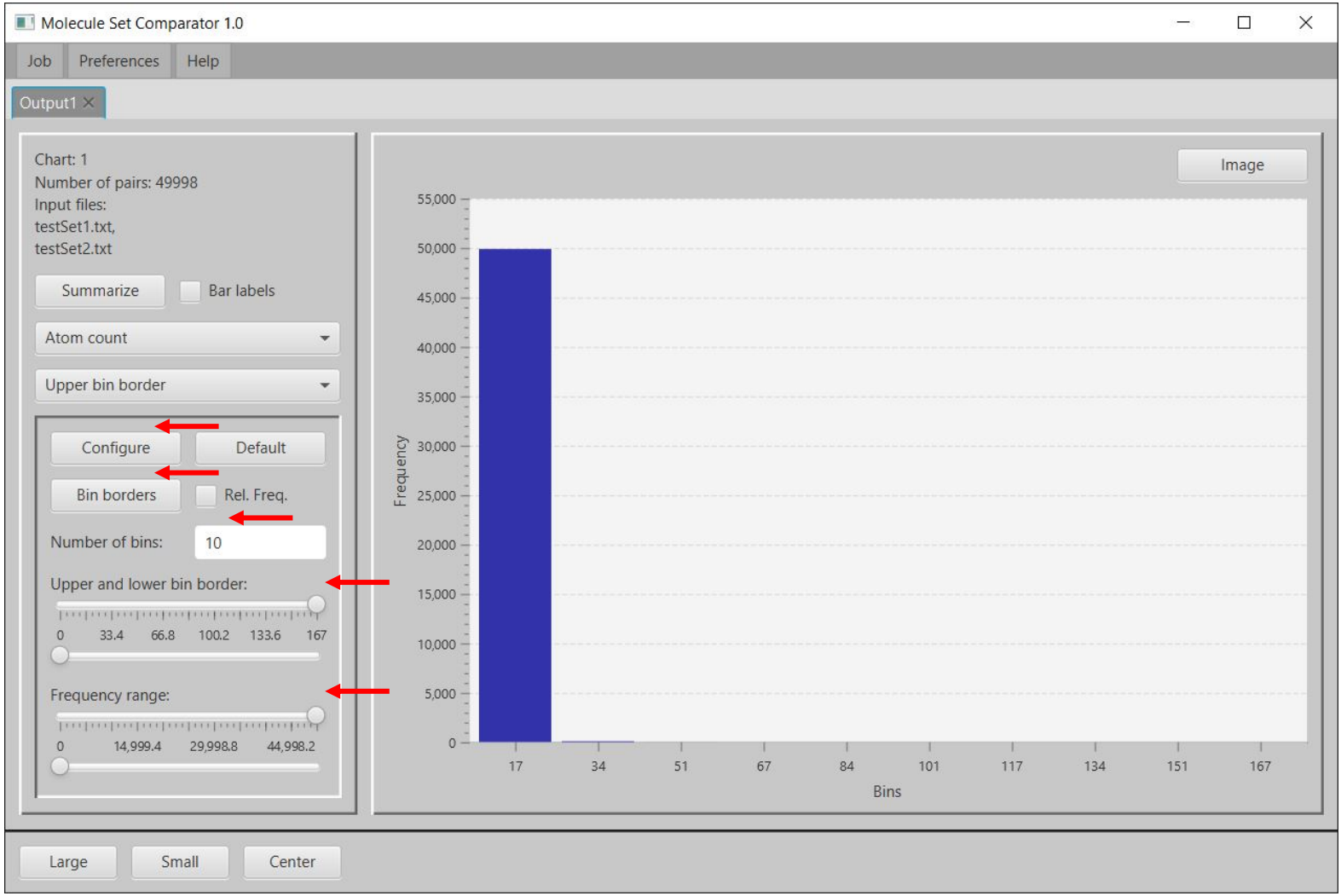
# Detail window

- To open the detail window, click on the marked bin.
- Use the arrow buttons to browse through the molecule pairs contained in this bin or use the text field to go to a specific position in the list.
- Save a list that contains the left molecule of every pair by pressing the **L list** button
- Select the **PubChem** fingerprint checkbox to calculate an additional Tanimoto coefficient
- Then close the *"Molecule pairs of bin 1"* window.



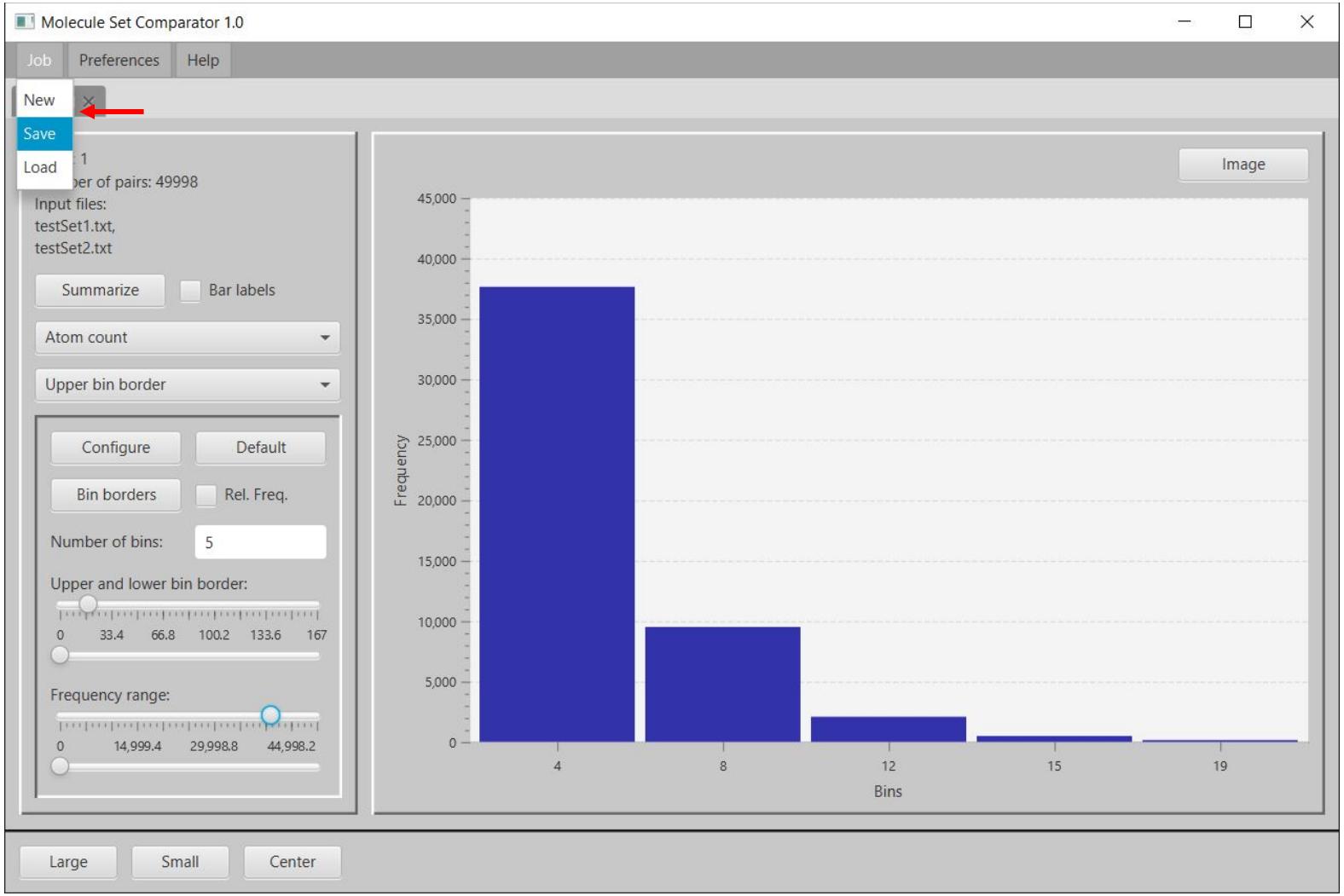
# Chart configuration

- Change the upper border of the last bin by using the provided slider.
- Change the range of the y-axis by using the provided slider.
- The bin borders and y-axis range can also be set explicitly by pressing the **Configure** or **Bin borders** buttons
- Change the number of bins to 5 by typing in the text field and hitting the enter key



# Saving the output

- To save the output, select **Job -> Save** in the menu bar.
- Select or create a folder where you want the output files to be saved.
- These results can be reloaded by selecting **Job -> Load** in the menu bar and selecting the corresponding folder.



# Changing the preferences

- Open the *"Other preferences"* dialog by choosing **Preferences -> Others** in the menu bar.
- Here:
  - The preferences for the number of parallel threads to be used for computations,
  - The default number of bins,
  - The number of molecule pairs to be saved when saving a job,
  - And the image quality for saved images can be set.