Molecule Set Comparator (MSC)
- A short introduction -

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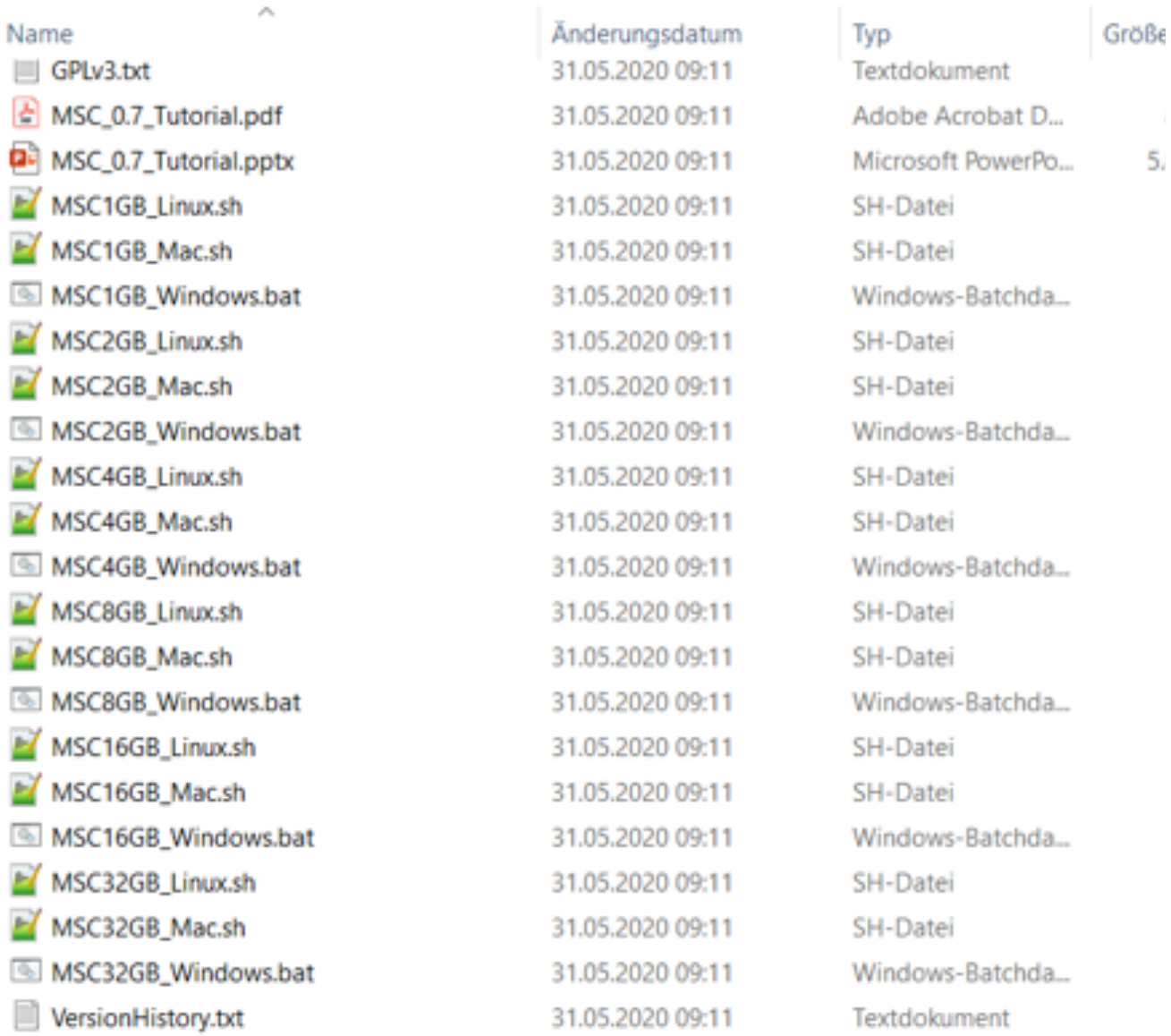
Starting the application

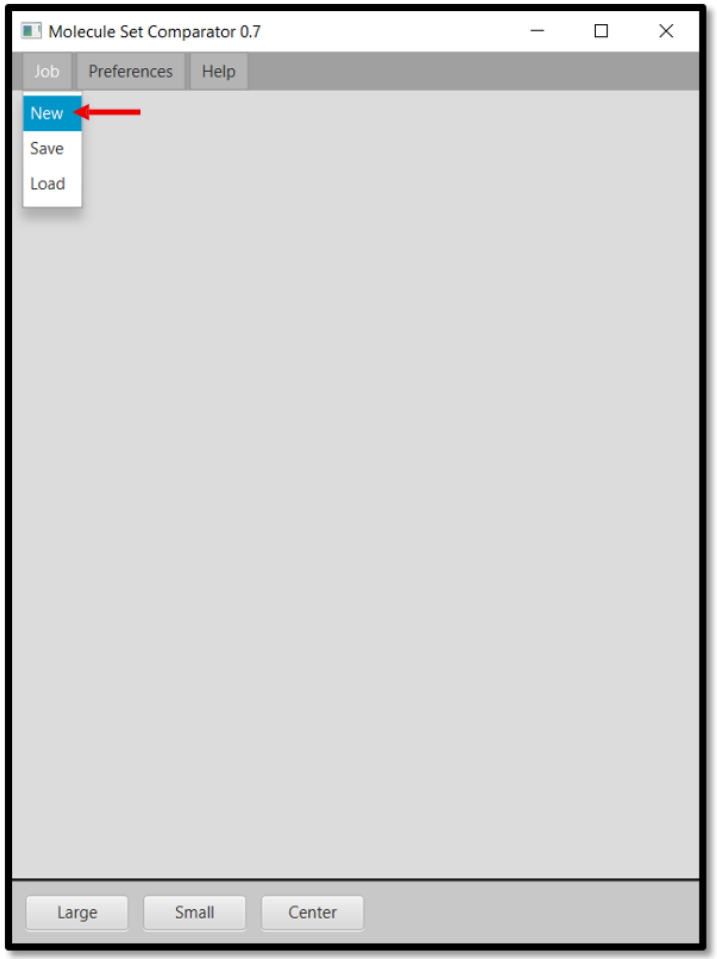
- Open the *“MSC_1.0”* folder.
- Select and execute one of *“MSC_?GB_<OS>”* files where <OS> should be your operating system and ? specifies the amount of RAM that must be allocated for the JVM in gigabytes.

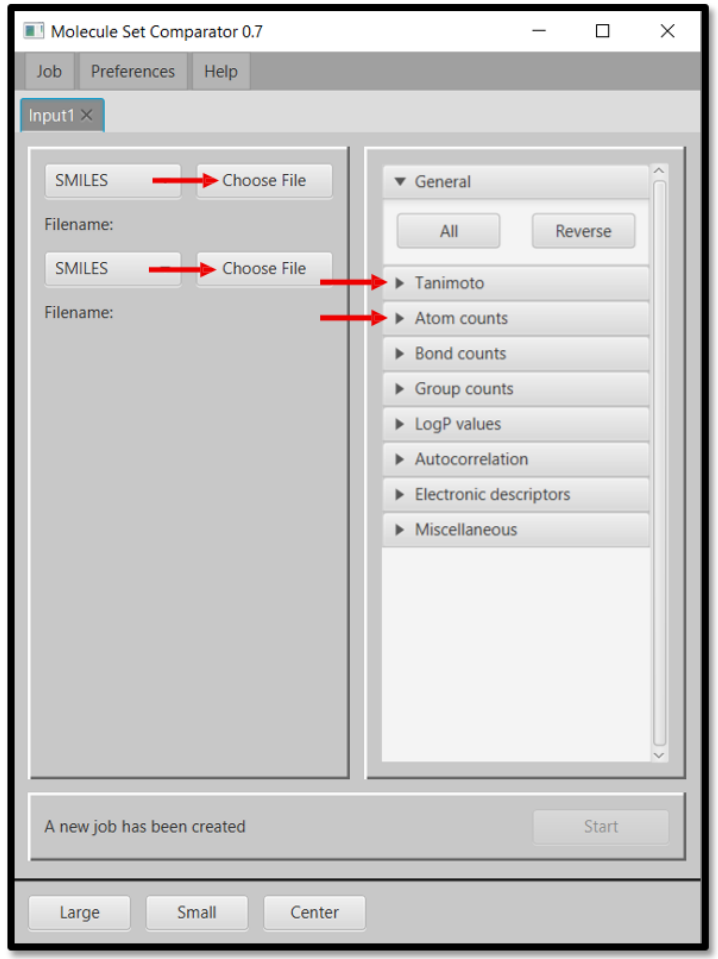


Name	Änderungsdatum	Typ	Größe
GPLv3.txt	31.05.2020 09:11	Textdokument	
MSC_0.7_Tutorial.pdf	31.05.2020 09:11	Adobe Acrobat D...	
MSC_0.7_Tutorial.pptx	31.05.2020 09:11	Microsoft PowerPo...	5.
MSC1GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC1GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC1GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
MSC2GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC2GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC2GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
MSC4GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC4GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC4GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
MSC8GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC8GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC8GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
MSC16GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC16GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC16GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
MSC32GB_Linux.sh	31.05.2020 09:11	SH-Datei	
MSC32GB_Mac.sh	31.05.2020 09:11	SH-Datei	
MSC32GB_Windows.bat	31.05.2020 09:11	Windows-Batchda...	
VersionHistory.txt	31.05.2020 09:11	Textdokument	

Initializing a new job

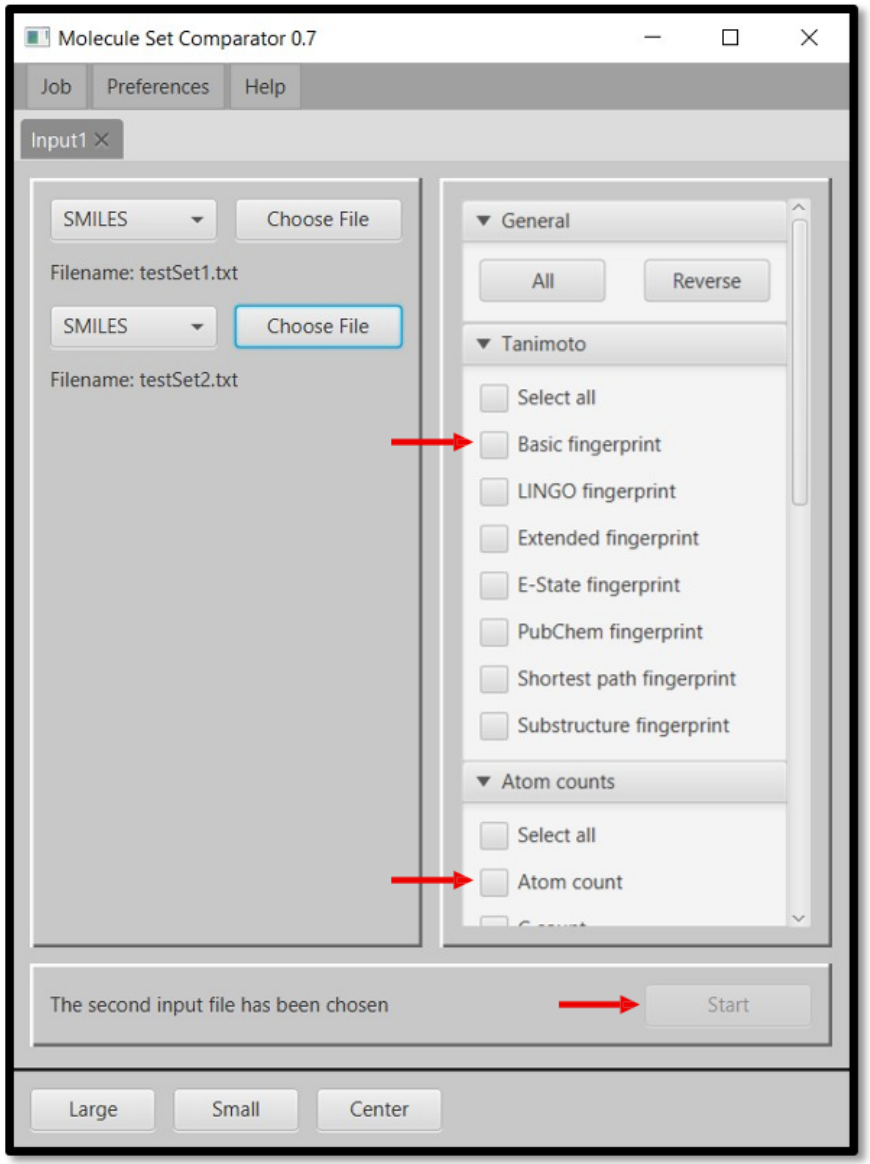
- Create a new job by choosing **Job -> New** in the menu bar.
- Then click on **Choose File** button.
- Navigate to the *"TestSets"* folder under the MSC folder and select the *"testSet1.txt"* file.
- Repeat the same steps to select the *"testSet2.txt"* file.
- Finally, press the **Tanimoto** and **Atom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





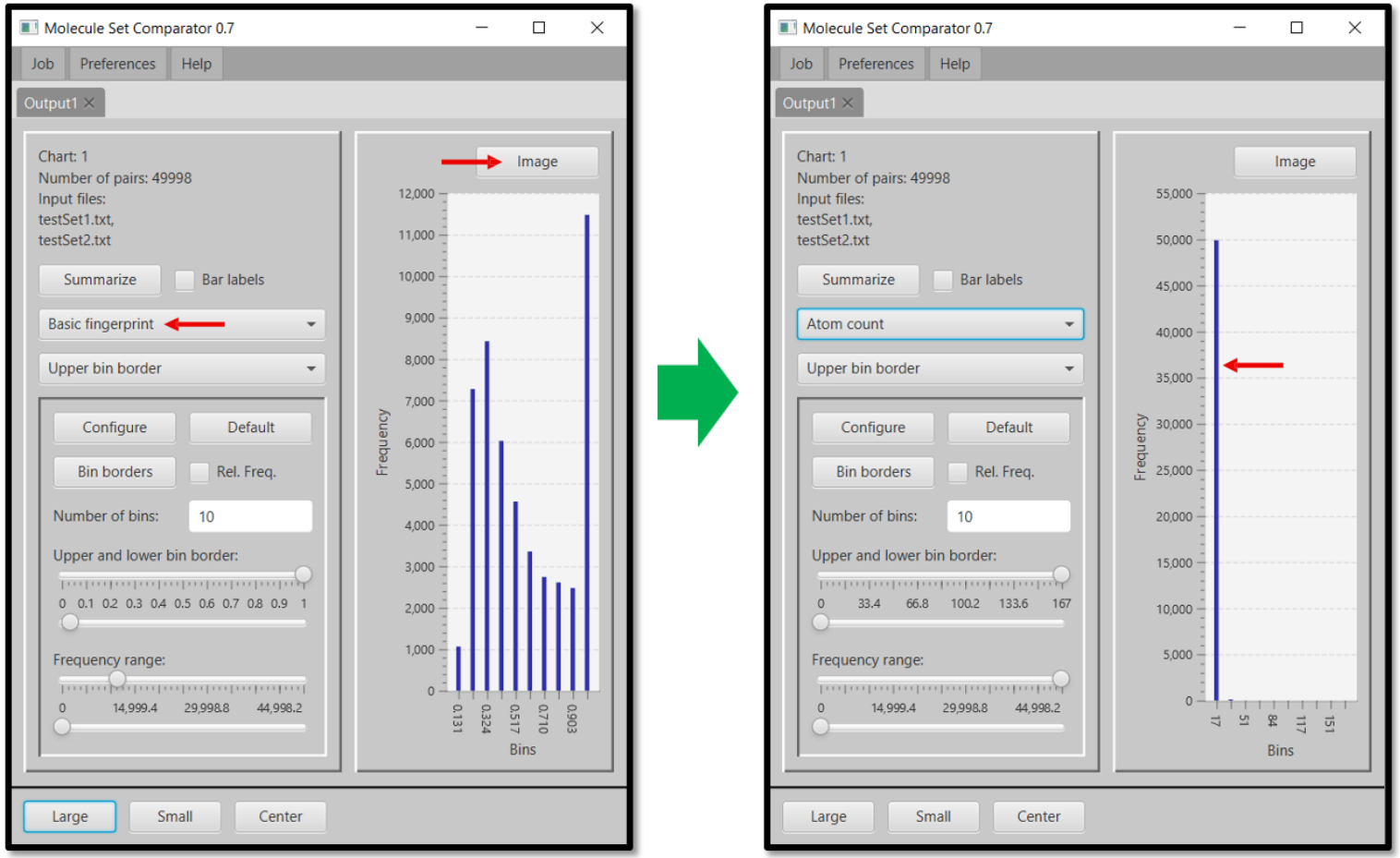
Initializing a new job

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



The output tab

- You can save the charts as PDF files by clicking on the Image button.
- Switching to the next descriptor can be done using the drop down menu.
- To get more fine detailed information you can click on the bins.



Detail window

- Use the arrow buttons to browse through the molecule pairs or use the text field to go to a specific position in the list.
- To save a list of molecules that contains the molecule in the visualized in the left side , click on the **L list** button.
- For more information, additionally you can select the **PubChem fingerprint** checkbox to calculate another Tanimoto coefficient.
- To get back to the previous window, close the *“Molecule pairs of bin 1”* window.

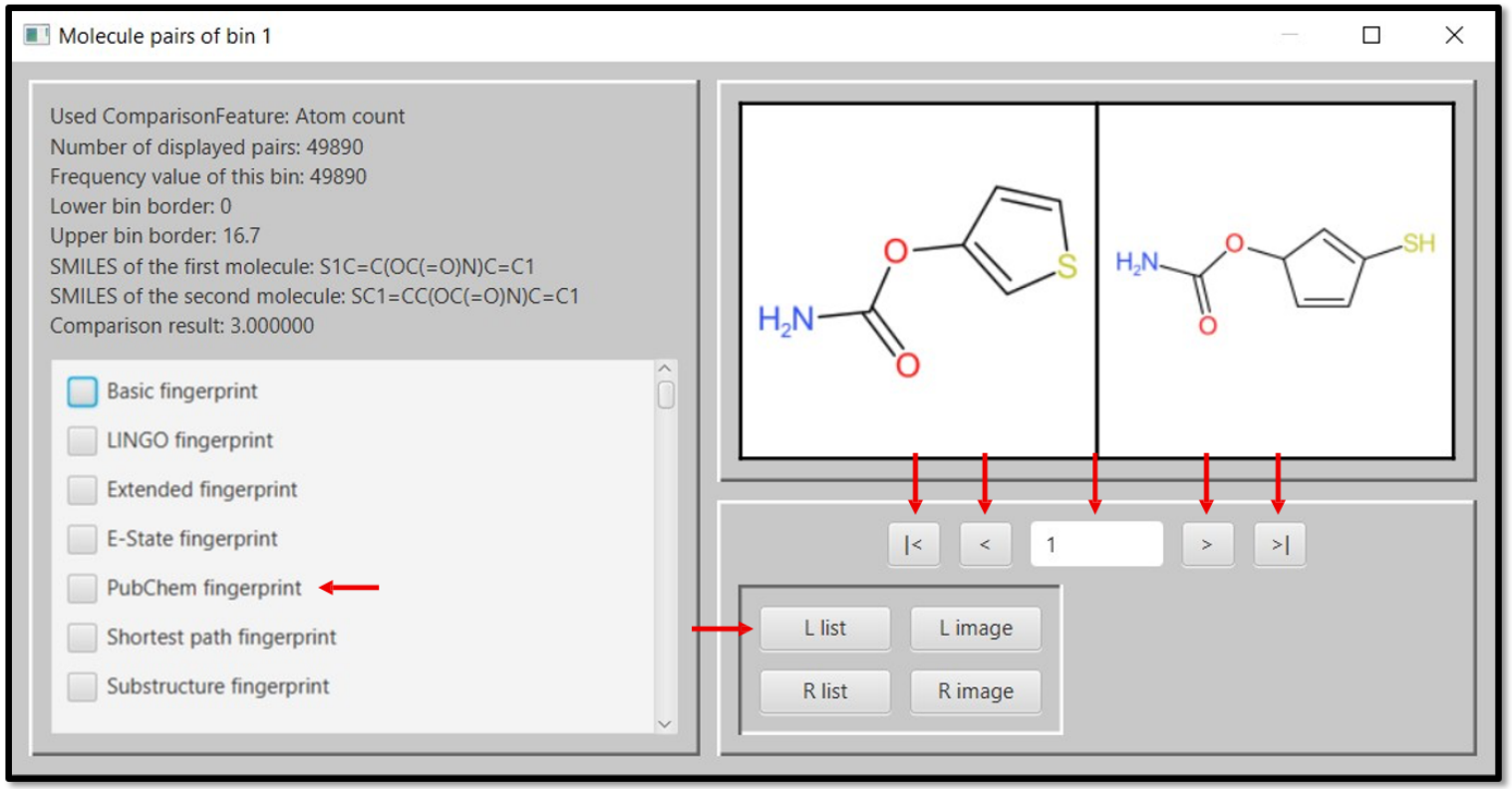
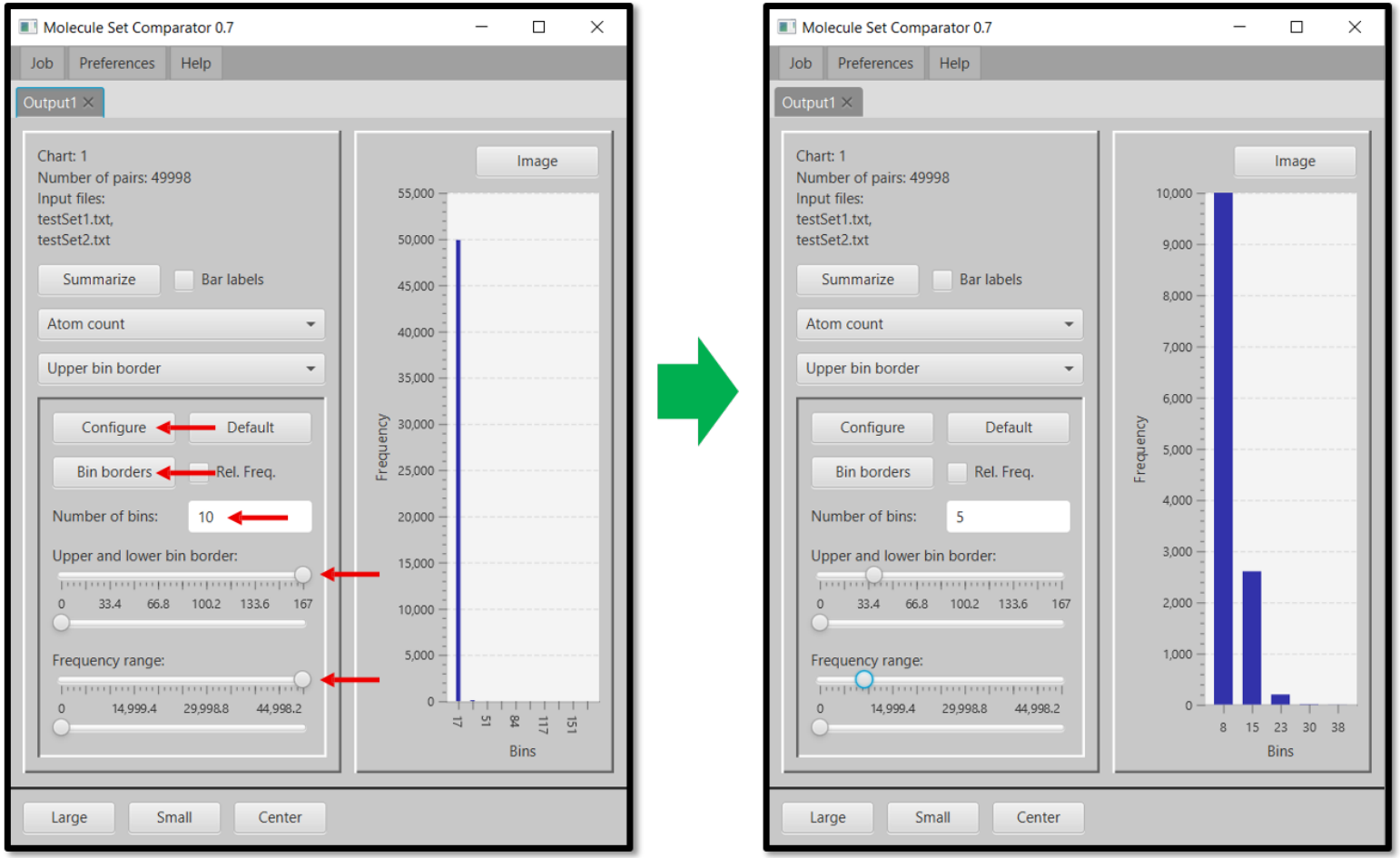


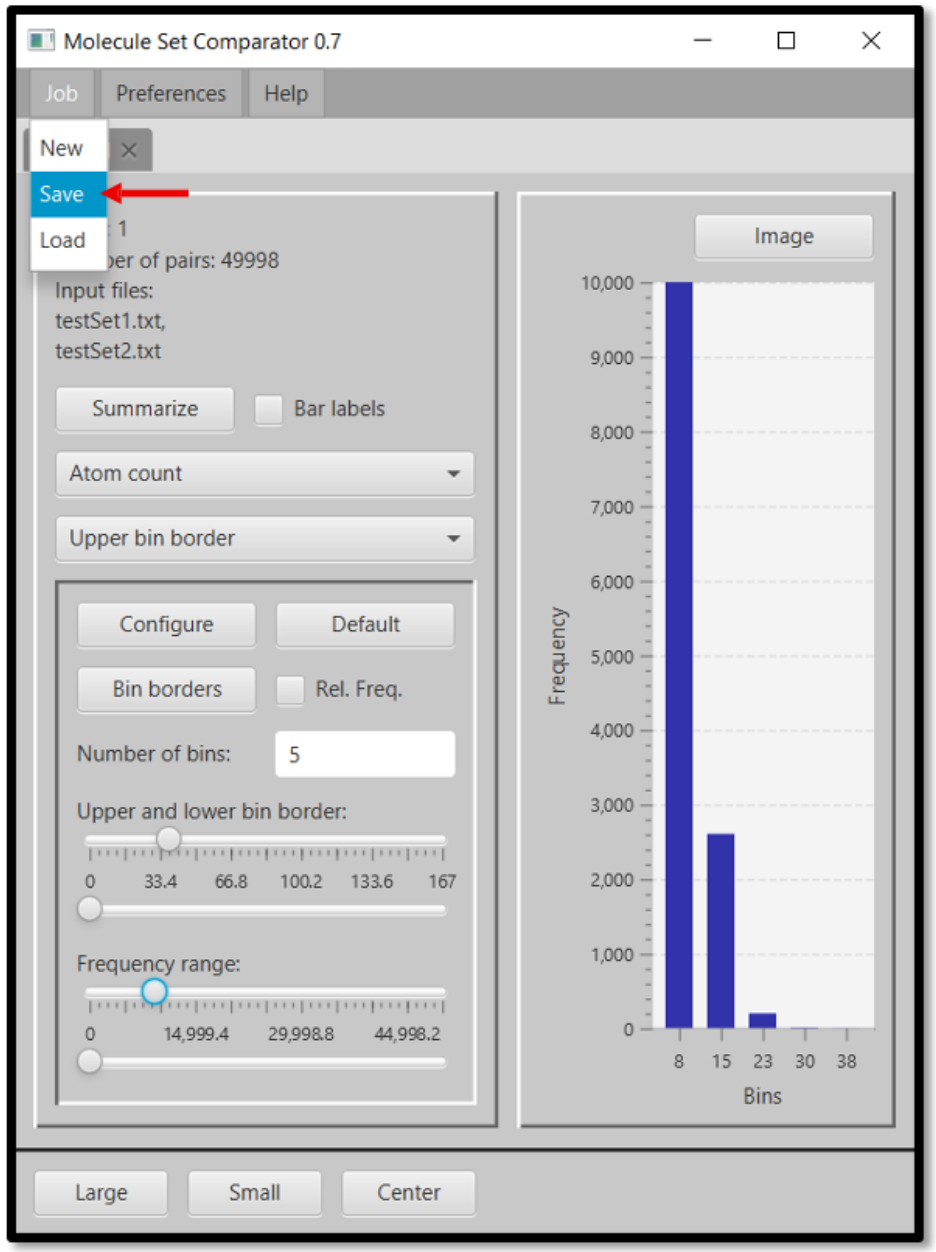
Chart configuration

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



Saving the output

- To save the output ,select **Job -> Save** in the menu bar.
- Select or create a folder where you need the output files to be saved.
- These results can be loaded back 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 we save a job .
  - And the image quality can be set.