Using SIRIUS for compound annotation:

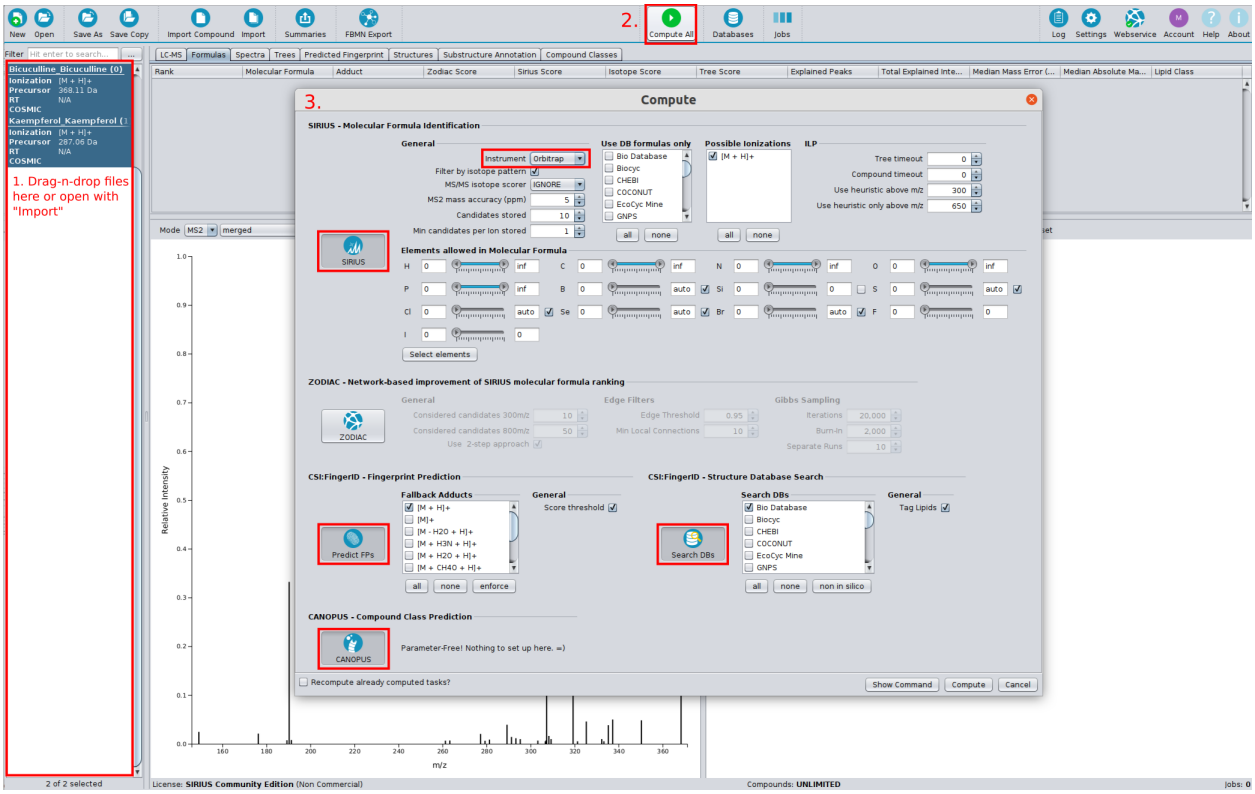
The full set of documentation including videos, a book chapter and workshops can be found on the Sirius webpage

The following is a very abridged tutorial on using SIRIUS/CSI:FingerID/Canopopus for compound structure prediction

***Tutorial/Demo data from:

(https://boecker-lab.github.io/docs.sirius.github.io/quick-start/#analyzing-multiple-compounds)***

SIRIUS's "Batch mode" corresponds to analyzing many compounds at once, each having one or more mass spectra. Obviously, you can also use this workflow to analyze a single compound.



Analyze multiple compounds in a view simple steps. Steps in figure do not directly correspond to detailed steps below.

1. Move the files `demo-data/ms/Bicuculline.ms` and `demo-data/ms/Kaempferol.ms` and from the demo data via Drag and Drop into the application window.

2. The two compounds are now displayed in the compound list.

3. Just check if the ionization and parent mass is correctly annotated. You can change this values by right-clicking on the compound and then on *Edit*.

4. Click on the *Compute All* button.

5. Select SIRIUS.

6. You can now select the allowed elements, the instrument type as well as the maximal allowed mass deviation. Be aware that this settings will be used for all imported compounds

7. Choose *Orbitrap* in the instrument field and press *OK*

8. Select *Predict FPs* to predict the compounds' molecular fingerprints with CSI:FingerID.

9. Select *Search DBs* to search compounds in a structure database with CSI:FingerID. (turn on the different databases, click non in silicp)

10. Select *CANOPUS* to predict compound classes (database-free).

11. Click *Compute*.

12. A *gear* symbol occurs on the lower right corner of each compound. This means that the compound is part of a computation job.

13. Sometimes a computation might take a long time (e.g. for compounds with a lot of elements or very high masses). You can cancel running computations by selecting *Cancel All* in the toolbar.

14. Inspect results with the help of the *Formulas*, *Structure* and *Compound Classes* views. Structure and compound class annotations are always based on a selected molecular formula candidate of the compound. Even more details can be found by looking at the *Substructure Annotation* and *Predicted Fingerprint* views.