

---

# AEROSOLOMICS QUICK START GUIDE

---

This Quick Start Guide is intended to explain the basic aspects of using the *aerosolomics* database for Compound Discoverer (Thermo Fisher Scientific) and MZmine 3. The spectra were recorded using a high-resolution hybrid quadrupole-Orbitrap mass spectrometer equipped with a higher-energy collisional dissociation cell with stepped collision energies of 15, 30, and 45 eV. In general, a good agreement of the spectra of different instruments can be seen. However, if another instrument (or energies) were used, the parameters may need to be adjusted and the results interpreted with caution.

When using the database for your publications, please cite:

Thoma, M., Bachmeier, F., Gottwald, F. L., Simon, M., and Vogel, A. L.: Mass spectrometry-based *aerosolomics*: a new approach to resolve sources, composition, and partitioning of secondary organic aerosol, *Atmos. Meas. Tech. Discuss.* [preprint], <https://doi.org/10.5194/amt-2022-221>, in review, 2022.

## Download the *aerosolomics* database

To use the *aerosolomics* database, please download the “aerosolomics\_db.zip” folder for using Compound Discoverer (Thermo Fisher Scientific) or the “aerosolomics\_msp.zip” folder for using MZmine (v3.0 or later) from our [homepage](#). The folders consist of libraries for each chemical system studied.

A free demo version of Compound Discoverer is available on the Thermo Fisher Scientific [homepage](#) (please note that Compound Discoverer is only available for Microsoft Windows). MZmine 3 can be downloaded via [GitHub](#) (Microsoft Windows, Mac OS, and Linux).

---

For questions or comments please contact us:

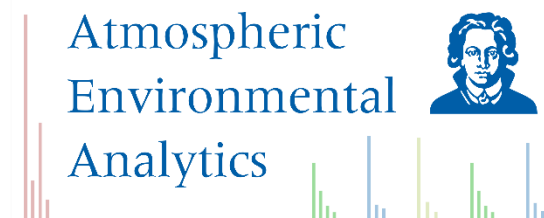
Institute for Atmospheric and Environmental Sciences

Research group: Atmospheric Environmental Analytics

Altenhöferallee 1, 60438 Frankfurt/Main

Prof. Dr. Alexander L. Vogel

[Aerosolomics@dlist.server.uni-frankfurt.de](mailto:Aerosolomics@dlist.server.uni-frankfurt.de)



## Application with Compound Discoverer

Before application of the *aerosolomics* database, the db-files must be imported into the “List and Libraries Manager”

(1). Open “Spectral Libraries” (2) and “Import ...” (3) the required files.

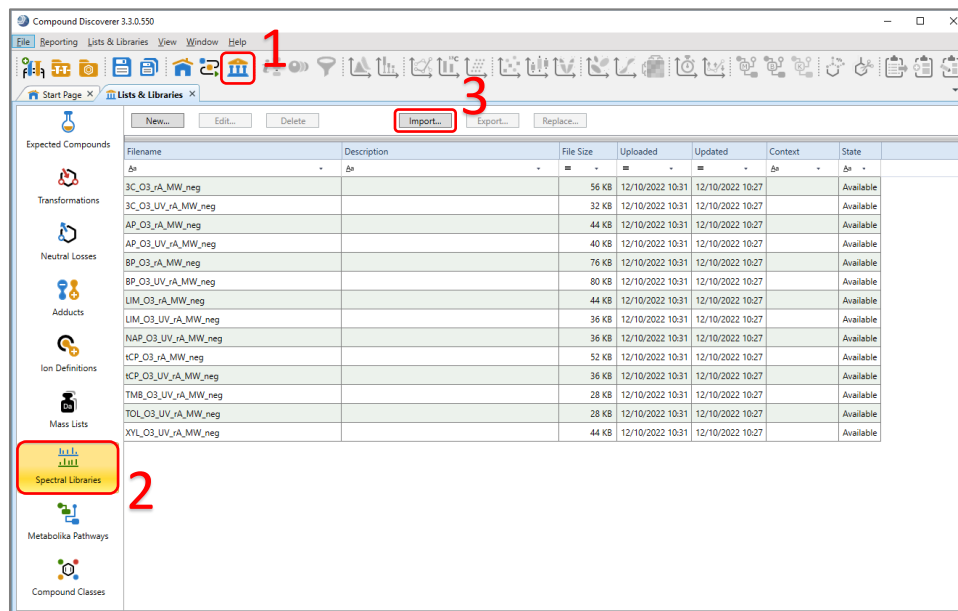


Figure 1. Compound Discoverer (v.3.3) List and Libraries Manager.

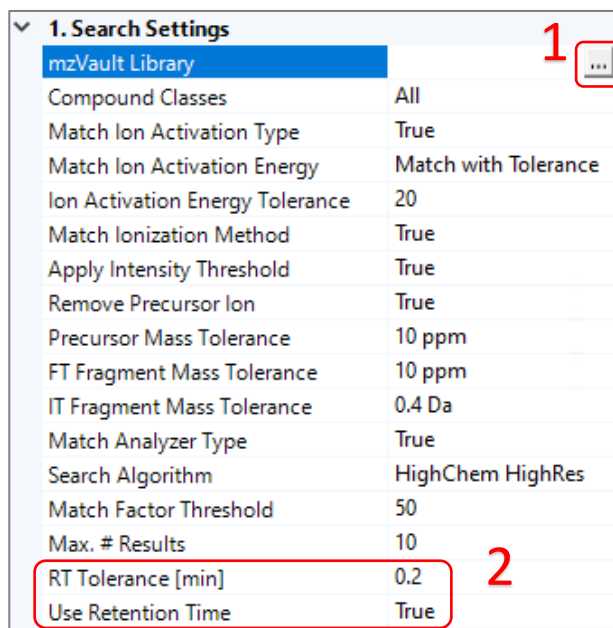


Figure 2. Proposed parameters of the “Search mzVault” node. The final settings depend on the devices and experimental settings being used.

To match fragmentation spectra of the database with those of the samples the “Search mzVault” node must be used in the workflow.

The required libraries can be selected by clicking the three points next to “mzVault Library” (1). Afterwards, the final settings can be made.

Note: Using the retention time (2) is not mandatory but increases the level of confidence for an identification. Isomeric structures often fragment in very similar ways, making identification difficult without retention time.

To include the outcome of the “Search mzVault” node in the results of the study you have to set one “Data Source” in the “Assign Compound Annotations” node to “mzVault Search”.

The outcome is implemented in the result table for each compound as well as in the “mzVault Results” tab.

## Application with MZmine (v.3.0 or later)

To use the database with MZmine 3, please download the “aerosolomics\_msp.zip” on our homepage. The msp-files can be imported into the software (“Raw data methods” → “Raw data import” → “Import spectral libraries”).



Figure 3. MZmine 3 (v.3.2.8) interface. Libraries can be imported via “Raw data import”.

To match the spectra of the database with your samples use the “Spectral library search” in your workflow (“Feature list methods” → “Annotation” → “Search spectra” → “Spectral library search”). Select the desired libraries (1) and make the desired setting of the parameters.

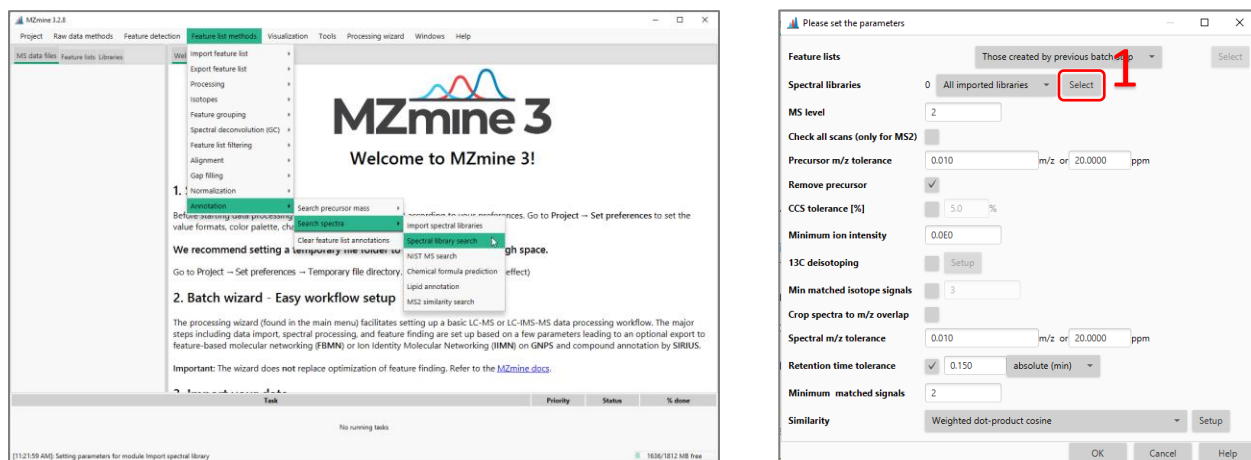


Figure 4. Left: Spectral library search with MZmine 3. Right: The final settings depend on the devices and experimental settings being used.

The results are implemented in the corresponding feature list. For MZmine newbies we recommend the “Processing wizard” to create a workflow with all needed features.