

User manual for

imCorrect ver. 1.0 beta3

Release date: August, 2024

About *imCorrect*

imCorrect was a software we developed for improvement of mass and relative isotopic abundance (RIA) accuracy by the consideration of the effects of noise level, signal stability and signal decay effects during the MS analysis.



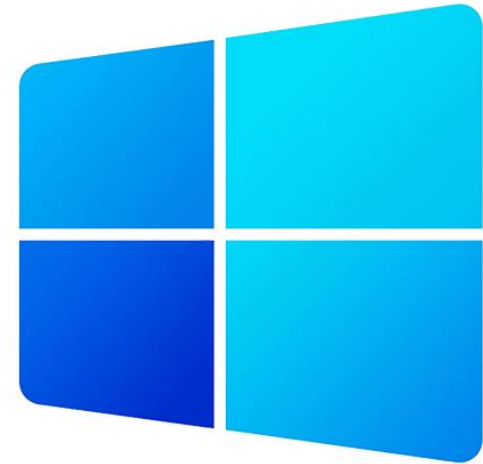
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1. System Requirements

Recommended requirements

- 4 or more CPU cores
- 16 GB or more RAM
- 64-bit Windows 10 or later (macOS is not available)



2. Installation

Prerequisites

- Visual C++ redistributable package (64-bit)
- .NET Framework 4.7.2 or later (64-bit)
- *imCorrect*
- *MSConvert*



- The successful running of *imCorrect* requires the installation of Visual C++ redistributable package and .NET Framework.
- A detailed guide for the installation of Visual C++ redistributable package and .NET Framework can be found in [Appendix A1 and A2](#).
- The raw data obtained from vendor format must be converted into .mzML format (please see [Appendix A3](#)) for successfully running in *imCorrect*.

Download Software and Example Data



DOWNLOADS

USER MANUAL

CONTACT US

REPORT ISSUES

Downloads

①

Software

[imCorrect \(ver. 1.0\)](#)

②

Example Data

Doped Lipids in Plant Cell Lysate Identified in MS analysis with Orbitrap Elite	raw	mzML
Plant Lipids Identified in MS analysis with Orbitrap Elite	raw	mzML
Plant Lipids Identified in MS analysis with IQ-X	raw	mzML

imCorrect can be downloaded from the following link:

https://msomics.abrc.sinica.edu.tw/imCorrect/?page_id=10

①

Download the **Software**

②

Download the **Example Data**, available in two formats (Thermo.raw and mzML), to freely test and verify the software

Fig-1. The page for downloading the software and example data

Checking the Download File

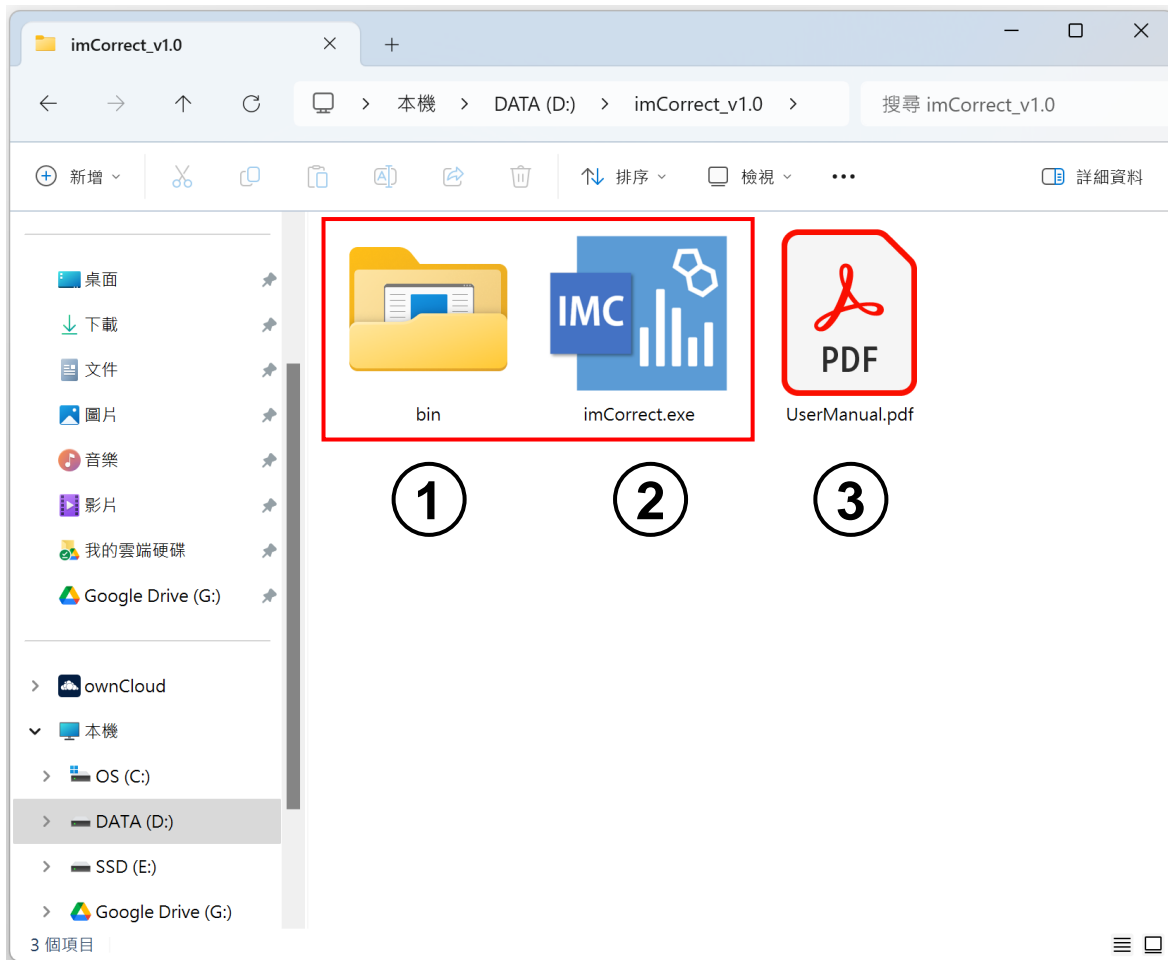


Fig-2. The items included in the *imCorrect* download folder

Once the download is complete, the folder will contain the following four items:

- ① **bin:** This folder contains the executable files of *imCorrect*.
- ② **imCorrect.exe:** The main program executable for *imCorrect*.
- ③ **UserManual.pdf:** A tutorial providing a guidance on how to use *imCorrect*.



- For successful execution of *imCorrect*, place the (1) “bin” folder, (2) “imCorrect.exe” file in the same directory.

3. Steps for the data processing within *imCorrect*

3-1. Launch the *imCorrect*

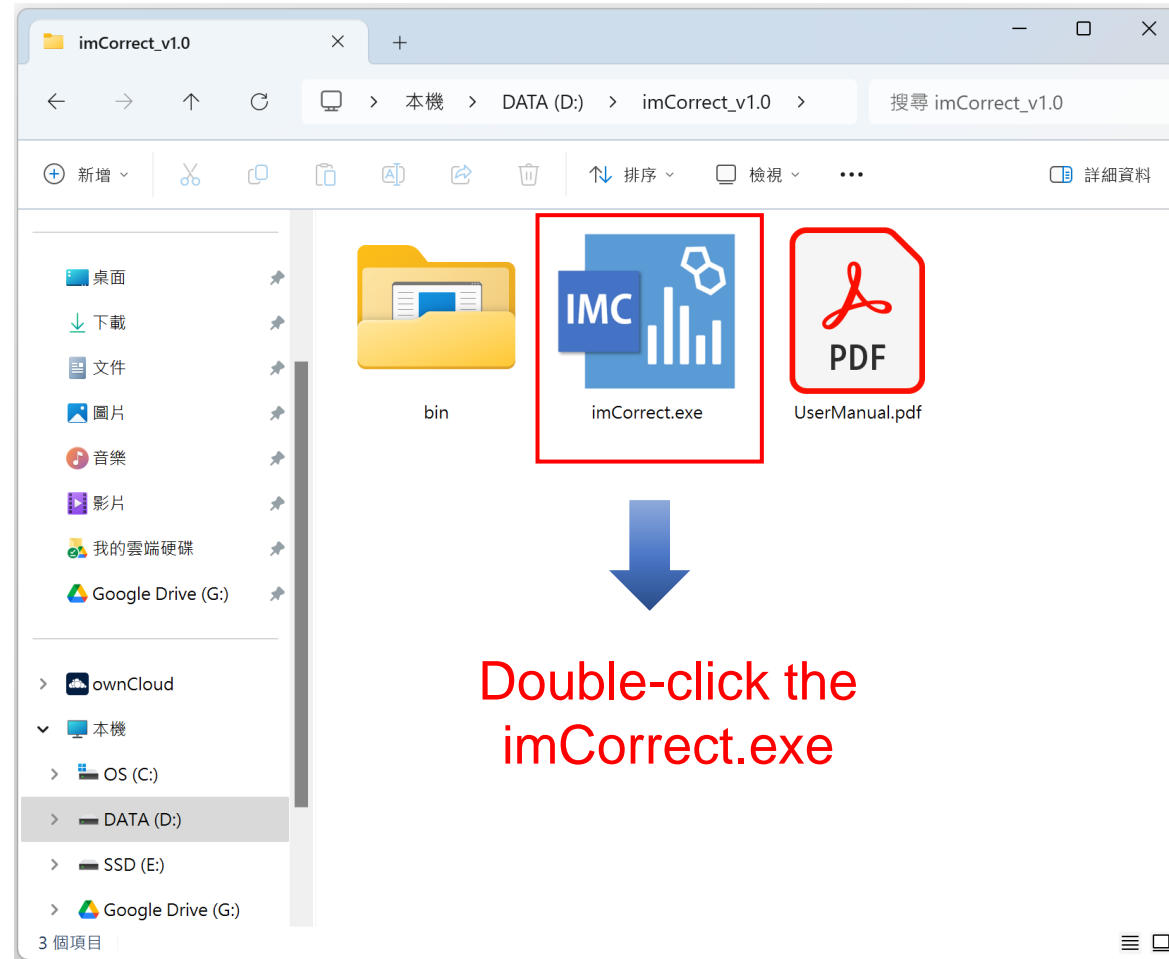


Fig-4. Starting the software

3-2. Data Processing (Function-1)

1 Data Processing Analysis

2 mzML File:

Browse Add Remove

D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_1.mzML
D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_2.mzML
D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_3.mzML
D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_4.mzML
D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_5.mzML
D:\mzML_doped_lipids\20210603_QC_D10_SPIKE_DE_MEASURE_461_Ref_ESI_POS_6.mzML

Parameter: Import Export

Common Parameters

Project Name TEST1

Mass Tolerance for MS Peak Detection 15 ppm

Mass Tolerance for Isotope Detection 5 ppm

RT Tolerance 10 seconds

Polarity Mode ☒ Positive ☐ Negative

Smoothing Setting

Noise Removal Setting

Mass and RIA Correction

Mass Correction ☒ Enable ☐ Disable Range \pm 100

RIA Correction ☒ Enable ☐ Disable

Reference

Compound NaAce

Browse

Error Correction ☒ Enable ☐ Disable

Retention Time Setting

Output Folder: Browse D:\imCorrect_v1.0

RUN

1 Select the “Data Processing”.

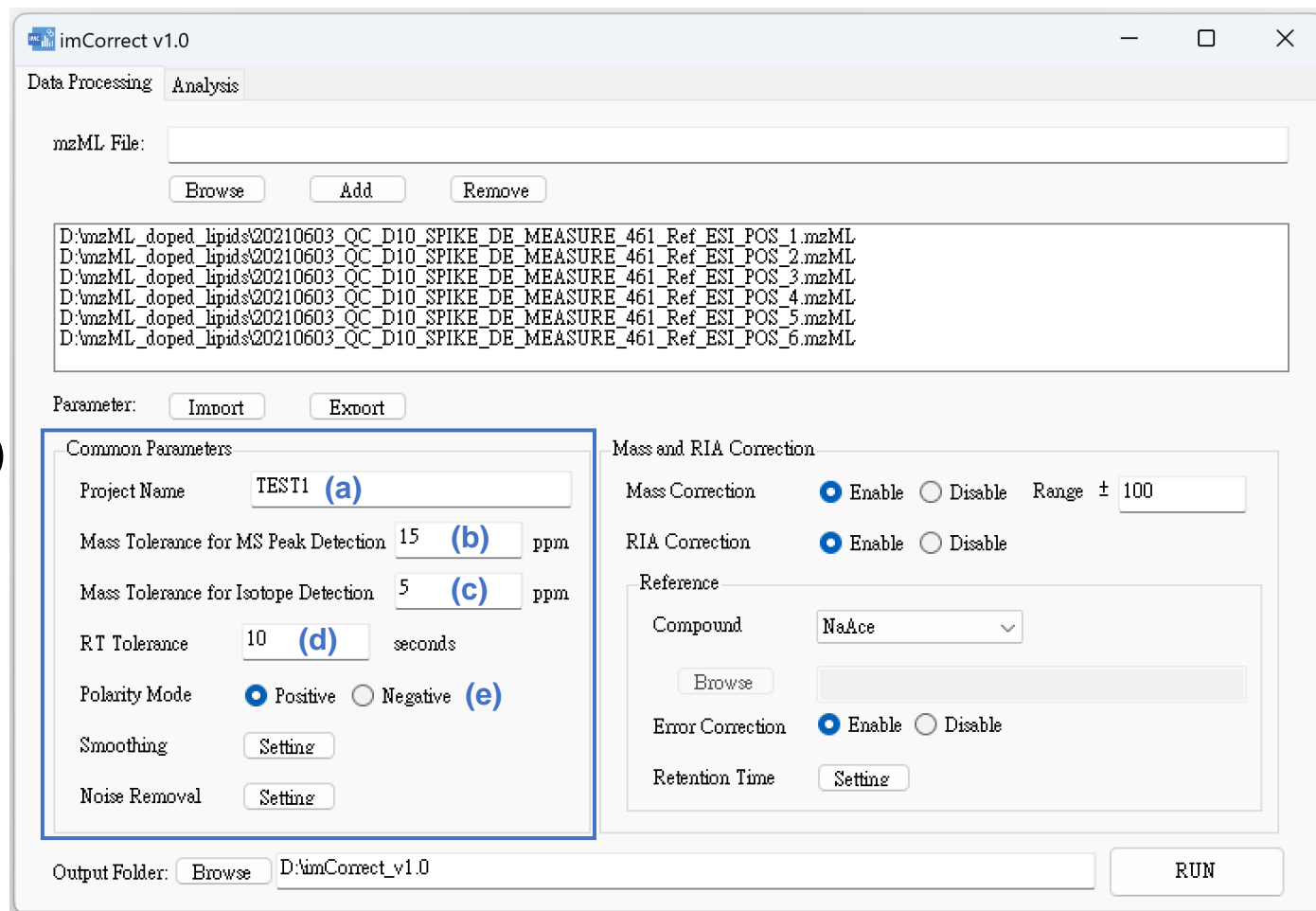
2 Click “Browse” to import the raw data file in [mzML](#) format.



As the mzML format was required, carefully refer to the parameter settings for data conversion in [MSconvert](#) provided in [Appendix A3](#).

Fig-5. Interface of “Data Processing” in *imCorrect*

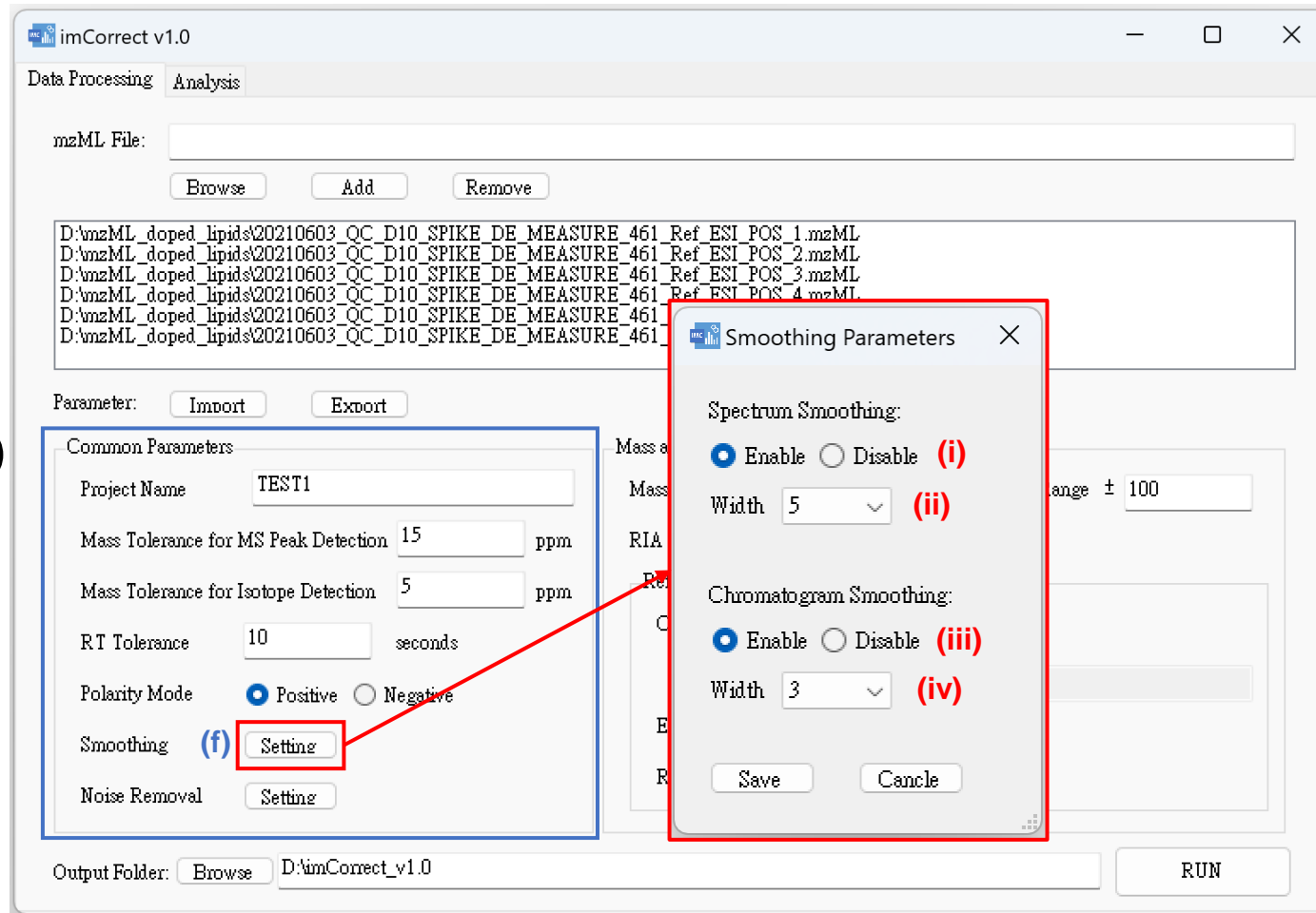
3-2. Data Processing (Function-1)



- ③ Set the common parameters:
- Specify a "Project Name" which will be automatically added as a prefix to the output file name. For example: **TEST1**_file name.
 - Set the "Mass Tolerance for MS Peak Detection" with ppm for the peak height of EIC search.
 - Set the "Mass Tolerance for Isotope Detection" with ppm for the isotopic envelopes detection.
 - Set the "RT Tolerance" with seconds for the isotopic envelopes detection.
 - Positive ion mode is default setting.

Fig-5. Interface of "Data Processing" in *imCorrect*

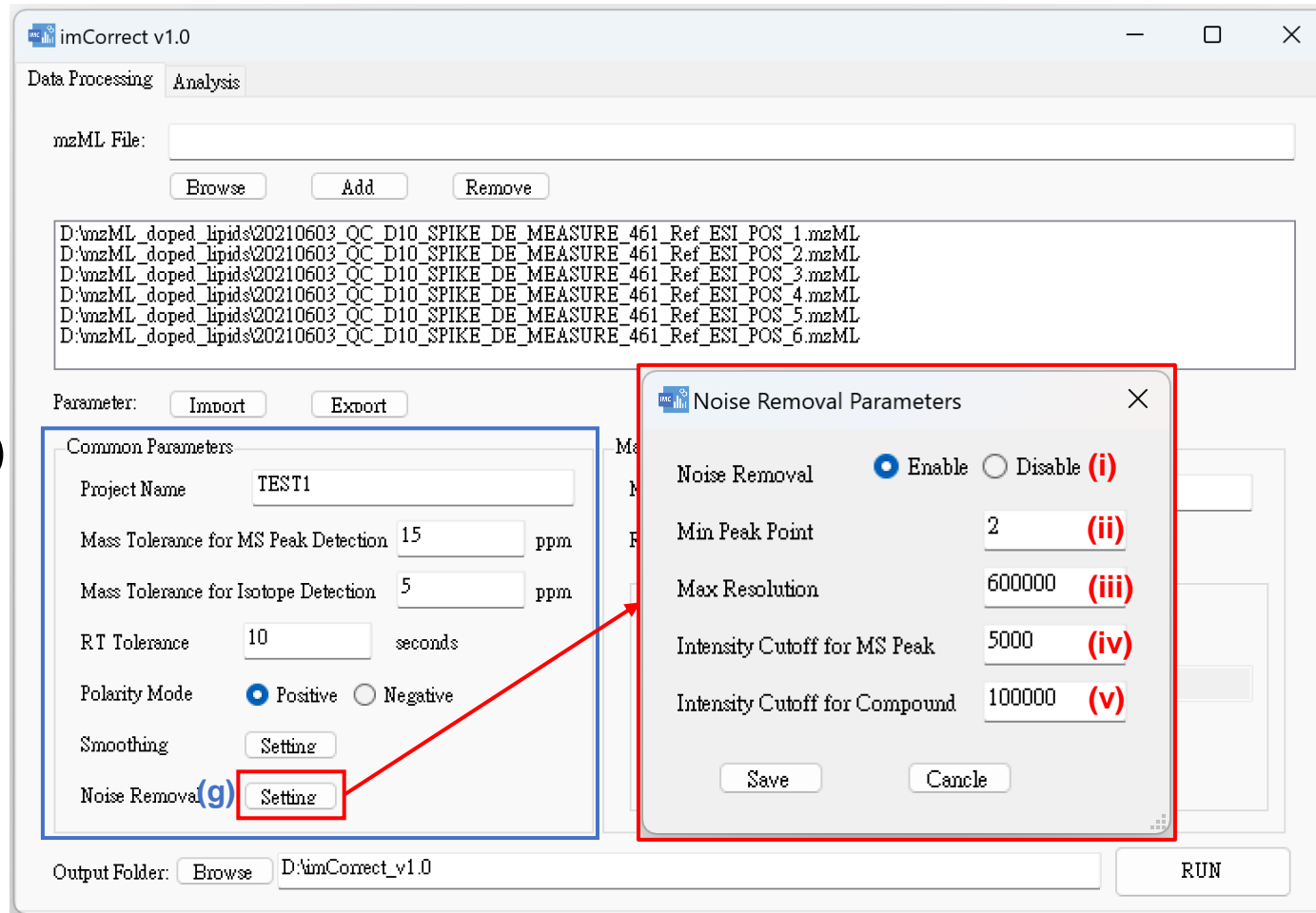
3-2. Data Processing (Function-1)



- ③ Set the common parameters:
- Click “Setting” to show the “Smoothing Parameters” form:
 - Enable or disable the “Spectrum Smoothing” function.
 - Set smoothing width for “Spectrum Smoothing” function.
 - Enable or disable the “Chromatogram Smoothing” function.
 - Set smoothing width for “Chromatogram Smoothing” function.

Fig-5. Interface of “Data Processing” in *imCorrect*

3-2. Data Processing (Function-1)



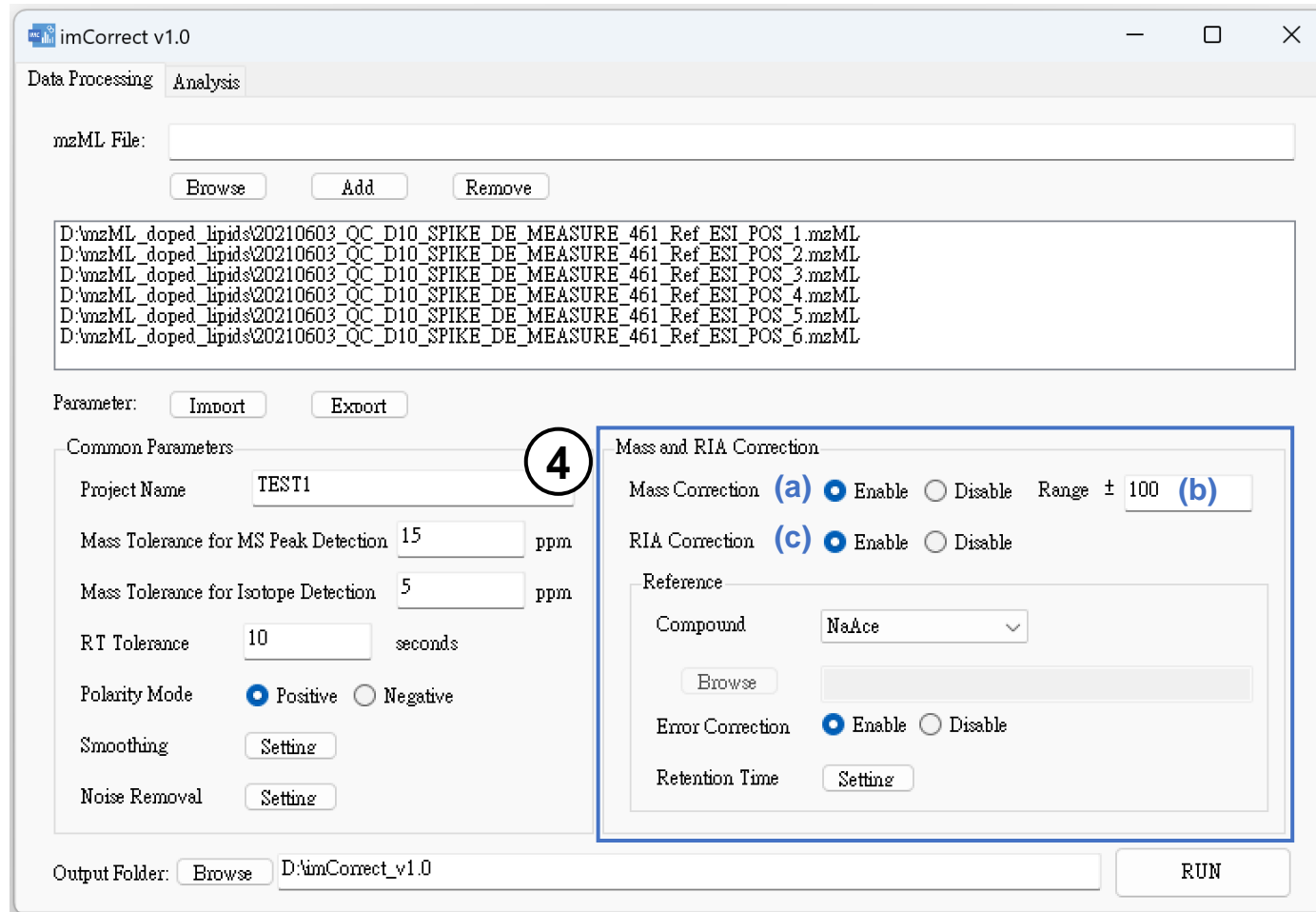
③ Set the common parameters:

g. Click “Setting” to show the “Noise Removal Parameters” form:

- Enable or disable the “Noise Removal” function.
- Set the “Min Peak Point” to remove noise peak by the number of peak point.
- Set the “Max Resolution” to remove noise peak by peak resolution.
- Set the “Intensity Cutoff for MS Peak” to remove noise peak by peak intensity.
- Set the “Intensity Cutoff for Compound” to remove detected compound by its intensity.

Fig-5. Interface of “Data Processing” in *imCorrect*

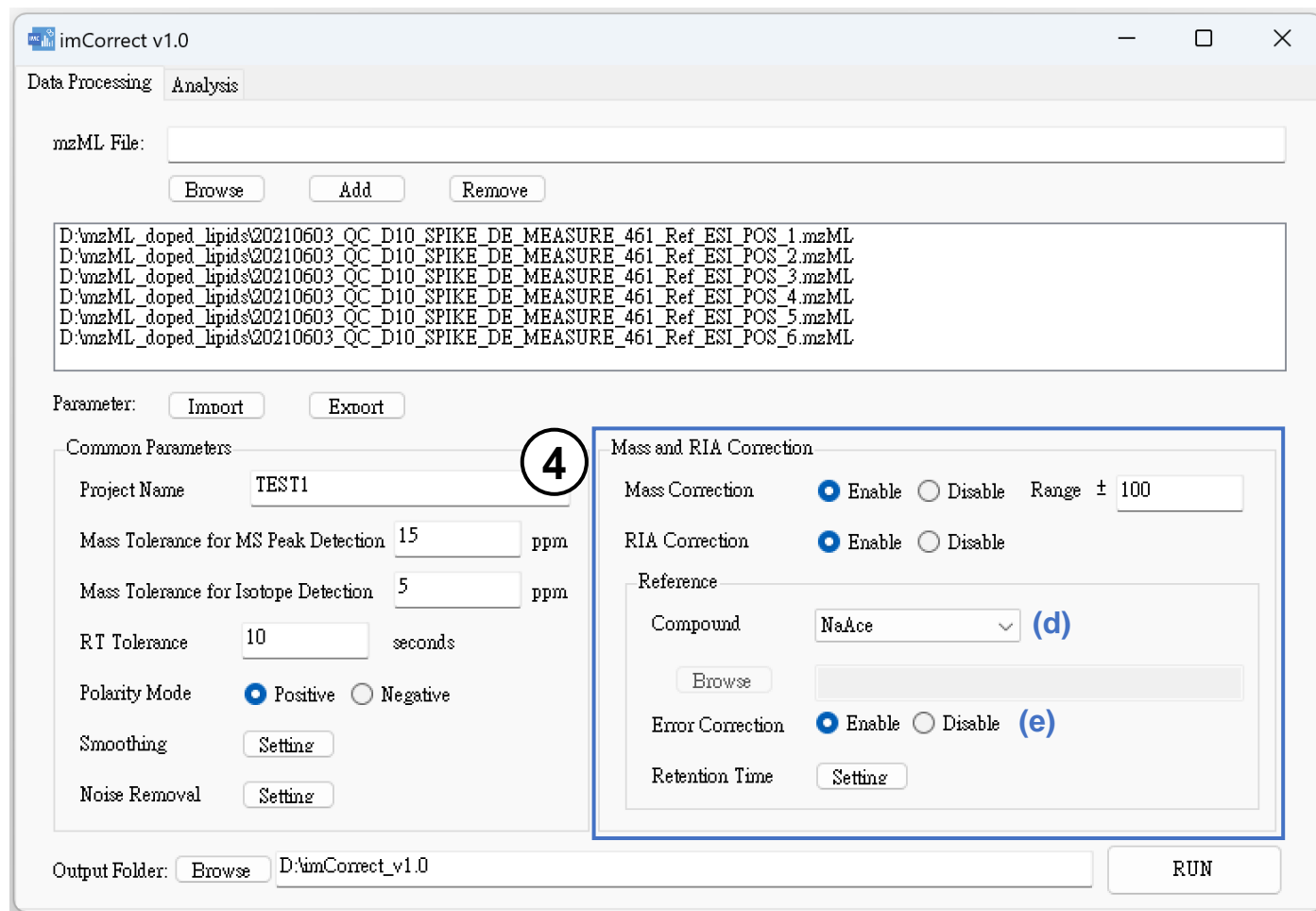
3-2. Data Processing (Function-1)



- ④ Set the parameters of “Mass and RIA Correction”:
- Enable or disable the “Mass Correction” function.
 - Set the mass range of reference selection for “Mass Correction” function.
 - Enable or disable the “RIA Correction” function.

Fig-5. Interface of “Data Processing” in *imCorrect*

3-2. Data Processing (Function-1)

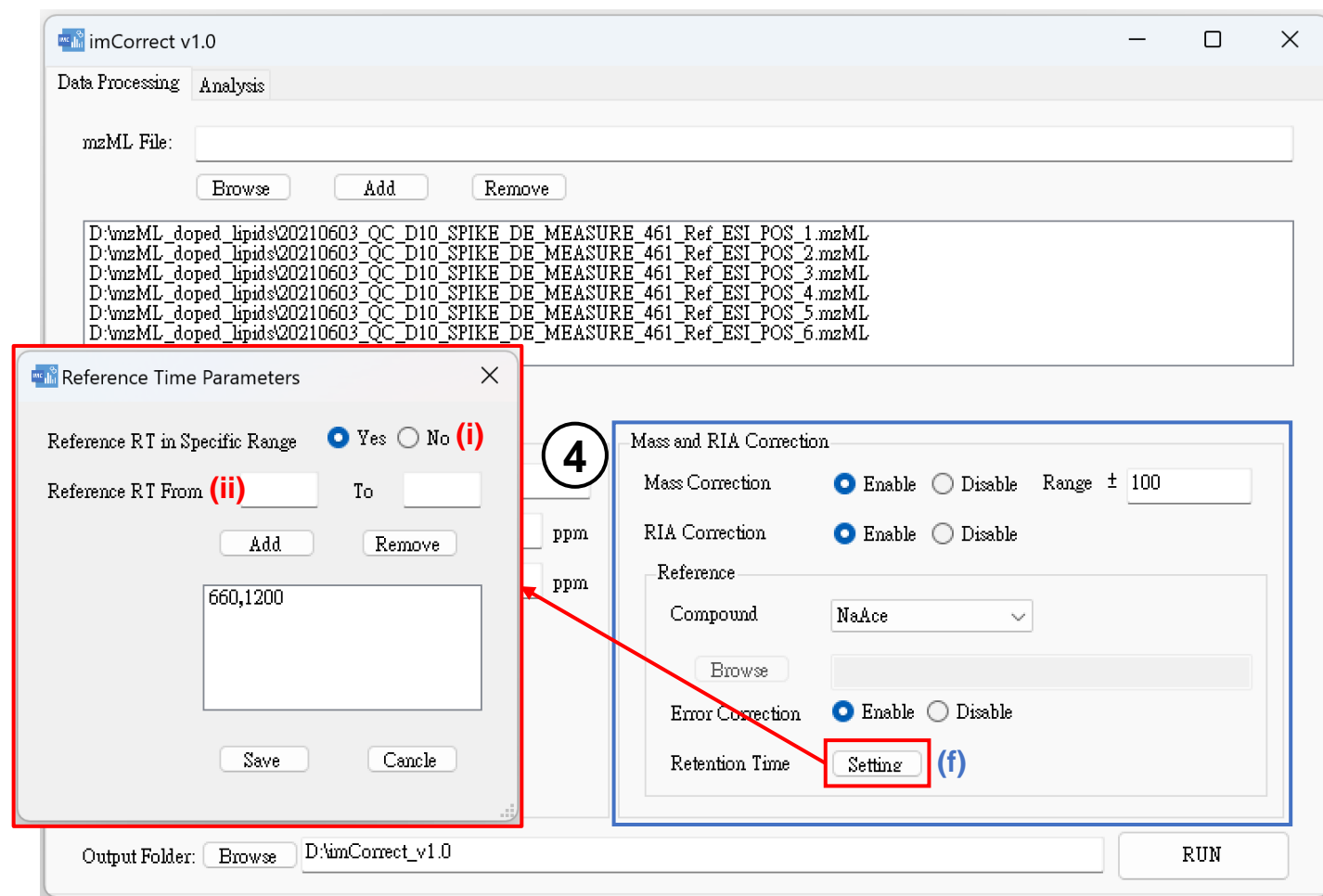


④ Set the parameters of “Mass and RIA Correction”:

- d. Select compound type of reference. Built-in parameters for NaAce and NaF. If use other types of compounds, their parameters can also upload. Please refer to the following link for the format.
- e. Enable or disable the “Error Correction” function for correction RIA error of reference signal due to dimer.

Fig-5. Interface of “Data Processing” in *imCorrect*

3-2. Data Processing (Function-1)

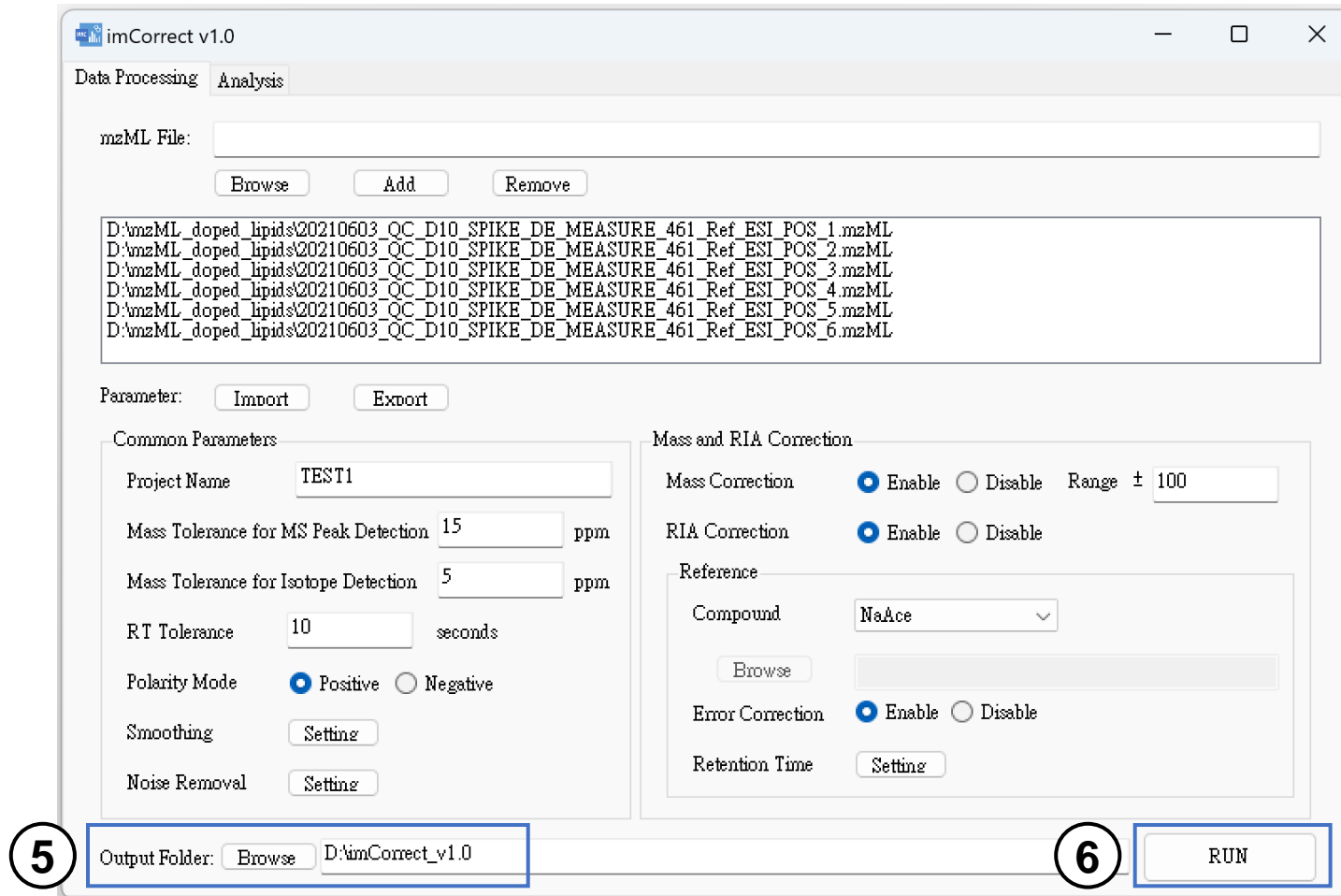


④ Set the parameters of “Mass and RIA Correction”:

- f. Click “Setting” to show the “Reference Time Parameters” form:
 - i. Select whether the RT of the reference is within a specific range. (Select “Yes” if you using external reference correction method; Select “No” if you using internal reference correction method, and the uploaded file needs to record the RT of each internal reference)
- ii. Editing the RT range of a reference signal

Fig-5. Interface of “Data Processing” in *imCorrect*

3-2. Data Processing (Function-1)

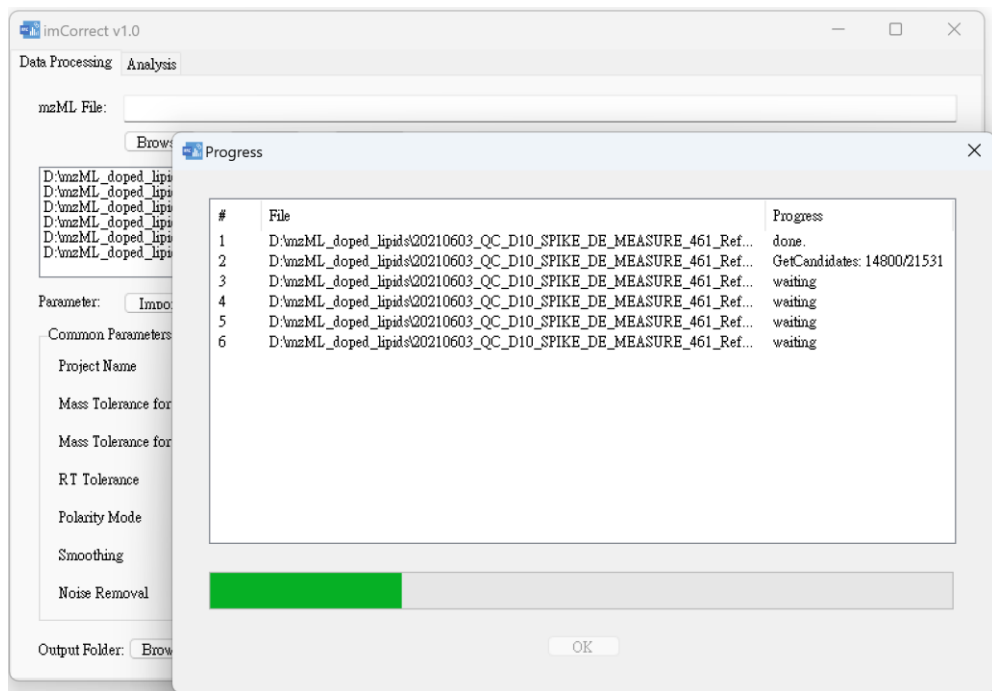


⑤ Specify the output path. (The output files will be in .CSV format.)

⑥ Click "RUN" to start execution.

Fig-5. Interface of “Data Processing” in *imCorrect*

When processing



Finished

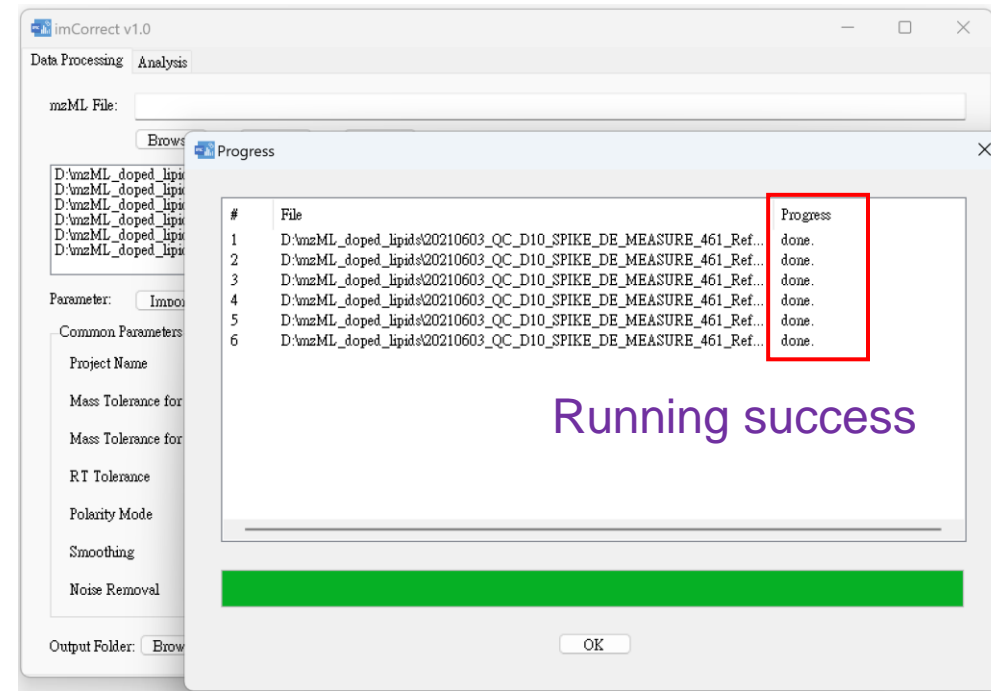


Fig-6. Display of the running progress during the execution

Fig-7. Display of the running completed

Output success

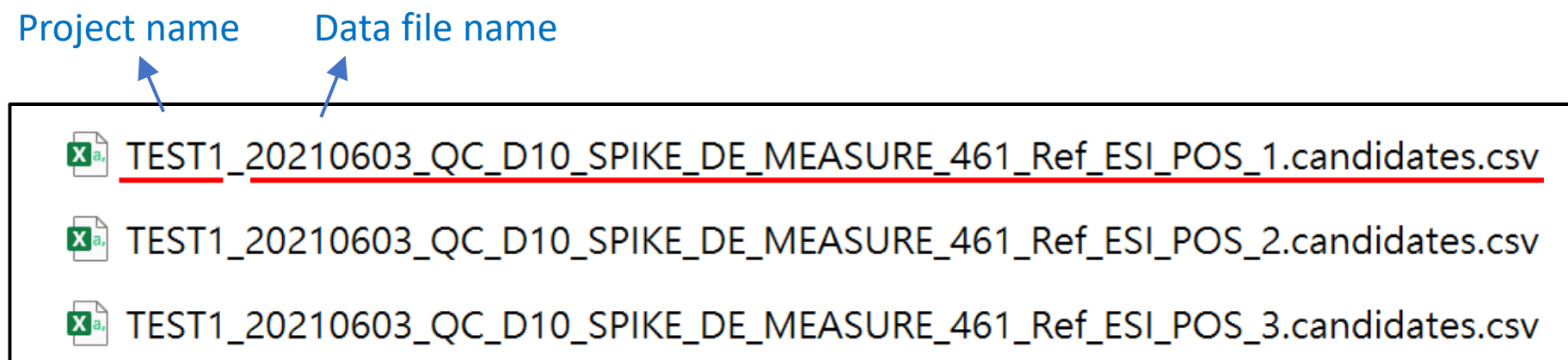
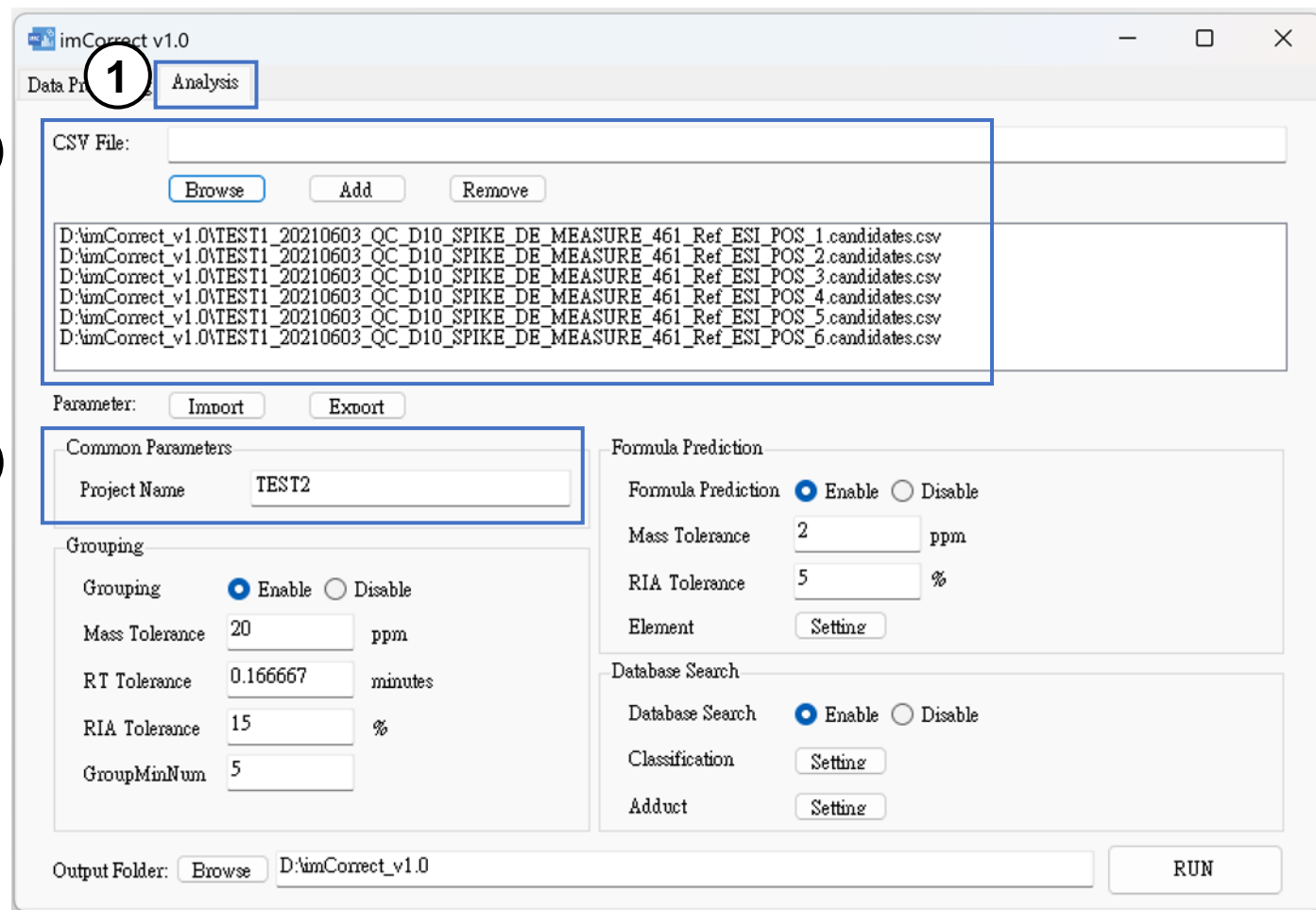


Fig-8. The results output in the specified output folder

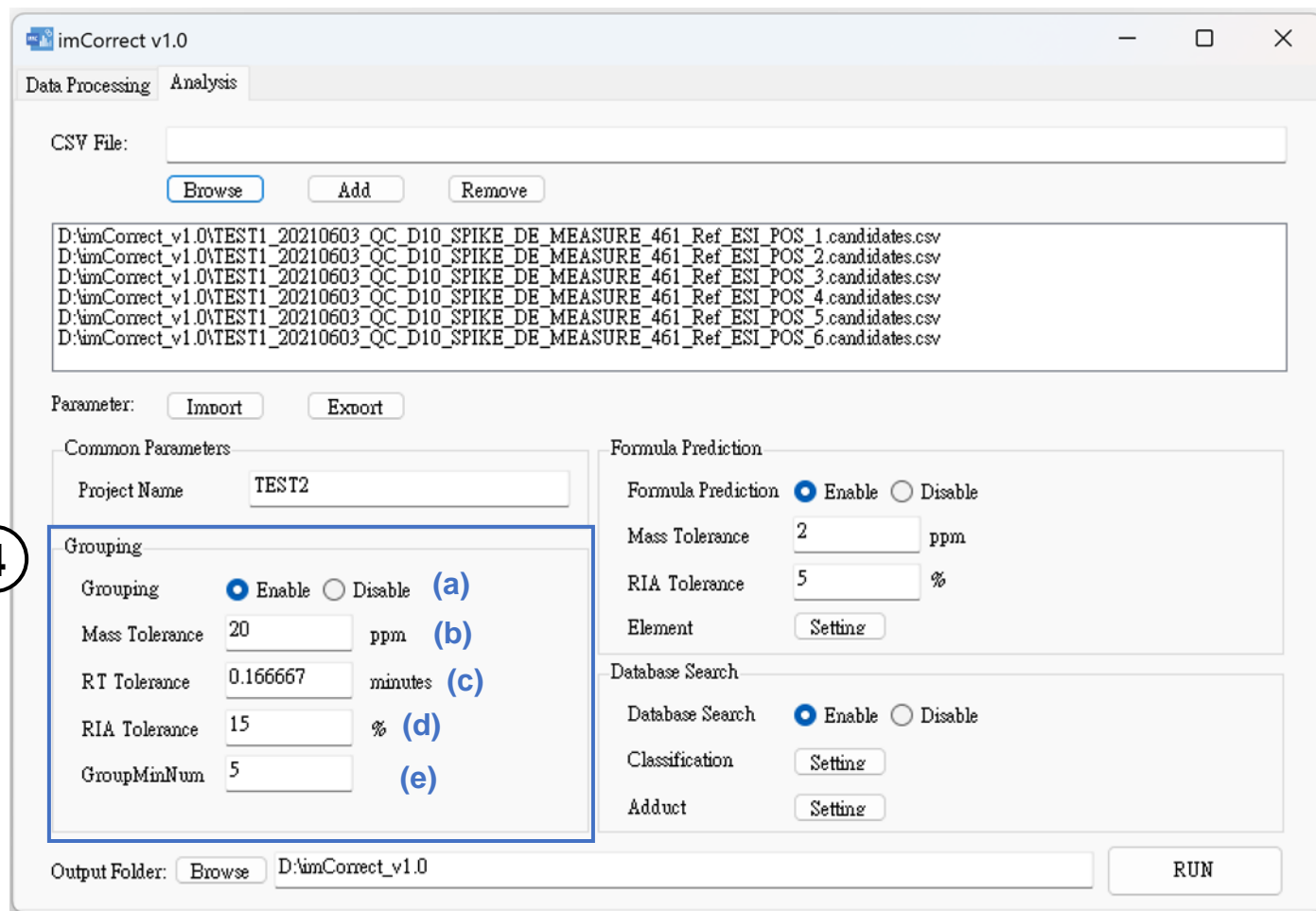
3-3. Analysis (Function-2)



- ① Select the “Analysis”.
- ② Click “Browse” to import the .CSV file that was generated from Data Processing (Function-1).
- ③ Specify a "Project Name" which will be automatically added as a prefix to the output file name. For example: TEST2_file name.

Fig-9. Interface of “Analysis” in *imCorrect*

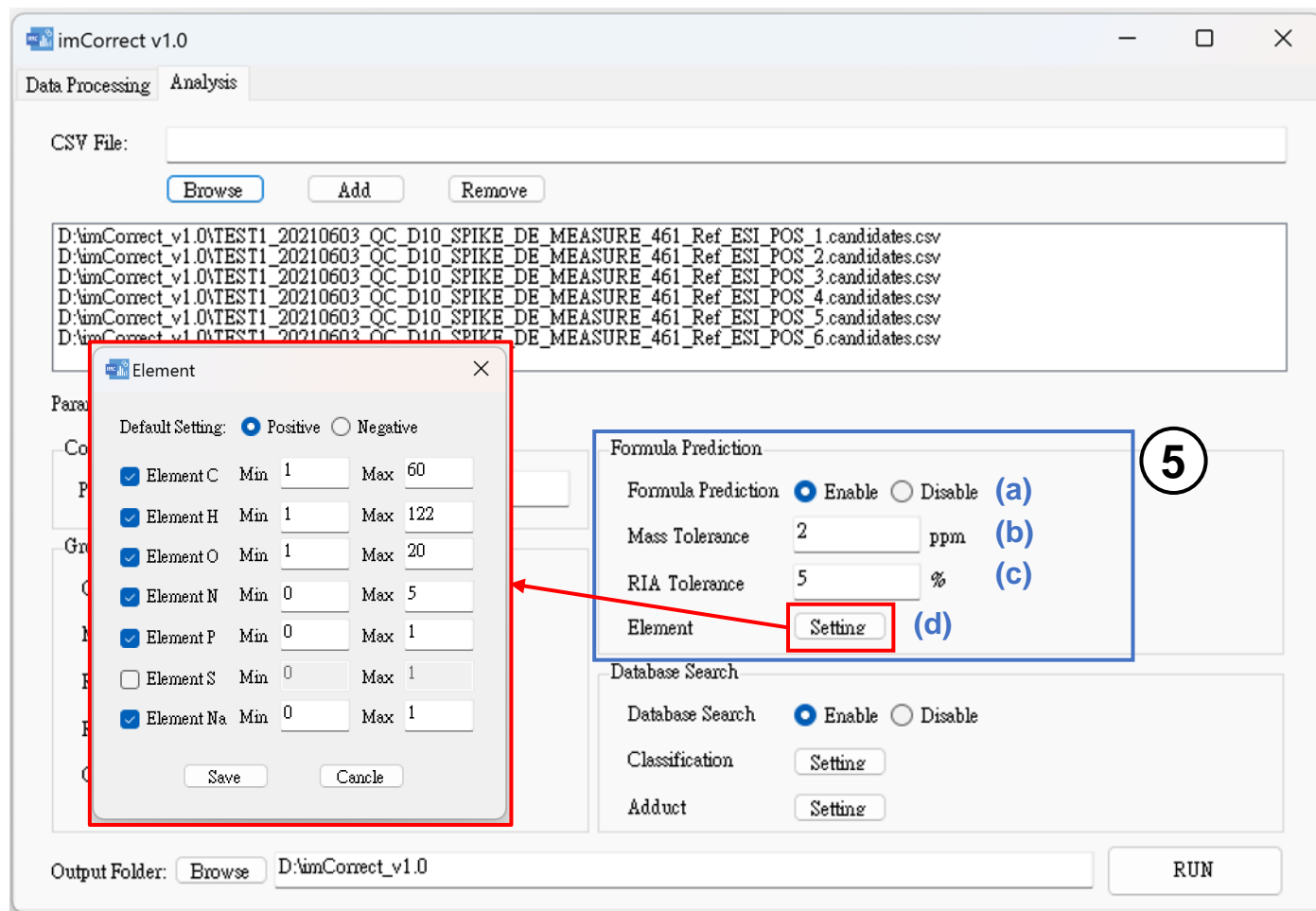
3-3. Analysis (Function-2)



- ④ Set the parameters of “Grouping”:
- Enable or disable the “Grouping” function.
 - Set the “Mass Tolerance” with ppm for the compound grouping from different repeats.
 - Set the “RT Tolerance” with minutes for the compound grouping from different repeats.
 - Set the “RIA Tolerance” with percentage for the compound grouping from different repeats.
 - Set the “GroupMinNum” for the compound grouping at least how many repeats are needed.

Fig-9. Interface of “Analysis” in *imCorrect*

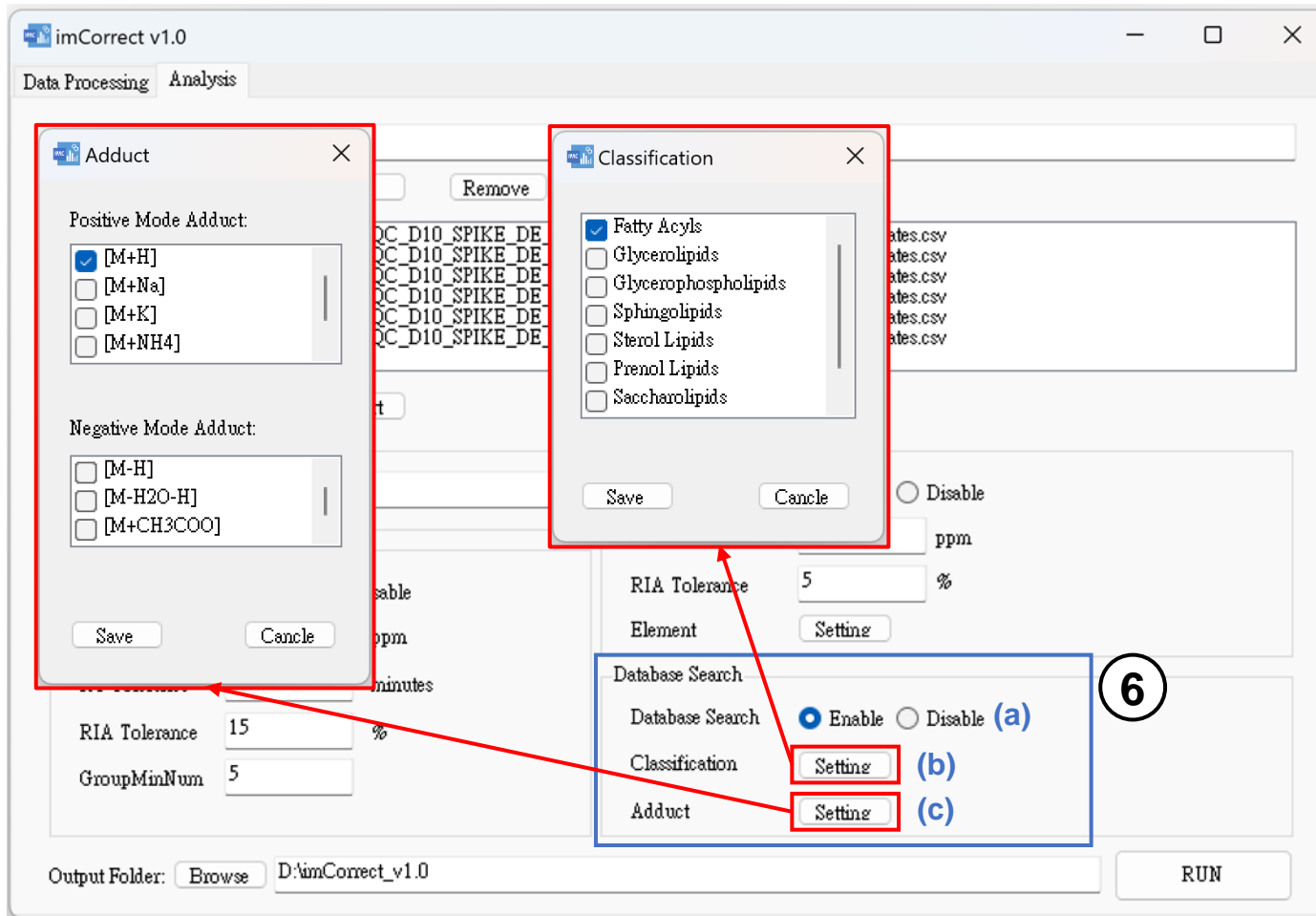
3-3. Analysis (Function-2)



- ⑤ Set the parameters of “Formula Prediction”:
- Enable or disable the “Formula Prediction” function.
 - Set the “Mass Tolerance” with ppm for compound formula prediction.
 - Set the “RIA Tolerance” with percentage for compound formula prediction.
 - Click “Setting” to show the “Element” form:
 - Positive ion mode is default setting.
 - Select the element type and their number range.

Fig-9. Interface of “Analysis” in *imCorrect*

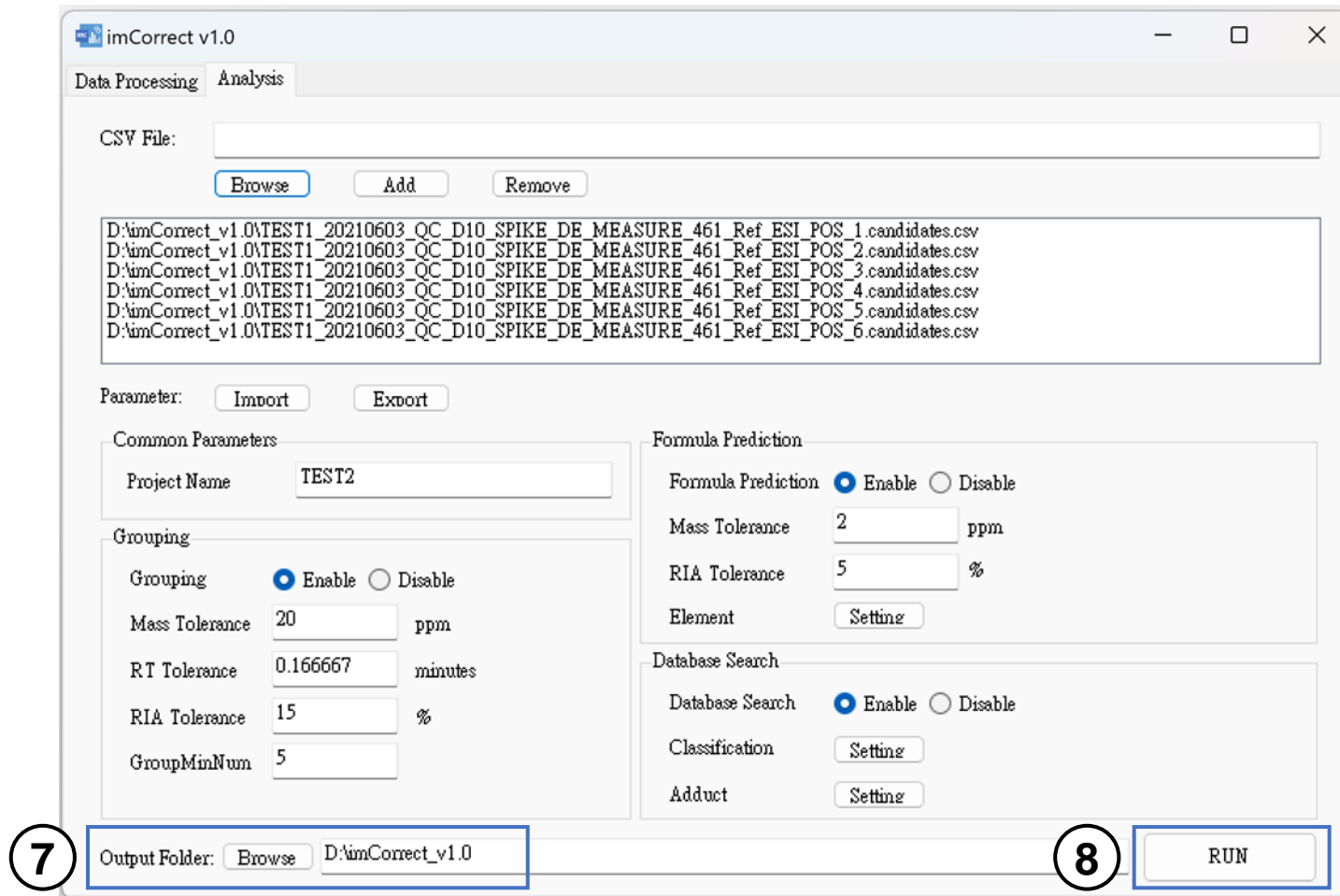
3-3. Analysis (Function-2)



- ⑥ Set the parameters of “Database Search”:
- Enable or disable the “Database Search” function.
 - Click “Setting” to show the “Classification” form:
 - Select the lipid type for database search.
 - Click “Setting” to show the “Adduct” form:
 - Select the adduct type for database search.

Fig-9. Interface of “Analysis” in *imCorrect*

3-3. Analysis (Function-2)



⑦ Specify the output path. (The output files will be in .CSV format.)

⑧ Click "RUN" to start execution.

Fig-9. Interface of "Analysis" in *imCorrect*

Finished

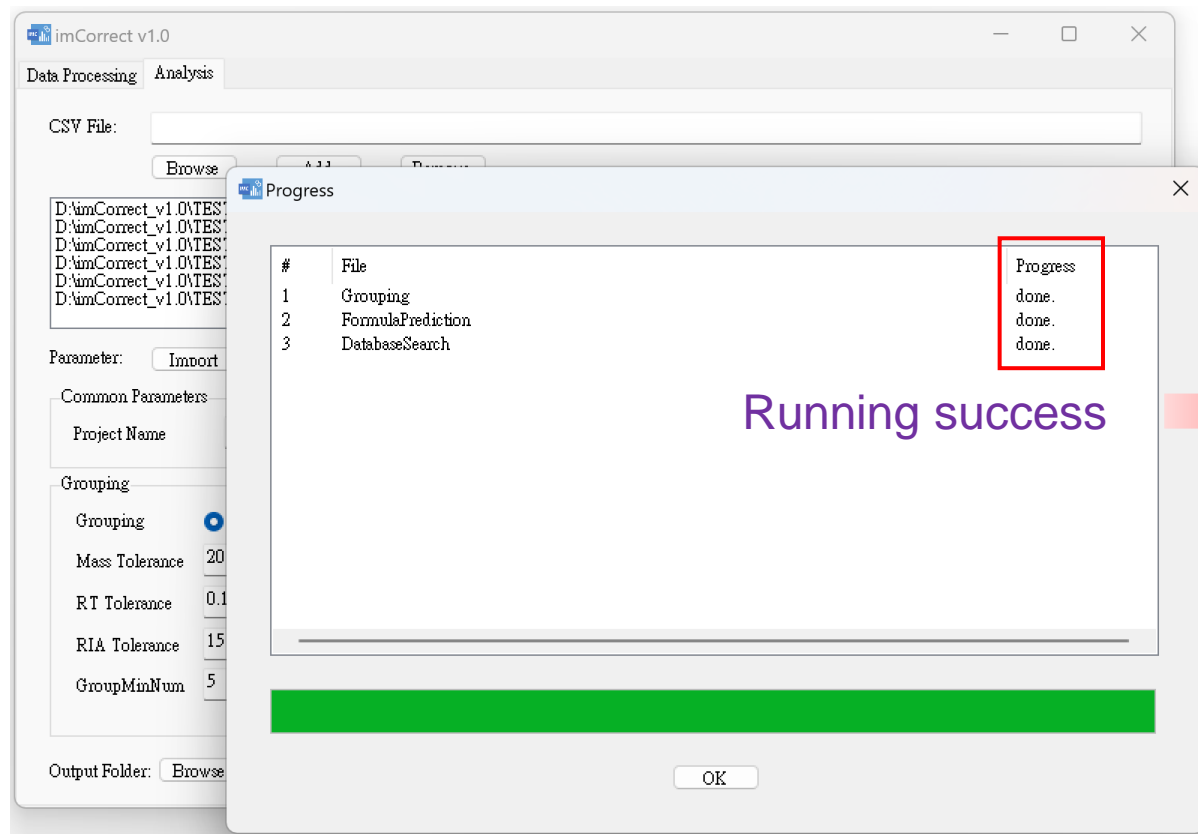


Fig-10. Display of the running completed

Output success

- [1] TEST2_group.csv (Grouping results of imported .CSV files)
- [2] TEST2_formula.csv (Formula prediction results of [1])
- TEST2_db.csv (Database search results of [2])

Fig-11. The results output in the specified output folder

4. Appendix-A1

Visual Studio 2015, 2017, 2019, and 2022

This table lists the latest supported English (en-US) Microsoft Visual C++ Redistributable packages for Visual Studio 2015, 2017, 2019, and 2022. The latest supported version has the most recently implemented C++ features, security, reliability, and performance improvements. It also includes the latest C++ standard language and library standards conformance updates. We recommend that you install this version for all applications created using Visual Studio 2015, 2017, 2019, or 2022.

Unlike older versions of Visual Studio, which have infrequent redistributable updates, the version number isn't listed in the following table for Visual Studio 2015-2022 because the redistributable is updated frequently. To find the version number of the latest redistributable, download the redistributable you're interested in using one of the following links. Then, look at its properties using Windows File Explorer. In the **Details** pane, the **File version** contains the version of the redistributable.

Architecture	Link	Notes
ARM64	https://aka.ms/vs/17/release/vc_redist.arm64.exe	Permalink for latest supported ARM64 version
X86	https://aka.ms/vs/17/release/vc_redist.x86.exe	Permalink for latest supported x86 version
X64	https://aka.ms/vs/17/release/vc_redist.x64.exe	Permalink for latest supported x64 version. The X64 Redistributable package contains both ARM64 and X64 binaries. This package makes it easy to install required Visual C++ ARM64 binaries when the X64 Redistributable is installed on an ARM64 device.

Download and install

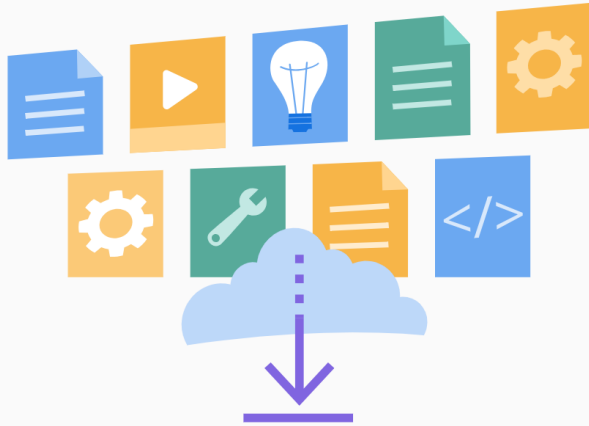
Fig-A1. The page for downloading Visual C++ redistributable package

Visual C++ redistributable package can be downloaded from the official website of Microsoft:
<https://learn.microsoft.com/en-us/cpp/windows/latest-supported-vc-redist?view=msvc-170>

4. Appendix-A2

Download .NET Framework 4.7.2

Not sure what to download? [See recommended downloads for the latest version of .NET.](#)



Runtime

Do you want to run apps? The runtime includes everything you need to run existing apps/programs built with .NET Framework.

[Download .NET Framework 4.7.2 Runtime →](#) **Download and install**

Developer Pack

Do you want to build apps? The developer pack is used by software developers to create applications that run on .NET Framework, typically using Visual Studio.

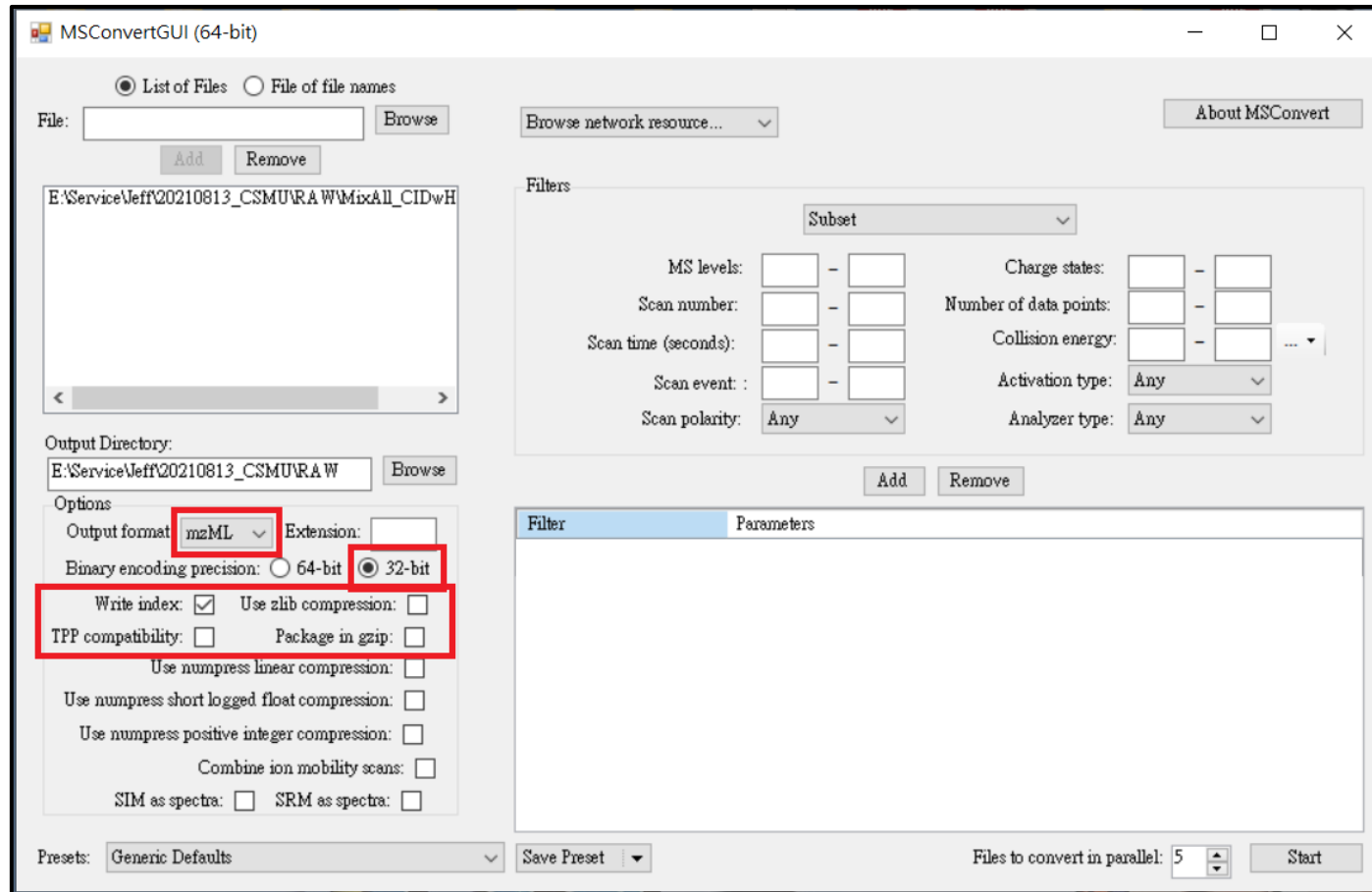
[Download .NET Framework 4.7.2 Developer Pack →](#)

Fig-A2. The page for downloading .NET Framework

.NET Framwork can be downloaded from the official website of Microsoft:

<https://dotnet.microsoft.com/en-us/download/dotnet-framework/net472>

4. Appendix-A3



MSConvert can be downloaded from the website:

<https://proteowizard.sourceforge.io/download.html>

Fig-A3. Recommended setting parameter for converting data from vendor's format to mzML

Report Issues

We welcome your feedback and comments, as they can greatly contribute to enhancing the development of the software.

If you encounter any issues with *imCorrect*, please include the following information in your issue report:

- (1) *The version of imCorrect.*
- (2) *Screenshots of error messages or unexpected results.*
- (3) *Any additional information that could help us better understand the challenges or bugs you're encountering.*

Please leave your feedback and comments at the following link:

https://msomics.abrc.sinica.edu.tw/imCorrect/?page_id=64



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