

## Quick Start Guide for BAFinder 2.0

### To start

For Windows64 system:

Open folder “BAFinder2\_windows64”, and double click “BAFinder2\_win64.exe”.

For macOS system:

Open folder “BAFinder2\_macosx”, in the sub-directory “Contents/MacOS”, find BAFinder\_macosx and double click it.

### Work with test data

Select the test data folder and library files, enter the parameters as shown in the screenshot below and click on the “Run” button. A processing bar will show up. The output should be same as the files in “3. Output \Result\_for\_test\_data” folder. It takes about 30 min on a PC with Intel(R) Xeon(R) W-2235 CPU and 64 GB RAM.

Open the “Final\_summary.csv” file to check the bile acids annotated. After filtering the annotation (“-BA” to get amino acid conjugated bile acids), confidence level (remove blank) and sample numbers (detected in at least 2 samples in one species), the result should be same as the Table S3 in the manuscript.

BAFinder 2.0

about

Input file folder in neg mode

G:\ProcessedData\1.Input\Neg\_human\_dog\_rat

Input file folder in pos mode

G:\ProcessedData\1.Input\Pos\_human\_dog\_rat

MS/MS library (MSP)

G:\ProcessedData\2.Library\insilico\_AABA\_and\_experimental\_BA\_recommend

(Optional) retention time library (txt)

G:\ProcessedData\2.Library\RT\_library\_for\_test\_only.txt

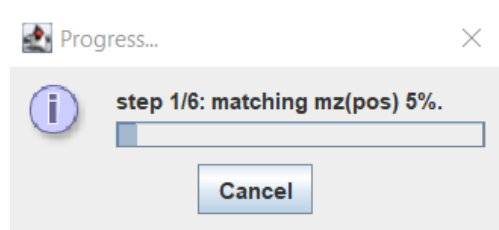
m/z tolerance (Da)  RT tolerance (min)

Output directory

G:\ProcessedData\3.Output

(Optional) custom conjugates import:

G:\ProcessedData\2.Library\Customized\_conjugate\_list.txt



For more information, please refer to the User Manual or contact mayan@nibs.ac.cn.