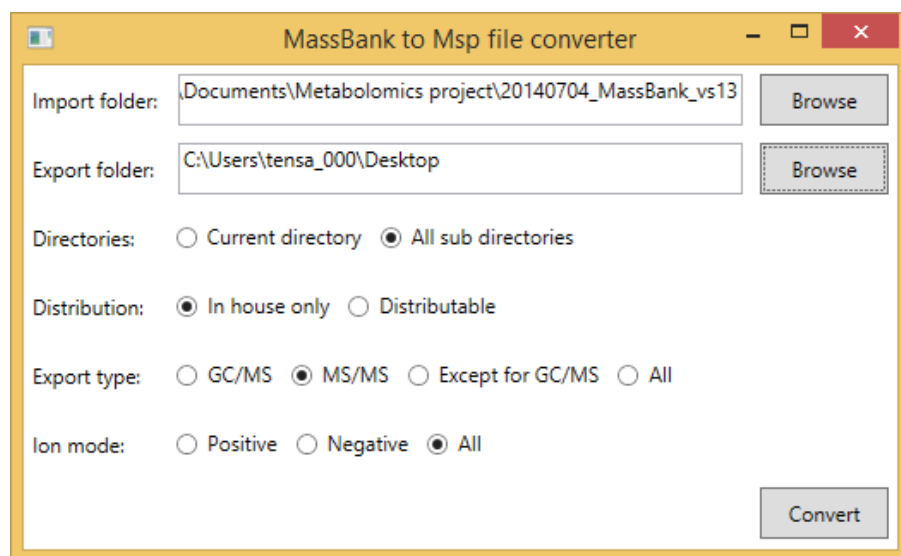


## MassBank to NIST MSP tutorial

### Objective

This program helps us to prepare NIST MSP format libraries applicable to a lot of programs (MS-DIAL, NIST MS Search, AMDIS) from MassBank records (also ReSpec). Merging each MassBank text file into MSP is actually easy for the programmers though, the end users (even me) are struggling to do this task. If you want other functions to extract MassBank records, please let us know ([hiroschi.tsugawa@riken.jp](mailto:hiroschi.tsugawa@riken.jp)).

### How to use the program



1. Select a directory which contains the text files of MassBank record.
2. Select an output directory.
3. Select your options. (Make sure some records, ex of Metabolon, cannot be re-distributed by CC BY-NC-ND)
4. Click convert.

### MassBank records

The mass spectrum libraries from standard compounds must be required for compound identifications. The end-users can easily confirm chromatogram peaks with spectrum DBs (in GCMS, the retention index should be also useful!). MassBank gives us all of spectrum records at no charge.

### Why developed?

Unfortunately, the MassBank records are not applicable yet to some programs utilized in metabolomics (MS-DIAL, AMDIS, NIST MS Search). On the other hand, the NIST MSP format is mostly available. That's why the MSP format file has to be prepared from MassBank records, but the MassBank records are still downloaded at the separated text files (see below). Therefore, we prepared the library converter from

MassBank records to MSP format since there is no tool so far...

