The download package contains the following files/folders:

GUI:

We highly recommend that the users use the GUI instead of the command line version. The GUI launcher along with a tutorial/manual has been included in the GUI folder.

binaries:

- The "**bin**" folder contains java class files necessary for running MaSS-Simulator. SimSpec.class is the main class file which the users will be needing.

Source files:

- All the source files can be found in the folder "**src**". If the users are having trouble running the compiled class files, fresh class files can be generated using the following command in source folder:

  javac SimSpec.java

Datasets:

- all the test datasets have been compressed into **datasets.tar.gz** file. Related files for each dataset have been contained in a separate folder. Files for modified and non-modified spectra have been separated. Each file which ending in "*mods*" refers to spectra corresponding to modified peptides, similarly "*nomods*" refers to spectra corresponding to non-modified peptides. Following are the details about what is contained in each file. Here * can be replaced with mods or nomods:

  - **analysis-*.txt:** this file contains details about SNR and peptide coverage for each ms2 spectrum.
  - **Experimental-*.ms2**: this file contains experimental spectra.
  - **Peptides-*.rst:** this file contains ground truth, peptides corresponding to each ms2 spectrum, indexed using scan-numbers.
  - **Simulated-*.ms2:** this file contains simulated spectra.
  - **Theoretical-*.ms2:** this file contains theoretical spectra.

Manual.pdf:

- This manual briefly discusses how the simulator can be configured using the configuration file.

Modifications.ptm

- This is the default file which contains details about the variable and static modifications which need to be simulated.

Params.txt

- This is the default configuration file.

Please contact us for support and any feedback at: fsaeed@fiu.edu