Important Notes regarding the SpectrumMerger Software:

Installation

To "install" the Software, simply copy all the files contained in this folder into a folder on your PC. The program will not work, if either of the dlls (MathNet.Iridium.dll or XRawfile2[_x64].dll) is missing.

Functionality

The SpectrumMerger Software can be used to consolidate .raw files where separate id- and quan-scans have been recorded for each precursor. This is done by detecting for each precursor the two scans belonging together and merging the reporter ion area from the quan-scan into the id-scan. The merging is done by copying a selected m/z-range from the id-scan overwriting a selected m/z-range in the quan-scan.
For each processed .raw file the resulting merged scans are assembled in an .mgf file having the same name that is stored in the directory of the .raw file.

Usage

The interface is very simple, as there are only a few settings to be made (see Figure 1). To perform the merging simply follow these steps:

1. Click on **Select RAW File(s)** (see Figure 1) to choose the files you want to analyze.
2. Using the up-down control **From (m/z)** choose the m/z-range in which the reporter ions can be found in the quan-scan.
3. Select the range in the id-scan that should be overwritten: **To (m/z)**.

   The selection of a quantitation method fills in the values in the **From** and **To** fields corresponding to the respective reporter ion range. This only defines the ranges to be considered for the merging. The method does not necessarily need to be the one the sample has been prepared with.
   Note that, of course, both intervals need to have the same size.
4. Configure the **Activation Type**, **Collision Energy** and **Isolation Width** for both the id- and quan-scans. If this information is not correct the scan cannot be distinguished and the merging cannot be done.
5. Click the **Merge** button to start the process.

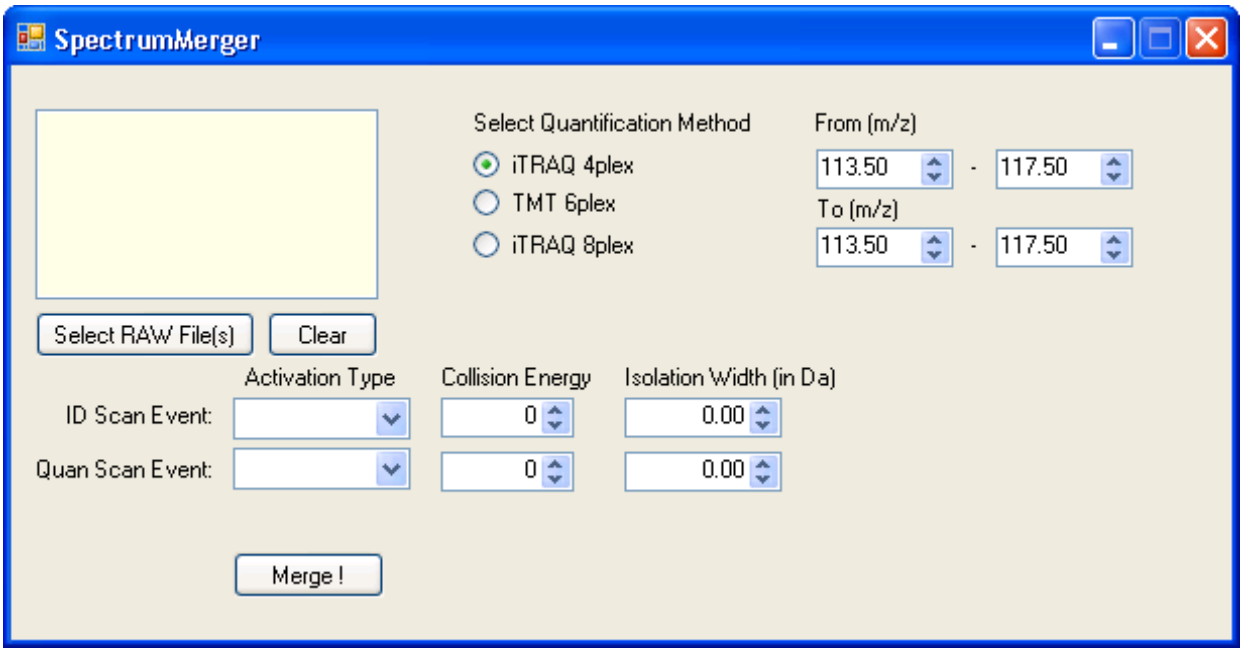

Figure 1: Interface of the SpectrumMerger Software