MSFileReader-MATLAB API

Joshua Goldford

11-13

1 Introduction

Thermo MATLAB API is a MATLAB package for the import of profile scan data from the .RAW files generated from Thermo Fisher mass spectrometers. This document is meant to clarify the installation requirements and usage for this package.

2 Preliminaries and Compilation

Before use, it is important the the following are installed on your 64 bit (32 bit) Windows machine:

1. **MATLAB MEX** and a C++ compiler
2. **MS File Reader** from Thermo Fisher Scientific.

Find and copy the full path to **Xrawfile2_x64.dll** (**Xrawfile2_x32.dll**); you will have to change line 10 in each .cpp file in the **source** subdirectory. Compile .cpp files using **mex** command and place **.mex64** (**.mex32**)files in the **mex** subdirectory. Make sure this is is included in your path when running MATLAB.

3 Usage

To import Profile scans into MATLAB, run the function **getRawData.m** with the path to the .RAW file as an input. The output is the structure containing:

1. **RT**: $1 \times N$ array with retention time associated to each N scas.
2. **scan**: $1 \times N$ structure containing the following fields:

(a) **reads**: total number of data points = M

(b) **mz**: $1 \times M$ measurement mass to charge ratio

(c) **intensity**: $1 \times M$ measurement intensity

(d) **noise** $1 \times M$ measurement noise