

# Thermo MATLAB API

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## 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.

## 2 Preliminaries and Compilation

Before use, it is important the the following are installed on your 64 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**; you will have to change line 10 in each .cpp file in the **source** subdirectory. Compile .cpp files using **mex** commmand and place **.mex64** files in the **mex** subdirectory. Make sure this is included in your matlab 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