

Loads2Chrom.exe – Help file

Summary: This folder contains **Loads2Chrom.m**, a MATLAB m-file and **Loads2Chrom.exe**, a standalone executable program that runs in the Windows environment. Both convert chemometric model loadings (e.g. PARAFAC, MCR) from matrix to *.mpl format, for use in the chromatography software OpenChrom. **Loads2Chrom.m** runs within a licensed version of MATLAB. **Loads2Chrom.exe** runs on Windows operating systems with the free MATLAB Compiler Runtime (MCR) version 7.17 installed. Mpl-files can be imported into OpenChrom and compared with reference peaks in NIST mass spectral databases via its Peak Identification Batch Editor. This folder also contains **netCDFload.m**, a MATLAB m-file that loads netCDF files containing GC-MS data to MATLAB, and converts the data to two-way array (elution time x mass spectra).

Procedure for using the MATLAB mfiles:

- (1) Place **Loads2Chrom.m** and **netCDFload.m** in a folder that is located on the MATLAB path
- (2) For instructions, type '**help loads2chrom**' or '**help netCDFload**' in the command window.

Note that netCDFload requires MATLAB R2011a or later.

Procedure for using the standalone executable:

To use the executable, place your text files containing model loadings in the folder called **OpenChromData**. When you double-click on **Loads2Chrom.exe**, matching mpl files will be created in the same folder.

- (1) Unzip Loads2Chrom.zip on your computer. Choose the correct version for your computer architecture. This is either 32-bit (x86) or 64-bit (x64).
- (2) Place your C and S loadings in tab-delimited text files located in the folder OpenChromData. Be sure that the loadings adhere to the formatting described below. Three examples are provided in Example1-3.txt.
- (3) Install the **Matlab Compiler Runtime** (MCR 7.17) if it is not already installed. To do this, double-click on Loads2Chrom.exe. This extracts the MCR Installer from the archive, along with all the files that make up the MCR. Once all the files have been extracted, the MCR Installer starts automatically. Alternatively, download the installer from the web at <http://www.mathworks.com/products/compiler/mcr/index.html>
- (4) Once MCR is installed, double-clicking on **Loads2Chrom.exe** will result in mpl files created in the OpenChromData folder. One mpl file will be created to match each model contained in this folder.

Detail:

INPUT DATA: All *.txt files in the folder /OpenChromData. These must conform to a specific format. Each file contains the elution and mass spectral loadings for a single model, stored in **tab-delimited text format**.

The text files contain [C S] for a single model where:

- C is a column of elution times (in milliseconds) and nFac columns of elution loadings corresponding to each peak.
- S is a column of m/z and nFac columns of mass spectral loadings corresponding to each peak.

Thus a model with nFac factors has 2*(nFac+1) columns of data. See Example1.txt and Example1.mpl containing loadings for a 3 component PARAFAC model.

Note that elution times in C must be in milliseconds and must be rounded to the nearest whole millisecond. Also, MATLAB Compiler Runtime (MCR) version 7.17 (R2012a) must be installed to execute this program. For further detail on MCR, see <http://www.mathworks.com/products/compiler/>

OUTPUT DATA: *.mpl files are created to match the matrix loading files.

Processing implemented by Loads2Chrom:

Processing includes the following steps:

- negative parts of elution spectra are set to zero
- m/z=0 are ignored.
- data are formatted to conform with requirements of OpenChrom

Reference:

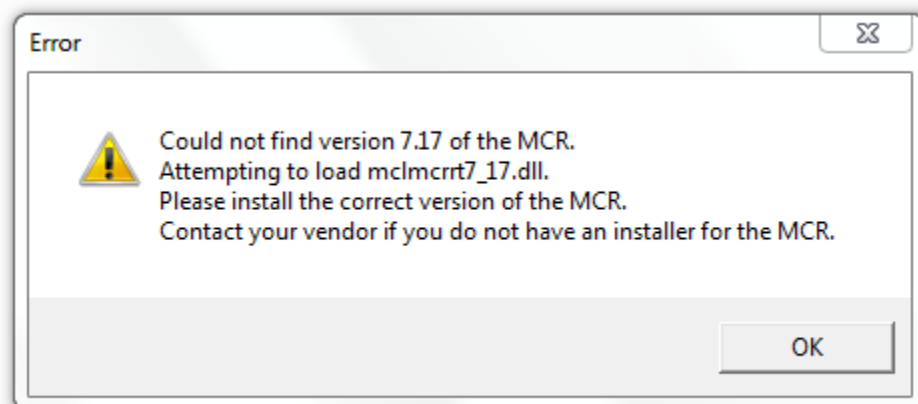
K.R. Murphy, P. Wenig, G. Parcsi, T. Skov, R.M. Stuetz. Characterizing odorous emissions using new software for identifying peaks in chemometric models of gas chromatography - mass spectrometry datasets. Chem Intel Lab Sys (in press). DOI: 10.1016/j.chemolab.2012.07.006

Contact: krm@unsw.edu.au

Questions and Troubleshooting

Q: Can I run the executable on a Linux operating system?

A: Yes, provided that you are also running a Windows emulator. If you get the exception below, you may need to manually install the correct version of MCR (either Win32 or Win64) from the web site first.



Q: Do I need a MATLAB license to install MCR

A: No, you do not. If you are being asked for license information when you attempt to download MCR it may be because you are trying to download the licensed compiler instead of the free compiler runtime. The MCR is found at <http://www.mathworks.com/products/compiler/mcr/index.html>

Q: Does it matter which version of MCR I install? Can I install the most recent one instead?

A: Yes it matters. The executable only works with MCR version 7.17.