

July 6, 2017

## **MRspa (Magnetic Resonance s processing and analysis)**

### **Initial Setup:**

Add the full pathname where you install MRspa in your Matlab startup file.

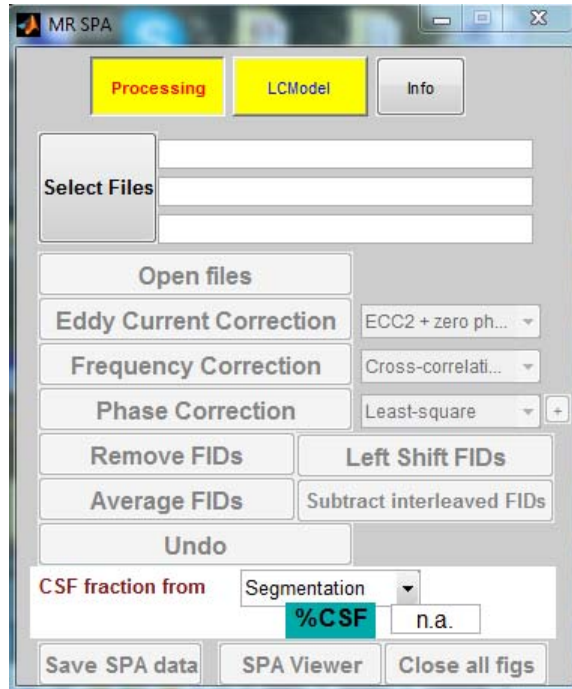
To start the program, execute MRspa.

*NOTE:* Current version does not support spaces in filenames and pathnames.

### **First time use:**

First time you run MRspa, you will be prompted to enter 1) the name of the host computer where the LCModel license is installed and 2) the exact LCModel license holder name (refer to LCModel manual for more info), and 3) the location of the LCModel executable file. If MRspa is run under Windows, there will be an additional step, i.e. 4) to enter the user's home directory path on the linux machine where LCModel is installed.

## Processing Tab (preprocessing of MRS data before LCModel analysis)



### Select files

- 1) Dicom , Siemens RAW, Bruker or Varian data format

Select the metabolite file/folder (water suppressed data)

Water reference file/folder for ECC correction

Water reference file/folder for absolute quantification

- 2) SPA files (change "Files Filter" for selection)

This is used to add several SPA files. In general, performing a frequency correction is enough before summing the data.

### Open files

Load data picked up using the "Selected files" button. Note that this does not load the "Water TEs" files which are processed independently when clicking the %CSF button.

### Eddy current, Frequency and Phase Corrections

Different algorithms are available to perform these specific corrections. In most cases using the default option is sufficient.

#### Remove FIDS

Remove selected individual FIDs from the metabolite data

#### Average FIDS

This is used only if there is not enough SNR in single scans to perform scan-to-scan frequency correction. This option allows averaging of data in small blocks before frequency correction. For example, a set of 128 scans can be averaged into 32 blocks of 4 scans each, and then frequency correction can be performed on these 32 blocks.

#### Undo

Undo previous processing steps, starting with the most recent one. To view all the processing steps carried out, move arrow over the Undo button.

#### CSF fraction from

1) Water TEs: Use button to select water files acquired at different TEs.

%CSF: Determine the CSF fraction by performing a bi-exponential fit of water data at different TEs. The user needs to enter an assumed value for T2csf.

2) Segmentation: Enter %CSF which was obtained using MRI segmentation

#### Save SPA data

Processed summed spectrum, water reference for quantification and CSF fraction are saved in .spa format. In addition, all the processing steps performed on the dataset are saved into this file except if zero-order phase correction was done. Do **NOT** use "Save as" button on the "SPA viewer" window to save the data, else spectrum will be saved with the display LB and GF filters.

## SPA viewer

This button opens a new window to

View individual/sum spectrum

Perform zero-order phase correction

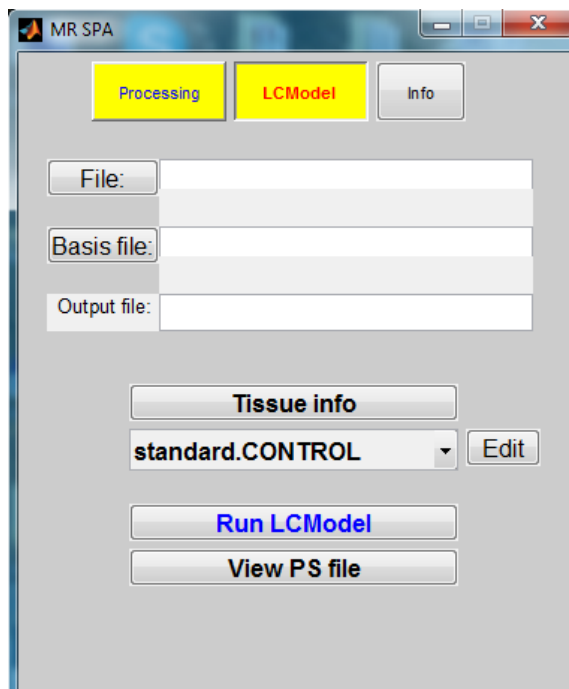
Measure linewidth of metabolites

Determine SNR

Save spectra (as displayed with LB and GF values) in Varian or EPS format

## **LCModel Tab:**

LCModel analysis can be carried out on a single .spa file or multiple .spa files (i.e. batch analysis).



### File

Load .spa, .batch or .COORD file (change "Files Filter" for selection)

Multiple .spa files can be selected. In this case, MRspa will generate a .batch file (user-input filename) containing a list of the selected .spa files. The name of the saved .batch file will be shown in this entry.

Selecting LCMODEL fitted .COORD files allow to view the measured spectrum, fitted spectrum, baseline, residual or individual metabolite fits.

### Basis file

Select Basis set file to use during LCMODEL analysis.

For easy file selection, it is recommended to copy your .BASIS file in a directory called *basis-sets* located in the MRspa directory.

### Output file

Single file mode: If the entry is left blank, MRspa will assign the output filename to that of the input "SPA file".

Batch mode: This entry will display "Batch mode". For each dataset, the output filename will correspond to the filename of the starting .spa file.

#### Tissue info

For absolute concentration, the following parameters are required: TE, T2 water (user defined or fitted T2 value obtained during processing step from CSF calculation), T2 metabolite, %CSF fraction, %water content and %CSF water content.

Single file mode: If the .spa file contains the CSF fraction (calculated during the Processing steps), the "CSF fraction (%)" entry will display its value. Otherwise this entry will be empty and will need to be entered manually.

Batch mode: The "CSF fraction (%)" entry is omitted in the input parameters and MRspa assume that all .spa files contain the CSF info. Another way to include the CSF fraction info is to edit the .batch file and add the CSF fraction value at the end of each line. *Important:* the latter option will ignore any CSF fraction value contained in the .spa file.

#### .CONTROL file

Select CONTROL file from the popup list. All .CONTROL files are located in a directory called CONTROL located in MRspa.

#### Edit

Edit the selected control file in order to modify/add input parameters used by LCMoDel.

Ok button: This will save any changes made in memory ONLY and these changes will apply only for the current LCMoDel analysis. To reload the control file, reselect the file from popup menu list.

Discard button: Discard any changes and use the previous control parameters in memory

Save as button: This option will save the parameters in a new control file.

#### Run LCMoDel

This step will run LCMoDel only after these files (RAW, .CONTROL, .H2O, ...) were successfully created. If LCMoDel fails, a message will display the error codes corresponding to the problem.

#### View PS file

View the output .PS file generated by LCMoDel. This option is only available in single file mode analysis

#### Metab conc Table

Generate a table from all datasets which contains data on abs concentration and CRLB. The table is saved as xx\_conc.txt where xx is the name of the batch file (see "SPA file" above) and this file is located in the same directory where the .batch file was saved. This table can be imported directly into Excel as a text file. Note that this option is only available in batch mode analysis.