



Data Manipulation Software

© 2010 Grup d'Aplicacions Biomèdiques de la RMN (GABRMN)

Table of Contents

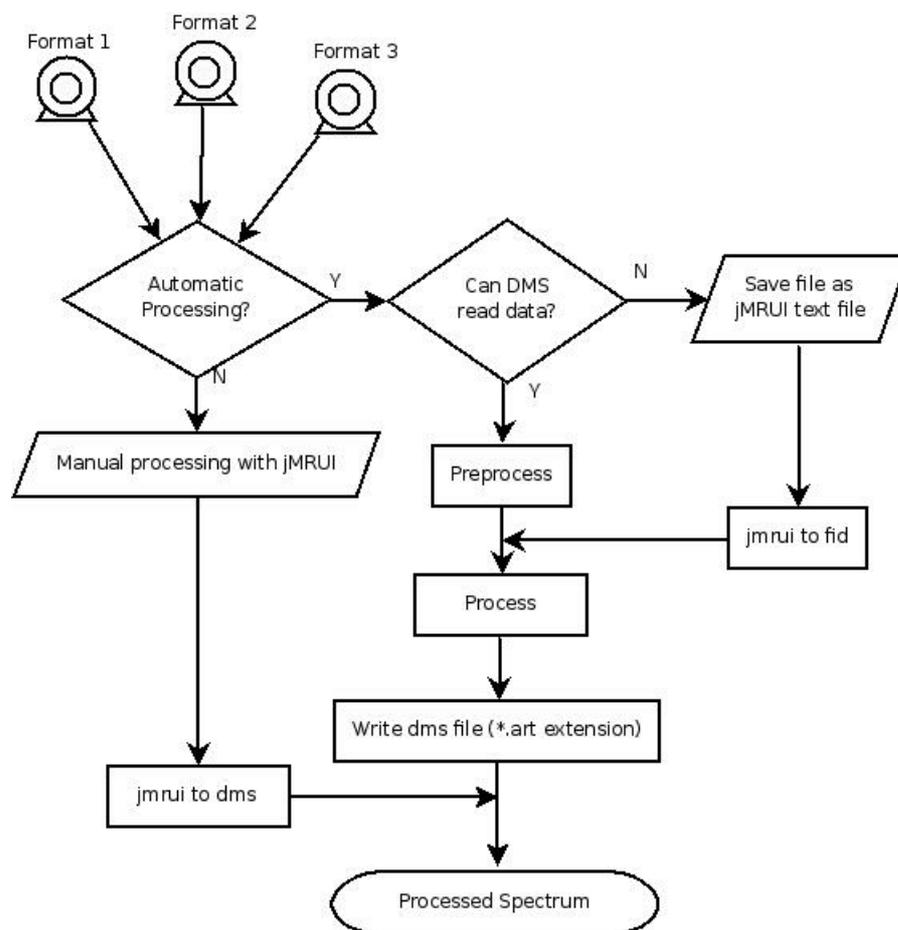
1 Introduction	3
2 Raw files	4
3 Canonical format	5
4 How do I use it?	7

1 Introduction

The Data Manipulation Software (DMS) is a tool developed along the last ten years first by the University of Sussex, in the context of the [INTERPRET](#) European project and later by the GABRMN, from 2003 onwards. The DMS is able to read raw data files from Single Voxel MR scanners and to process them automatically.

Since each manufacturer has their particular way to export MRS data, a canonical format to represent the MRS was needed independently of the machine, number of points and sweep width. The INTERPRET canonical format (DMS format) works for single voxel data (originally at 1.5T) and it has 512 points to represent the range between 7.1 to -2.7 ppm. The DMS format has the art extension and it is a simple ASCII text file.

The user is encouraged to keep in mind the following scheme about the use of the DMS.



The DMS can automatically process only some types of [raw data files](#). If the file version or manufacturer is not listed below in section 2, the user can use JMRUI as a format converter to export MRS data in text format (See JMRUI

section in [raw files](#) part).

2 Raw files

Unprocessed MRS data from the following manufacturers and formats can be processed by the system:

- Raw data directly exported from Philips scanners (sdat/spar).
- Raw data directly exported from a GE scanner up to version 9X, in SAGE format (Pxxxx file with an accompanying shf file or alternatively a sdf/shf pair of files).
- Raw data directly exported from Siemens scanners (Numaris 4 - raw extension)
- JMRUI text file. [JMRUI](#) can be used as a format reader in case that data comes from another version or manufacturer not listed above.

For all MRS types, you should provide enough information in order to correctly process and load the case.

Please be careful with the options.

Although automated alignment check-up is carried out by the processing algorithm, you may want to double check it in case of uncommon spectral patterns. The creatine resonance should appear at 3.034 ± 0.004 ppm. If creatine is not visible, total choline should appear at 3.210 ± 0.004 ppm. If not, manual realignment of the processed file may be needed.

Philips:

In order to process and classify raw data files with the DSS, please check that you have both metabolite (water suppressed) and water (unsuppressed water) acquisitions and that you have the corresponding spar/sdat pairs for each of these. Ensure that all are located in the same directory. This is mandatory for the INTERPRET data manipulation software (DMS) to be able to process your files. Secondly, you have to name your files in a specific way: [filename_metabolite].[spar/sdat] for the metabolite acquisitions and [filename_water].[spar.sdat] for the unsuppressed water acquisitions. The "filename" should not contain any blank spaces or characters such as "_".

Siemens:

In order to process and classify raw data files from Siemens, please check that you have both metabolite (water suppressed) and water (unsuppressed water) *.raw data files, and ensure that they are located in the same directory. This is mandatory for the INTERPRET data manipulation software (DMS) to process your files. The second issue is the file name: your files must be renamed with the following convention: [filename_metabolite].raw for the metabolite file and [filename_water].raw for the water file. The "filename"

should not contain any blank spaces or characters such as “_”.

GE:

Raw data directly exported from GE scanners (up to 9X version)

- For the Sage formats that have metabolite (suppressed water) and water (unsuppressed water) and sdf/shf pairs of files, be sure that the files are in the same directory and are named according to the following convention: [filename_metabolite].[sdf/shf] and [filename_water].[sdf/shf].
- For the PROBE files, be sure that both the PROBE file and the accompanying shf file are in the same directory and that have the same filename (P [filename] and P[filename].shf). The “filename” should not contain any blank spaces or characters such as “_”.

JMRUI:

JMRUI is an independent program that can easily perform MR analysis (<http://sermn02.uab.cat/mrui>). It can read a wide variety of raw data files from different scanner vendors and versions of their softwares. This capability can be exploited using JMRUI as a 'format converter'. The user can open his/her case and save it as text file without any processing in order to store the acquisition signal in it. This is specially important in raw data files obtained in scanners with multi-channel coils where the files have to be manually consolidated in order to obtain a single acquisition file. Be careful to save each file (one for metabolites, one for water signals) in text format with *.txt extension using the JMRUI.

3 Canonical format

The DMS performs some processes over the time-domain signals in order to produce a single spectrum. The process is composed by the ten steps listed below:

1. Compute the water line width using one lorentzian over the unsuppressed water fid.
2. Apply the Quality algorithm (Klose algorithm: Deconvolution of metabolite fid with its unsuppressed water fid).
3. Henkel - Lanczos Singular Value Decomposition (HLSVD) filter of the residual water signal in the metabolite fid (Using 10 lorentzians).
4. Apply a lorentzian apodisation resulting in a line broadening of 1 Hz.
5. Do the Fast Fourier Transform, with zero-filling up to 819 points if the spectrum has less than 819 data points.
6. Correct the spectrum baseline offset, taking as a reference points in the [-2ppm, -1ppm] and [9ppm, 11ppm] regions.
7. Compute the maximum Signal/Noise ratio in the [0ppm, 3.4ppm] region taking as a reference the [9ppm, 11ppm] noise.

8. Set to zero all points in the region [4.33ppm, 5.1ppm] and then normalise the spectrum intensities in the region [7.1ppm, -2.7ppm] to unit length.
9. Save the spectrum in a DMS format (ASCII text file with art extension).
10. Align the 'art' file and save it in the '_aligned.art' file.

The alignment process adds zeros to the beginning or to the end of the spectrum and removes the same number of data points of the opposite part in order to correct the desired peak to the expected position. Alignment is based on the following algorithm:

1. Search Choline, Creatine and Lipid peaks at 3.21, 3.03, and 1.29 ppm respectively. Each peak is searched in a range near the expected position point (± 4 or 5 data points). One point will be a peak only if its height is greater than the height of the contiguous points on the left and right sides.
2. If the Creatine peak is found and:
 - 2.1. If the Choline peak is found and its height is greater than 3 times the Creatine height then align the spectrum using the Choline reference.
 - 2.2. If the Lipid peak is found and its height is greater than 10 times the Creatine height then align the spectrum using the Lipid reference.
 - 2.3. If the two previous conditions are not satisfied then align the spectrum using the Creatine reference.
3. If the Creatine peak is not found, but the Choline peak is found and:
 - 3.1. The Lipid peak is found and its height is greater than 10 times the Choline, then align the spectrum using the the Lipid reference.
 - 3.2. If the previous condition is not satisfied then align the spectrum using the Choline reference.
4. If neither the Creatine nor the Choline peaks are found but the Lipid peak is present then align the spectrum using the Lipid reference.
5. If none of the three peaks is found in the ranges expected then the spectrum can not be aligned automatically and is left unchanged.

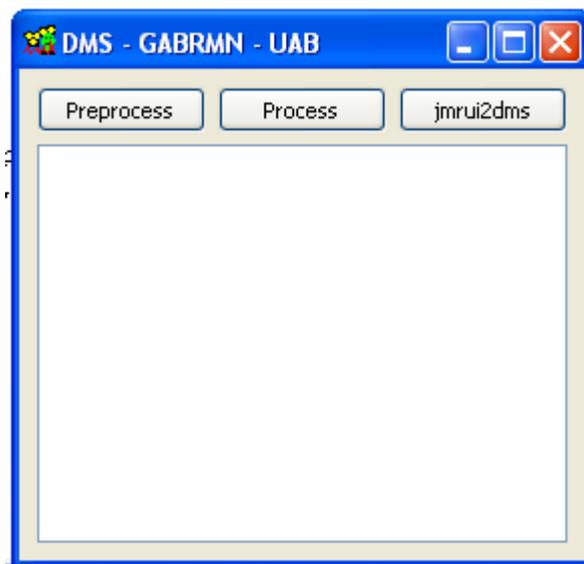
The resulting spectrum is formed by 512 points and represents the region between 7.1 ppm and -2.7 ppm. All spectra obtained using the DMS have the same characteristics and they can be compared or analyzed in the same way as files obtained from a single scanner. The DMS is the tool to make multi-scanner analysis.

The described process in this section is similar to the one described in Tate et al. 2006[1] with enhancements. This processing provides a good quality spectrum in a wide range of cases but if the results are unexpected, please consider a manual processing for the case with another tool like JMRUI and convert it to the DMS format with the jmrui2dms tool provided with the DMS gui.

[1] Tate, A.R., et al., Development of a decision support system for diagnosis and grading of brain tumours using in vivo magnetic resonance single voxel spectra. *NMR Biomed*, 2006. 19(4): p. 411-34.

4 How do I use it?

The DMS has a minimalist graphical user interface with 3 buttons and a text area.



The function of each button is as follows:

- Left button: Clicking in this button, the user can select the file to be 'Preprocessed'.
- Middle button: Clicking in this button, the user can select the file to be 'Processed'.
- Right button: It is used to invoke the method to convert a manually processed JMRUI text file into the 'canonical' DMS format.

'Pre-process' reads the raw data files and creates another set of intermediary files, one for the metabolite and another for the water signal. These files have the *.fid extension and contain only one free induction decay signal (FID). If there are several individual FIDS, they are summed. These intermediary files solve the format number and platform incompatibilities and put the relevant information into the same format without any manufacturer dependencies.

'Process' is the application of all mathematical steps described in the [Canonical format](#) section in order to obtain a 'canonical spectrum'. Please be careful to select the respective *.fid files obtained from the 'Pre-process' step.

Output files will be created in the same folder where the original files are.

Log information about the process applied to the files will appear in the text area provided.

It has to be taken into account that if the DMS is able to process the target files automatically, the right output file is named '*_aligned.art'. If the user uses the DMS to convert a manually processed file into DMS format, the right output file is named '*_fromJMRUI.art'.

For further information or support contact to dms@gabrmn.uab.es

Back Cover