# Macromolecule data collection

This repository contains a number of pre-processed macromolecule (metabolite-nulled) spectra in Varian format (sometimes converted from Siemens format), acquired at different field strengths from different mammals, including human. These data are represented in Figure 1 of the recently published consensus on macromolecule acquisition and handling.
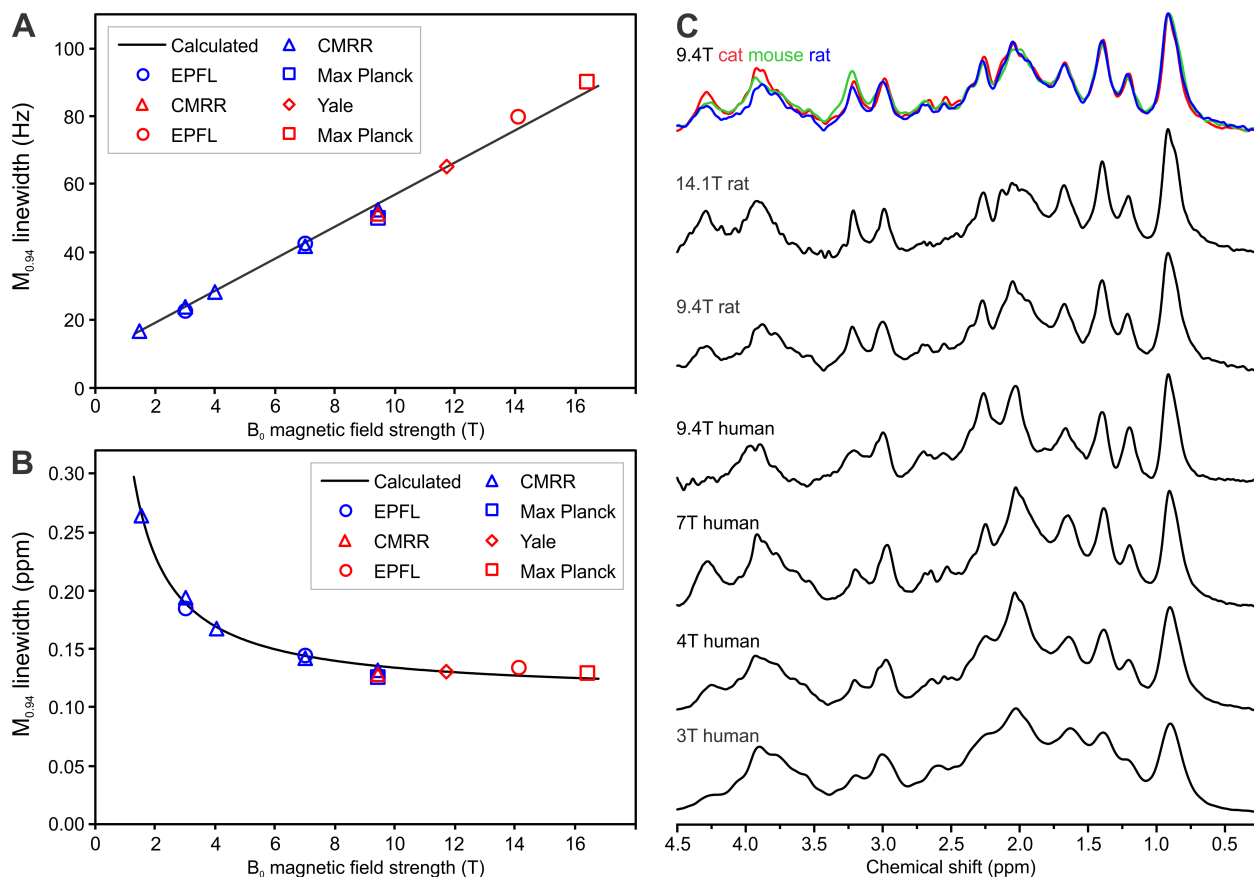
(adapted from: C Cudalbu, KL Behar, PK Bhattacharyya, W Bogner, T Borbath, RA de Graaf, R Gruetter, A Henning, C Juchem, R Kreis, P Lee, H Lei, M Marjanska, R Mekle, S Murali-Manohar, M Považan, V Rackayova, AM Wright, D Simicic, J Slotboom, Z Starčuk, J Starčukova, BJ Soher, I Tkáč, S Williams, M Wilson, L Xin, V Mlynárik. Contribution of macromolecules to brain 1H MR spectra: Experts' consensus recommendations. NMR Biomed (2020, in revision))

MM data have been acquired from multiple subjects, frequency-corrected, summed, and the residual water and 3.93 ppm Cr/PCr peak were removed.

The following MM spectra are included in this repository:

Field strength (T)	Localization	TE [ms]	Type	Author
3	STEAM	8	Human	Dinesh Deelchand
4	STEAM	4	Human	Ivan Tkáč
7	STEAM	6	Human	Ivan Tkáč
9.4	sLASER	24	Human	Anke Henning
9.4	STEAM	2	Rat	Ivan Tkáč
9.4	STEAM	2	Mouse	Ivan Tkáč

Field strength (T)	Localization	TE [ms]	Type	Author
9.4	STEAM	2	Cat	Ivan Tkáč
14.1	SPECIAL	2.8	Rat	Cristina Cudalbu

In addition, the repository contains two conventional single-subject 1H-MRS spectra from the human occipital cortex:

Field strength (T)	Localization	TE [ms]	Type	Author
4	STEAM	4	Human	Ivan Tkáč
7	STEAM	6	Human	Ivan Tkáč

Importing data

All of the above data can be imported with a Varian import function of your choice. For example, Jamie Near's FID-A toolbox includes the function `io_loadspec_varian.m`. The following set of code snippets can serve as a starting point:

```
filename = 'MM_database/9.4T_MM_rat_STEAM_CMRR.fid';
MM_rat = io_loadspec_varian(filename);
```

The loader will likely prompt you to provide the dimensions of the data - entering `1` for the time dimension, `2` for the average dimension, and `0` for all other dimensions will do the trick:
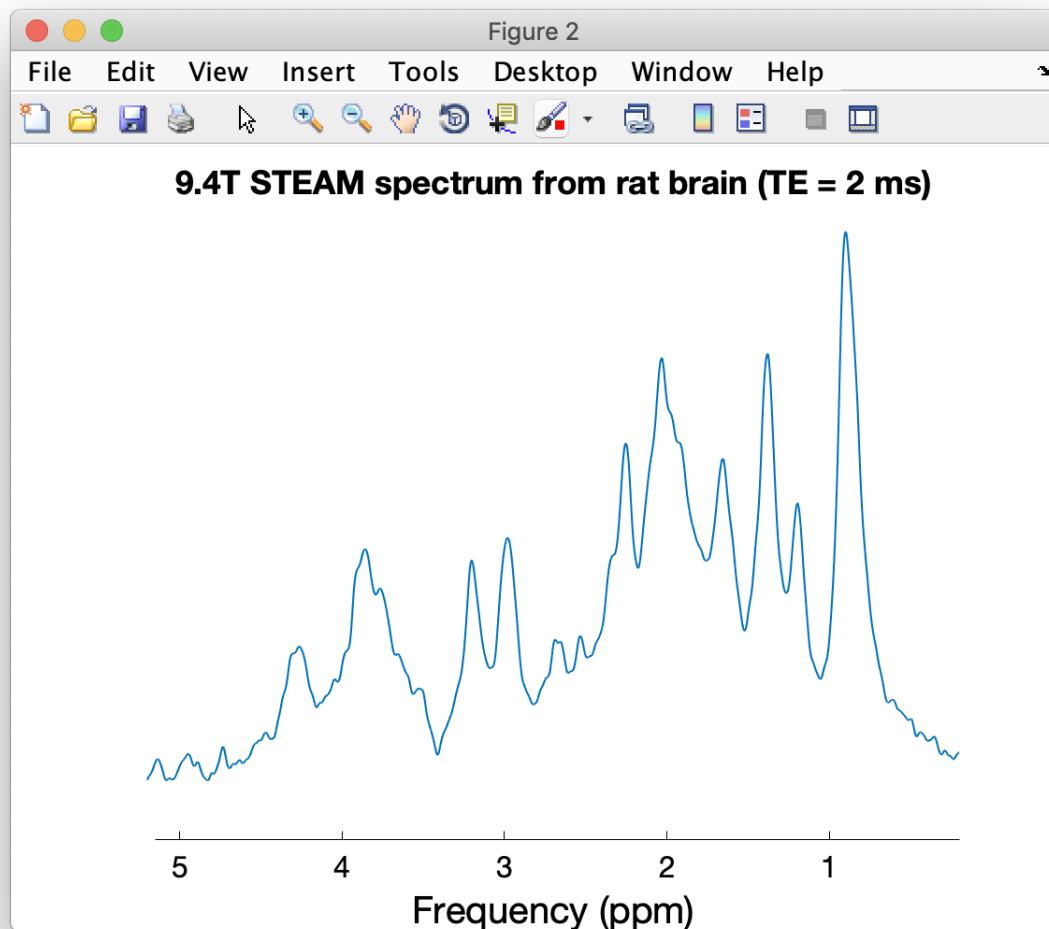
```
THE SIZE OF THE DATA ARRAY IS:  2048 x 1

Now please identify each of the data dimensions.  Note, if any two
data dimensions have the same array index, you will also need to
specify whether they are interleaved or not.  For example, if averages
and coils are both indexed in the 2nd dimension of the array, please
answer '2' below for both averages and coils, and then answer 'y' or 'n' to
the question about whether they are interleaved or not.

Which is the time dimension? (Usually it is '1'):  1
Which is the coils dimension? ('0' for none):  0
Which is the averages dimension? ('0' for none):  2
Which is the subspecs dimension? ('0' for none):  0
Any extra dimensions not listed above?  ('0' for none):  0
```

You can then plot the data using the FID-A `op_plotspec` function:

```
op_plotspec(MM_rat, 0.2, 5.2, 'Frequency (ppm)', '', '9.4T STEAM spectrum from rat brain (TE = 2 ms)');
```

Acknowledgements