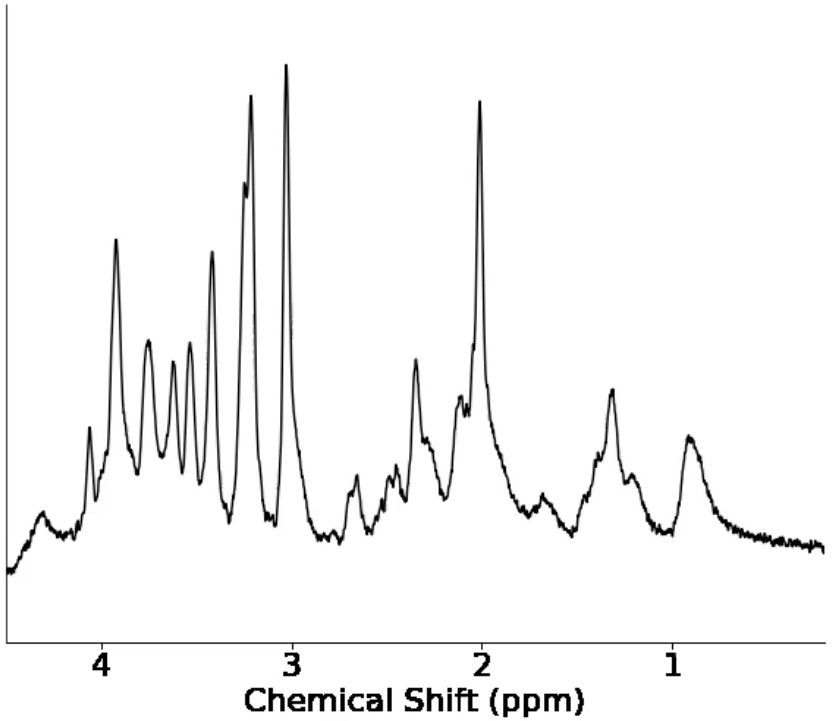
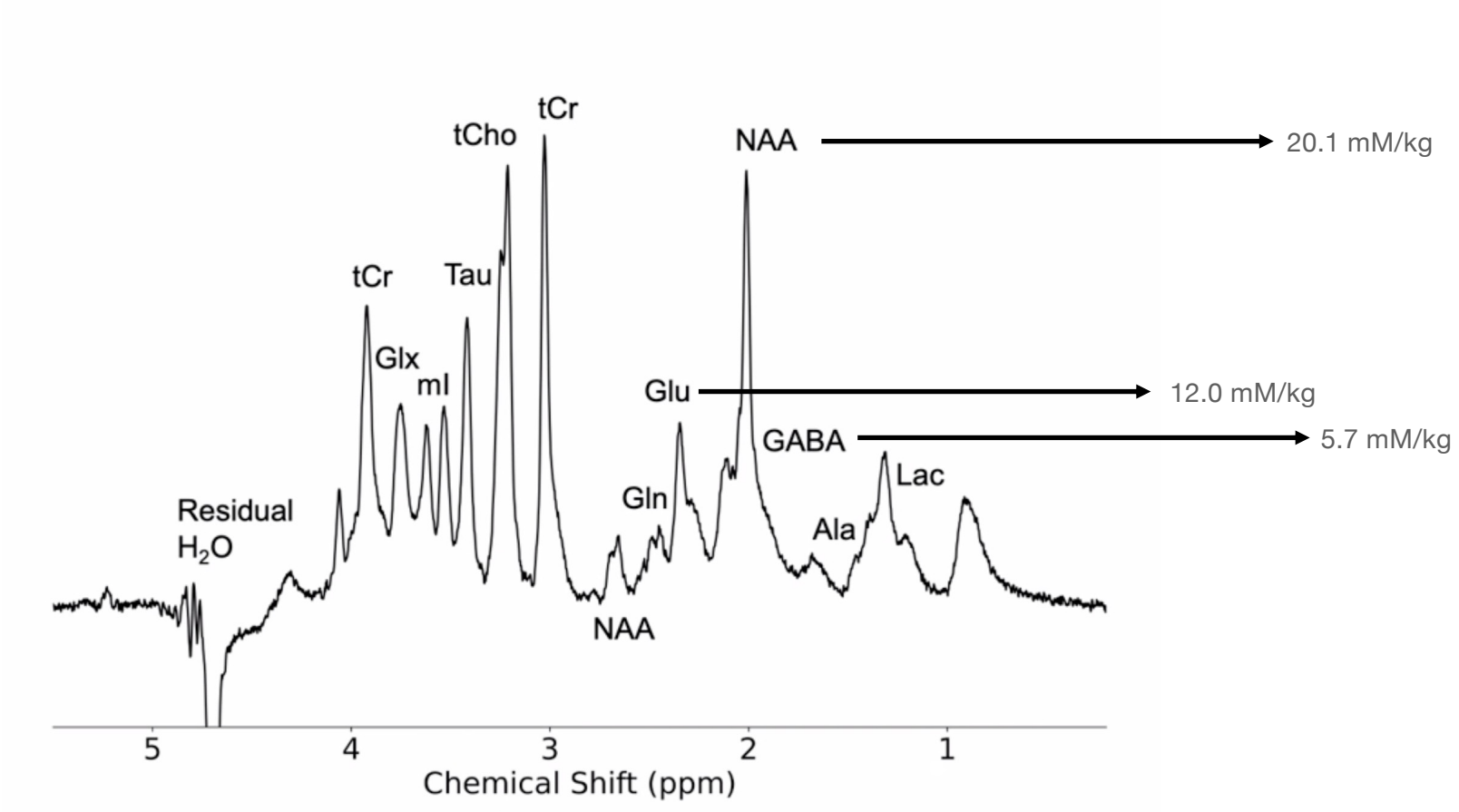
FSL-MRS – Tools for Magnetic Resonance Spectroscopy



III. Fitting

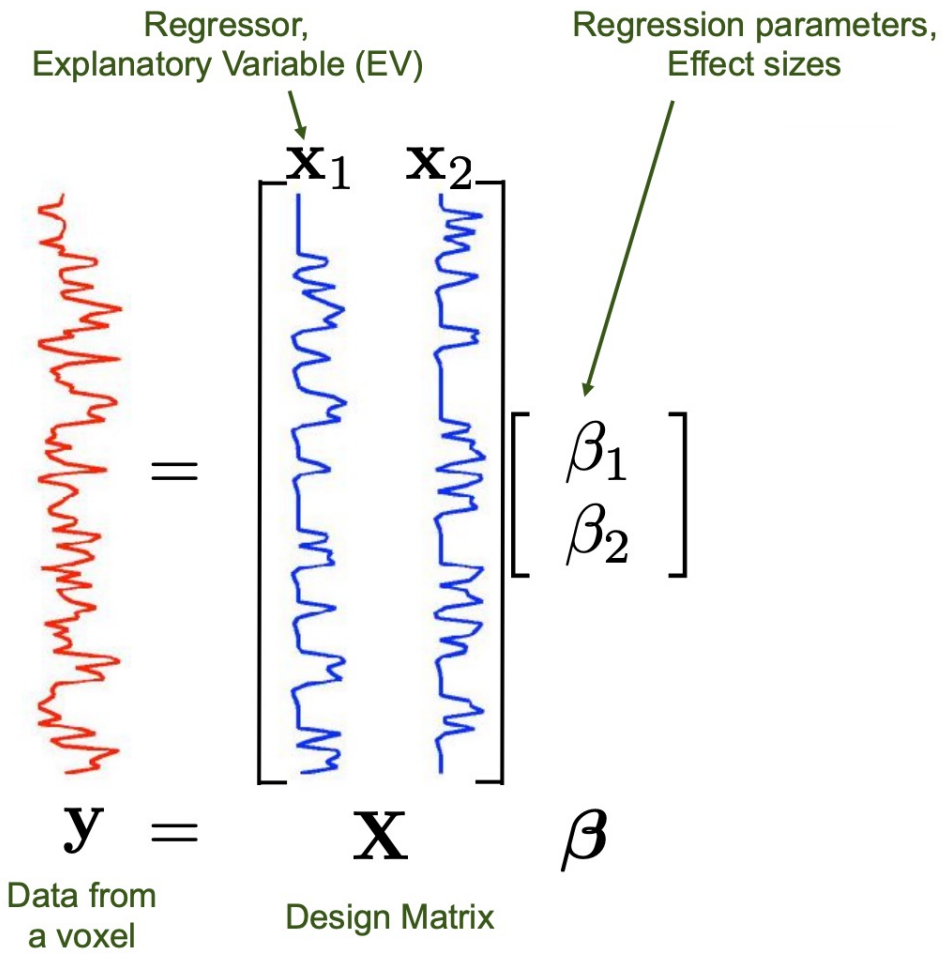
Goal of MRS fitting

Metabolite quantification



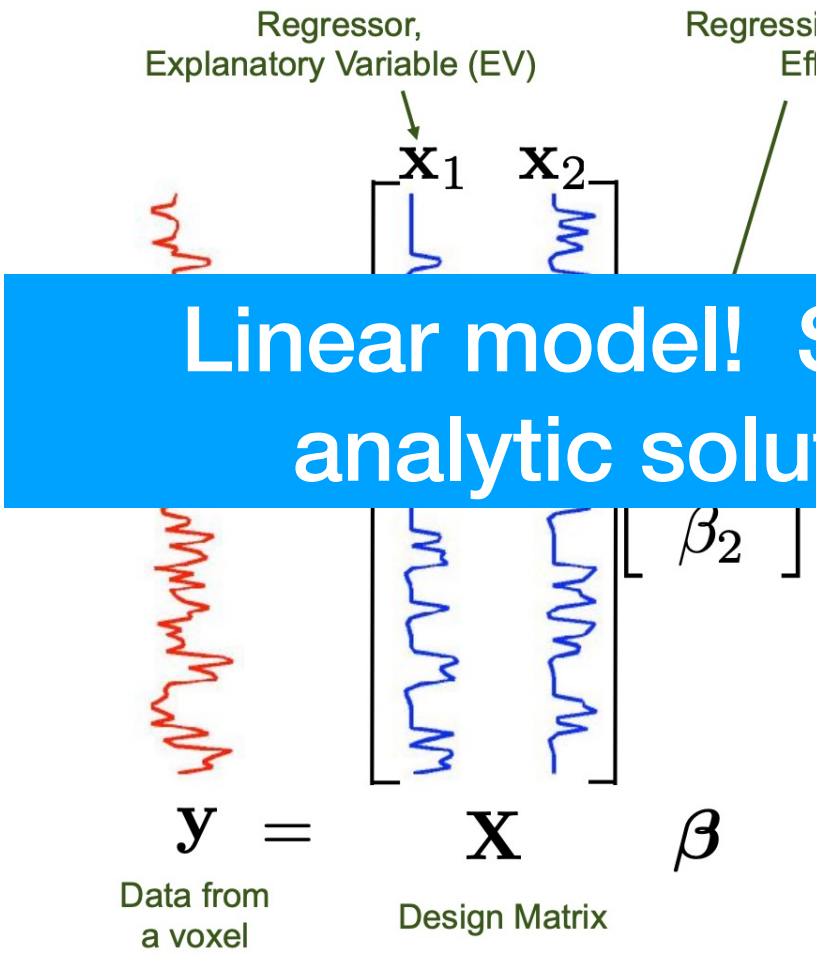
Remember the GLM?

For task FMRI

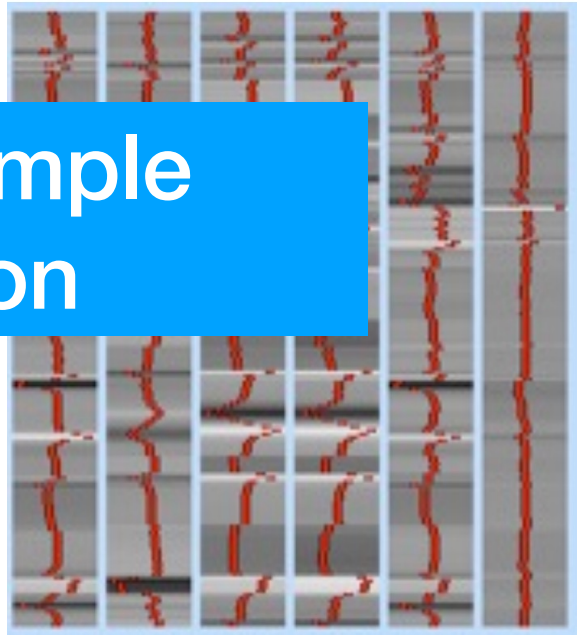


Remember the GLM?

For task FMRI



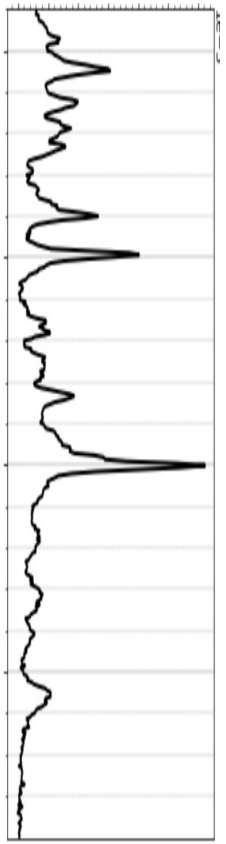
Linear model! Simple analytic solution



Motion regressors (confounds)

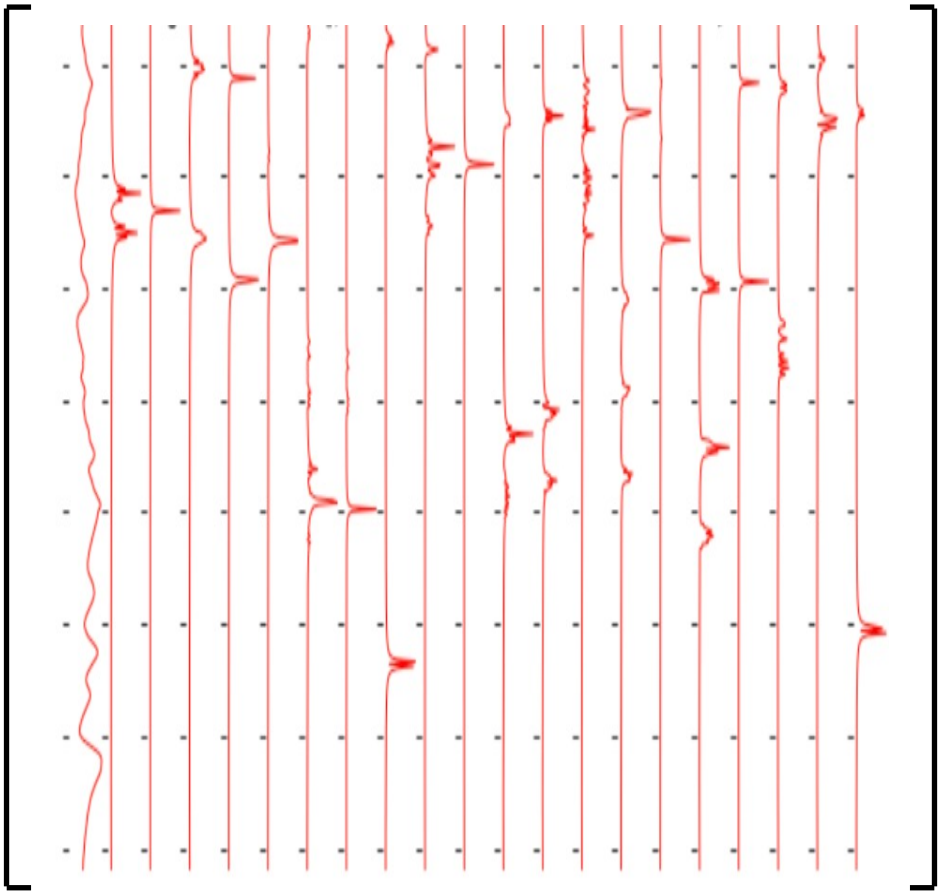
MRS Modelling is also a GLM

Spectrum (complex)



=

Basis (design matrix)



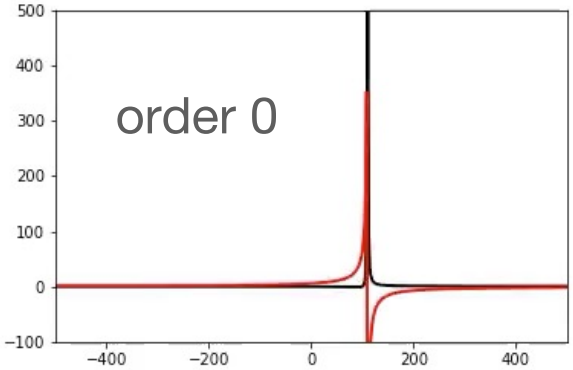
Concentrations

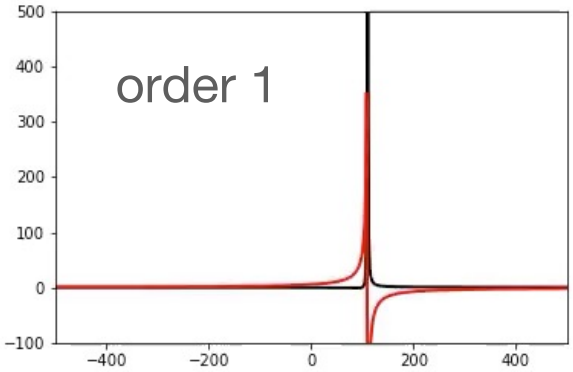
$$\begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{bmatrix}$$

Each metabolite has its own spectrum

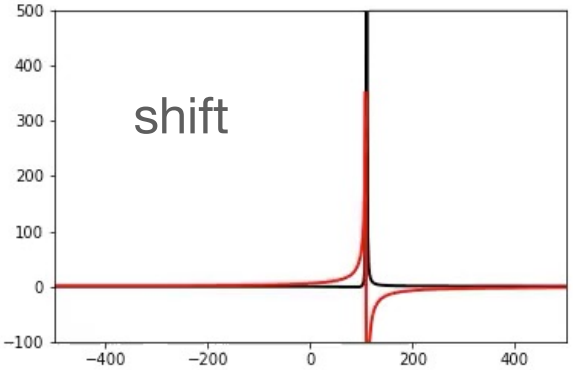
But with "Confound" modelling

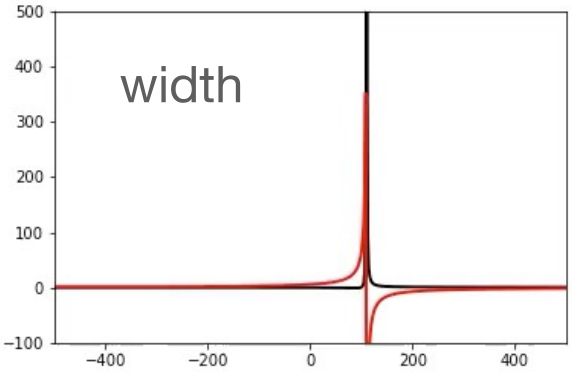
Phase



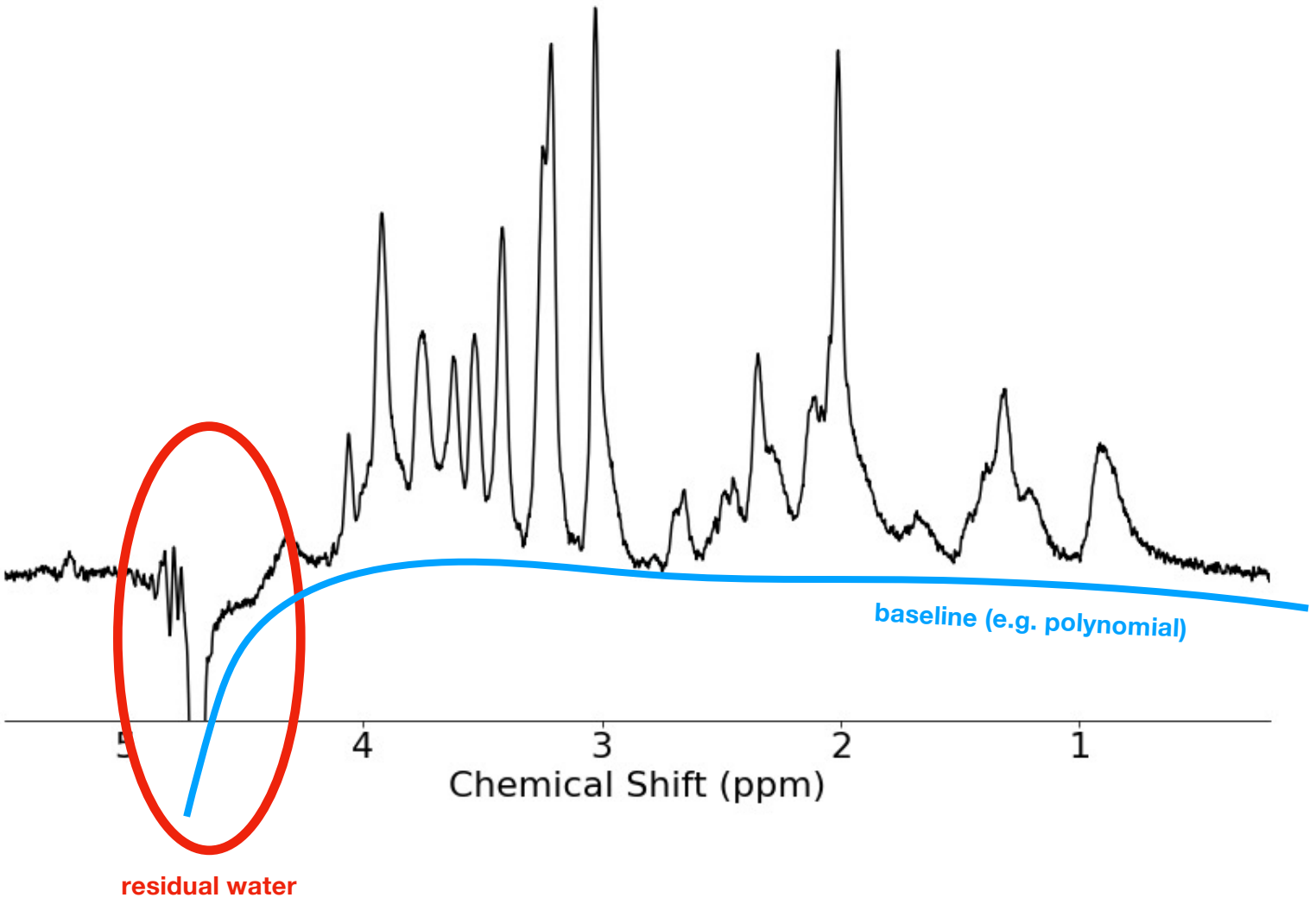


Line shape



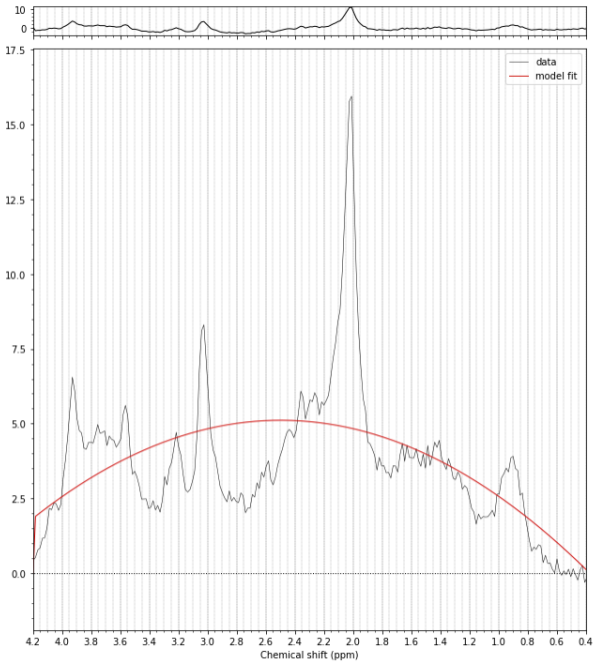


Other confounds (baseline)

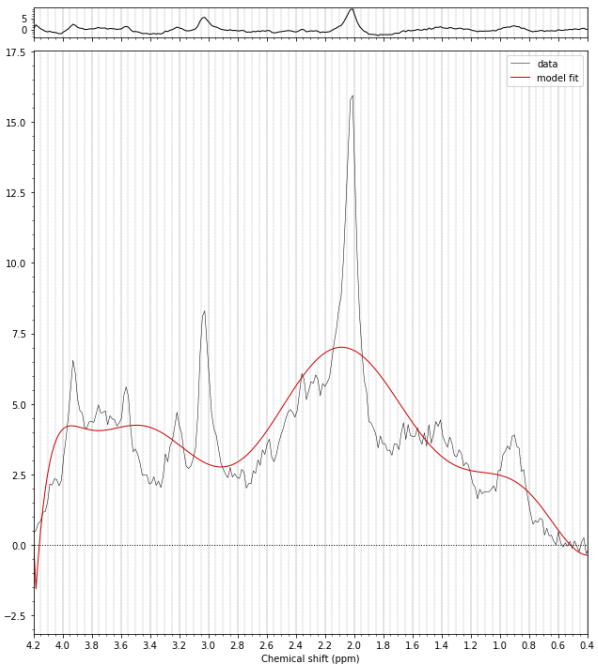


Beware of overfitting!

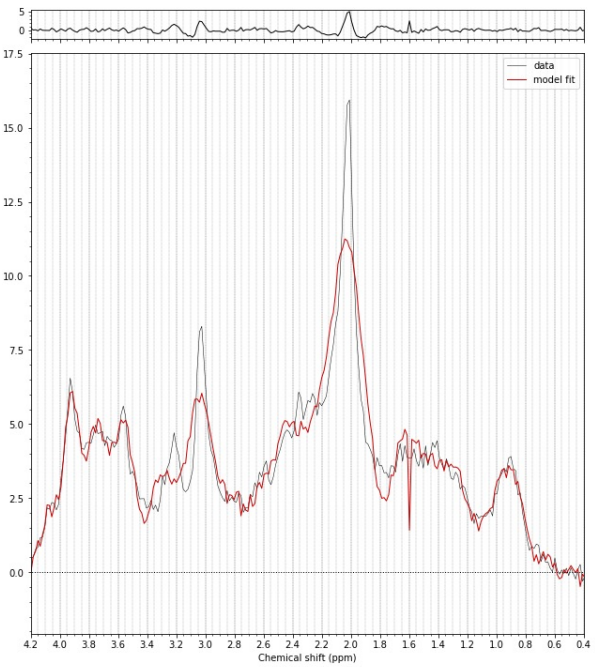
order = 2



order = 10



order = 50



The model

$$S(\nu) = B(\nu) + e^{-j(\Phi_0 + \nu\Phi_1)} \sum_{g=1}^{N_g} \sum_{k=1}^{N_m} c_{k,g} \Im \left[m_k(\tau) e^{-\tau(\gamma_g + j\epsilon_g)} \right]$$

- $S(\nu)$: complex Spectrum
- $B(\nu)$: Baseline
- $e^{-j(\Phi_0 + \nu\Phi_1)}$: Phase (0th and 1st order)
- $c_{k,g}$: Concentrations
- $m_k(\tau)$: Basis "spectra"
- $e^{-\tau(\gamma_g + j\epsilon_g)}$: Line shifting and broadening

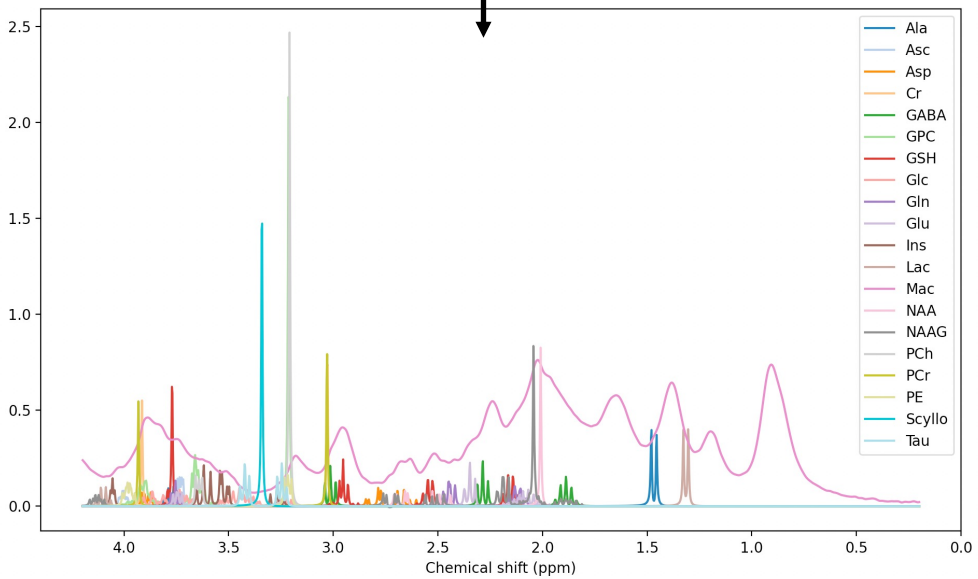
Nonlinear model! Requires Optimisation

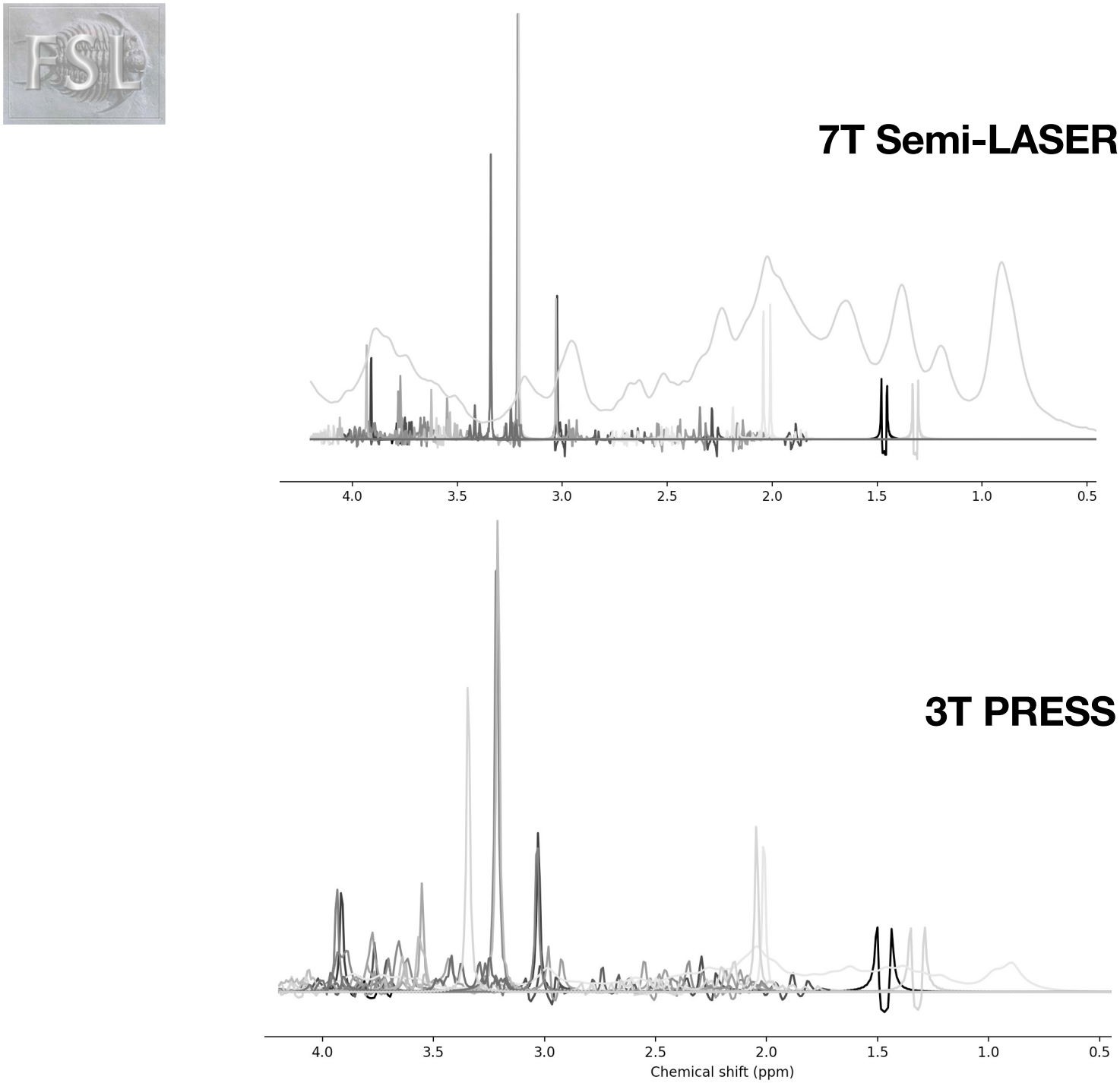
Constructing the basis

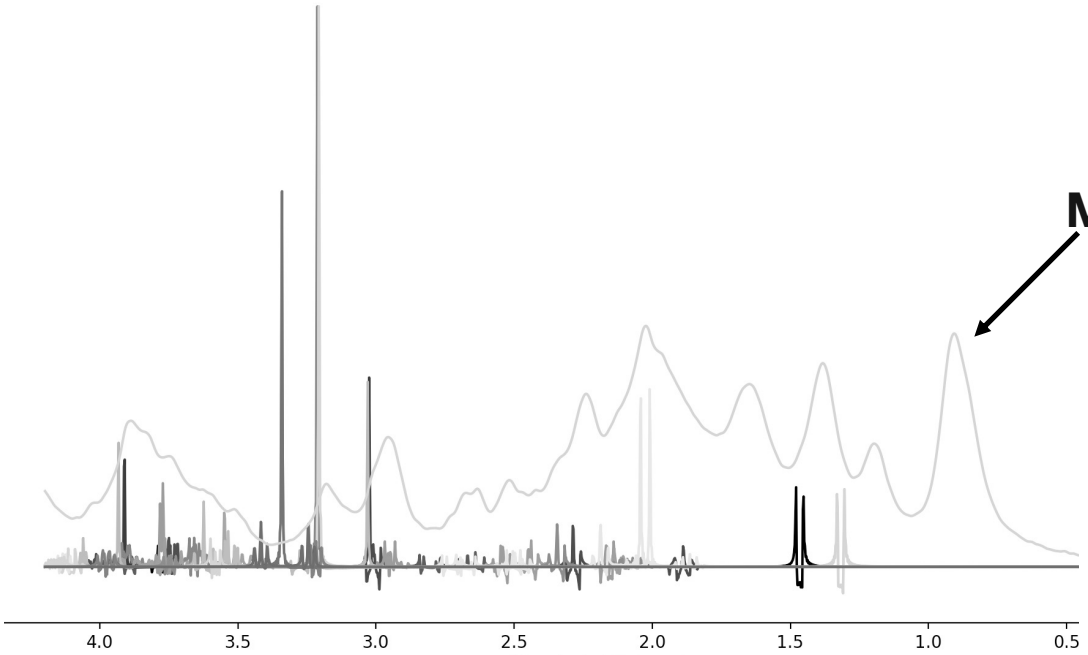
Spin system (metabolite)

Sequence (Gradients and RF pulses)

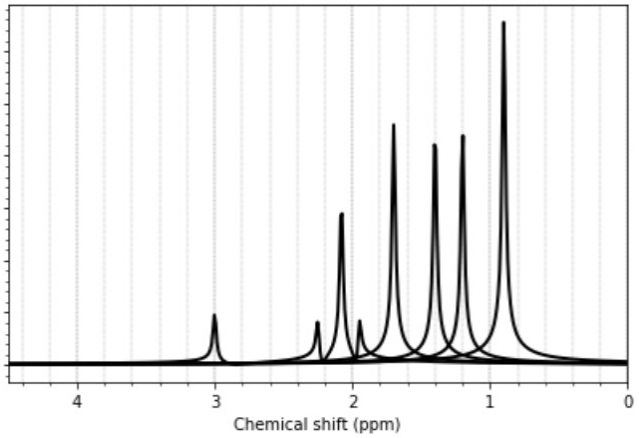
Density Matrix Simulator




7T Semi-LASER
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
3T PRESS
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
Chemical shift (ppm)



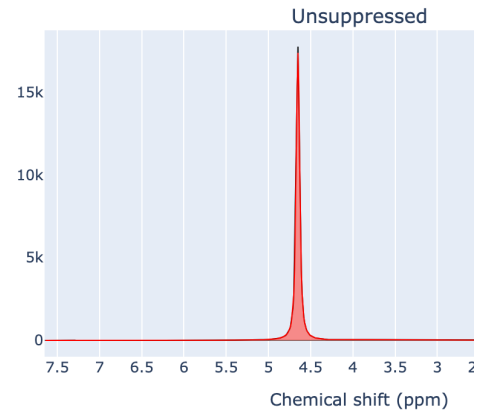
- Measured (with a similar sequence, nulling metabolite signal)
- Simulated (approximate)

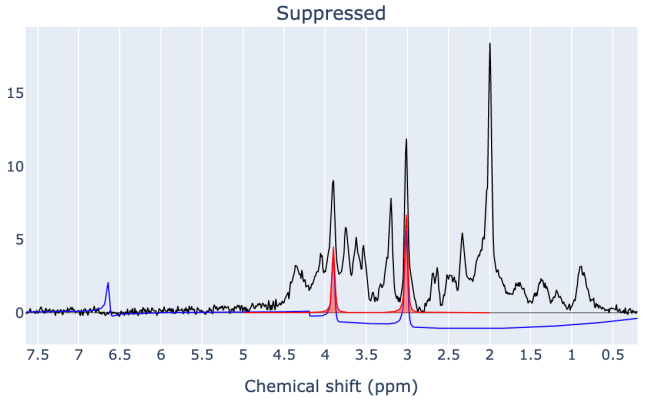


Quantitation

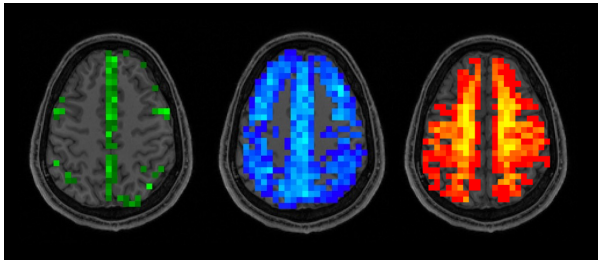
Calibrated measurements

- Water reference data
- Ref metabolite (e.g. tCr)





- Tissue partial volume (FAST)



- Relaxation parameters (typically from literature)

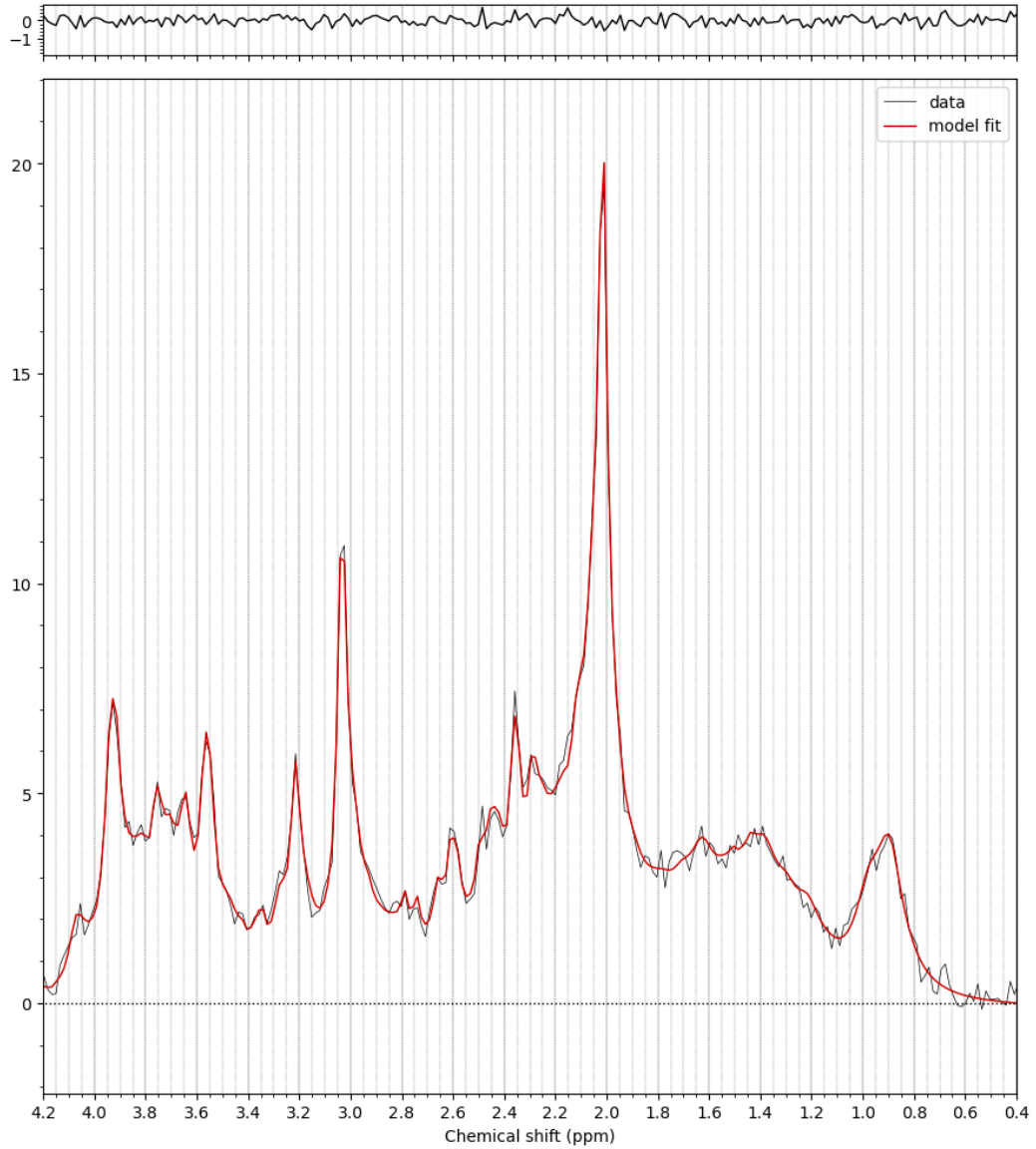
```
STANDARD_T1 = { '3T':{'H2O_WM':0.97, # Ref: 1-6
                      'H2O_GM':1.50, # Ref: 1-6
                      'H2O_CSF':4.47, # Ref: 4
                      'METAB':1.29}, # Ref: 2, 7-9
                '7T':{'H2O_WM':1.21, # Ref: 1-6
                      'H2O_GM':2.05, # Ref: 1-6
                      'H2O_CSF':4.43, # Ref: 4
                      'METAB':1.43}} # Ref: 2, 7-9

STANDARD_T2 = { '3T':{'H2O_WM':0.073, # Ref: 1,3,10-11
                      'H2O_GM':0.088, # Ref: 1,3,10-11
                      'H2O_CSF':2.030, # Ref: 12
                      'METAB':0.194}, # Ref: 7-9,13-15
                '7T':{'H2O_WM':0.055, # Ref: 1,3,10-11
                      'H2O_GM':0.050, # Ref: 1,3,10-11
                      'H2O_CSF':1.050, # Ref: 12
                      'METAB':0.131}} # Ref: 7-9,13-15
```

Examples of fits

Good fit

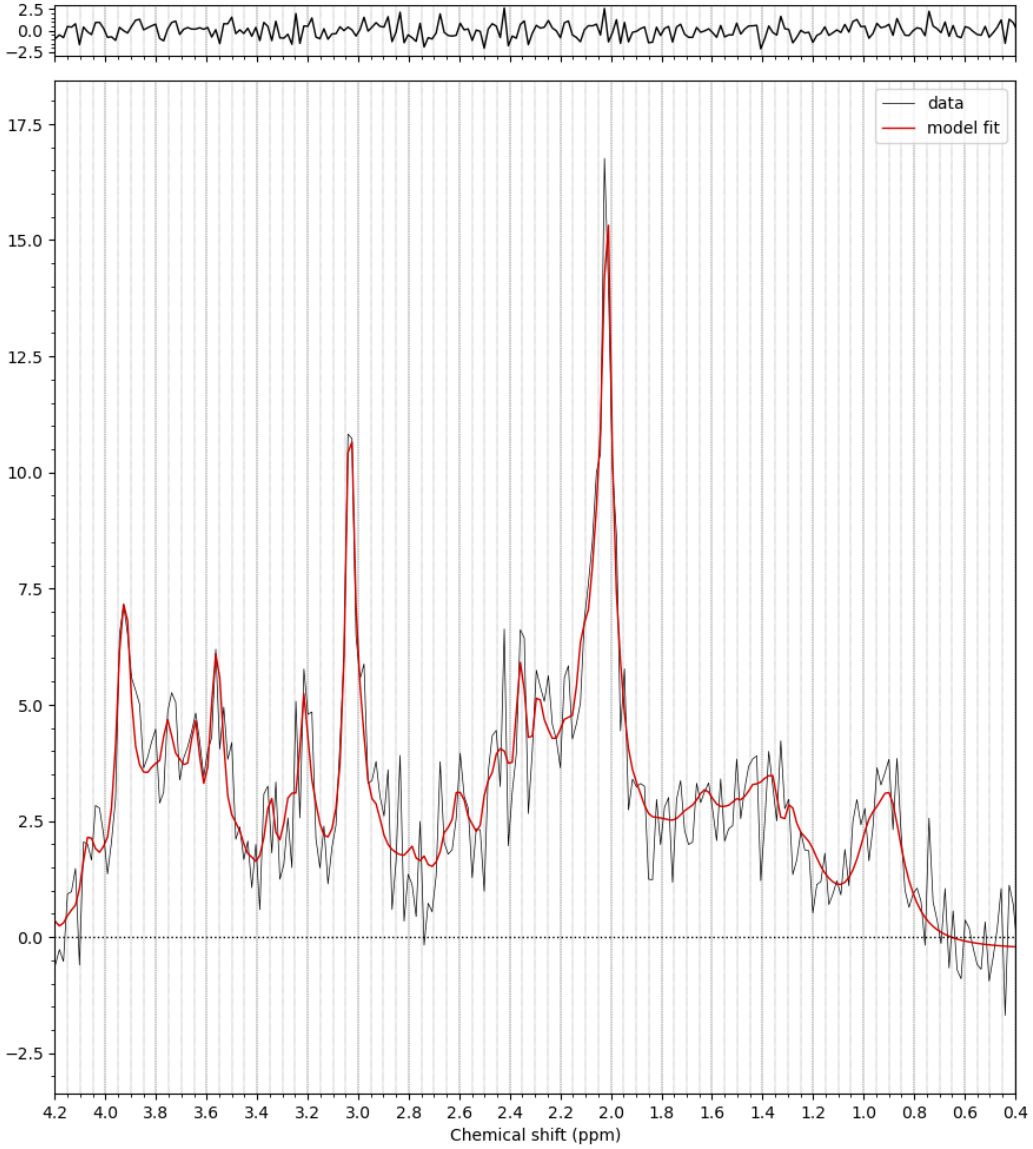
SNR: 38;
FWHM: 5.4 Hz
tNAA: 1.5%
Glx: 4.0%
Ins: 5.8%



Examples of fits

Low SNR

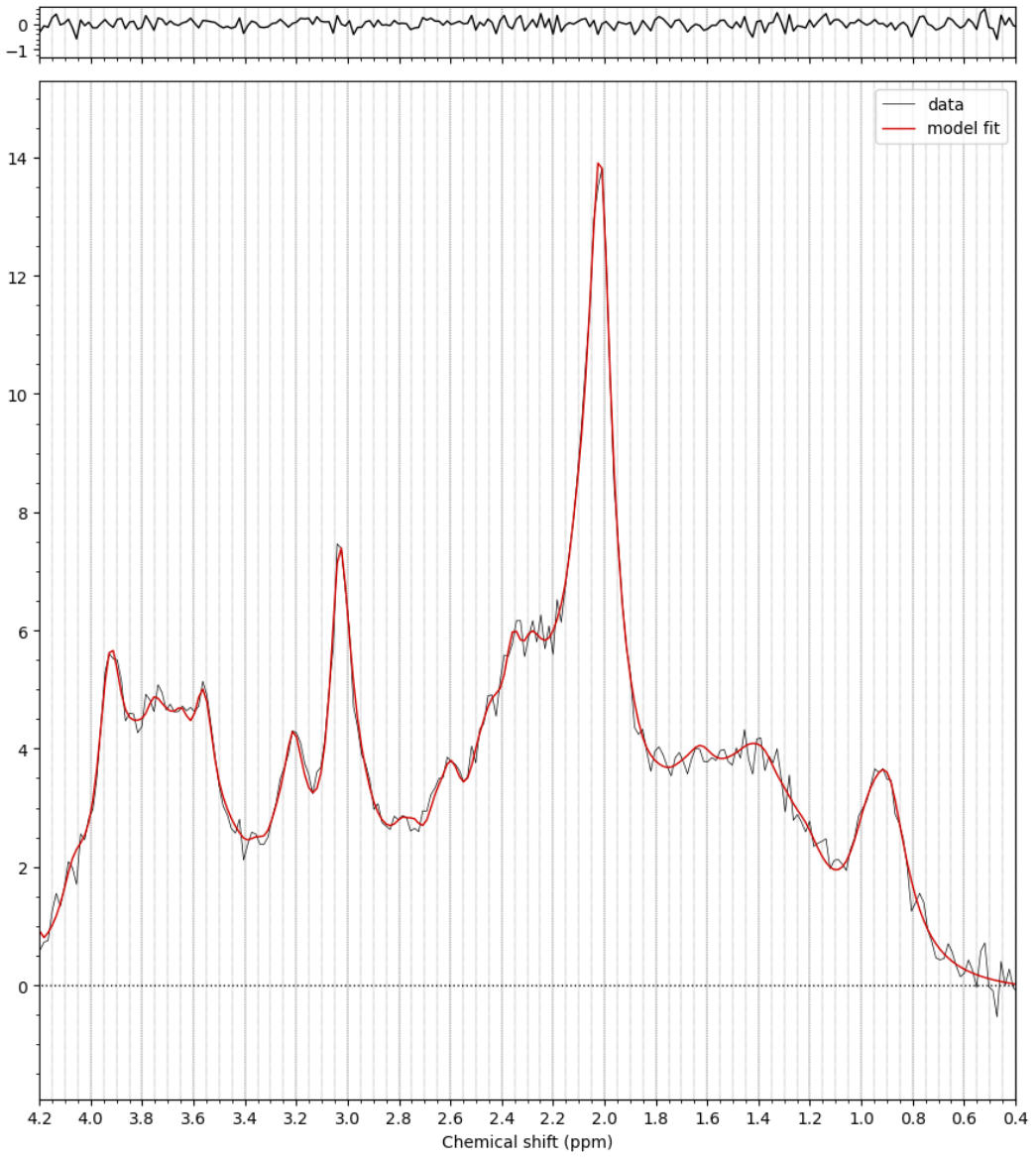
SNR: 8
FWHM: 5.6 Hz
tNAA: 6.9%
Glx: 15.8%
Ins: 19.1%



Examples of fits

Poor linewidth

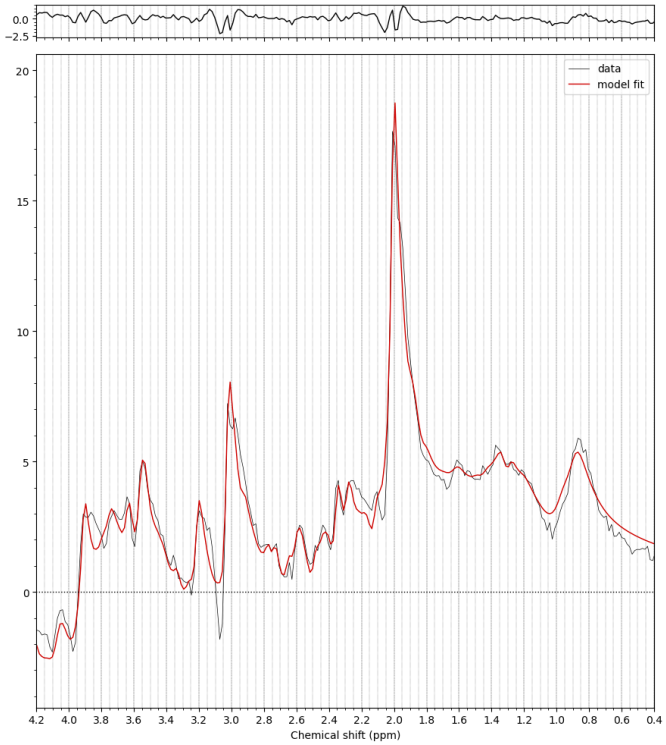
SNR: 23
FWHM: 11.1 Hz
tNAA: 2.4%
Glx: 4.6%
Ins: 8.9%



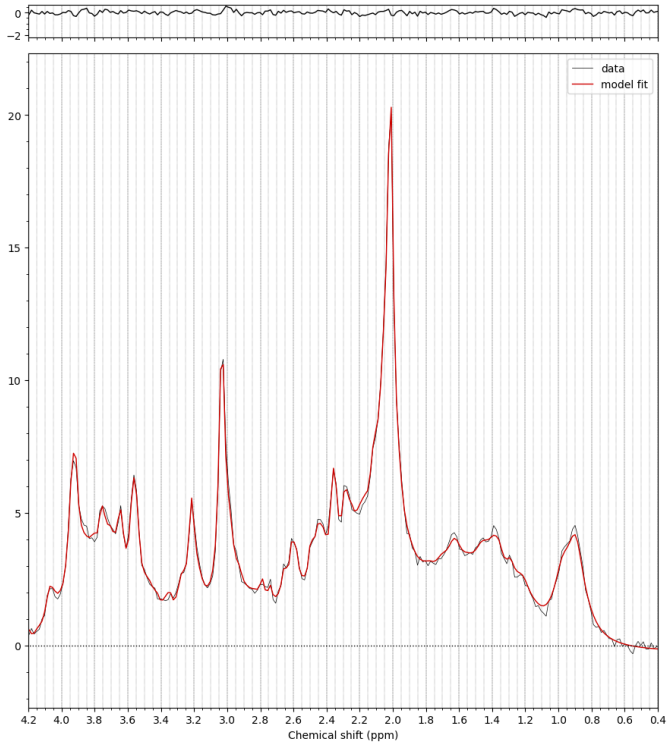
Look at your data!

Eddy currents

SNR: 47;
FWHM: 7.8 Hz
tNAA: 3.4%
Glx: 11.5%
Ins: 11.2%

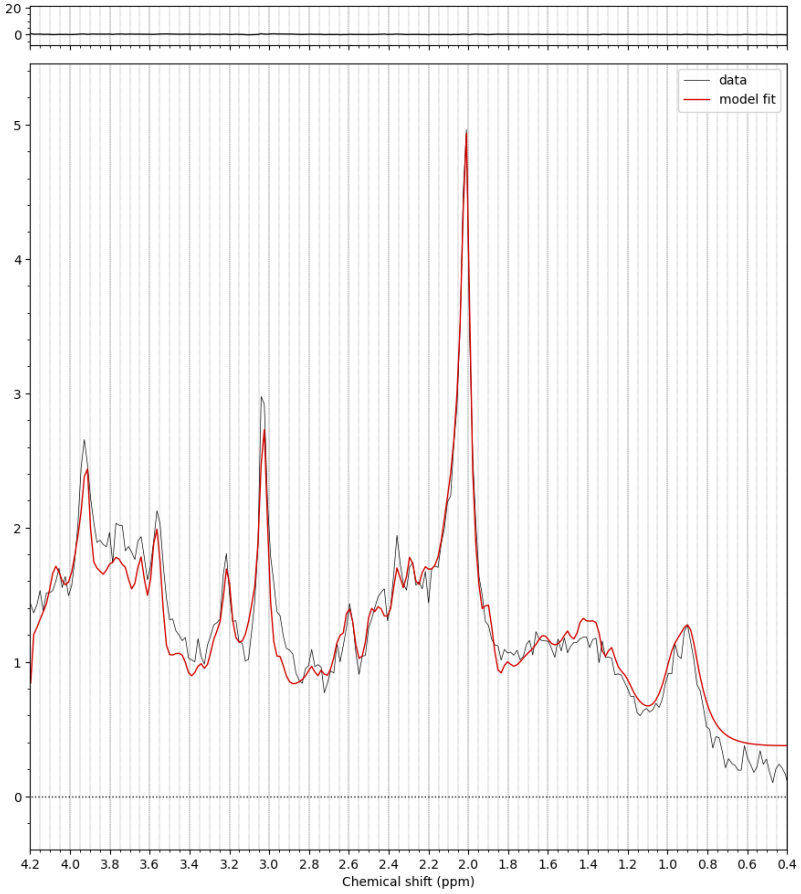


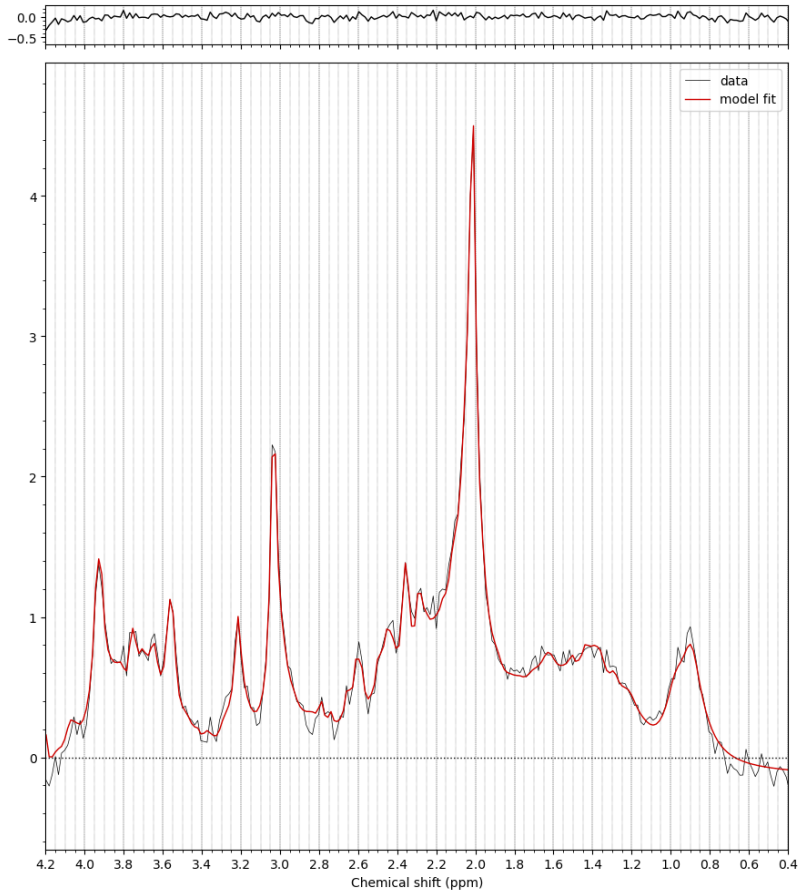
SNR: 73;
FWHM: 5.3 Hz
tNAA: 1.0%
Glx: 2.9%
Ins: 3.8%



Look at your data!

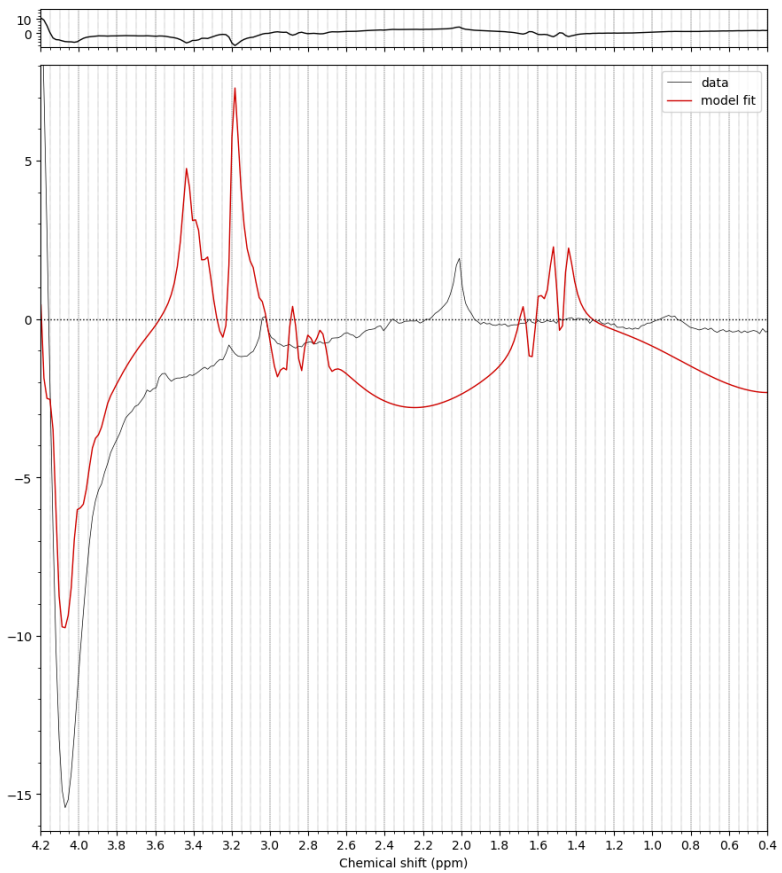
Residual water

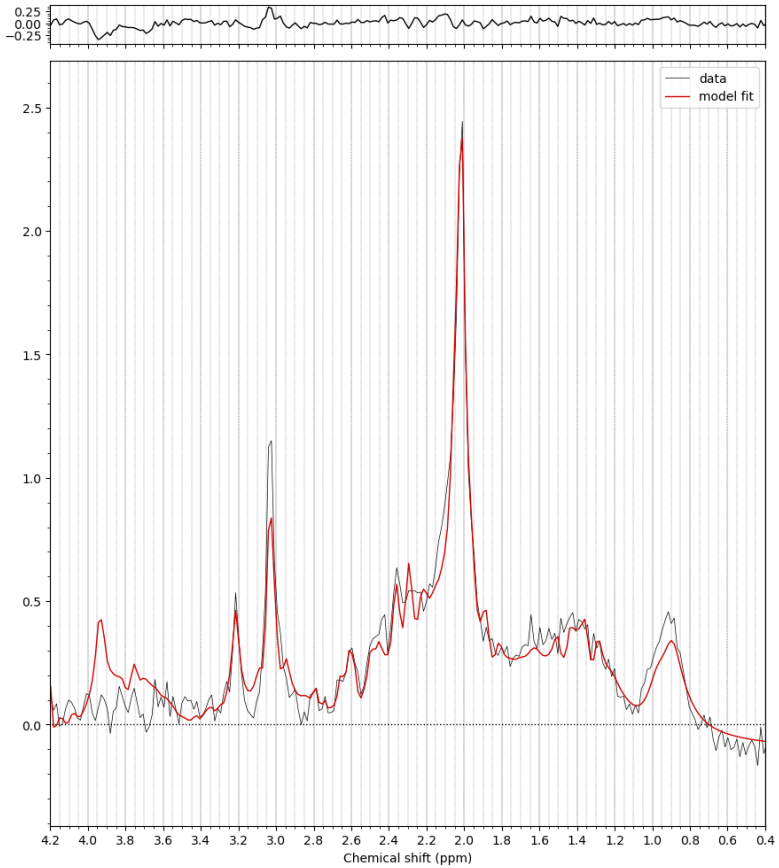




Look at your data!

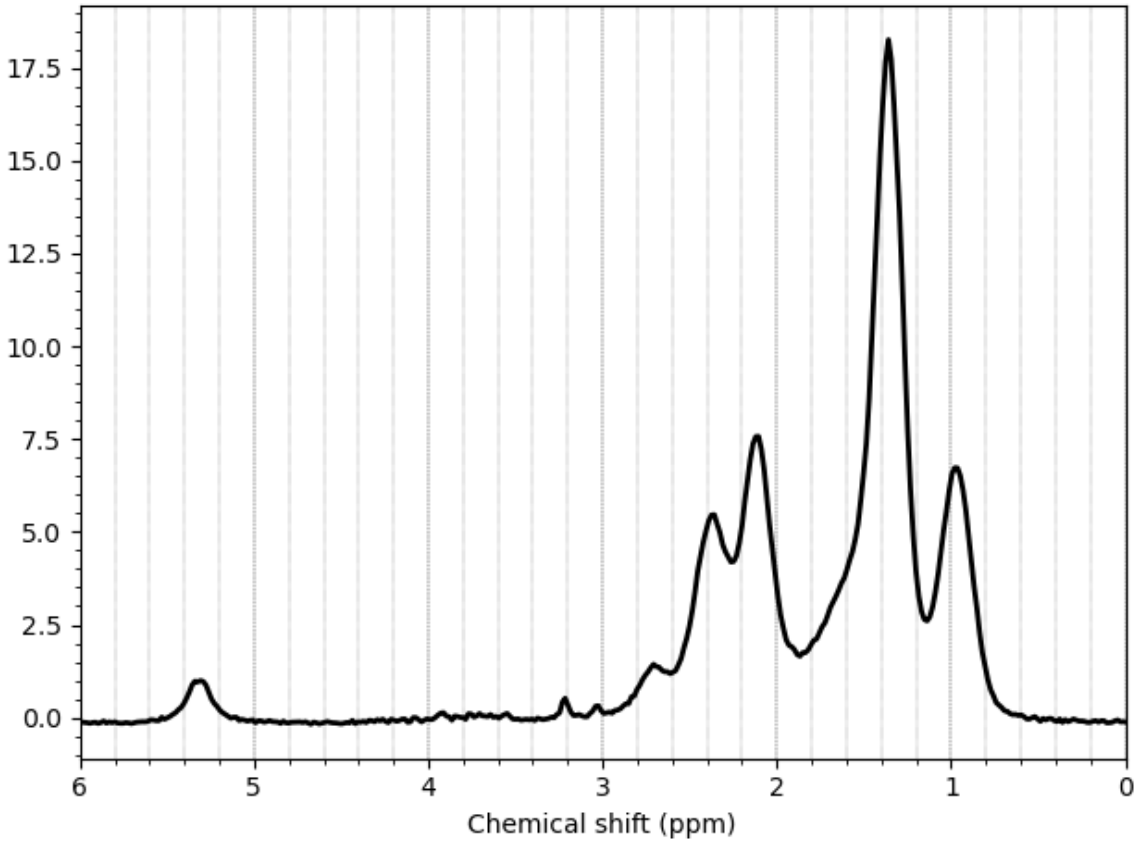
Residual water





Look at your data!

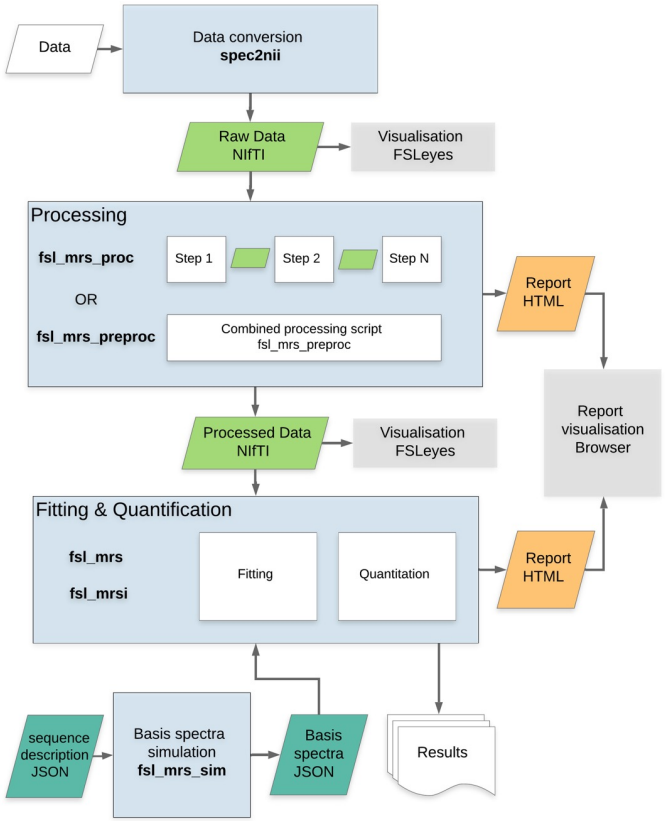
Lipids



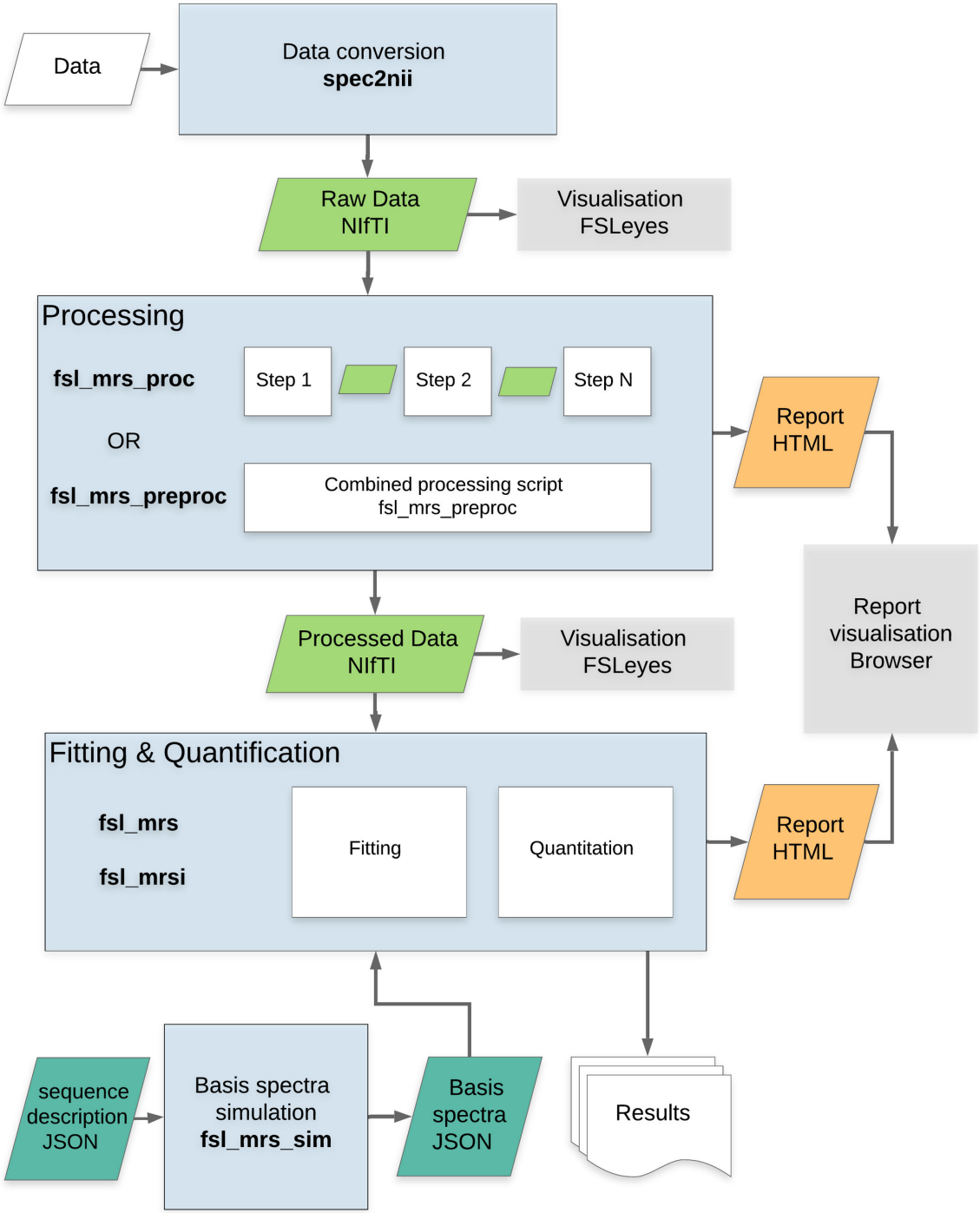
A quick pause for questions

Up next: FSL-MRS Tools

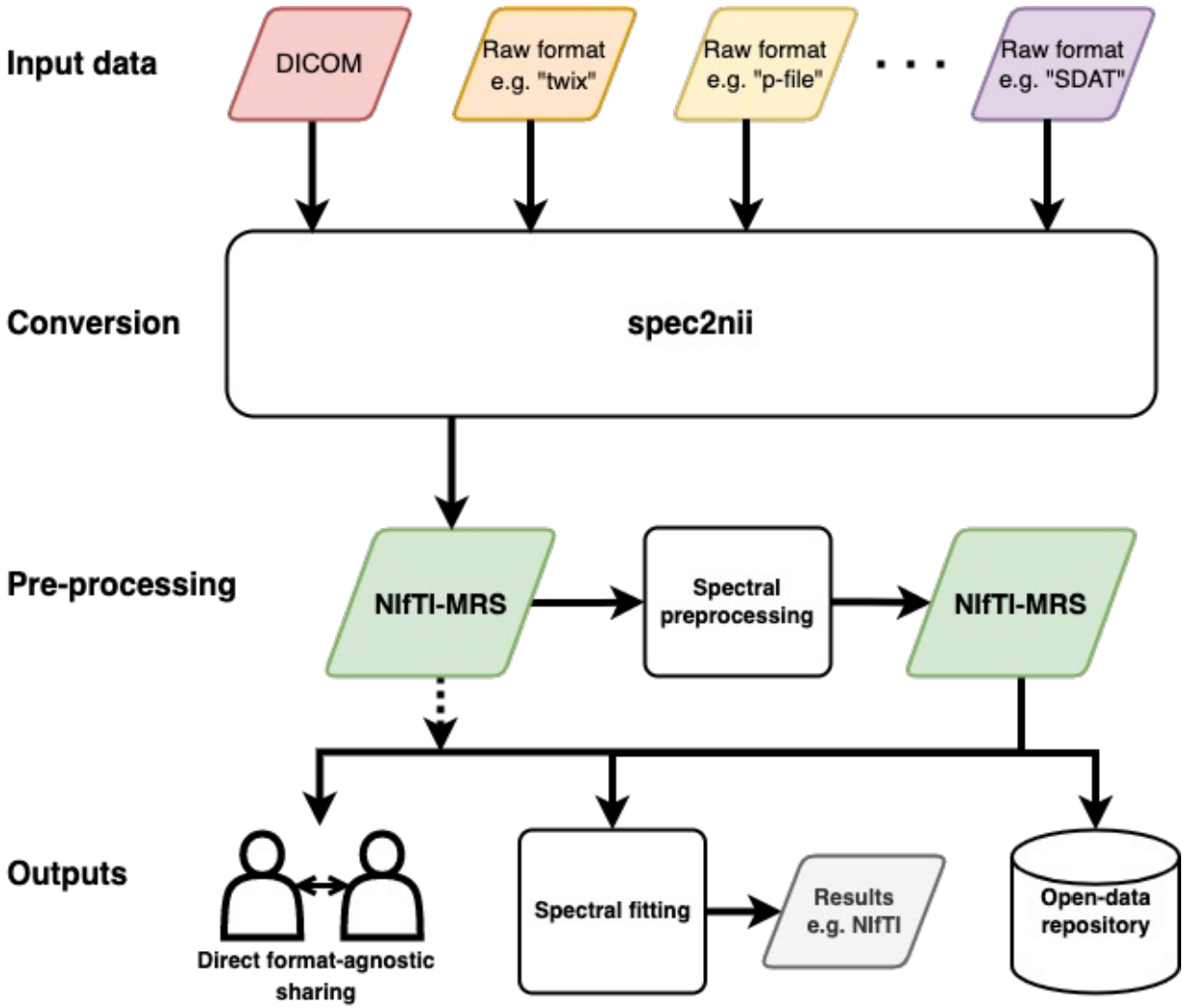
FSL-MRS – Tools for Magnetic Resonance Spectroscopy



IV. FSL-MRS tools


Data
Data conversion
spec2nii
Raw Data
NIfTI
Visualisation
FSLeyes
Processing
fsl_mrs_proc
Step 1
Step 2
Step N
OR
fsl_mrs_preproc
Combined processing script
fsl_mrs_preproc
Report
HTML
Report
visualisation
Browser
Processed Data
NIfTI
Visualisation
FSLeyes
Fitting & Quantification
fsl_mrs
fsl_mrsi
Fitting
Quantitation
Report
HTML
sequence
description
JSON
Basis spectra
simulation
fsl_mrs_sim
Basis
spectra
JSON
Results

Data conversion



https://doi.org/10.1002/mrm.29418

Data conversion

github.com/wtclarke/spec2nii

spec2nii

pypi v0.4.7 | python 3.7 | 3.8 | DOI 10.5281/zenodo.5907960

Currently supported formats

This table lists the currently supported formats. I have very limited experience with Philips and GE formats. Please get in touch if you are willing to help add to this list and/or supply validation data.

Format	File extension	SVS	CSI	Automatic orientation
Siemens Twix	.dat	Yes	No	Yes
Siemens DICOM	.ima / .dcm	Yes	Yes	Yes
Siemens RDA	.rda	Yes	No	Yes (WIP)
Philips	.SPAR/.SDAT	Yes	No	Yes
Philips	.data/.list	Yes	No	Yes
Philips DICOM	.dcm	Yes	No	Yes (WIP)
GE	.7 (pfile)	Yes	Yes	Yes
UIH DICOM	.dcm	Yes	Yes	Yes
Bruker	2dseq	Yes	Yes	Yes
Bruker	fid	Yes	Yes	Yes (WIP)
Varian	fid	Yes	No	No (WIP)
LCModel	.RAW	Yes	No	No
jMRUI	.txt	Yes	No	No
jMRUI	.mrui	Yes	No	No
ASCII	.txt	Yes	No	No

Pre-processing

`fsl_mrs_preproc` – One-stop pre-processing for SVS

`fsl_mrs_proc` – Run individual modular processing steps

- `coilcombine`
- `average`
- `align`
- `ecc`
- `remove`
- `phase`
- …

`fsl_mrs_preproc_edit` – One-stop pre-processing for edited SVS. **Warning**! WIP

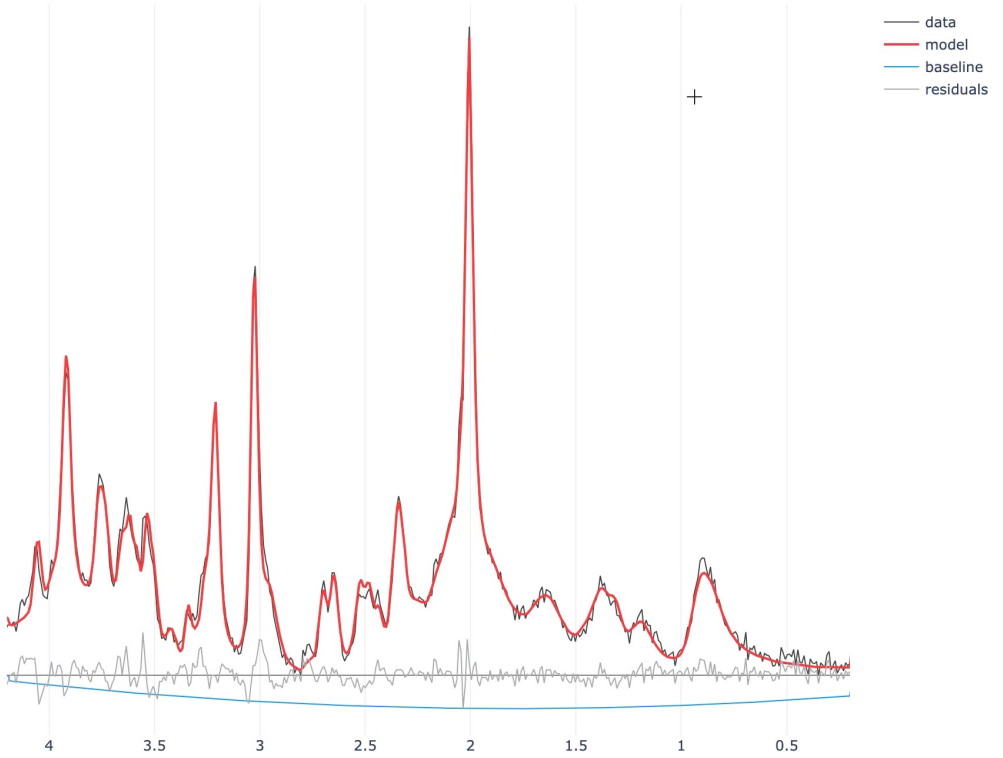
Fitting

Single spectra: `fsl_mrs`

Output: .csv + interactive report

Summary

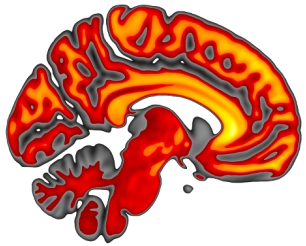
Metab	mMol/kg	%CRLB	/Cr+PCr
Ala	0.22	77.6	0.02
Asc	1.25	50.3	0.11
Asp	1.3	47.4	0.11
Cr	6.96	9	0.61
GABA	1.17	37.9	0.1
GPC	1.54	21.2	0.13
GSH	1.98	13.1	0.17
Glc	0.55	80	0.05
Gln	0.73	52	0.06
Glu	11.2	4.9	0.97
Ins	9.22	4.2	0.8
Lac	0.97	39.2	0.08
Mac	0.87	2.6	0.08
NAA	15.49	2.9	1.35
NAAG	1.72	18.1	0.15
PCh	0.47	56	0.04
PCr	4.54	14	0.39
PE	2.21	25.8	0.19
Scyllo	0.93	15.8	0.08
Tau	2.29	20.6	0.2
Cr+PCr	11.5	3.1	1

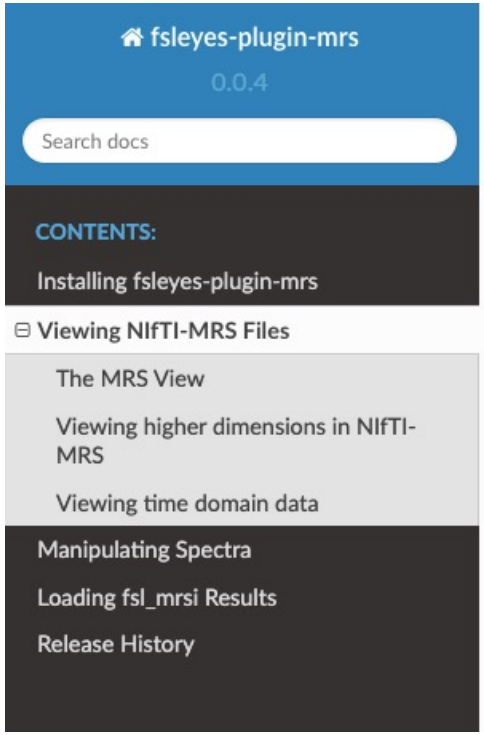


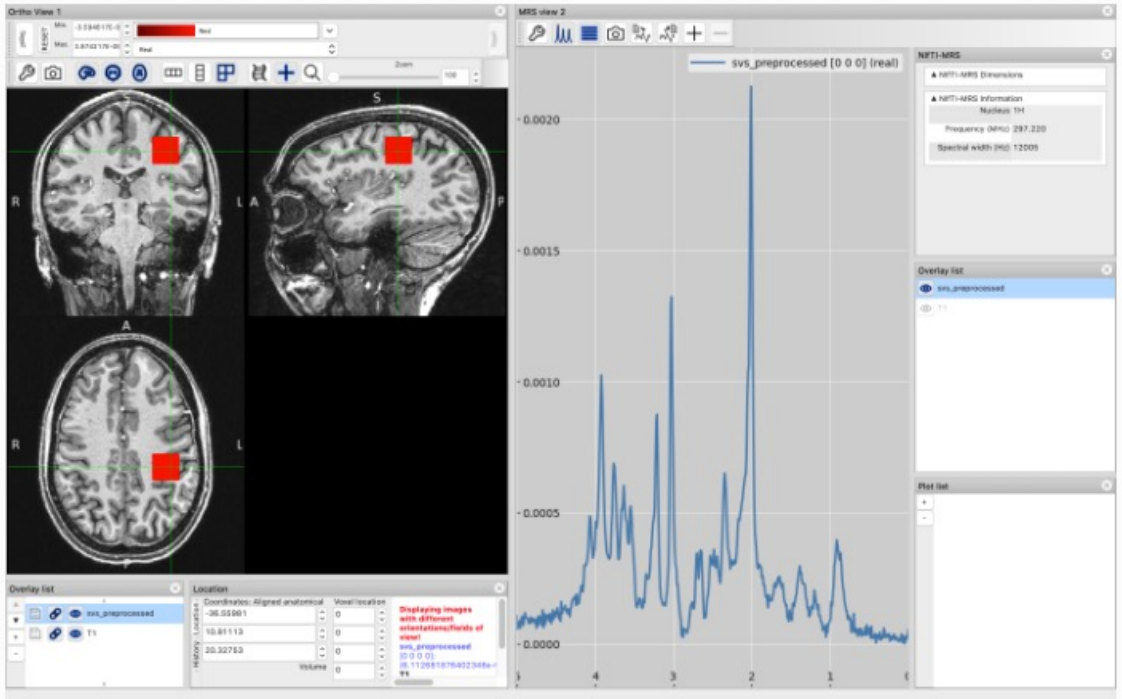
Fitting

MRSI: `fsl_mrsi`

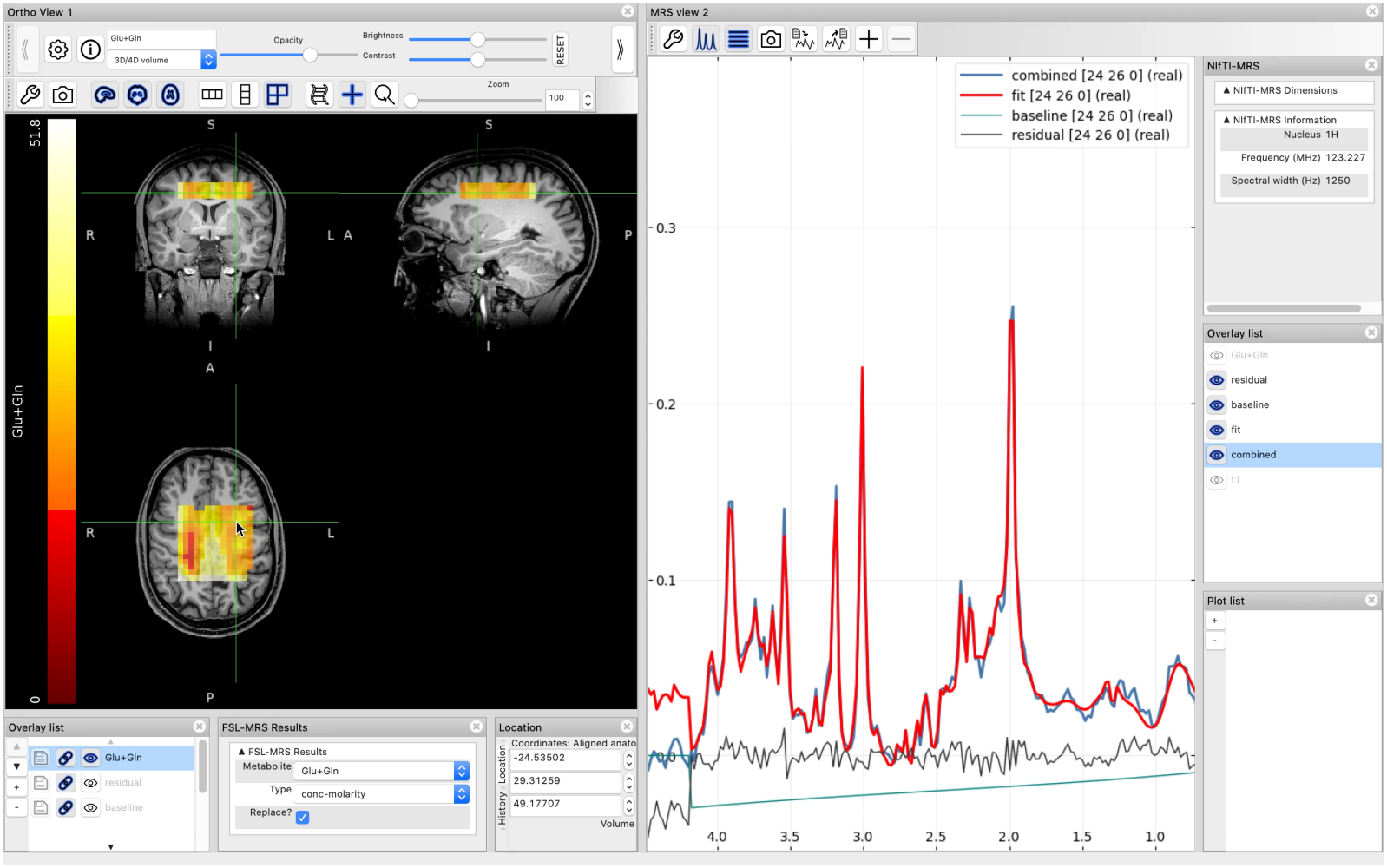
Output: NIfTI files (.nii), to be viewed in fsleyes…







Visualisation



+ basic viewer: `mrs_tools vis my_data.nii.gz`

Other tools

1. Simulation of basis spectra: `fsl_mrs_sim`
2. Basis spectra manipulation: `basis_tools`
3. Data manipulation: `mrs_tools`
4. Tissue segmentation: `svs_segment, mrsi_segment`
5. *New* Summary statistics: `fsl_mrs_summarise`

Tools can run through interactive Python API

Please Update!

fsl-mrs.com

```
conda update -c conda-forge -c defaults \
-c https://fsl.fmrib.ox.ac.uk/fsldownloads/fslconda/public/ \
fsl_mrs
```

FSL-MRS Release History

This document contains the FSL-MRS release history in reverse chronological order.

2.0.3 (Wednesday 21st September 2022)

- Fixed bug in results / QC that only ran QC over default ppm region.
- Improved loading and ID of file types.
- Fixed bug in packaged example data loader.
- Improved textual help in fsl_mrs_preproc and fsl_mrs_proc for inappropriate data.