

MRS Postprocessing & Quantification

NeuroMET Virtual MR Spectroscopy Workshop, May 27th 2021

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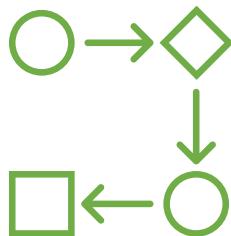


JOHNS HOPKINS
SCHOOL *of* MEDICINE

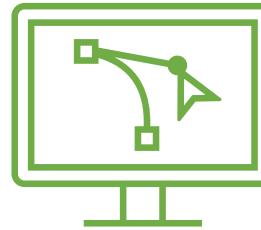


Kennedy Krieger Institute
UNLOCKING POTENTIAL

Contents



Modern MRS data analysis workflow



Software overview

... this guide is rather incomplete:

- Many different ways to acquire and analyze MRS data
- Reproducibility and validation are areas of concern
- Field is rapidly shifting towards open practices

2019-2021: Expert consensus efforts

Advanced single voxel ^1H magnetic resonance spectroscopy techniques in humans: Experts' consensus recommendations

Gülin Öz ✉, Dinesh K. Deelchand, Jannie P. Wijnen, Vladimír Mlynárik, Lijing Xin, Ralf Mekle, Ralph Noeske, Tom W.J. Scheenen, Ivan Tkáč, the Experts' Working Group on Advanced Single Voxel ^1H MRS

B_0 shimming for in vivo magnetic resonance spectroscopy: Experts' consensus recommendations

Christoph Juchem ✉, Cristina Cudalbu, Robin A. de Graaf, Rolf Gruetter, Anke Henning, Hoby P. Hetherington, Vincent O. Boer

Motion correction methods for MRS: experts' consensus recommendations

Ovidiu C. Andronescu ✉, Pallab K. Bhattacharya, Wolfgang Bogner, In-Young Choi, Aaron T. Hess, Phil Lee, Ernesta M. Meintjes, M. Dylan Tisdall, Maxim Zaitsev, André van der Kouwe

^{31}P magnetic resonance spectroscopy in skeletal muscle: Experts' consensus recommendations

Martin Meyerspeer ✉, Chris Boesch, Donnie Cameron, Monika Dezortová, Sean C. Forbes, Arend Heerschap, Jeroen A.L. Jenesos, Hermien E. Kan, Jane Kent, Gwenaël Layec, Jeanine J. Prompers, Harmen Reyngoudt, Alison Sleigh, Ladislav Valkovič, Graham J. Kemp, Experts' Working Group on ^{31}P MR Spectroscopy of Skeletal Muscle ... See fewer authors ^

Proton magnetic resonance spectroscopy in skeletal muscle: Experts' consensus recommendations

Martin Kršák ✉, Lucas Lindeboom, Vera Schrauwen-Hinderling, Lidia S. Szczepaniak, Wim Derave, Jesper Lundbom, Douglas Befroy, Fritz Schick, Jürgen Machann, Roland Kreis, Chris Boesch

Advanced magnetic resonance spectroscopic neuroimaging: Experts' consensus recommendations

Andrew A. Maudsley ✉, Ovidiu C. Andronescu, Peter B. Barker, Alberto Bazzi, Wolfgang Bogner, Anke Henning, Sarah J. Nelson, Stefan Posse, Dikoma C. Shungu, Brian J. Soher

Magnetic resonance spectroscopy in the rodent brain: Experts' consensus recommendations

Bernard Lanz ✉, Alireza Abaei, Olivier Braissant, In-Young Choi, Cristina Cudalbu, Pierre-Gilles Henry, Rolf Gruetter, Fırat Kara, Kejal Kantarci, Phil Lee, Norbert W. Lutz, Małgorzata Marjańska, Vladimír Mlynárik, Volker Rasche, Lijing Xin, Julien Valette, the Experts' Working Group on Magnetic resonance spectroscopy in the rodent brain ... See fewer authors ^

Spectral editing in ^1H magnetic resonance spectroscopy: Experts' consensus recommendations

In-Young Choi ✉, Ovidiu C. Andronescu, Peter Barker, Wolfgang Bogner, Richard A. E. Edden, Lana G. Kaiser, Phil Lee, Małgorzata Marjańska, Melissa Terpstra, Robin A. de Graaf

Terminology and concepts for the characterization of in vivo MR spectroscopy methods and MR spectra: Background and experts' consensus recommendations

Roland Kreis ✉, Vincent Boer, In-Young Choi, Cristina Cudalbu, Robin A. de Graaf, Charles Gasparovic, Arend Heerschap, Martin Kršák, Bernard Lanz, Andrew A. Maudsley, Martin Meyerspeer, Jamie Near, Gülin Öz, Stefan Posse, Johannes Slotboom, Melissa Terpstra, Ivan Tkáč, Martin Wilson, Wolfgang Bogner ... See fewer authors ^

Preprocessing, analysis and quantification in single-voxel magnetic resonance spectroscopy: experts' consensus recommendations

Jamie Near ✉, Ashley D. Harris, Christoph Juchem, Roland Kreis, Małgorzata Marjańska, Gülin Öz, Johannes Slotboom, Martin Wilson, Charles Gasparovic

Minimum Reporting Standards for in vivo Magnetic Resonance Spectroscopy (MRSinMRS): Experts' consensus recommendations

Alexander Lin, Ovidiu Andronescu, Wolfgang Bogner, In-Young Choi, Eduardo Coello, Cristina Cudalbu, Christoph Juchem, Graham J. Kemp, Roland Kreis, Martin Kršák, Phil Lee, Andrew A. Maudsley, Martin Meyerspeer, Vladimír Mlynárik, Jamie Near, Gülin Öz, Aimie L. Peek, Nicolaas A. Puts, Eva-Maria Ratai, Ivan Tkáč, Paul G. Mullins ✉ ... See fewer authors ^

MRSHub – one centralized resource



Home Software & Code Forum Data Links News About

Welcome to the MRSHub!

The MRSHub is a curated collection of resources for the analysis of magnetic resonance spectroscopy data. It is maintained by the Committee for MRS Code and Data Sharing of the MR Spectroscopy Study Group of the International Society for Magnetic Resonance in Medicine (ISMRM).

[We are actively seeking contributions! If you are interested in advancing open science in MRS, please see our MRSHub User Guide!](#)



Software & Code

The MRSHub code repository collects software packages and functions to process, manipulate, analyse, and display MRS data.

[To the MRSHub code listing](#)

Forum

The MRSHub forum is a place for the MRS community to seek support, exchange ideas, ask questions, and collaborate.

[To the MRSHub forum](#)

Data

The MRSHub data repository collects MRS datasets for demonstration and testing of new methods.

[To the MRSHub data listing](#)

Modern MRS data analysis workflow

From scanner to publication



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Methodological consensus on clinical proton MRS of the brain: Review and recommendations

Martin Wilson , Ovidiu Andronesi, Peter B. Barker, Robert Bartha, Alberto Bizzì, Patrick J. Bolan, Kevin M. Brindle, In-Young Choi, Cristina Cudalbu, Ulrike Dydak, Uzay E. Emir, Ramon G. Gonzalez, Stephan Gruber, Rolf Gruetter, Rakesh K. Gupta, Arend Heerschap, Anke Henning, Hoby P. Hetherington, Petra S. Huppi, Ralph E. Hurd, Kejal Kantarci, Risto A Kauppinen, Dennis W. J. Klomp, Roland Kreis, Marijn J. Kruiskamp, Martin O. Leach, Alexander P. Lin, Peter R. Luijten, Małgorzata Marjańska, Andrew A. Maudsley, Dieter J. Meyerhoff, Carolyn E. Mountford, Paul G. Mullins, James B. Murdoch, Sarah J. Nelson, Ralph Noeske, Gülin Öz, Julie W. Pan, Andrew C. Peet, Harish Poptani, Stefan Posse, Eva-Maria Ratai, Nouha Salibi, Tom W. J. Scheenen, Ian C. P. Smith, Brian J. Soher, Ivan Tkáč, Daniel B. Vigneron, Franklyn A. Howe ... [See fewer authors](#) ^

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Jamie Near , Ashley D. Harris, Christoph Juchem, Roland Kreis, Małgorzata Marjańska, Gülin Öz, Johannes Slotboom, Martin Wilson, Charles Gasparovic

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Raw MRS data

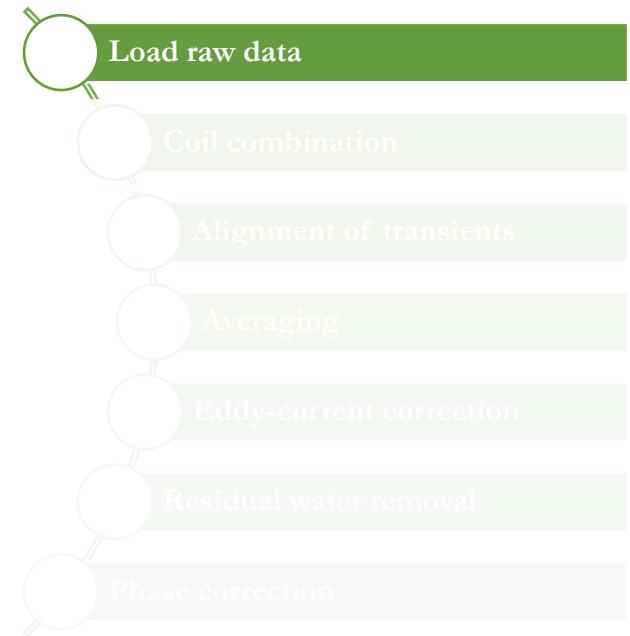
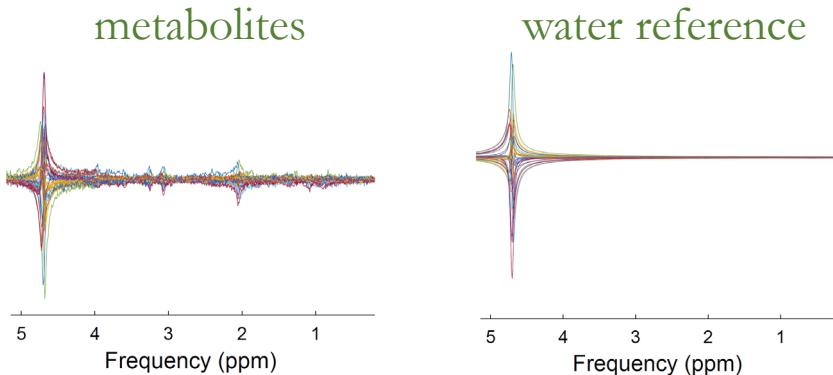
Vendor	File extension	Coils combined?	Averaged?	Contains voxel geometry?
Philips	.sdat /.spar	Yes	Depends	Yes
	.data /.list	No	No	No
Siemens	.rda	Yes	Depends	Yes
	.twix	No	No	Yes
GE	.7	Depends	Depends	Yes
DICOM	.dcm (.ima)	Yes	Depends	Yes
NIfTI	.nii	No	No	Yes

- "Depends" ... on sequence developer, software version, exam card settings
- **Recommendation:** Export a format that conserves individual transients!

Preprocessing

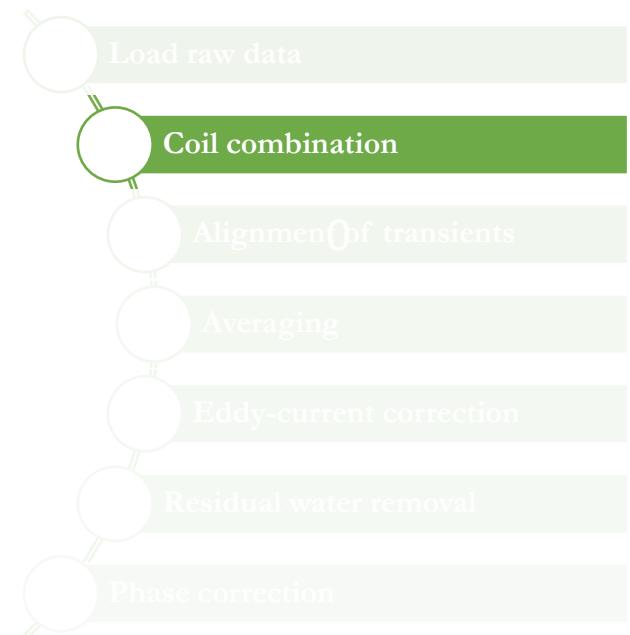
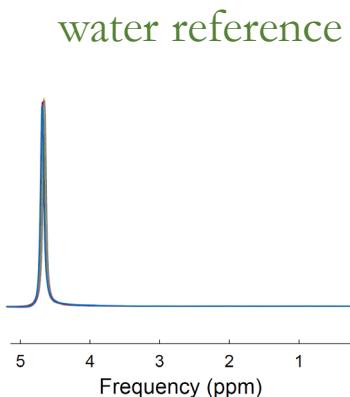
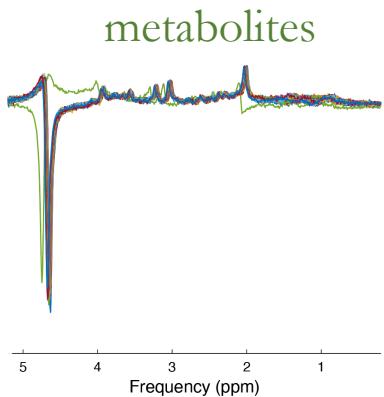
- **Preprocessing:** Preparing raw data into a signal that will be modeled
- Operations depend on the raw data format

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sub-01_PRESS30_w.dat	10/13/2020 10:19 AM	DAT File	39,415 KB



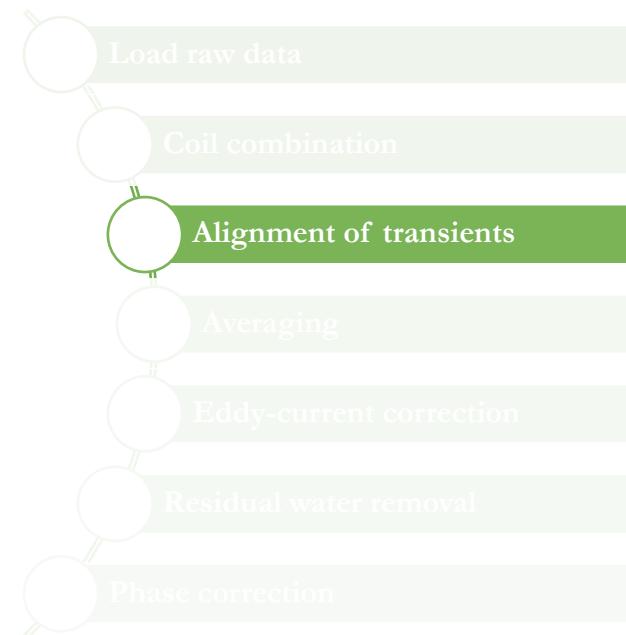
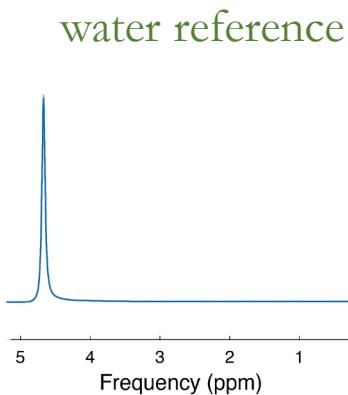
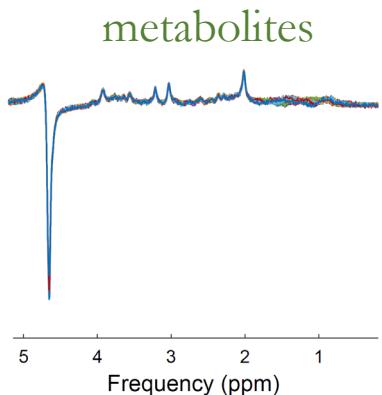
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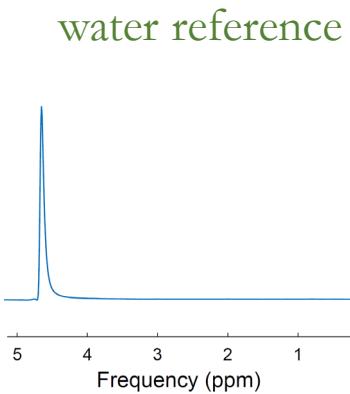
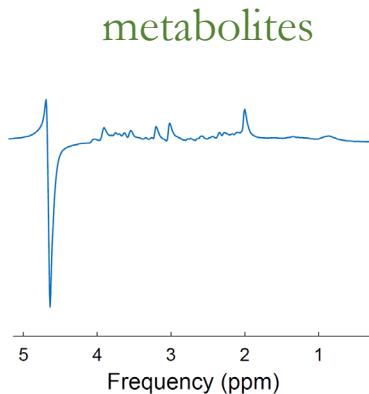
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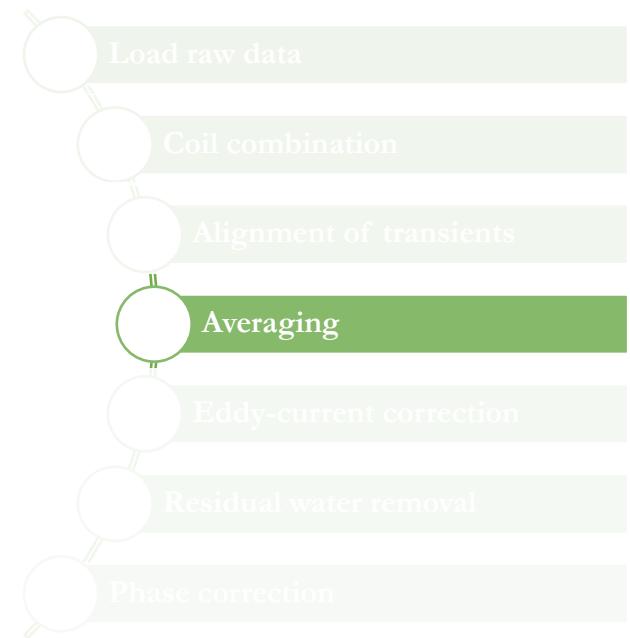


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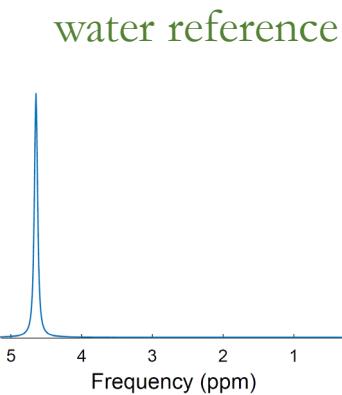
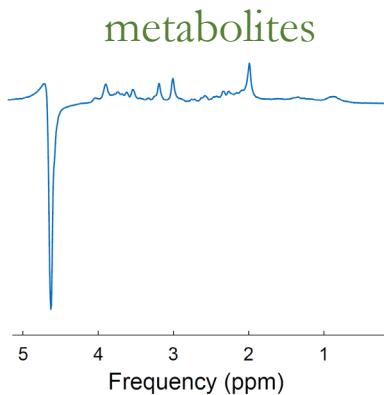


I have added a little bit of eddy-current artefact here...

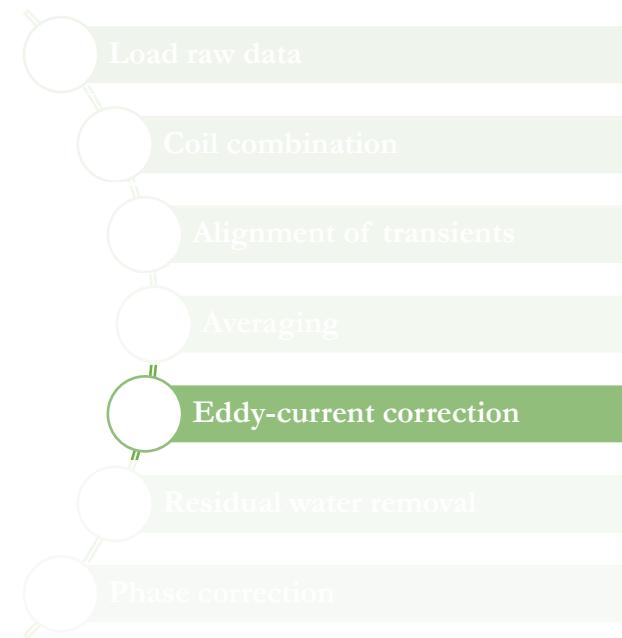


Preprocessing

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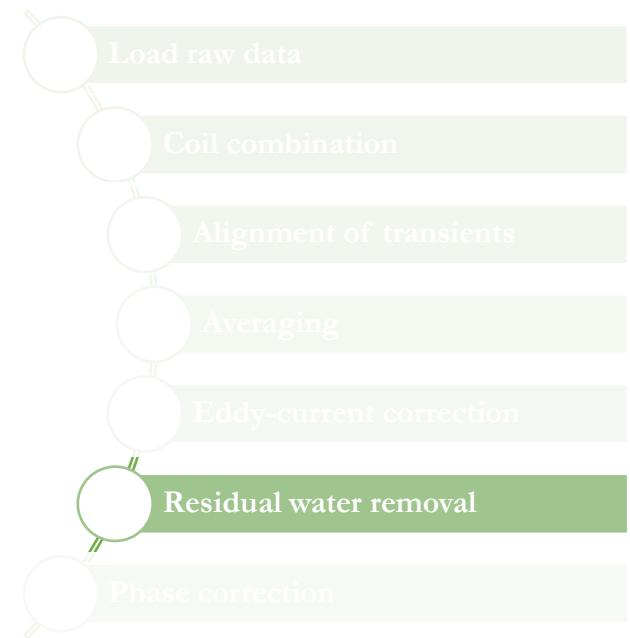
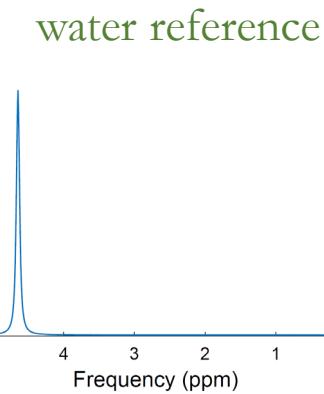
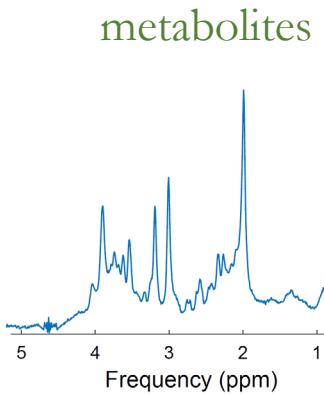


... which the eddy-current correction removes again.



Preprocessing

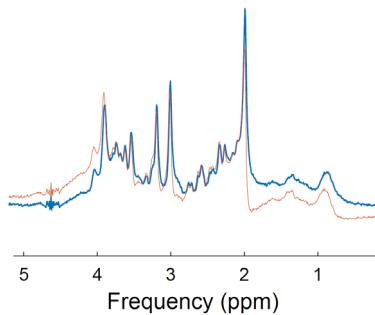
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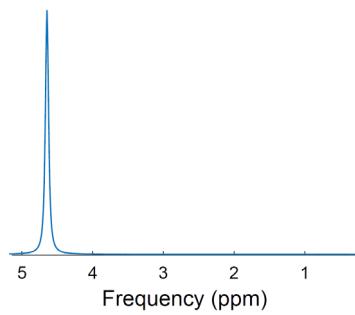
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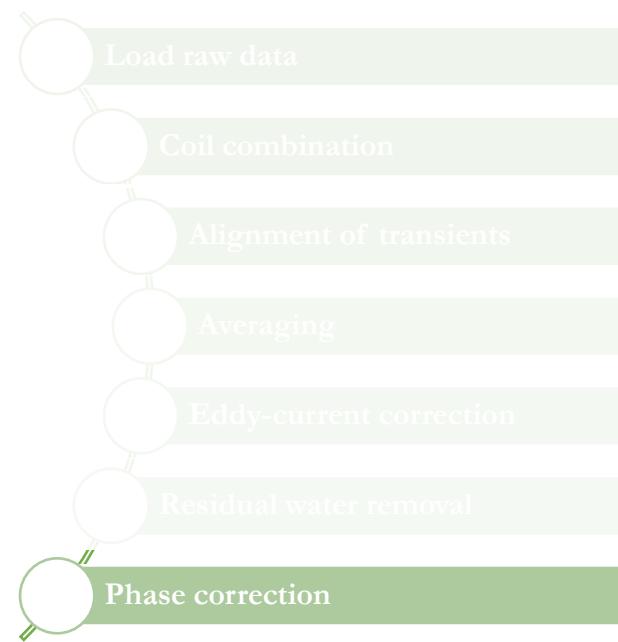
metabolites



water reference



Some additional alignment of frequency and phase happens at this point for spectral editing experiments.

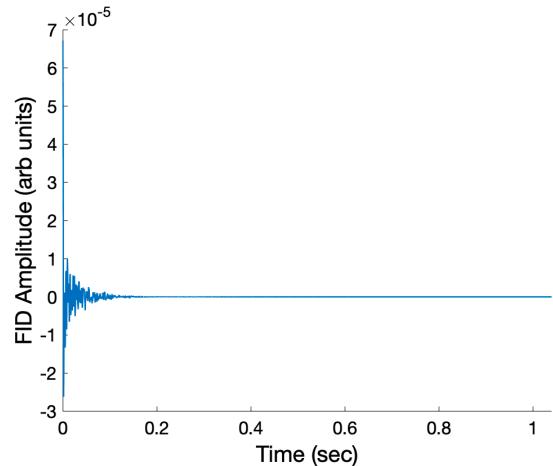
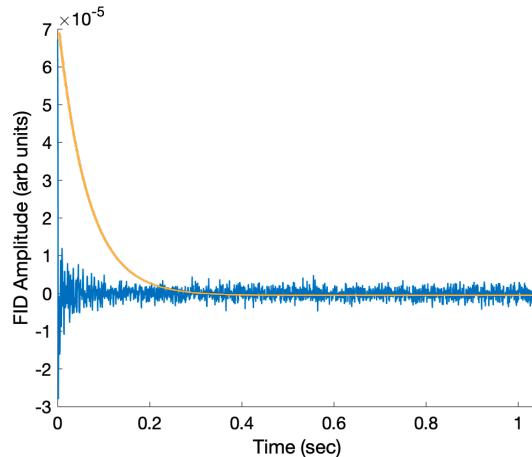


Operations for visualization

- Linebroadening improves the apparent SNR
- Zero-filling improves the apparent spectral resolution
- **Not recommended** for use with linear-combination modeling

Linebroadening /
apodization

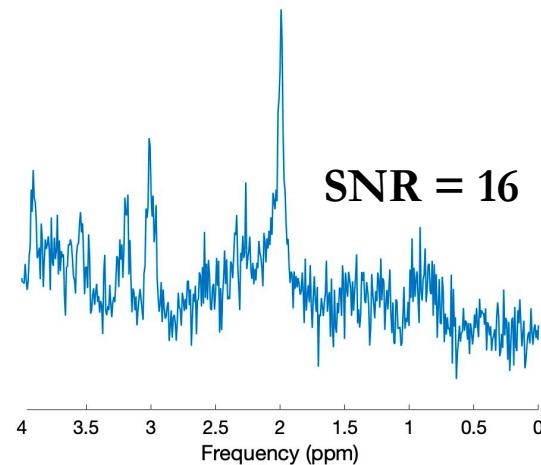
Zero-filling



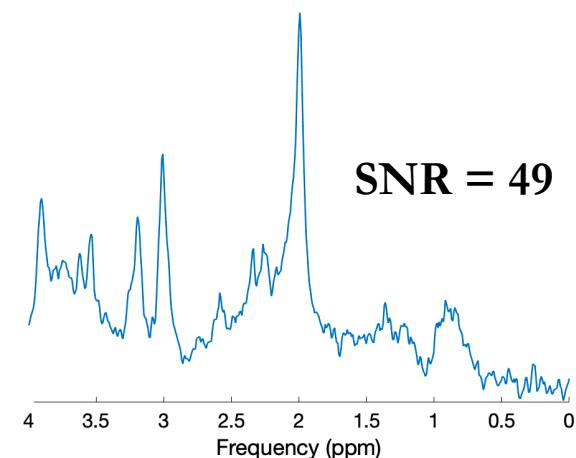
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Linebroadening /
apodization



Zero-filling

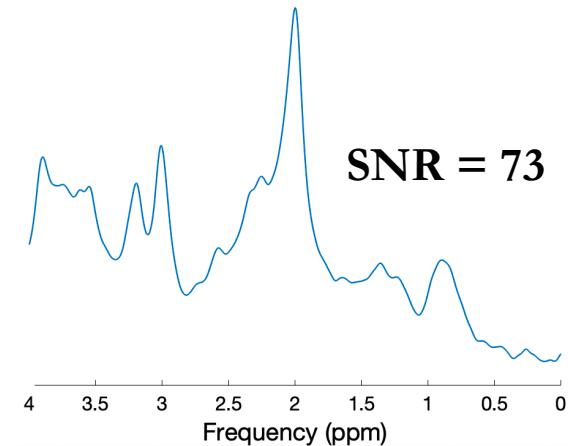
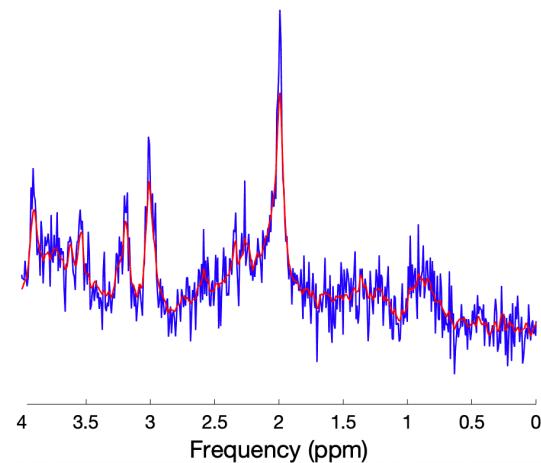


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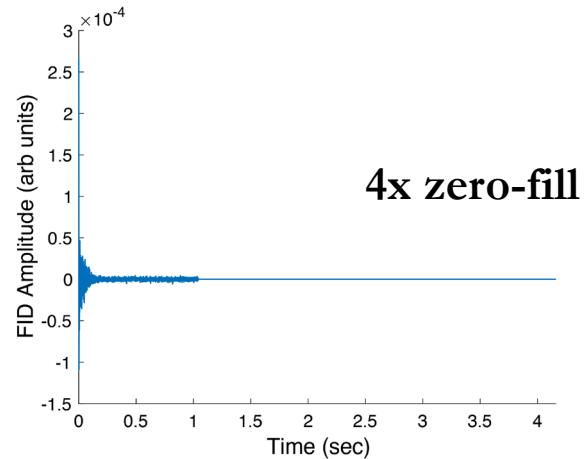
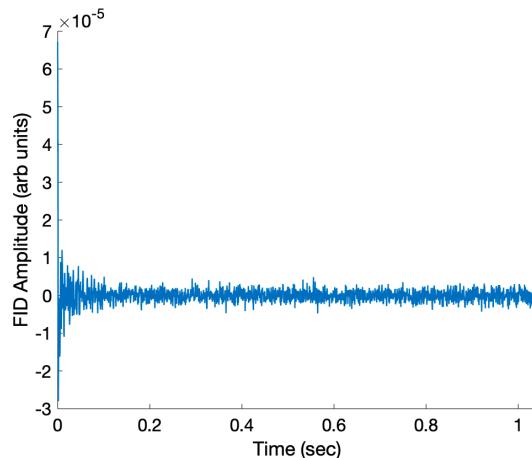
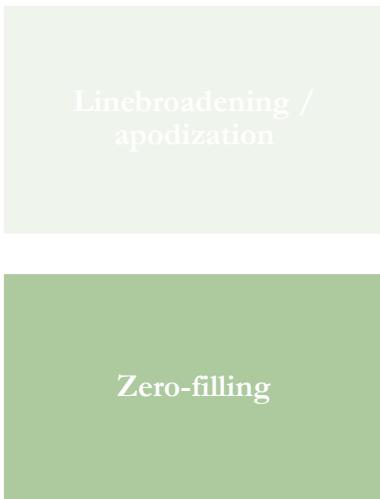
Linebroadening /
apodization

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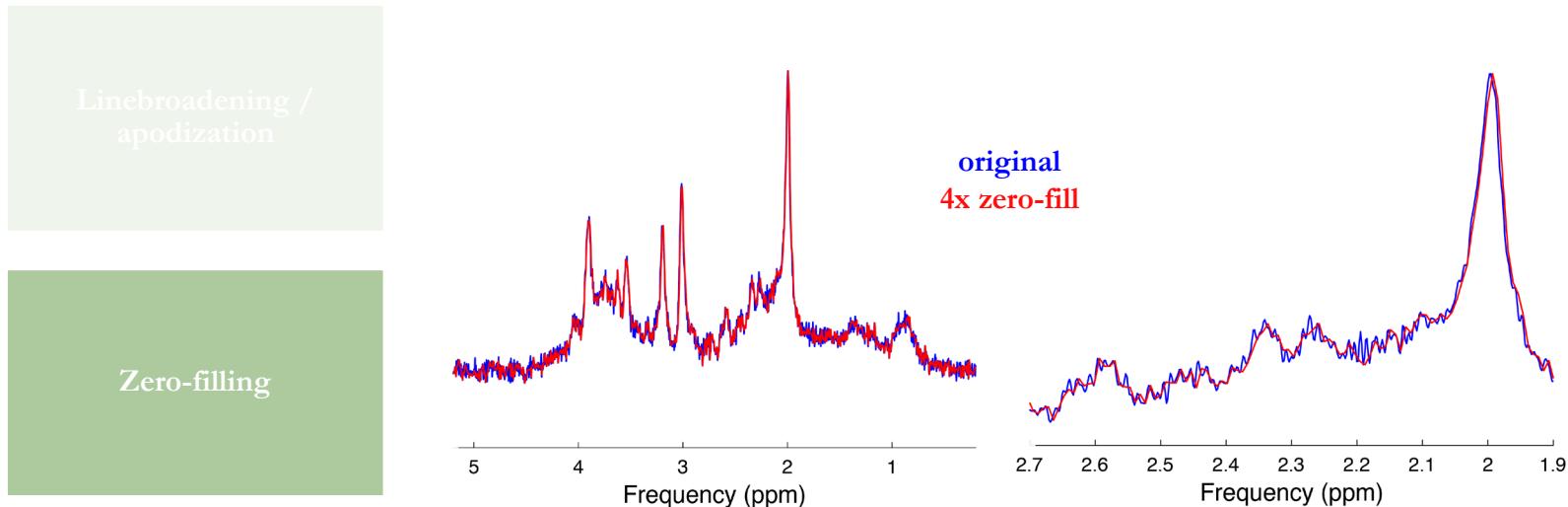
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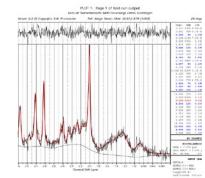
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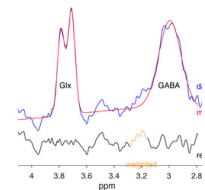
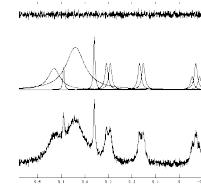


Modeling

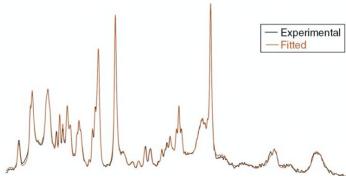
- **Modeling:** Extract quantitative estimates of signal amplitudes from the spectrum



Peak fitting



Linear-combination modeling

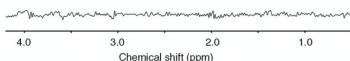


Weighted sum of (usually simulated) metabolite basis functions

- Model parameters account for...
 - Lineshape (Gauss/Lorentz)
 - frequency and phase shifts

... complicated by:

- Signal overlap
- Broad (short-T₂) macromolecular and lipid signals



LCModel



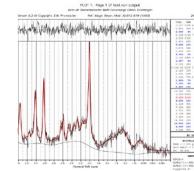
TARQUIN



FSL-MRS

jMRUI
QUEST
AQSES

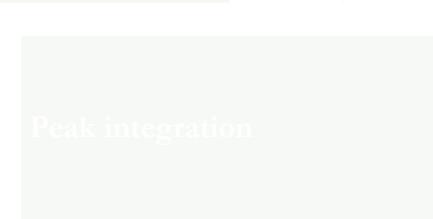
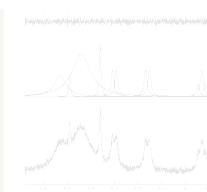
Recommended for most ¹H-MRS
brain applications



Linear-combination modeling

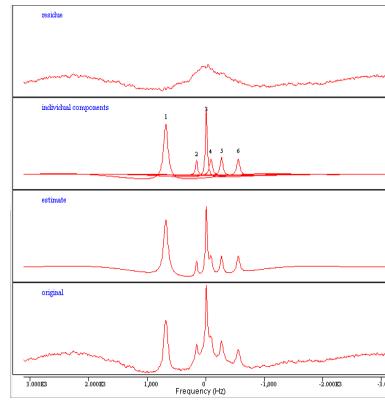


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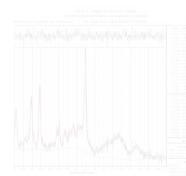
Peak integration

Peak fitting

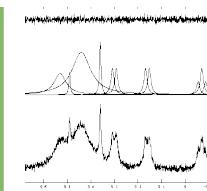


Weighted sum of single peaks

- Prior knowledge (AMARES, VOIGT)
 - Chemical shifts
 - Relative amplitude
 - Phase
 - Lineshape (Gauss/Lorentz/Voigt)
- Baseline terms



Linear-combination modeling

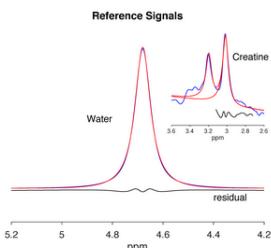
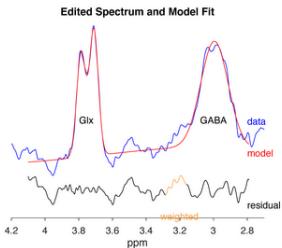


Peak integration

Rather suited for sparse data, i.e. little spectral overlap (long TE, spectral editing, ^{31}P , ^{13}C)



Peak integration

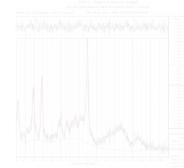


Estimation of area under the curve

- Directly by adding up data points
- Integration of a model to the data



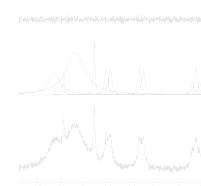
Only recommended for very sparse data, with little spectral overlap or background signal



Linear-combination modeling



Peak fitting

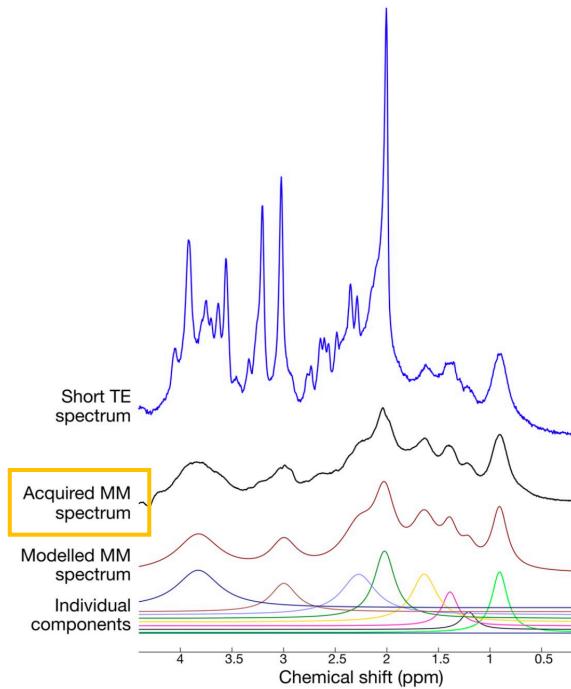


Peak integration



Macromolecules

- MM signals should be included in the model, ideally measured (or parametrized)



Acquired MM

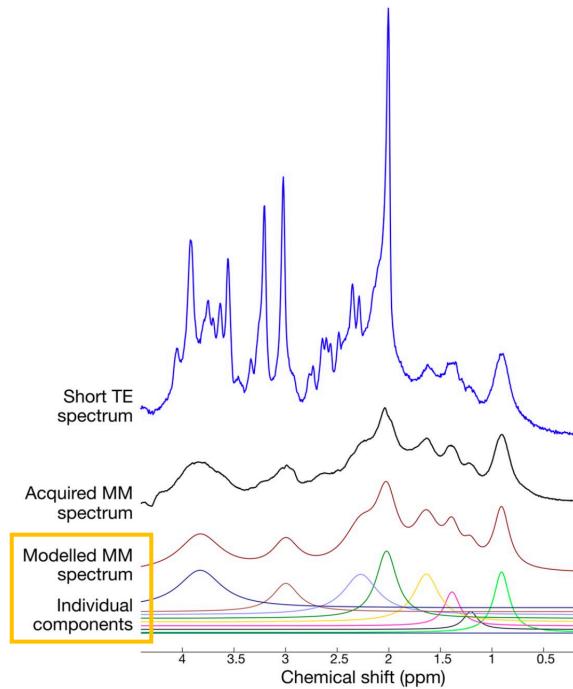
- Should match sequence & TE
- Few MM spectra are publicly available
- Check MRSHub

Modelled MM

- Parametrized components
- Defaults used in some software
- May be inadequate

Macromolecules

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Acquired MM

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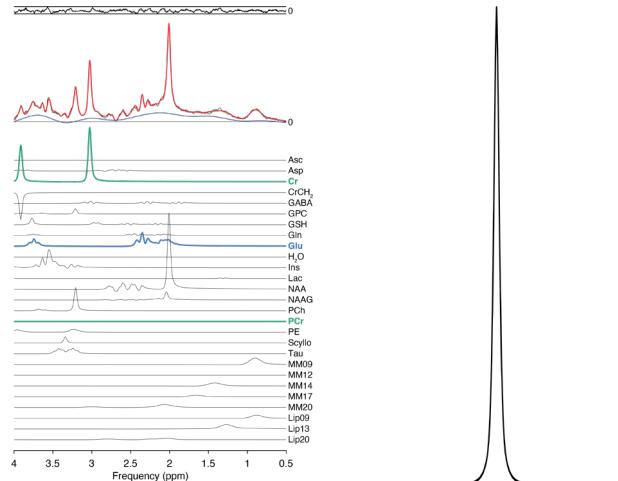
Modelled MM

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- May be inadequate

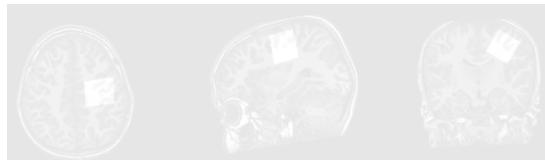
Quantification

- **Quantification:** Converting model parameters into quantitative estimates

Metabolite & water amplitudes



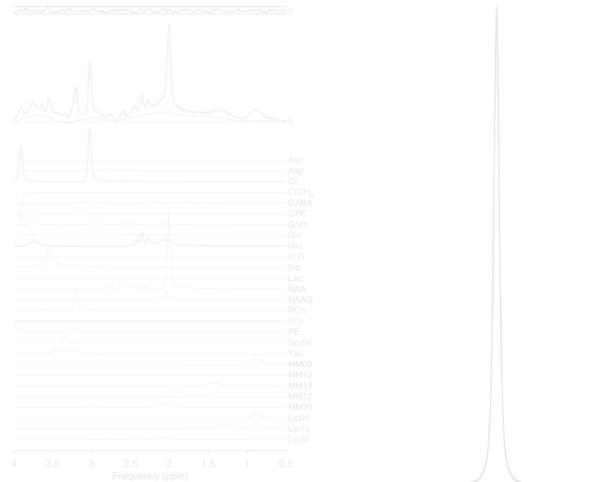
Tissue volume fractions



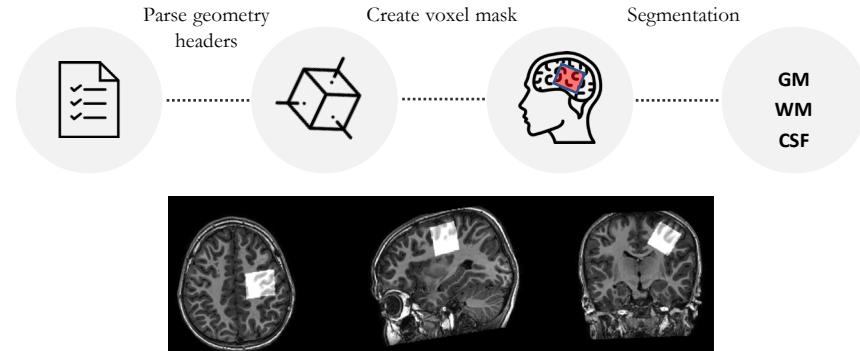
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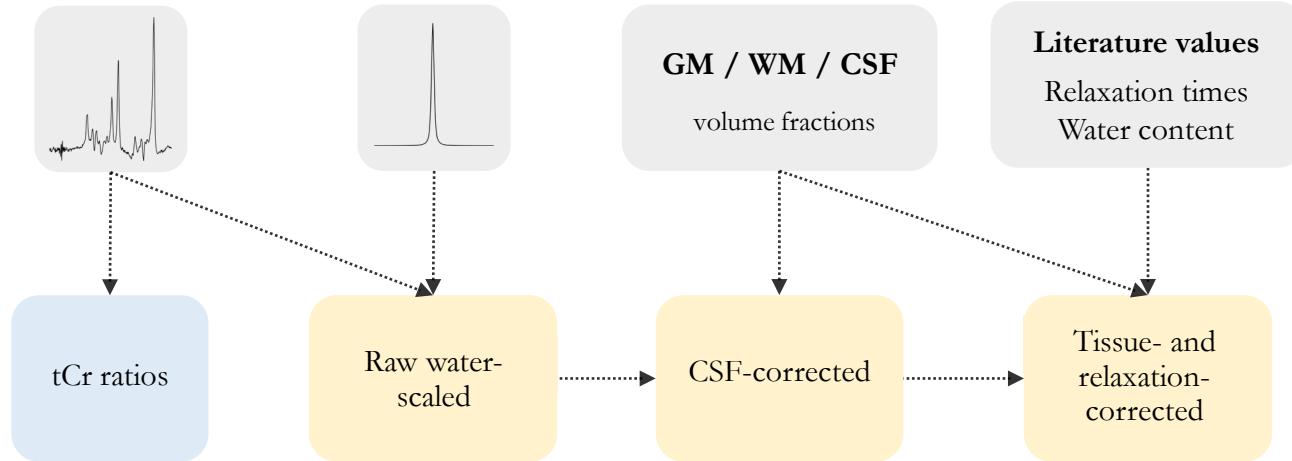
Metabolite & water amplitudes



Tissue volume fractions

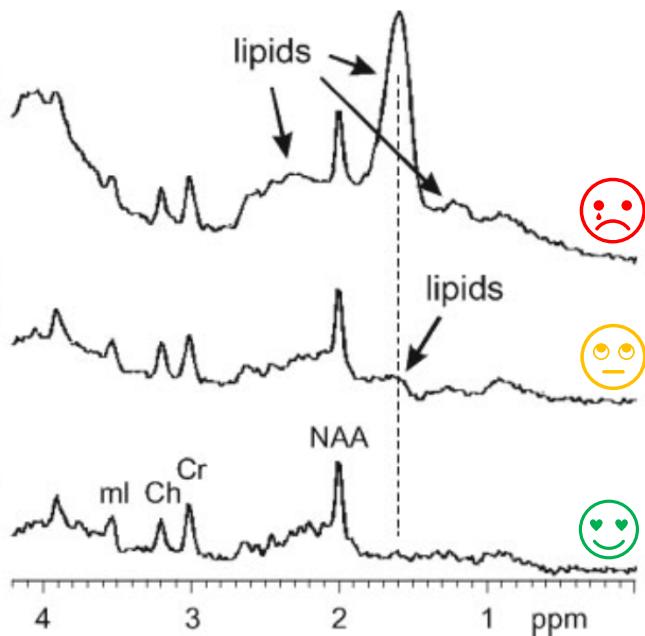


Quantification



- Report tCr ratios and tissue-relaxation-corrected metabolite estimates
- Strong effects on metabolite estimates should appear regardless of reference

Quality assessment



Data quality

Visual inspection

Lipid contamination

“Ghosts”

Residual water

Quality metrics

Signal-to-noise ratio (SNR)

Linewidth (FWHM)

Modeling quality

Visual inspection

Model looks like data

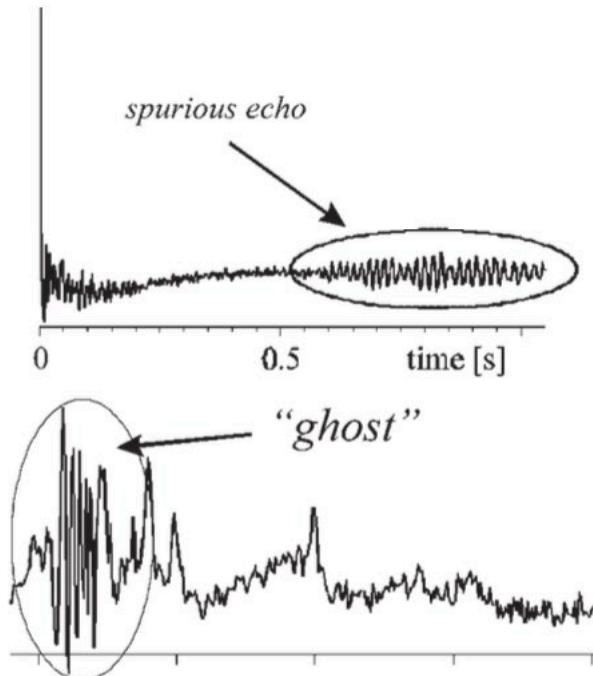
Noise-like residual

Quality metrics

Cramér-Rao lower bounds

Goodness of fit

Quality assessment



Data quality

Visual inspection

Lipid contamination

“Ghosts”

Residual water

Quality metrics

Signal-to-noise ratio (SNR)

Linewidth (FWHM)

Modeling quality

Visual inspection

Model looks like data

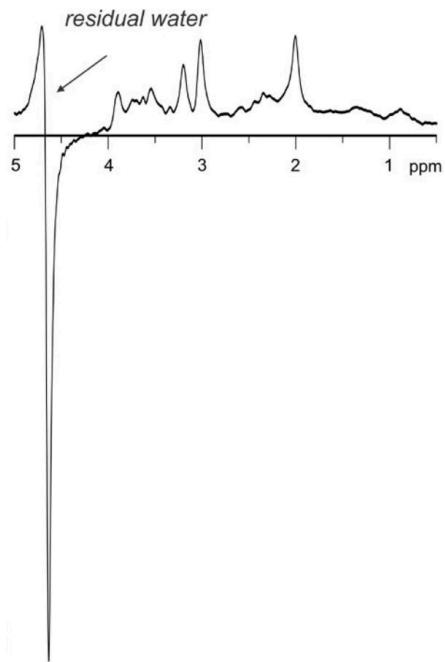
Noise-like residual

Quality metrics

Cramér-Rao lower bounds

Goodness of fit

Quality assessment



Data quality

Visual inspection

Lipid contamination

“Ghosts”

Residual water

Quality metrics

Signal-to-noise ratio (SNR)

Linewidth (FWHM)

Modeling quality

Visual inspection

Model looks like data

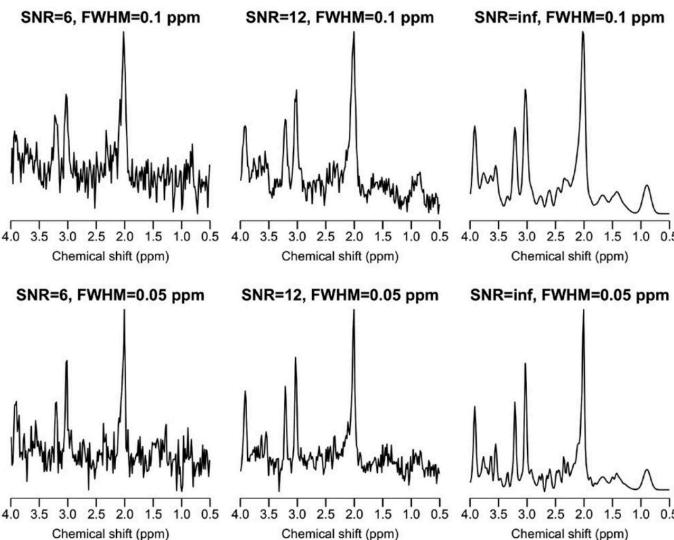
Noise-like residual

Quality metrics

Cramér-Rao lower bounds

Goodness of fit

Quality assessment



Data quality

Visual inspection

Lipid contamination

“Ghosts”

Residual water

Quality metrics

Signal-to-noise ratio (SNR)

Linewidth (FWHM)

Modeling quality

Visual inspection

Model looks like data

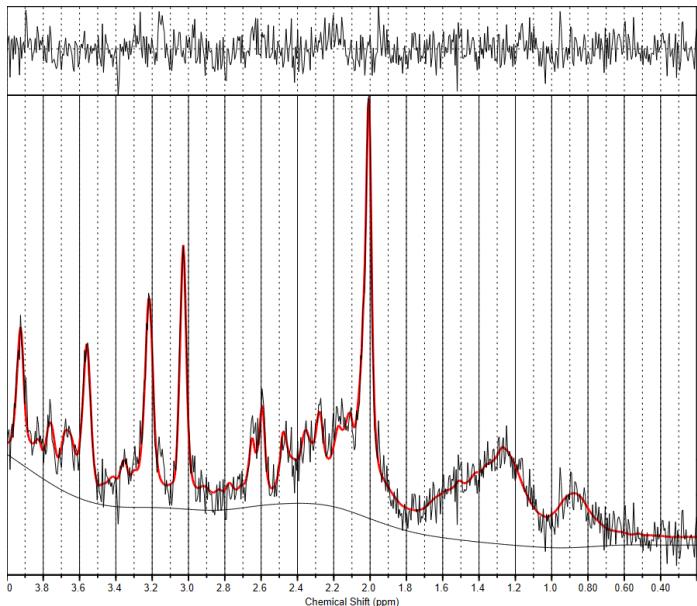
Noise-like residual

Quality metrics

Cramér-Rao lower bounds

Goodness of fit

Quality assessment



Data quality

Visual inspection
Lipid contamination
“Ghosts”
Residual water

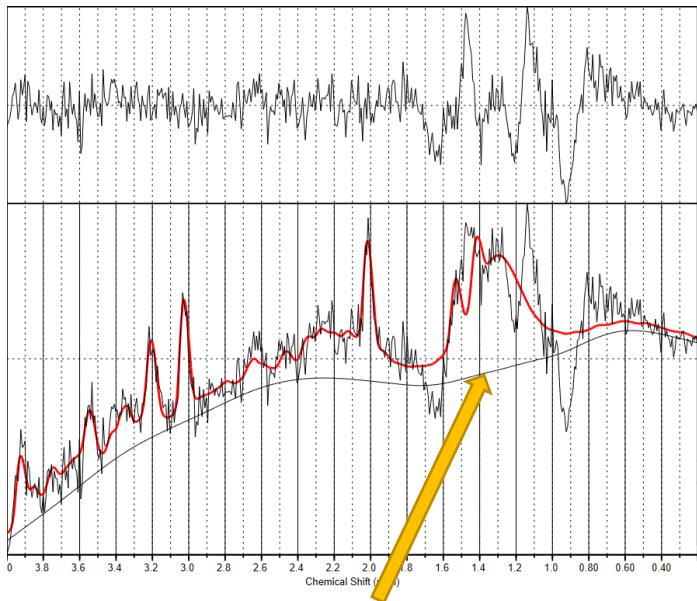
Quality metrics
Signal-to-noise ratio (SNR)
Linewidth (FWHM)

Modeling quality

Visual inspection
Model looks like data
Noise-like residual

Quality metrics
Cramér-Rao lower bounds
Goodness of fit

Quality assessment



Data quality

Visual inspection
Lipid contamination
“Ghosts”
Residual water

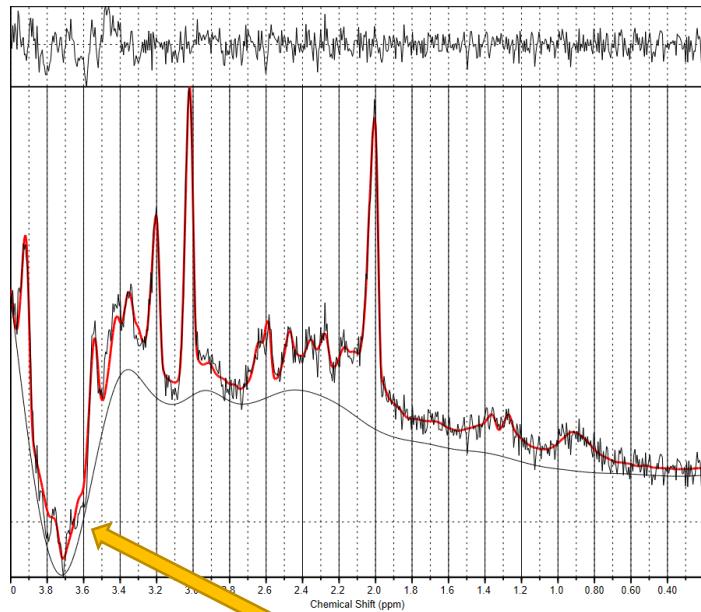
Quality metrics
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Modeling quality

Visual inspection
Model looks like data
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Goodness of fit

Quality assessment



Data quality

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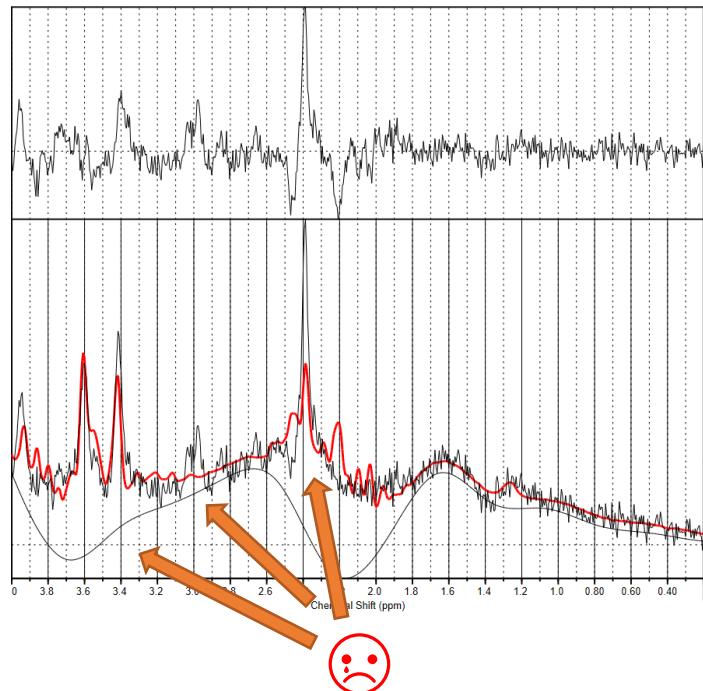
Quality metrics
Signal-to-noise ratio (SNR)
Linewidth (FWHM)

Modeling quality

Visual inspection
Model looks like data
Noise-like residual

Quality metrics
Cramér-Rao lower bounds
Goodness of fit

Quality assessment



Data quality

Visual inspection
Lipid contamination
“Ghosts”
Residual water

Quality metrics
Signal-to-noise ratio (SNR)
Linewidth (FWHM)

Modeling quality

Visual inspection
Model looks like data
Noise-like residual

Quality metrics
Cramér-Rao lower bounds
Goodness of fit

Quality assessment

Cramér-Rao lower bounds (CRLB)

- Estimate of minimal uncertainty in model parameter estimation
- Essentially, they are local derivatives of the model function
- Under ideal conditions, they are identical with the standard deviation
- ... but usually, conditions are not identical:

between estimated CRLBs, true CRLBs and standard deviations. Here we demonstrate that, although the CRLBs are theoretically truly a lower bound on the standard deviation (not an equality) for the problem typically encountered in quantification, they are still an adequate approximation to standard deviation as long as the model perfectly characterizes the data. In the case when the macromolecule basis deviates from the measured macromolecules it was shown that the CRLBs can deviate from standard deviations by approximately 50% for *N*-acetylaspartic acid, creatine and glutamate and of the order of 100% or more for myo-inositol and γ -aminobutyric acid. In the case when the model perfectly reflects the data the CRLBs are within approximately 10% of standard deviations for all metabolites. The result of the CRLB being

Data quality

Visual inspection
Lipid contamination
“Ghosts”
Residual water

Quality metrics
Signal-to-noise ratio (SNR)
Linewidth (FWHM)

Modeling quality

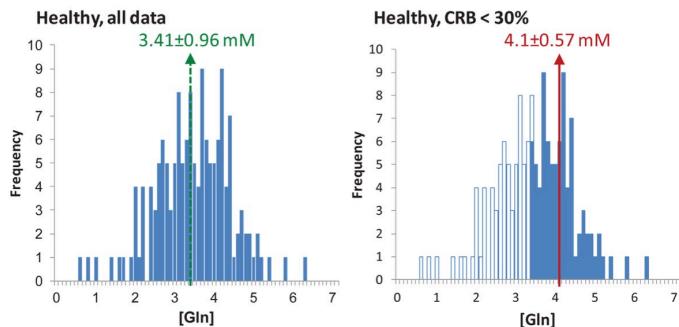
Visual inspection
Model looks like data
Noise-like residual

Quality metrics
Cramér-Rao lower bounds
Goodness of fit

Quality assessment

Cramér-Rao lower bounds (CRLB)

- Relative CRLB [%] often used to discard datasets, but that introduces bias against low levels:



- Better practice:
 - Use absolute CRLB
 - Use CRLB as a weighting factor in statistical analysis

Data quality

Visual inspection
Lipid contamination
“Ghosts”
Residual water

Quality metrics
Signal-to-noise ratio (SNR)
Linewidth (FWHM)

Modeling quality

Visual inspection
Model looks like data
Noise-like residual

Quality metrics
Cramér-Rao lower bounds
Goodness of fit

Quality assessment

Goodness of fit

- Not all modeling tools return CRLB
- Other estimates of modeling quality:
 - SD of residual
 - Max/min residual amplitude
 - $SD(\text{residual})/SD(\text{noise})$

Data quality

Visual inspection

Lipid contamination

“Ghosts”

Residual water

Quality metrics

Signal-to-noise ratio (SNR)

Linewidth (FWHM)

Modeling quality

Visual inspection

Model looks like data

Noise-like residual

Quality metrics

Cramér-Rao lower bounds

Goodness of fit

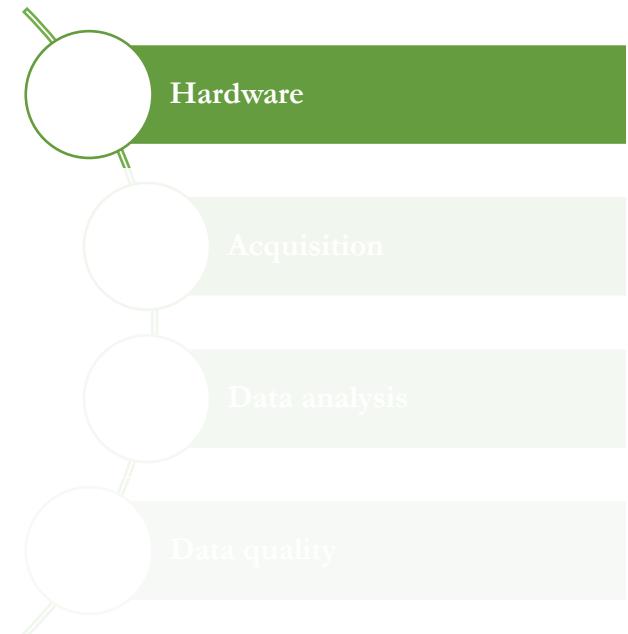
Reporting

Minimum Reporting Standards for in vivo Magnetic Resonance Spectroscopy (MRSinMRS): Experts' consensus recommendations

Alexander Lin, Ovidiu Andronesci, Wolfgang Bogner, In-Young Choi, Eduardo Coello, Cristina Cudalbu, Christoph Juchem, Graham J. Kemp, Roland Kreis, Martin Kršák, Phil Lee, Andrew A. Maudsley, Martin Meyerspeer, Vladamír Mlynárik, Jamie Near, Gülin Öz, Aimie L. Peek, Nicolaas A. Puts, Eva-Maria Ratai, Ivan Tkáč, Paul G. Mullins  ... See fewer authors 

1. Hardware

a. Field strength [T]	3 T
b. Manufacturer	Siemens
c. Model (software version if available)	Verio (VB17)
d. RF coils: nuclei (transmit/receive), number of channels, type, body part	32 channel head coil
e. Additional hardware	N/A

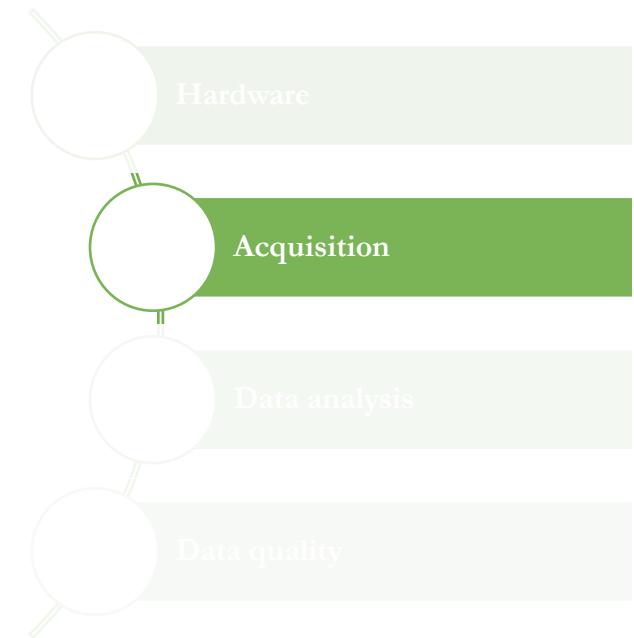


Reporting

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Alexander Lin, Ovidiu Andronesi, Wolfgang Bogner, In-Young Choi, Eduardo Coello, Cristina Cudalbu, Christoph Juchem, Graham J. Kemp, Roland Kreis, Martin Kršák, Phil Lee, Andrew A. Maudsley, Martin Meyerspeer, Vladamír Mlynárik, Jamie Near, Gülin Öz, Aimie L. Peek, Nicolaas A. Puts, Eva-Maria Ratai, Ivan Tkáč, Paul G. Mullins  ... See fewer authors ^

2. Acquisition	
a. Pulse sequence	3D localized correlated spectroscopy
b. Volume of interest (VOI) locations	Posterior cingulate gyrus
c. Nominal VOI size [cm ³ , mm ³]	3 × 3 × 3 cm ³
d. Repetition time (T_R), echo time (T_E) [ms, s]	T_R 1500 ms, initial T_E 30 ms, 0.8 ms increments
e. Total number of excitations or acquisitions per spectrum In time series for kinetic studies	64 increments with 8 averages per increment
i. Number of averaged spectra (NA) per time point	
ii. Averaging method (eg block-wise or moving average)	
iii. Total number of spectra (acquired/in time series)	
f. Additional sequence parameters (spectral width in Hz, number of spectral points, frequency offsets) If STEAM: mixing time (T_M) If MRS: 2D or 3D, FOV in all directions, matrix size, acceleration factors, sampling method	F1/F2: 2000 Hz/1250 Hz, 1024 points
g. Water suppression method	WET
h. Shimming method, reference peak, and thresholds for "acceptance of shim" chosen	Automated B_0 field mapping followed by manual shimming of water to <14 Hz
i. Triggering or motion correction method (respiratory, peripheral, cardiac triggering, incl. device used and delays)	N/A



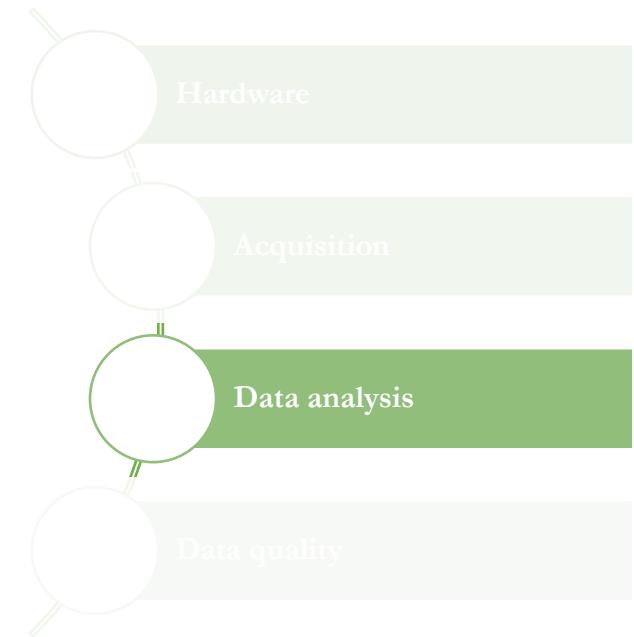
Reporting

Minimum Reporting Standards for *in vivo* Magnetic Resonance Spectroscopy (MRSinMRS): Experts' consensus recommendations

Alexander Lin, Ovidiu Andronesi, Wolfgang Bogner, In-Young Choi, Eduardo Coello, Cristina Cudalbu, Christoph Juchem, Graham J. Kemp, Roland Kreis, Martin Kršák, Phil Lee, Andrew A. Maudsley, Martin Meyerspeer, Vladamír Mlynárik, Jamie Near, Gülin Öz, Aimie L. Peek, Nicolaas A. Puts, Eva-Maria Ratai, Ivan Tkáč, Paul G. Mullins  ... See fewer authors ^

3. Data analysis methods and outputs

a. Analysis software	Felix-2007
b. Processing steps deviating from quoted reference or product	F2 domain (skewed sine-squared window, 2048 points, magnitude mode), F1 domain (sine-squared window, linear prediction to 96 points, zero-filling to 512 points, magnitude mode)
c. Output measure (eg absolute concentration, institutional units, ratio)	Ratio to creatine
d. Quantification references and assumptions, fitting model assumptions	Each spectrum was calibrated by setting the lysine cross peak (at 3.00-1.67 ppm) and specifying a constant 'number of contour levels' (set to 28), as well as a constant 'level multiplier' (defined as the difference between values of consecutive contour, set to 1.05).



Reporting

Minimum Reporting Standards for in vivo Magnetic Resonance Spectroscopy (MRSinMRS): Experts' consensus recommendations

Alexander Lin, Ovidiu Andronescu, Wolfgang Bogner, In-Young Choi, Eduardo Coello, Cristina Cudalbu, Christoph Juchem, Graham J. Kemp, Roland Kreis, Martin Kršák, Phil Lee, Andrew A. Maudsley, Martin Meyerspeer, Vladamír Mlynárik, Jamie Near, Gülin Öz, Aimie L. Peek, Nicolaas A. Puts, Eva-Maria Ratai, Ivan Tkáč, Paul G. Mullins  ... See fewer authors ^

4. Data quality

a. Reported variables (SNR, linewidth (with reference peaks))

SNR and linewidth not described

b. Data exclusion criteria

No subjects excluded

c. Quality measures of postprocessing model fitting (eg CRLB, goodness of fit, SD of residual)

No QA measures described

d. Sample spectrum

Figure 1

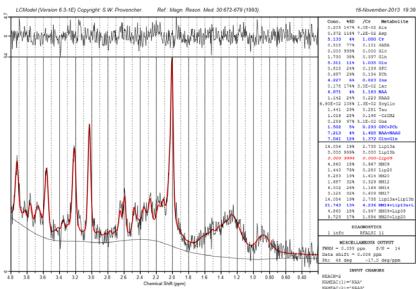


Software overview

The MRS software landscape 2021

- Recent years have seen many new (overwhelmingly open-source) tools for data processing, modeling, and quantification
- Processing and modeling remains a core focus of methodological research, and will be more consensus-oriented and collaborative
- Expect an increase in open-source methods and large-scale validation against synthetic data

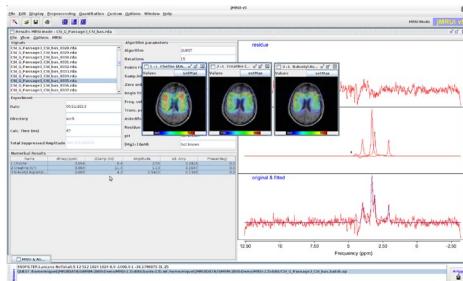
LCModel



LCModel

- Widely used, widely regarded as field standard
 - Commercial product (\$13,300) prior to February 2021
 - Now free & open-source, but discontinued development
 - Linux binaries (compiled by users for Windows & MacOS)
 - Automated analysis with many input parameters
 - Presets for brain, tumor, muscle, liver, CSF spectra
 - Core algorithm is fast & robust, but not well understood
 - Limited preprocessing
 - No tissue segmentation / correction

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
Tarquin	Yes	Yes	Yes	No	Win Linux Mac	C++
Vespa	Yes	Yes	Yes	No	All	Python
FID-A	Yes	Yes	No	No	All	MATLAB
Gannet	Yes	Yes	Yes	Yes	All	MATLAB
INSPECTOR	No	Yes	Yes	Yes	All	MATLAB
Osprey	Yes	Yes	Yes	Yes	All	MATLAB
spant	Yes	Yes	Yes	Yes	All	R
FSL-MRS	Yes	Yes	Yes	Yes	All	Python

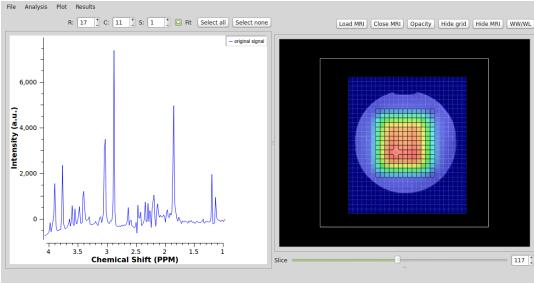


jMRUI

- Widely used
- Free license
- Uniquely focused on time-domain methods
- Many different spectral operations, interaction required
- Preprocessing somewhat limited
- Different fit algorithms (SVD, AMARES, QUEST, AQSES)
- Integrated basis set simulation (NMR-SCOPE-B)
- No tissue segmentation / correction

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
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FSL-MRS	Yes	Yes	Yes	Yes	All	Python

TARQUIN

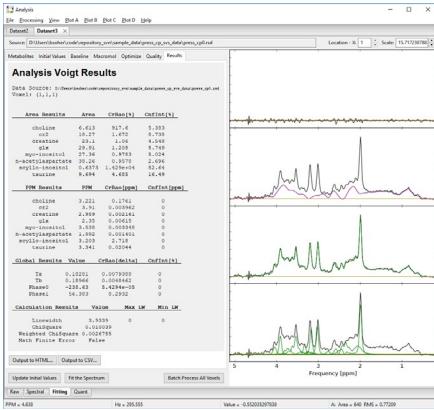


Tarquin

- Well-established free early LCModel alternative
- Automated preprocessing
- Internal calculation of basis sets
- No tissue segmentation

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
Tarquin	Yes	Yes	Yes	No	Win Linux Mac	C++
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Osprey	Yes	Yes	Yes	Yes	All	MATLAB
spant	Yes	Yes	Yes	Yes	All	R
FSL-MRS	Yes	Yes	Yes	Yes	All	Python

Vespa



Vespa

- Integrated open-source platform
- RF pulse design
- Full spectral simulations
- Creation of synthetic datasets
- Interactive processing and modeling
- No tissue segmentation, but volume fractions can be put in

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
Tarquin	Yes	Yes	Yes	No	Win Linux Mac	C++
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FSL-MRS	Yes	Yes	Yes	Yes	All	Python

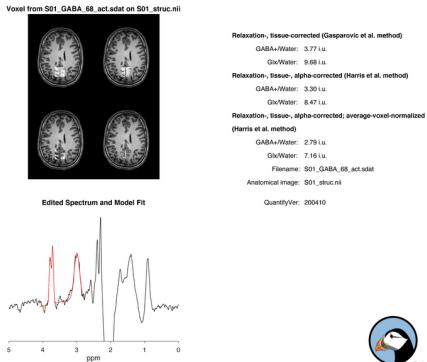
📁 FID-A_Documentation
📁 exampleData
📁 exampleRunScripts
📁 inputOutput
📁 processingTools
📁 rfPulseTools
📁 simulationTools
📄 .gitattributes
📄 LICENSE.txt
📄 README.md

FID-A

- Toolbox for processing and simulating MRS data
- Modular functions to construct processing pipelines
- Full spectral simulations and basis set generation
- Examples for processing and simulation pipelines
- No modeling or tissue segmentation functions

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
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Gannet

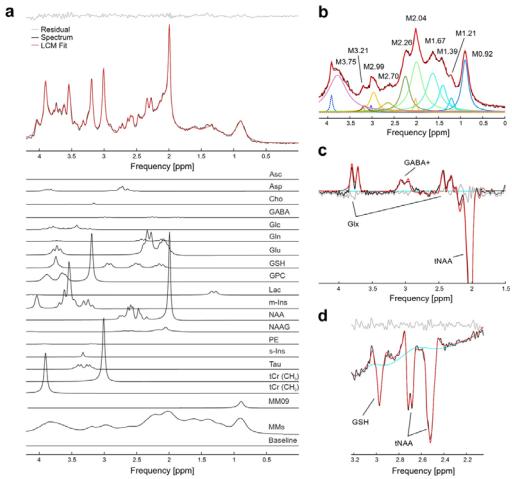


Gannet

- Toolkit for analyzing spectral-edited MRS data
- Automated preprocessing, modeling, and tissue-corrected quantification
- Peak integration based on Gaussian models
- Disclaimer: This is software I contributed to.

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
Tarquin	Yes	Yes	Yes	No	Win Linux Mac	C++
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INSPECTOR

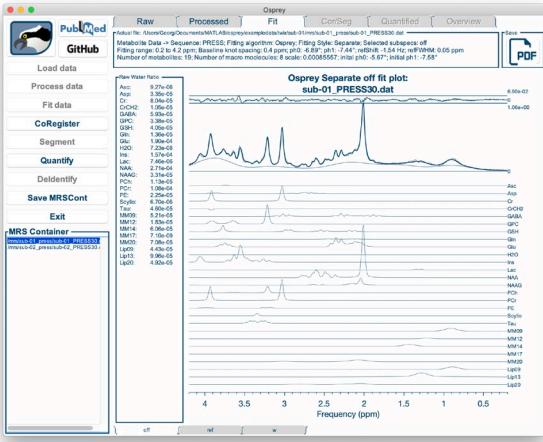


INSPECTOR

- Analysis software including flexible automated processing, linear-combination modeling, visualization, and tissue-corrected quantification
- Direct interface with basis set simulation software MARSS

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LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
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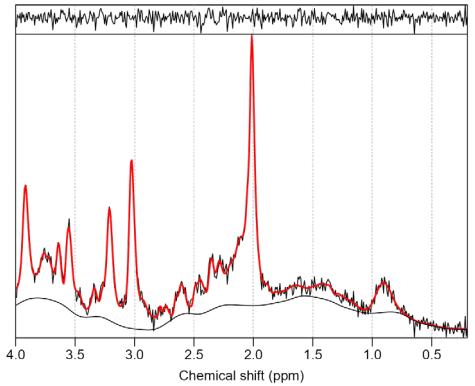
Osprey



Osprey

- Modular analysis software (using FID-A building blocks) including flexible automated processing, linear-combination modeling, visualization, and tissue-corrected quantification
- Disclaimer: This is software I develop and maintain.

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
Tarquin	Yes	Yes	Yes	No	Win Linux Mac	C++
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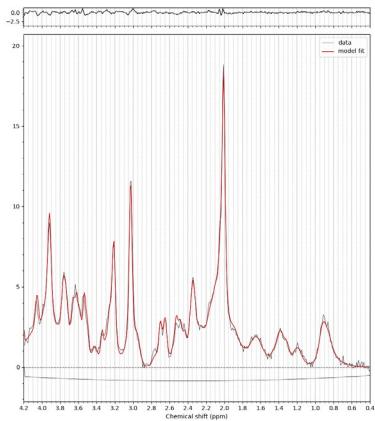


spant

- Modular set of tools to build automated analysis pipelines
- Includes functions for preprocessing, linear-combination modeling, tissue correction, visualization, and simulations

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
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FSL-MRS	Yes	Yes	Yes	Yes	All	Python

FSL-MRS



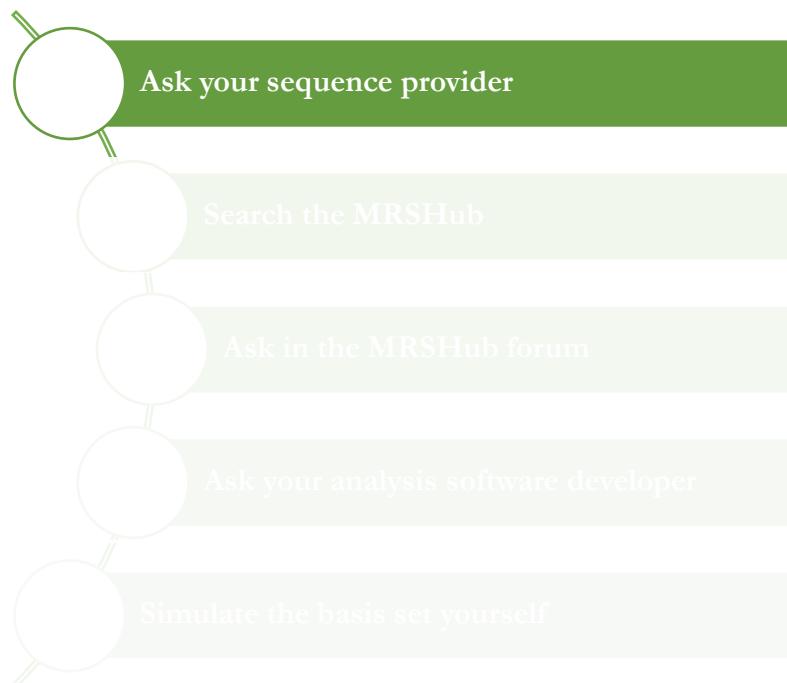
FSL-MRS

- Modular set of tools to build automated analysis pipelines
- Includes functions for preprocessing, linear-combination modeling, tissue segmentation, visualization, and simulations
- Interfaces directly with other FSL tools

Name	Open source?	Pre-processing	Modeling	Tissue segmentation	OS	Language
LCModel	Yes	Limited	Yes	No	Linux	FORTRAN77
jMRUI	No	Yes (limited)	Yes	No	Win Linux	JAVA
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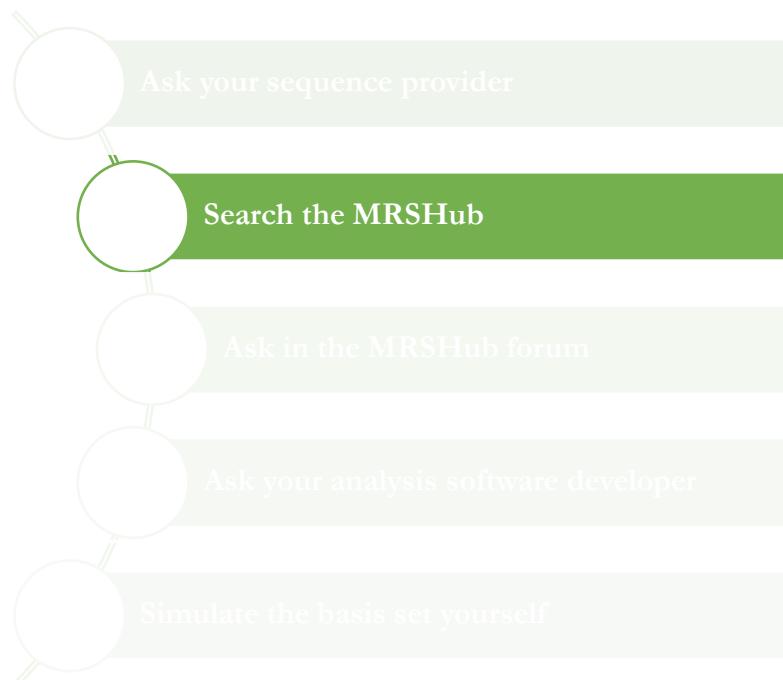
Where do I get a basis set?

Do not try to acquire an experimental basis set on the scanner with phantoms.



Where do I get a basis set?

Do not try to acquire an experimental basis set on the scanner with phantoms.



Basis sets for PRESS, STEAM and sLASER for multiple vendors [🔗](#)

These basis sets were generated using the exact waveforms, timings and 128^3 spatial points to appropriately accommodate the sidebands for each vendor/sequence combination. More details about the acquisition can be found in the reference below.

Basis sets for PRESS, STEAM and sLASER for multiple vendors

Developer Karl Landheer, Kelley Swanberg, Christoph Juchem

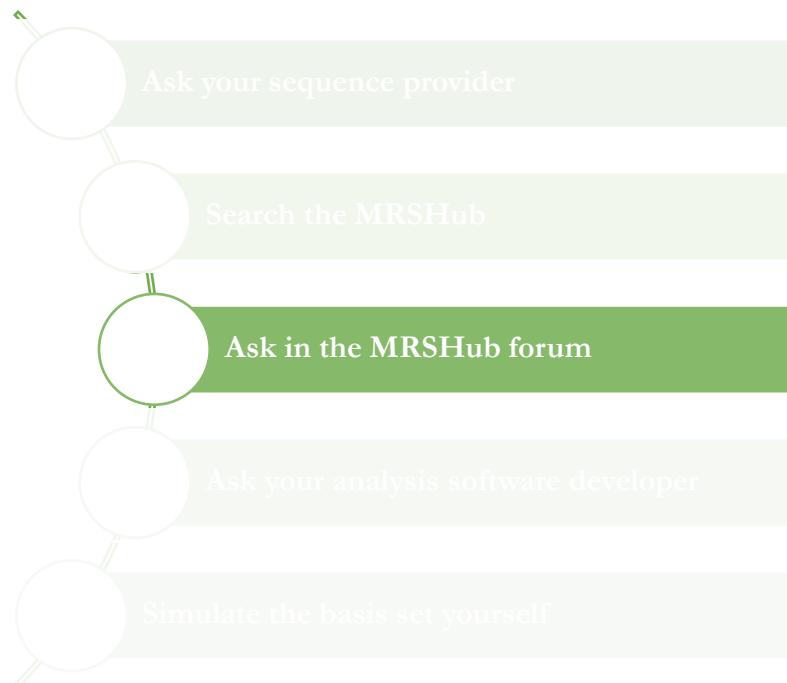
Format Both .RAW and .mat (INSPECTOR, readable in MATLAB) are provided. All files were generated using MATLAB

Sequence PRESS, sLASER, STEAM

License BSD3

Where do I get a basis set?

Do not try to acquire an experimental basis set on the scanner with phantoms.

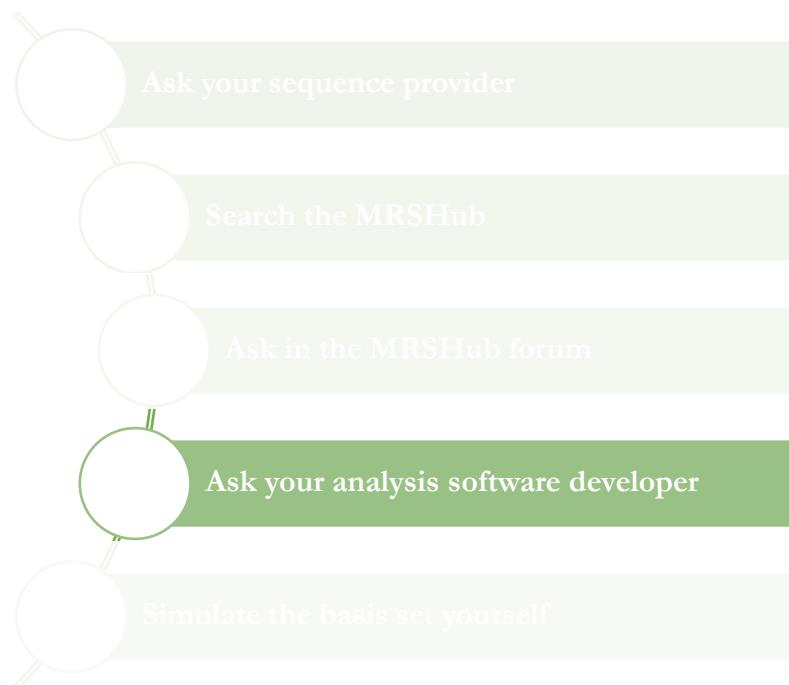


Basis set needed: Philips 3T MEGAPress
MMsuppr. GABA80
Basis Sets

4
Mar 16

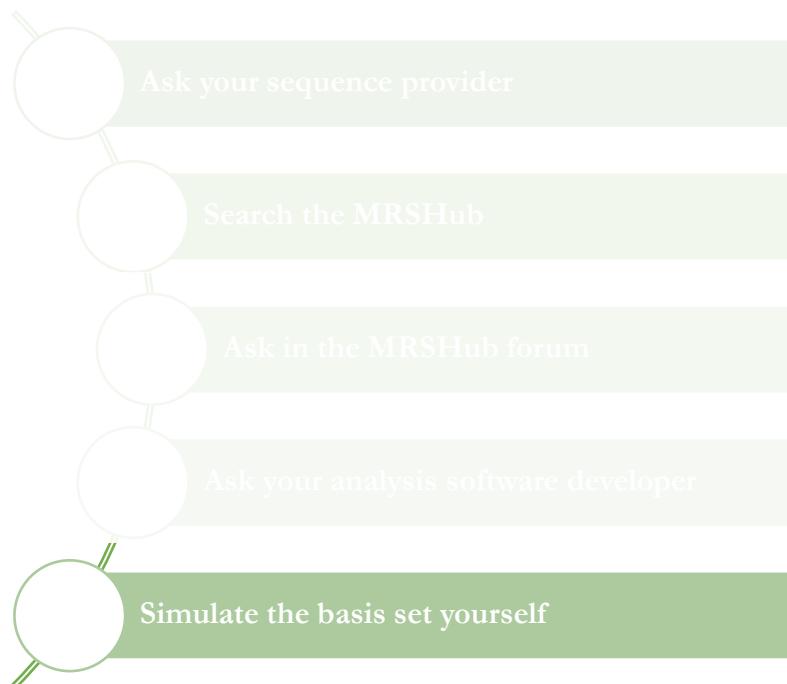
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Where do I get a basis set?

Do not try to acquire an experimental basis set on the scanner with phantoms.



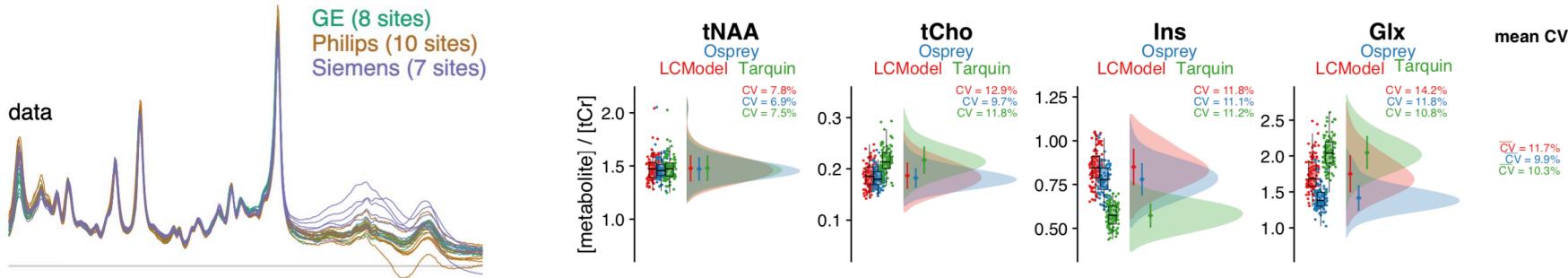
Various free simulation tools

- GAMMA
- FID-A
- MARSS / INSPECTOR
- NMR-SCOPEB
- Vespa
- FSL-MRS

Requires expert knowledge

- Pulse sequence timing
- Pulse waveforms (often not public)

Benchmarking comparison with common tools



- >270 PRESS spectra ($TE = 35$ ms) analyzed with **Osprey**, **LCModel**, **Tarquin**
- Substantial differences **between tools** even for major metabolites
- Choice of tool may introduce **substantial variance**

Final words



Build relationships with sequence and analysis software developers.



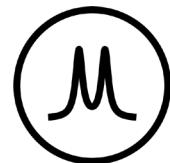
Be aware of new acquisition and analysis methods.



Different analyses will yield different results.
Be transparent.



Ask for help.



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