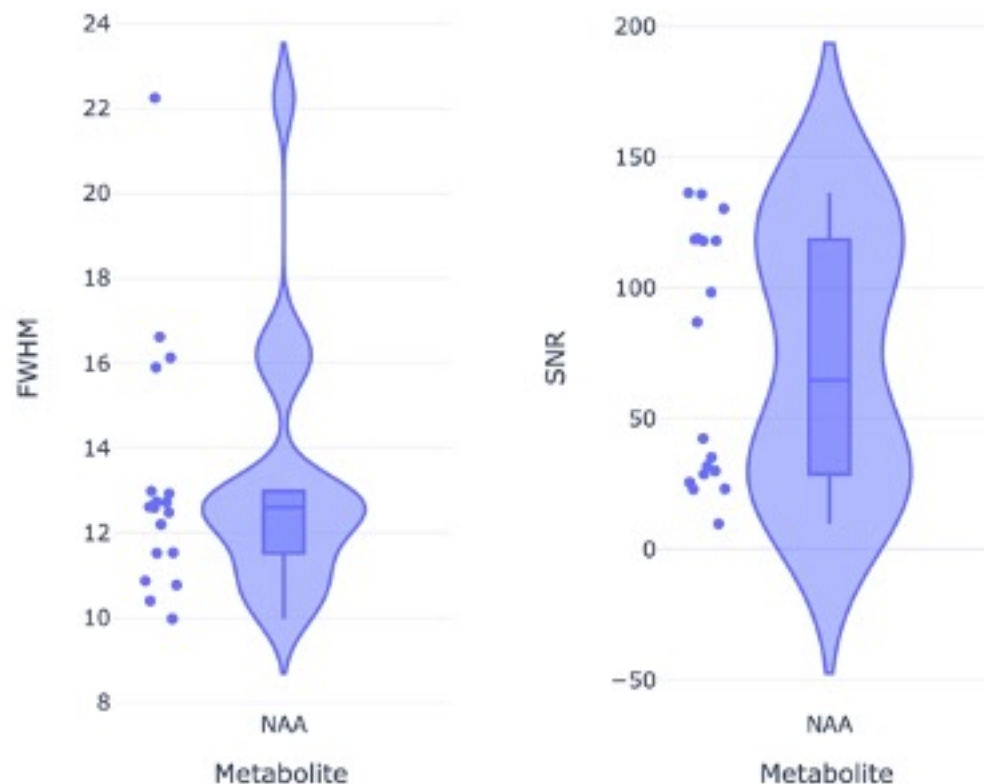




FSL-MRS – Tools for Magnetic Resonance Spectroscopy



IV. Data quality





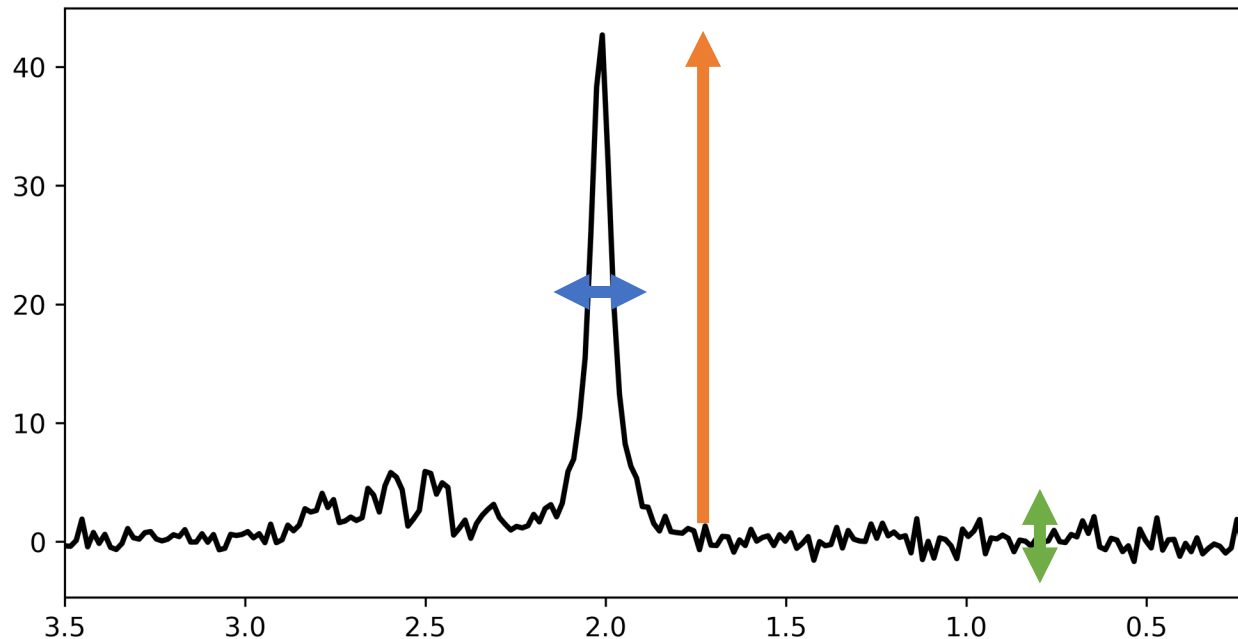
Quality Control (QC) metrics

Linewidth

Signal-to-noise ratio
(SNR)

Width of peak at half maximum

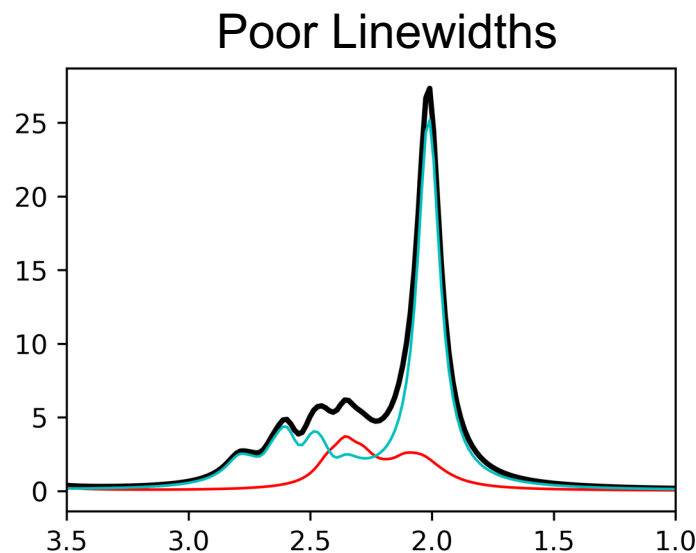
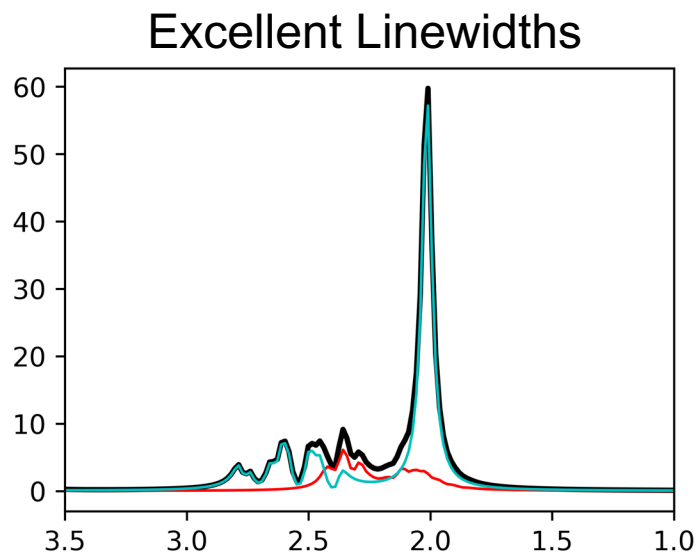
Height of peak / noise standard deviation





QC metrics: linewidth

Increasing linewidth decreases the separability of spectral peaks => greater correlation between fitted concentrations => greater uncertainty.



Comparable between studies/sites and consistently given as FWHM, but beware which peak used.





QC metrics: SNR

Many definitions of SNR are used. How do you measure signal? Noise?

- Noise: End of FID, spectral residual after fitting, signal-free spectral region, real/complex?
- Signal: First point of FID, a metabolite peak (which one? multiplet shape?), do you apply filtering first?

Compare apples with apples, not apples with poorly defined numbers from the literature.





Fit quality metrics

Cramér–Rao lower bound
(CRLB)

Estimated and best possible
uncertainty (standard deviation)
in metabolite concentrations
due to:

- 1) thermal noise, and
- 2) peak overlap

but not artifacts.

Metab	mMol/kg	CRLB	%CRLB	/Cr+PCr
Ala	0.4	0.23	58.4	0.04
Asc	4.03	0.35	8.7	0.37
Asp	2.11	0.67	31.9	0.19
Cr	6.08	0.43	7	0.56
GABA	0	0.39	999	0
GPC	3.34	0.15	4.5	0.31
GSH	1.92	0.18	9.4	0.18
Glc	1.06	0.39	36.3	0.1
Gln	1.14	0.35	31	0.11
Glu	6.26	0.34	5.4	0.57
Ins	14.28	0.29	2	1.31
Lac	1.91	0.23	12	0.17
Mac	13.96	0.76	5.4	1.28
NAA	10.76	0.26	2.5	0.99
NAAG	4.28	0.18	4.2	0.39
PCho	0.87	0.16	18.4	0.08
PCr	4.82	0.41	8.5	0.44
PE	0.27	0.5	182.1	0.02
Tau	2.2	0.3	13.8	0.2
sIns	0.5	0.07	14.8	0.05
Cr+PCr	10.9	0.25	2.3	1
NAA+NAAG	15.04	0.28	1.9	1.38
GPC+PCho	4.21	0.11	2.6	0.39
Glc+Tau	3.26	0.3	9.2	0.3





Relative vs. Absolute CRLB

MAGNETIC RESONANCE
IN MEDICINE

ISMIRM

ONE
COMMUNITY
FOR CLINICIANS
AND SCIENTISTS

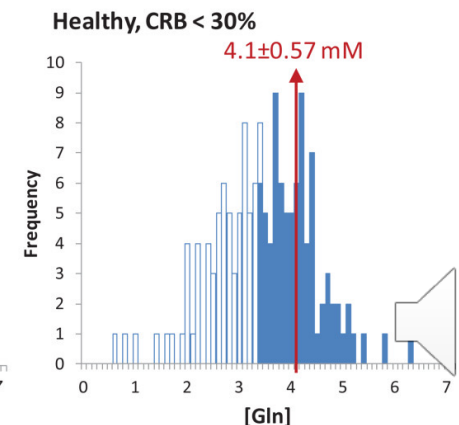
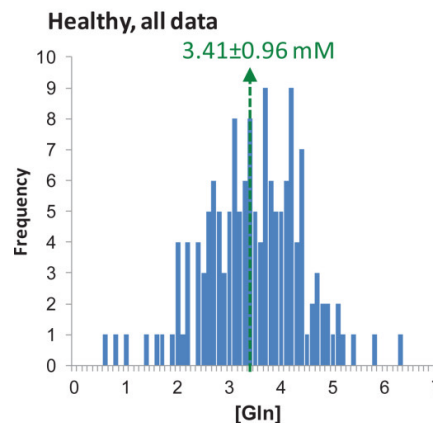
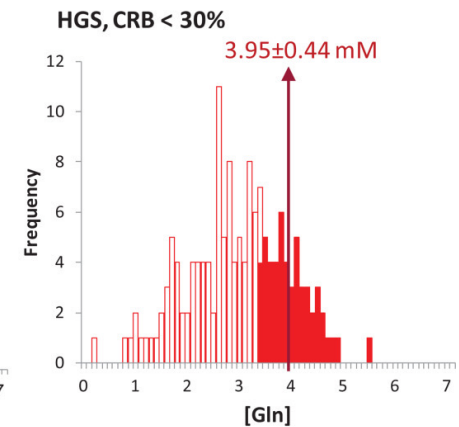
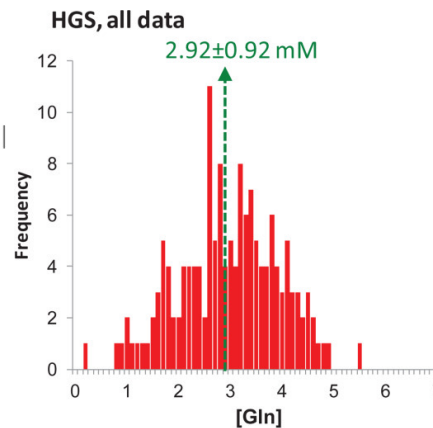
Mini-Review | Free Access

The trouble with quality filtering based on relative Cramér-Rao lower bounds

Roland Kreis

First published: 06 March 2015 | <https://doi.org/10.1002/mrm.25568>

Filtering data using relative CRLB (measured as percentage of concentration) can bias your results by excluding mostly low concentrations. Use absolute values!

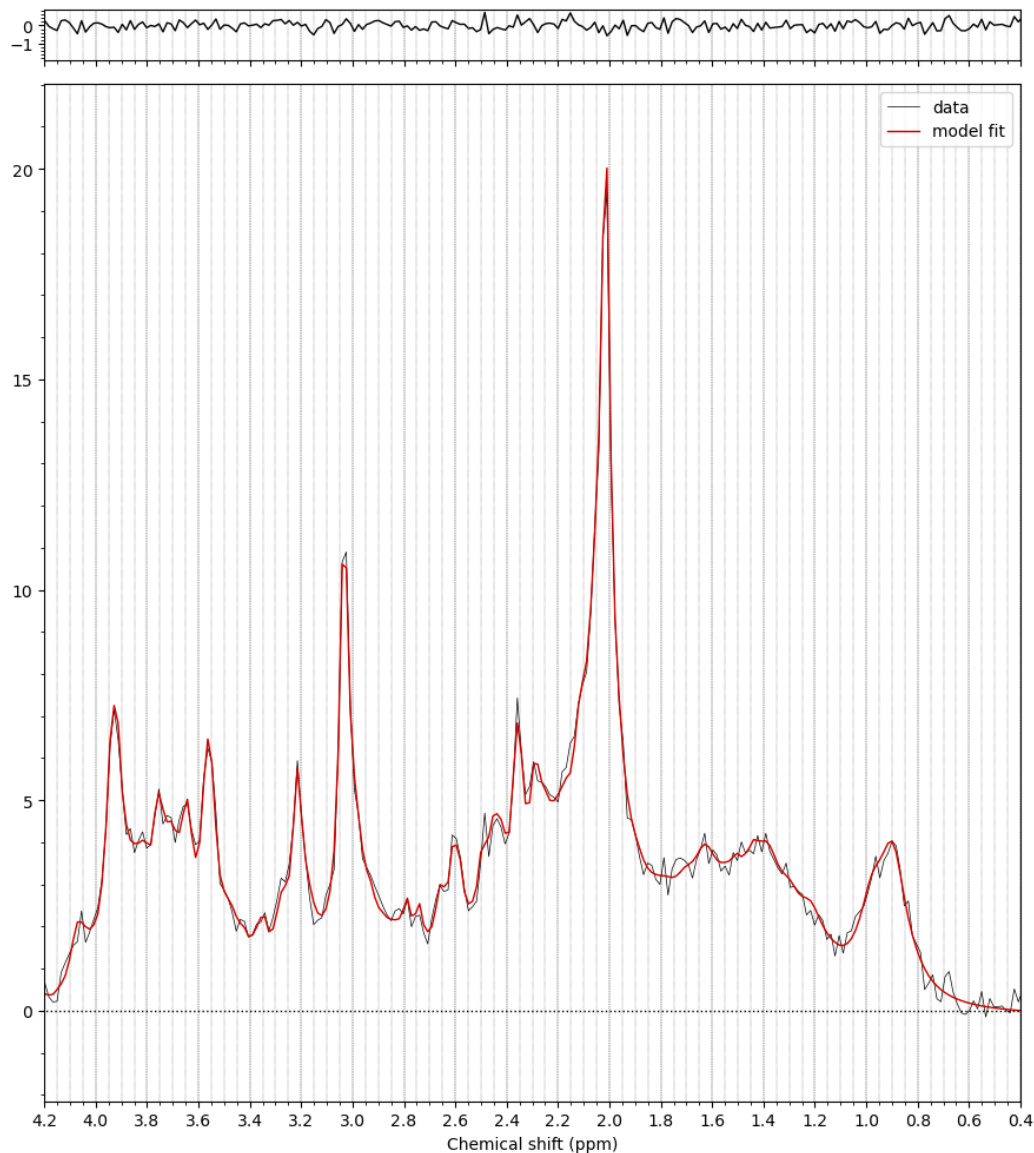




Examples of fits

Good fit

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





Examples of fits

Low SNR

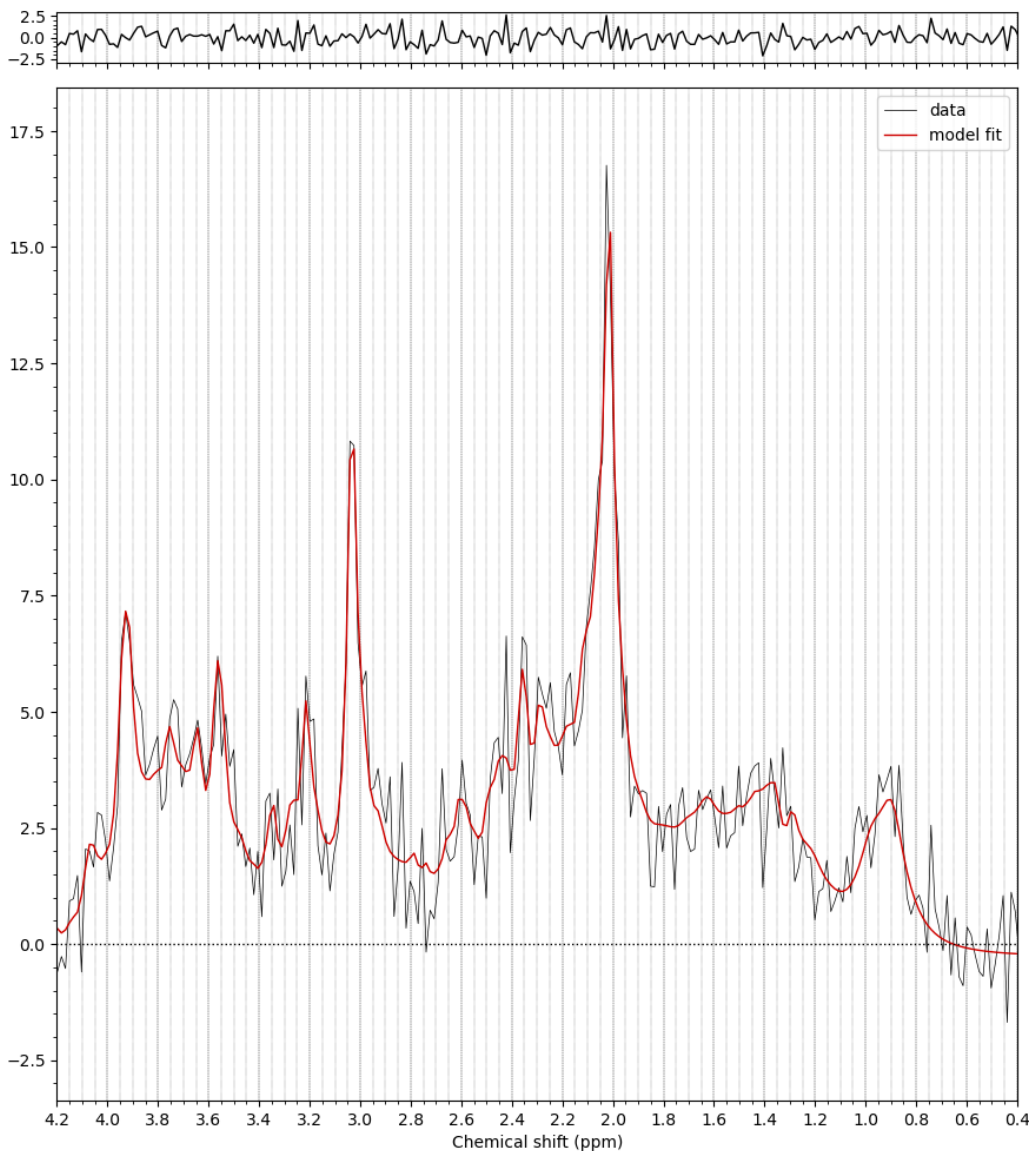
SNR: 8

FWHM: 5.6 Hz

tNAA: 6.9% (x 4.6)

Glx: 15.8% (x 4.0)

Ins: 19.1% (x 3.3)





Examples of fits

Poor linewidth

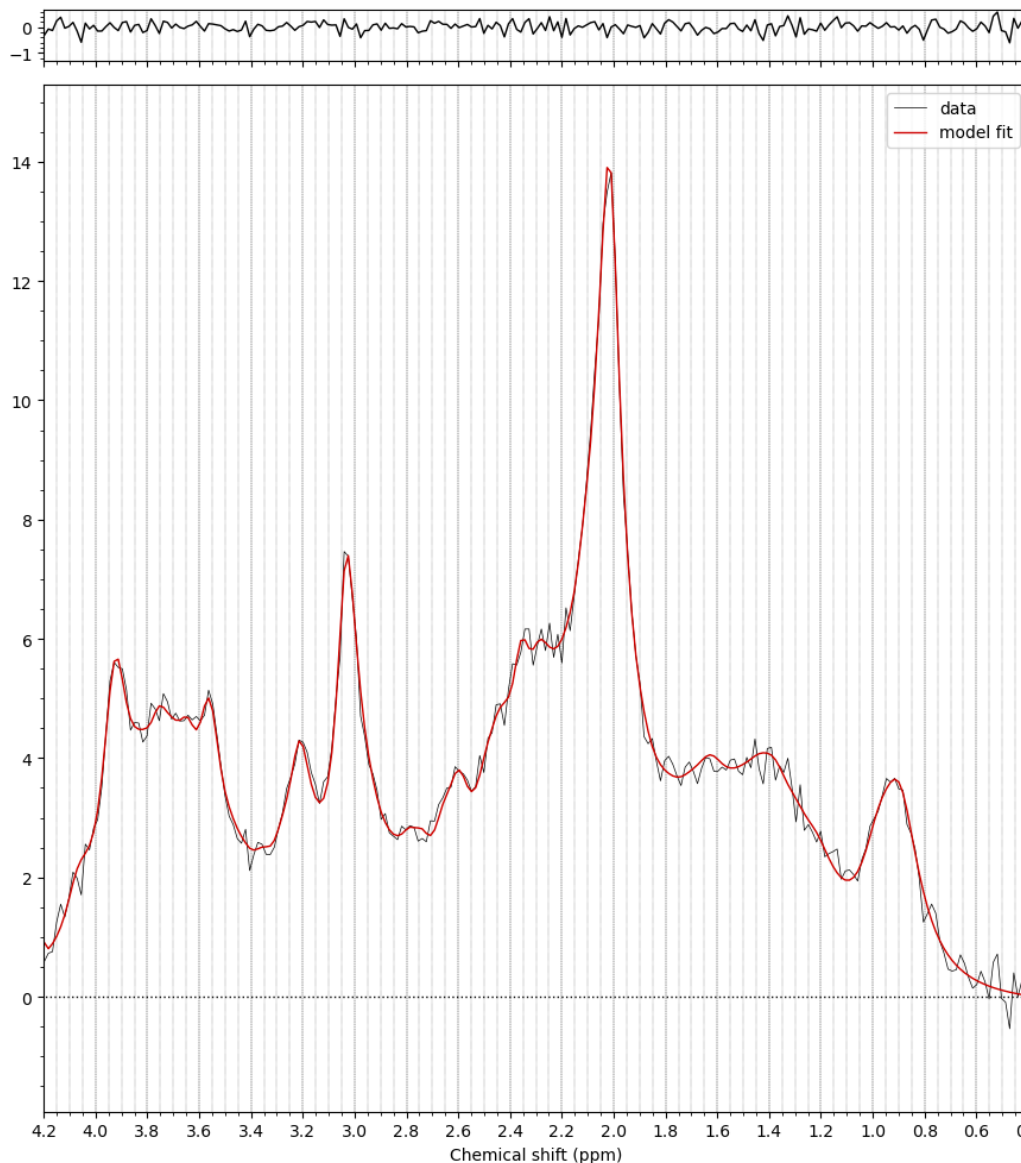
SNR: 23

FWHM: 11.1 Hz

tNAA: 2.4% (x 1.6)

Glx: 4.6% (x 1.2)

Ins: 8.9% (x 1.5)

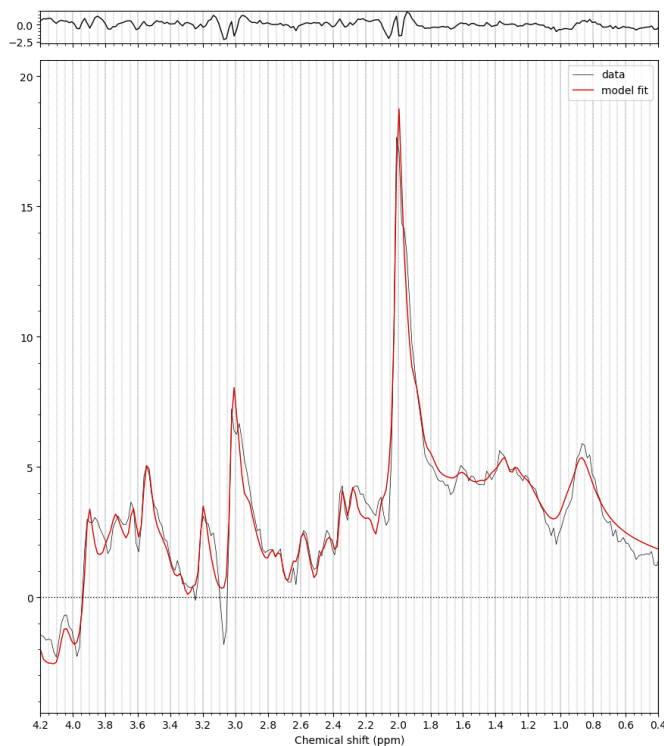




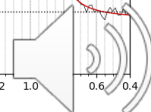
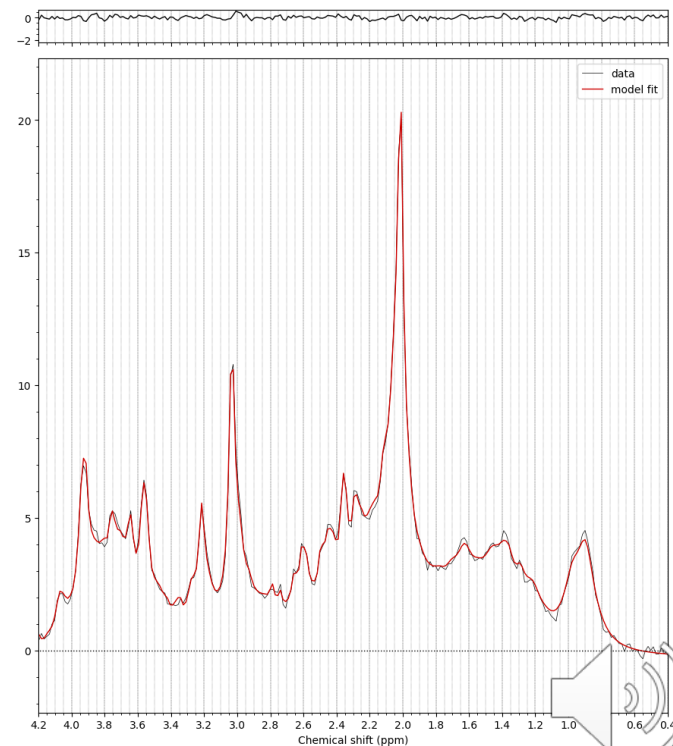
Look at your data!

Eddy currents

SNR: 47
FWHM: 7.8 Hz
tNAA: 3.4% (x 2.3)
Glx: 11.5% (x 2.9)
Ins: 11.2% (x 1.9)



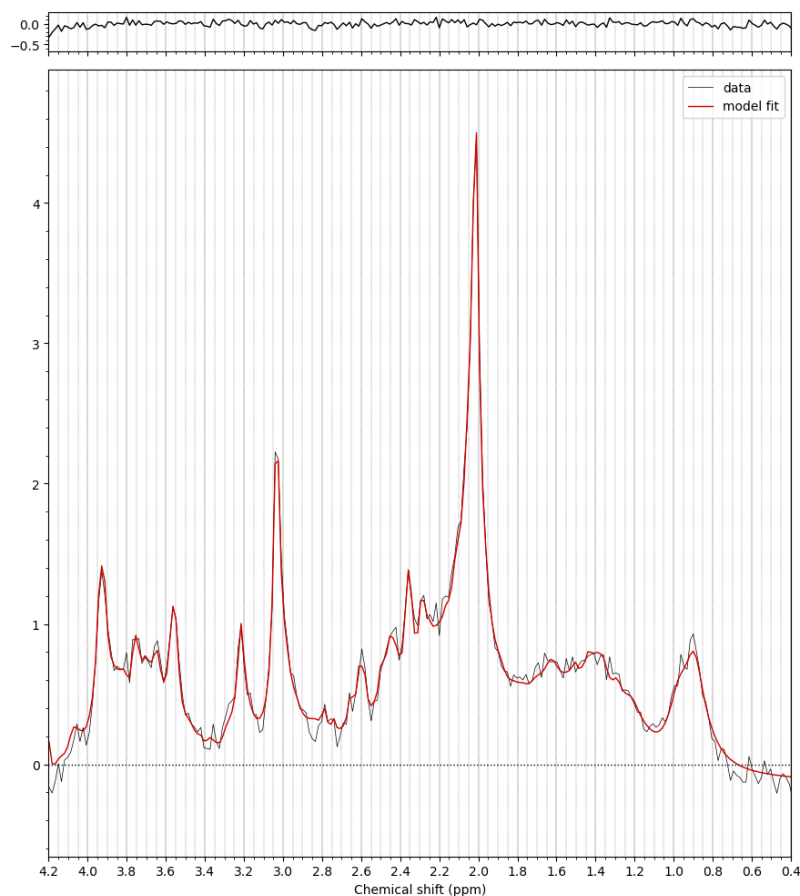
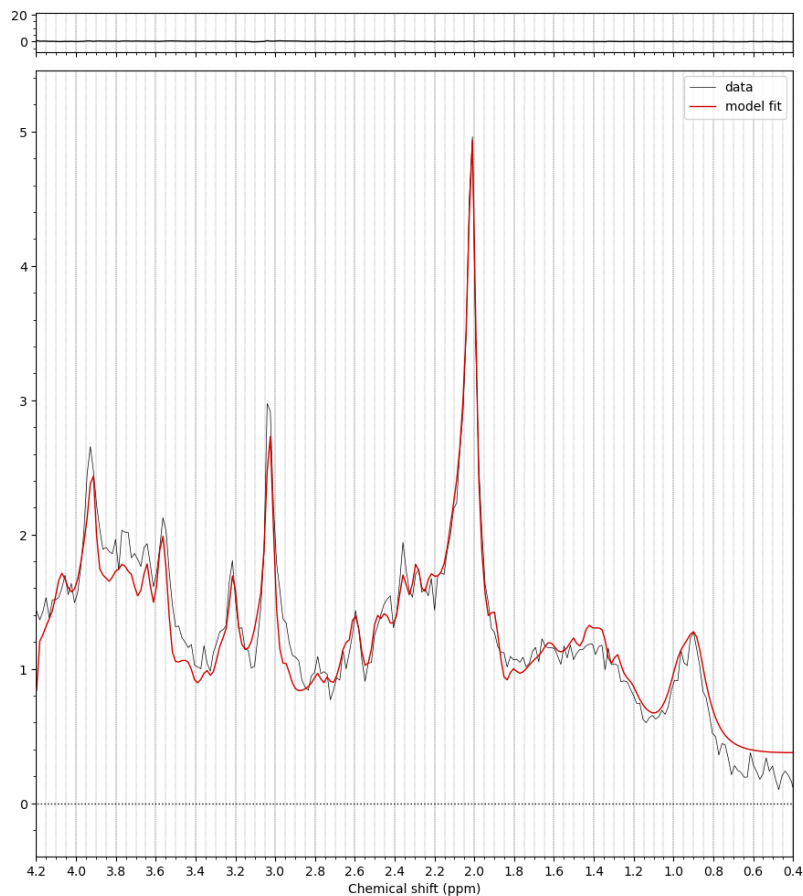
SNR: 73;
FWHM: 5.3 Hz
tNAA: 1.0%
Glx: 2.9%
Ins: 3.8%





Look at your data!

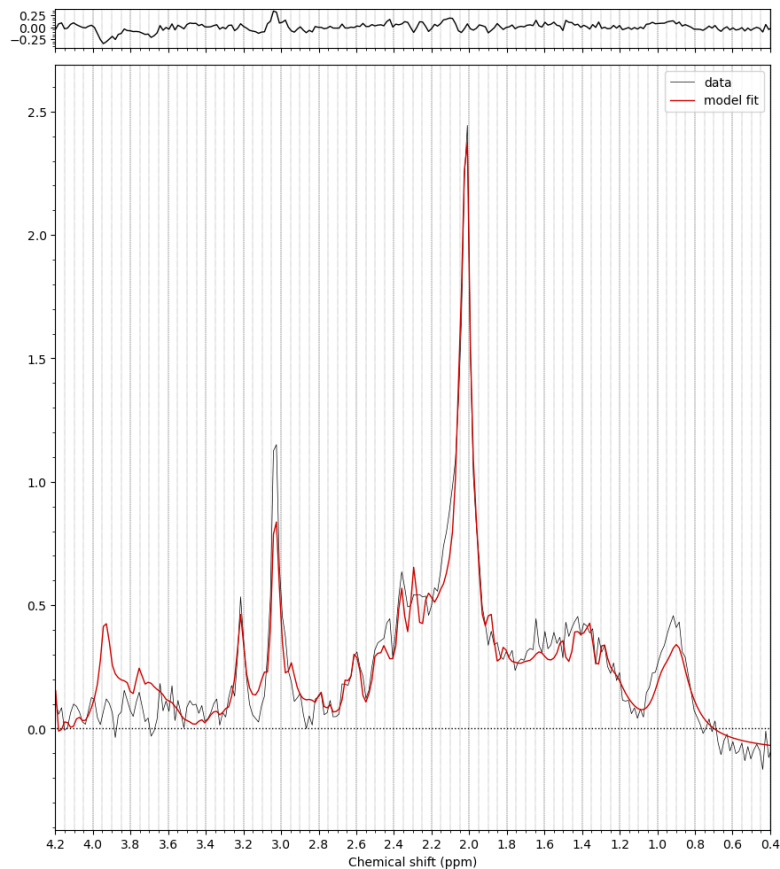
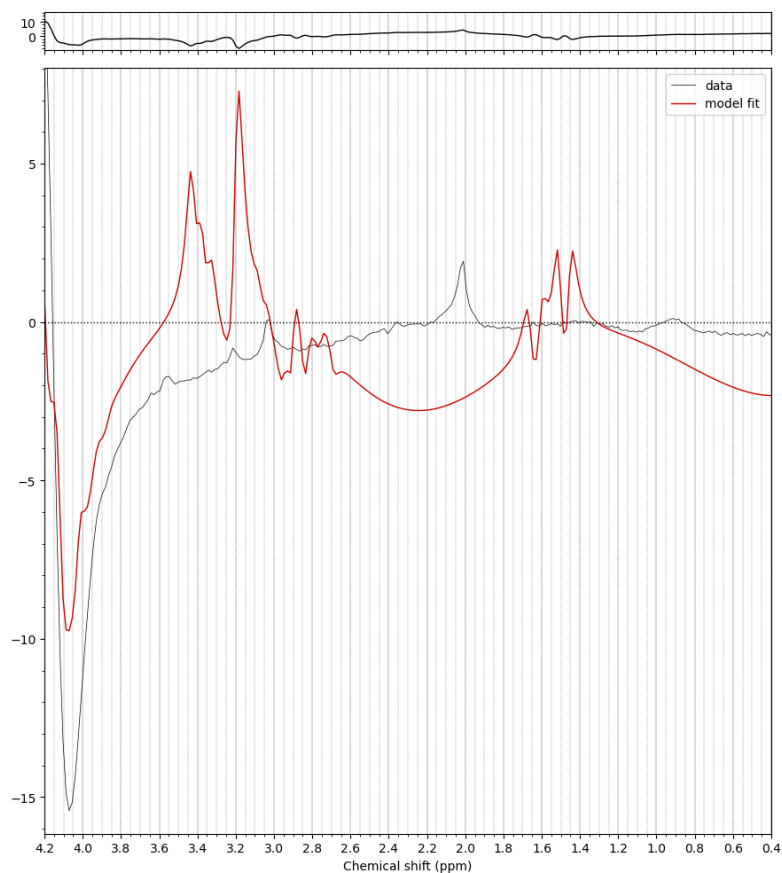
Residual water





Look at your data!

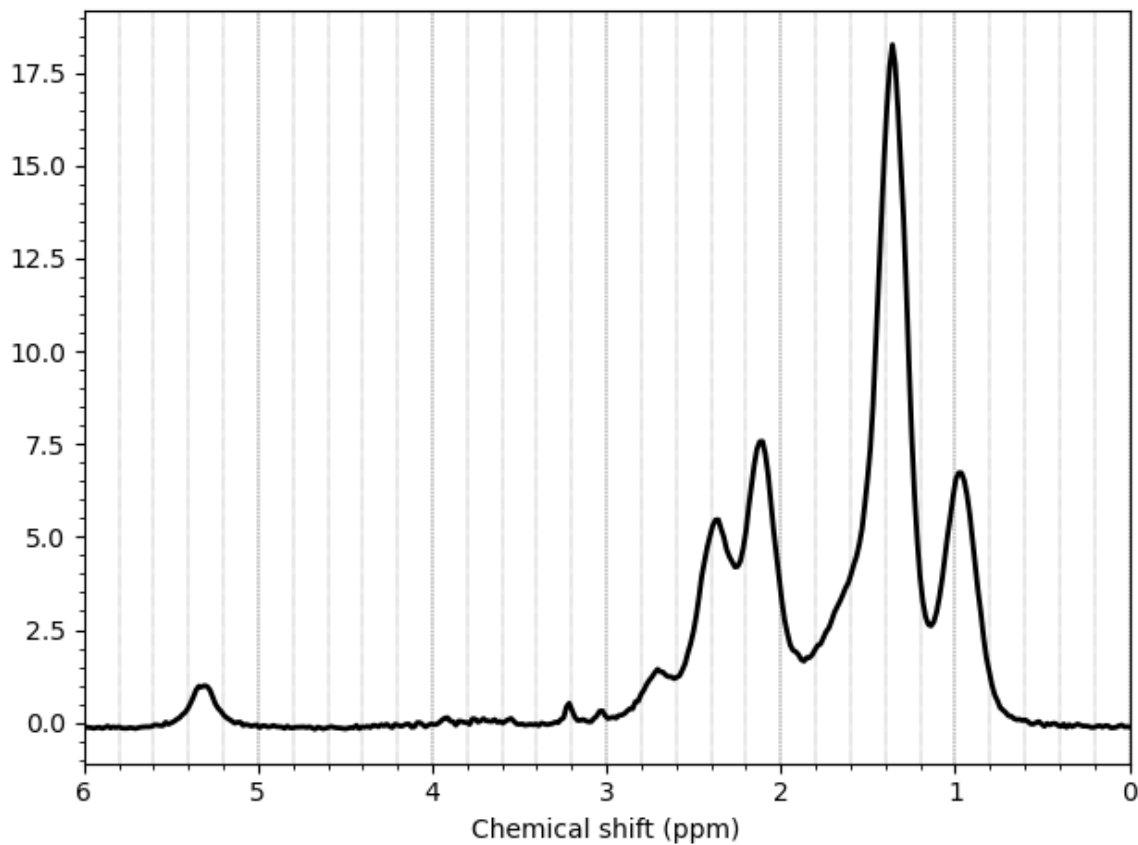
Residual water





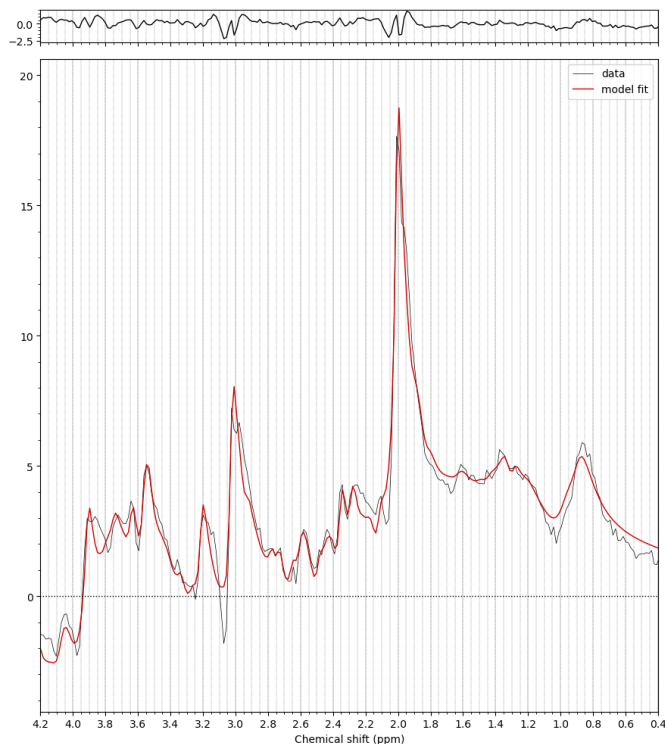
Look at your data!

Lipids





CRLB validity



CRLB not reliable
when model does
not represent data.

CRLB of metabolites still
“reasonable” in this example.



RESEARCH ARTICLE | [Full Access](#)

Are Cramér-Rao lower bounds an accurate estimate for standard deviations in in vivo magnetic resonance spectroscopy?

Karl Landheer, Christoph Juchem [✉](#)

First published: 19 April 2021 | <https://doi.org/10.1002/nbm.4521> | Citations: 6





Deciding cut-offs

Comparison with literature: linewidths, possibly SNR and CRLB

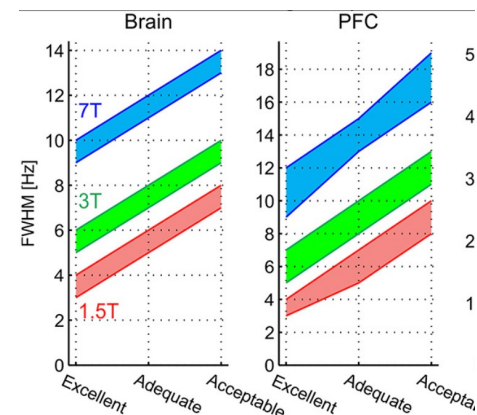


SPECIAL ISSUE REVIEW ARTICLE | [Full Access](#)

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

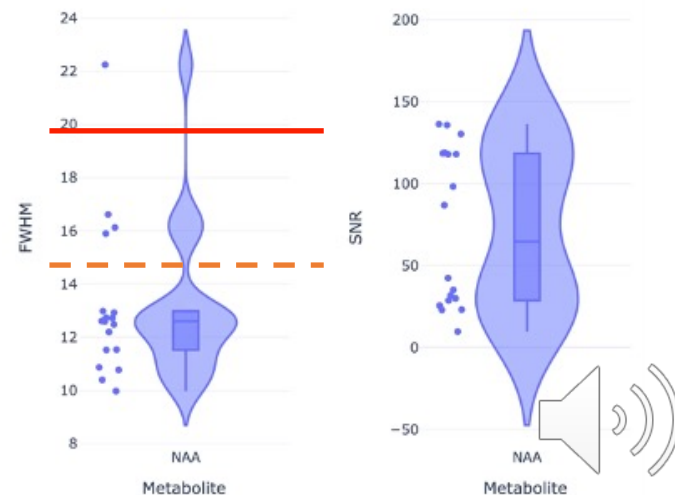
Christoph Juchem , Cristina Cudalbu, Robin A. de Graaf, Rolf Gruetter, Anke Henning,
Hoby P. Hetherington, Vincent O. Boer

First published: 28 June 2020 | <https://doi.org/10.1002/nbm.4350> | Citations: 30



Comparison with study population: linewidths, SNR and/or absolute CRLB

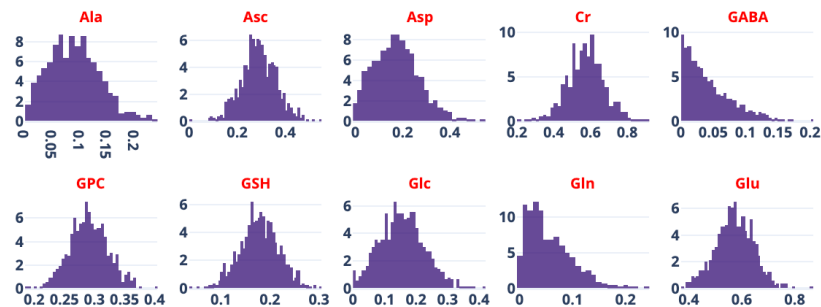
Exclude data based on comparing QC/fit metrics with study population or equivalent study population.



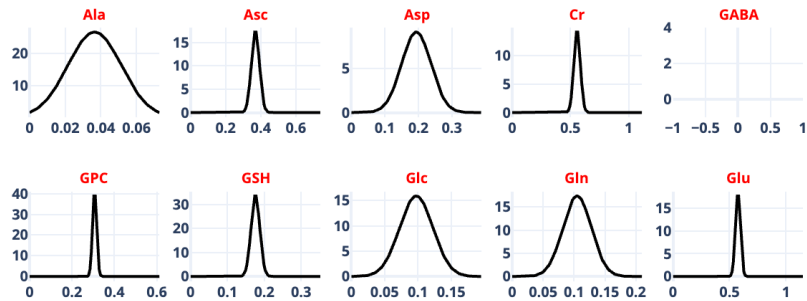


FSL-MRS outputs

MCMC marginal distributions (ref=Cr+PCr)



Approximate marginal distributions (ref=Cr+PCr)



Metab	mMol/kg	CRLB	%CRLB	/Cr+PCr
Ala	0.4	0.23	58.4	0.04
Asc	4.03	0.35	8.7	0.37
Asp	2.11	0.67	31.9	0.19
Cr	6.08	0.43	7	0.56
GABA	0	0.39	999	0
GPC	3.34	0.15	4.5	0.31
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Gln	1.14	0.35	31	0.11
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Cr+PCr	10.9	0.25	2.3	1
NAA+NAAG	15.04	0.28	1.9	1.38
GPC+PCho	4.21	0.11	2.6	0.39
Glc+Tau	3.26	0.3	9.2	0.3

QC parameters

Metab	SNR	FWHM (Hz)
Ala	0.6	24.8
Asc	5.3	19.7
Asp	0.9	70.0
Cr	17.7	14.2
GABA	0.0	0.0
GPC	29.0	14.2
GSH	4.2	17.3
Glc	1.0	40.4
Gln	1.1	27.9
Glu	7.0	24.3
Ins	20.2	46.7

QC and fit quality (CRLB) metrics are given in the summary.csv, qc.csv and concentrations.csv outputs as well.

