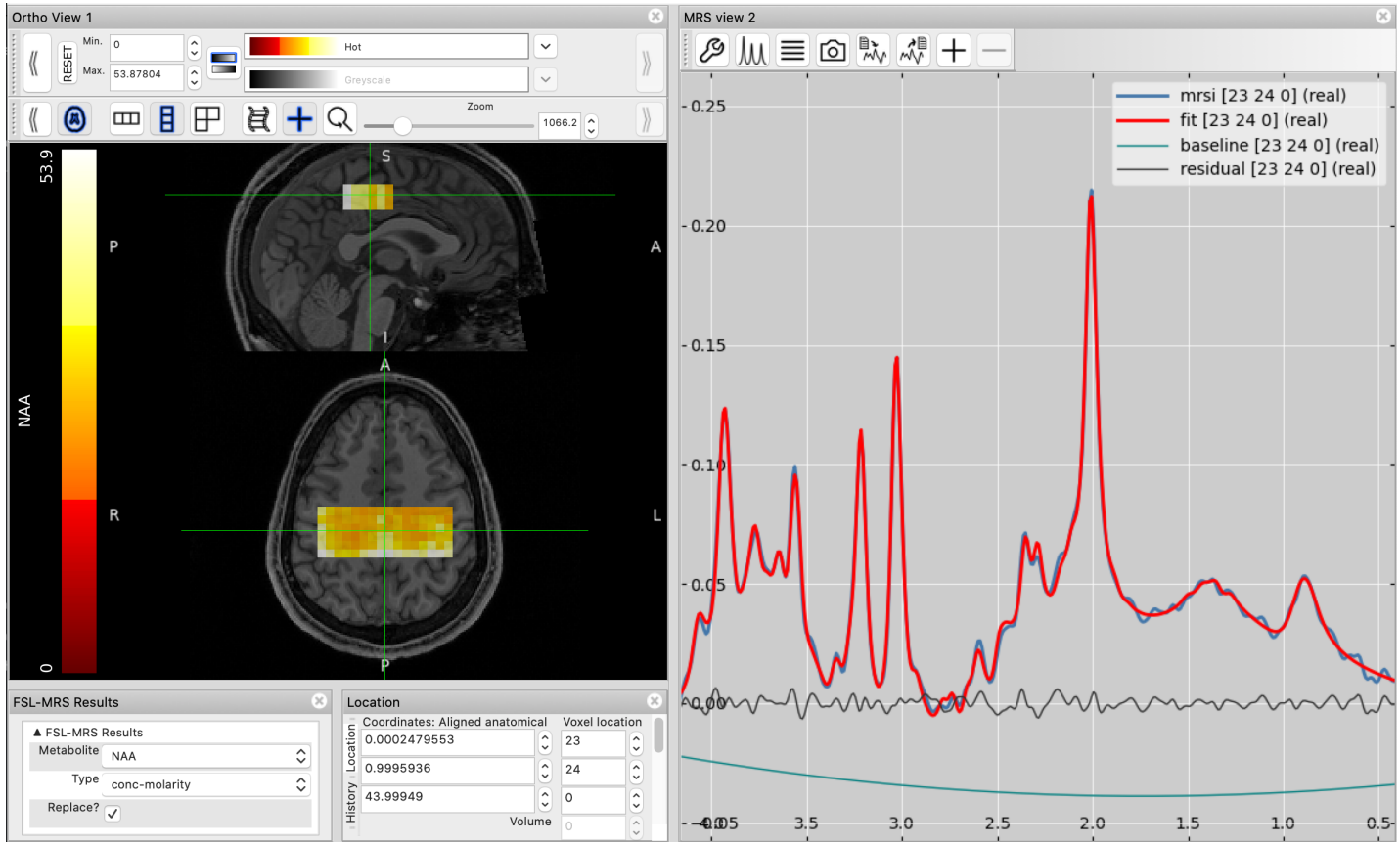
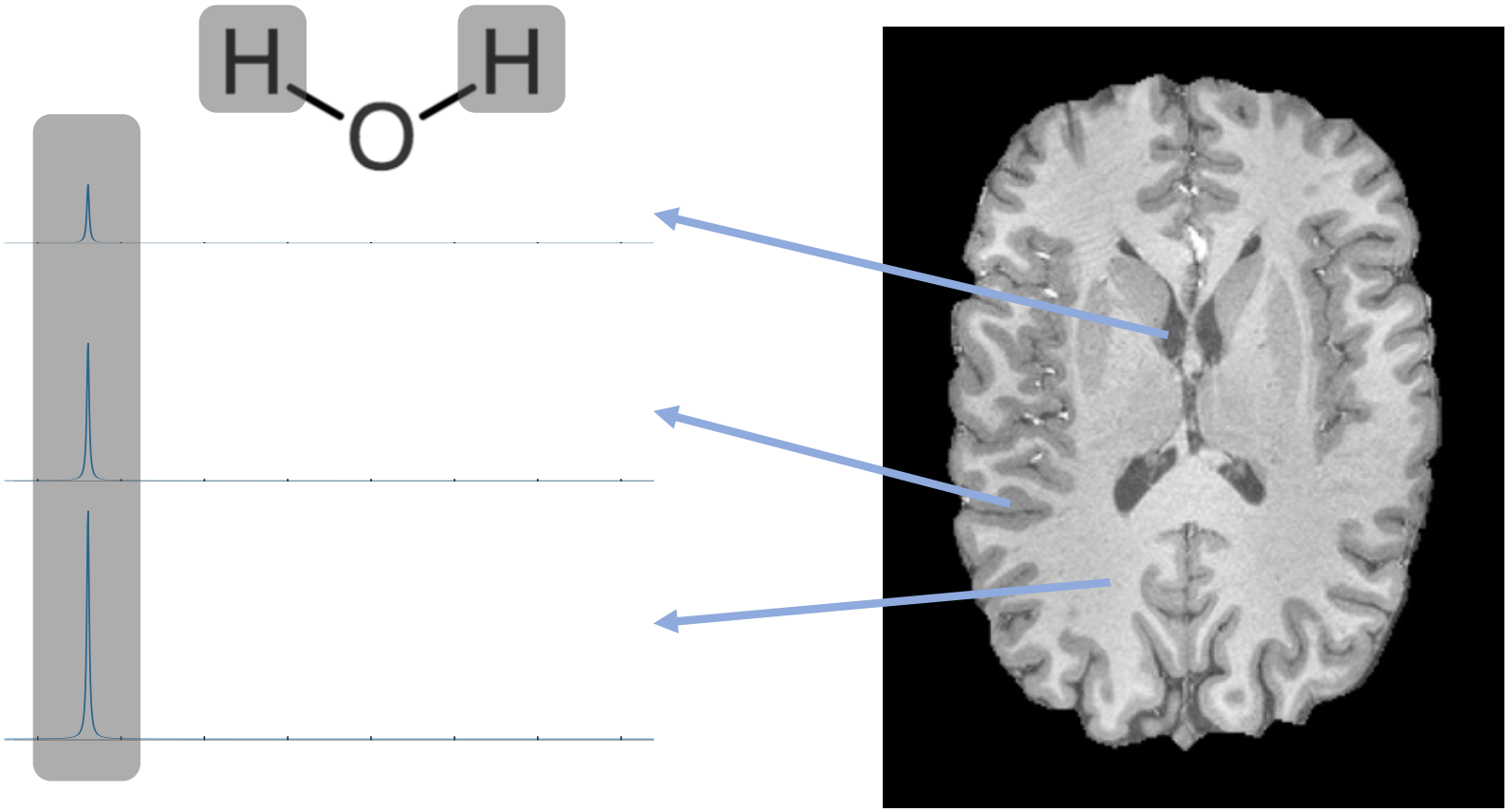
FSL-MRS – Tools for Magnetic Resonance Spectroscopy



Introduction to MRS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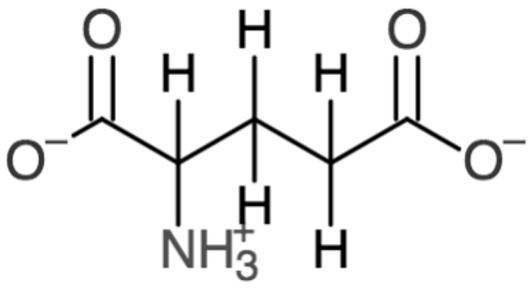
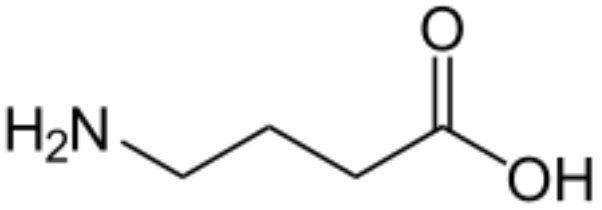
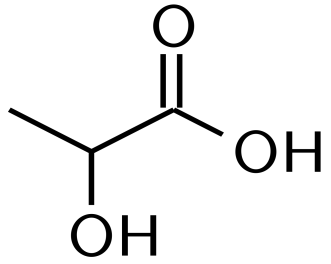


Glutamate

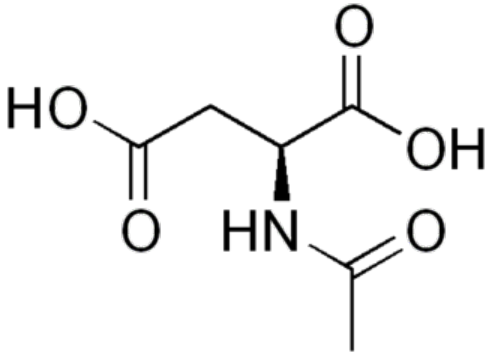
GABA

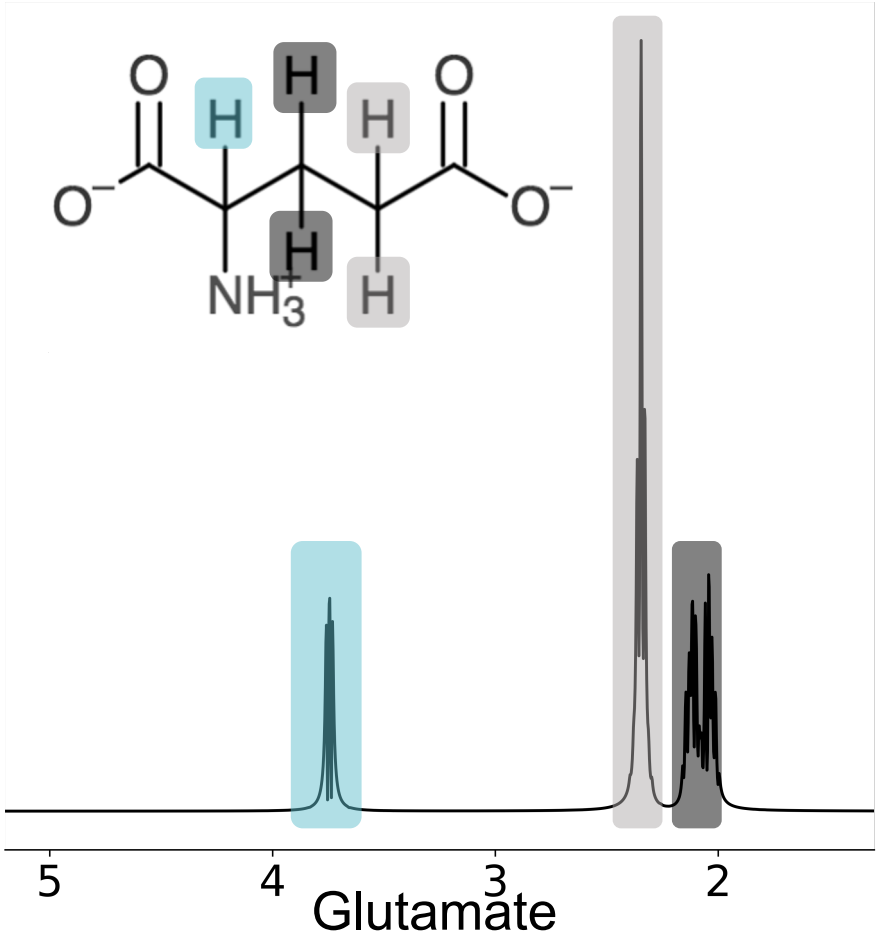


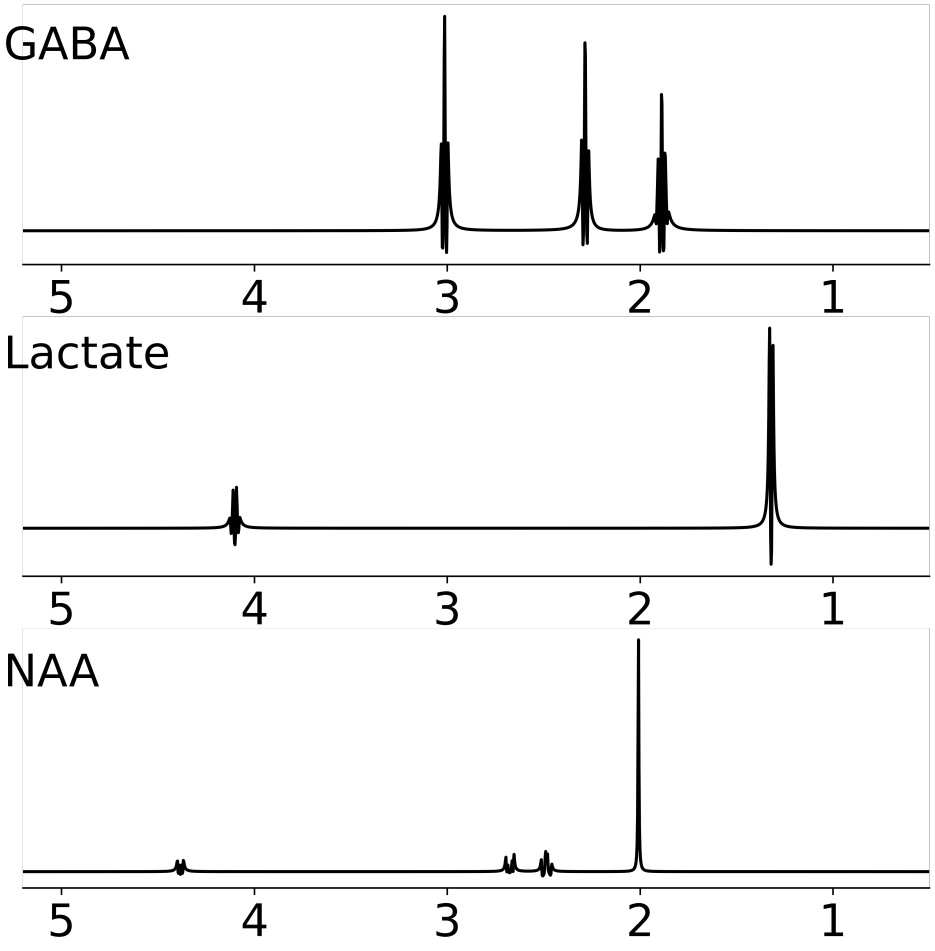
Lactate



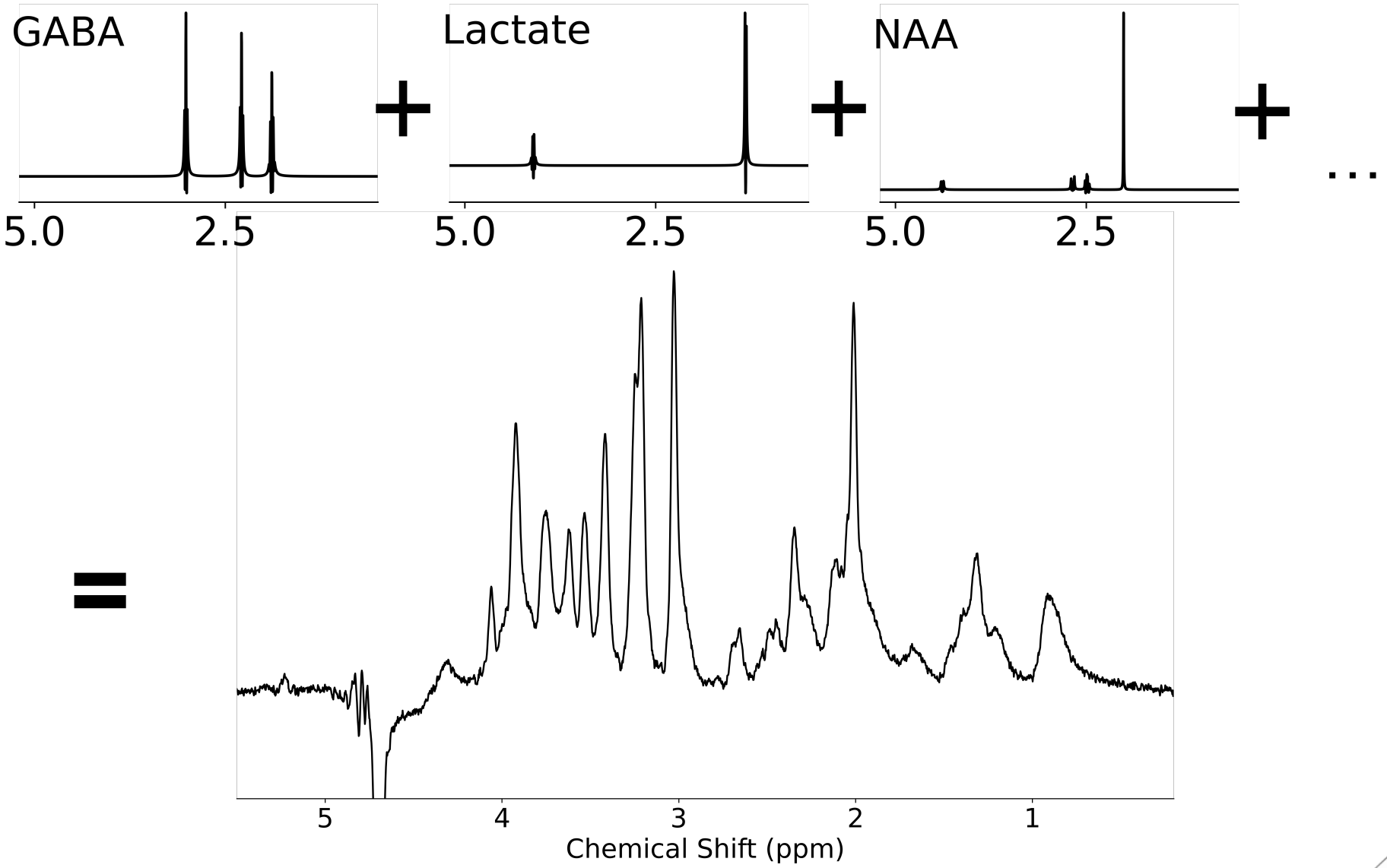
NAA

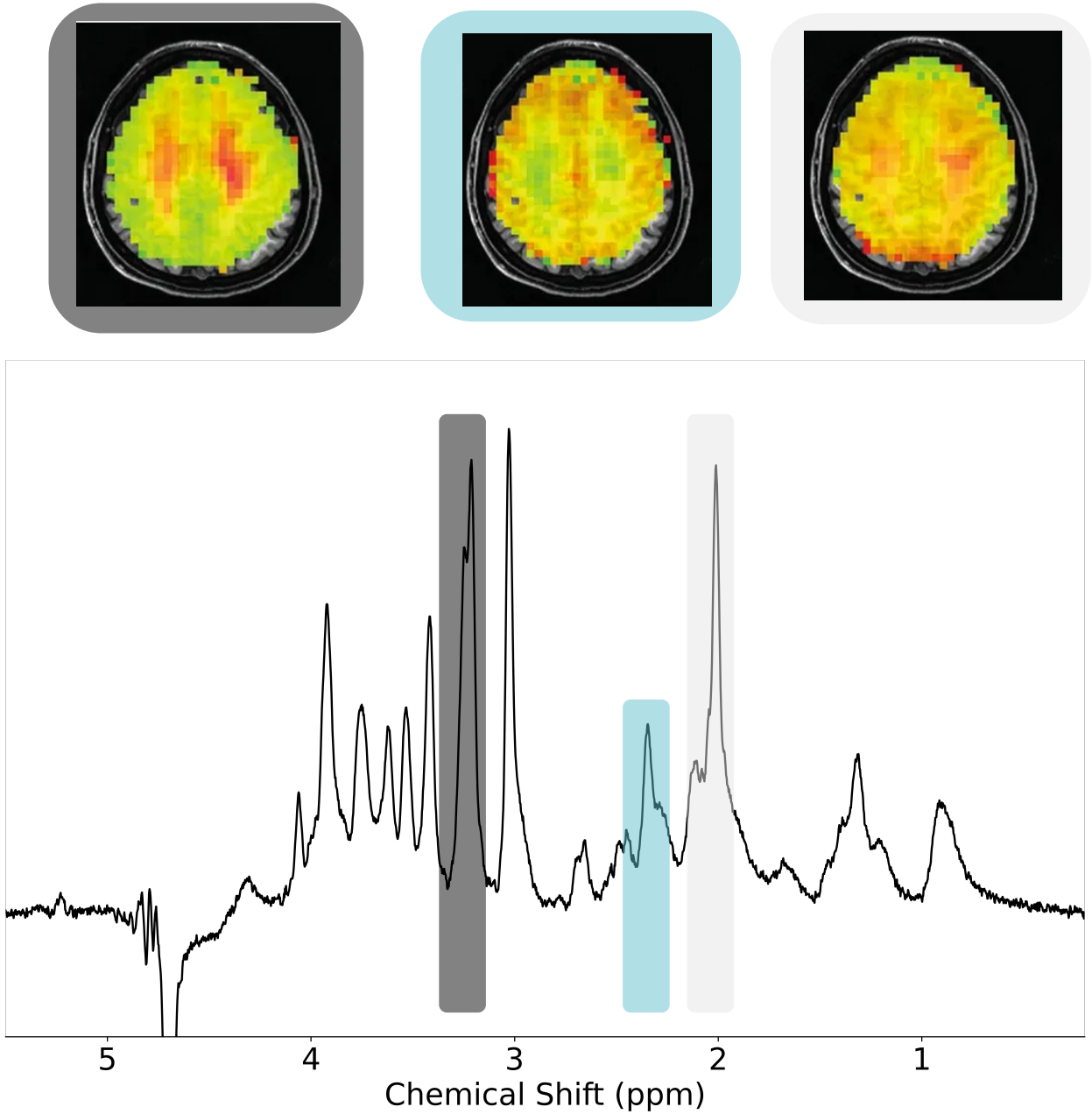






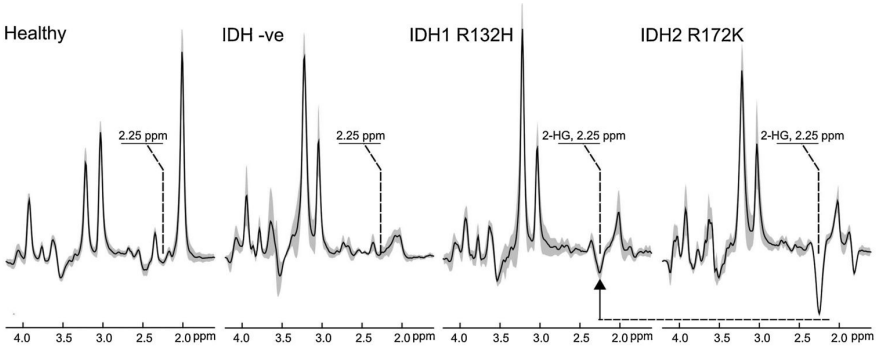
+ 15 other metabolite “fingerprints”


GABA
Lactate
NAA
5.0
2.5
5.0
2.5
5.0
2.5
5
4
3
2
1
Chemical Shift (ppm)


5
4
3
2
1
Chemical Shift (ppm)

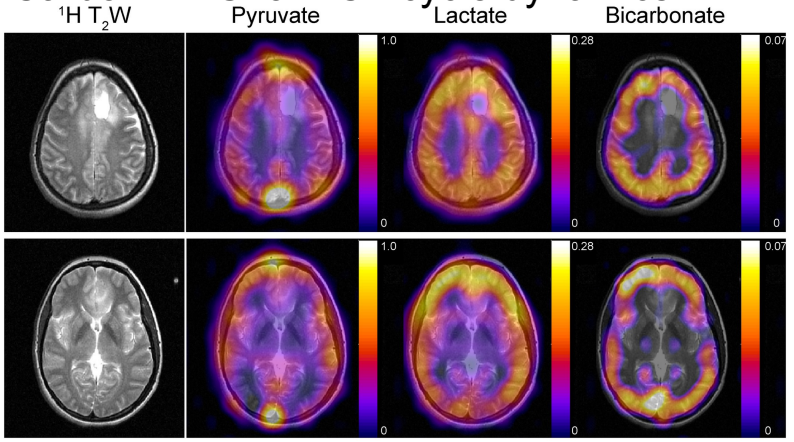
Many uses of MRS

Proton MRS for metabolic profile



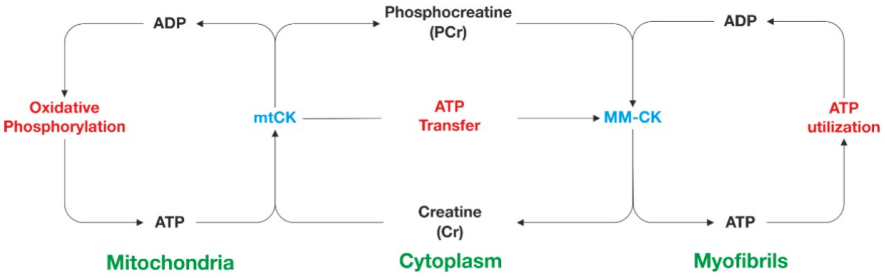
Emir et al. Cancer Res. 2016 Jan 1;76(1):43-9.

Carbon MRS for TCA cycle dynamics

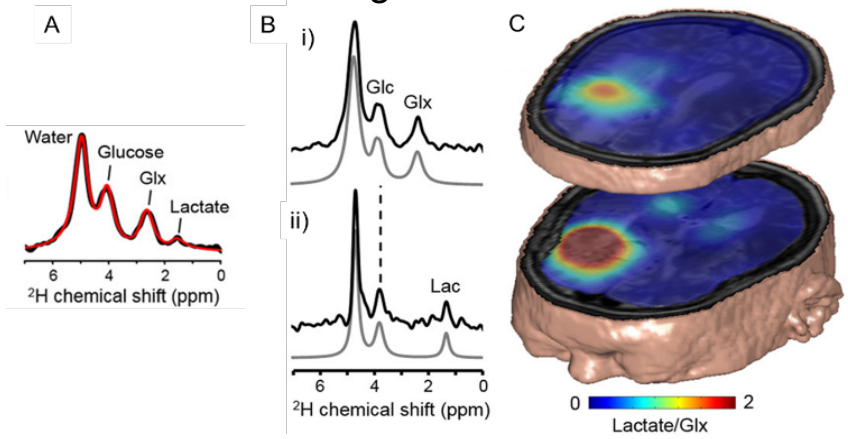


Gordon et al MRM 81(4) 2702-2709

Phosphorus MRS for oxidative phosphorylation



Deuterium MRS for glucose metabolism



Henk M. De Feyter et al. Sci Adv 2018;4:eaat7314

Visible Neurochemicals

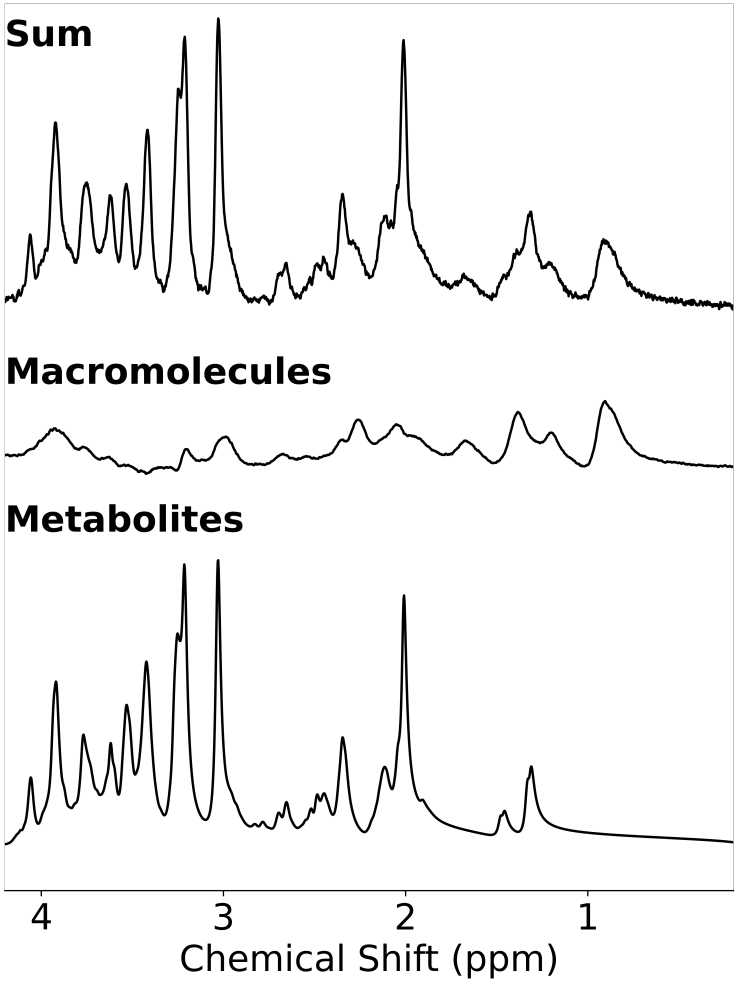
- Water ~10000 times larger
- Lipids – artefactual or pathological

✓ Metabolites with >1 mM concentration

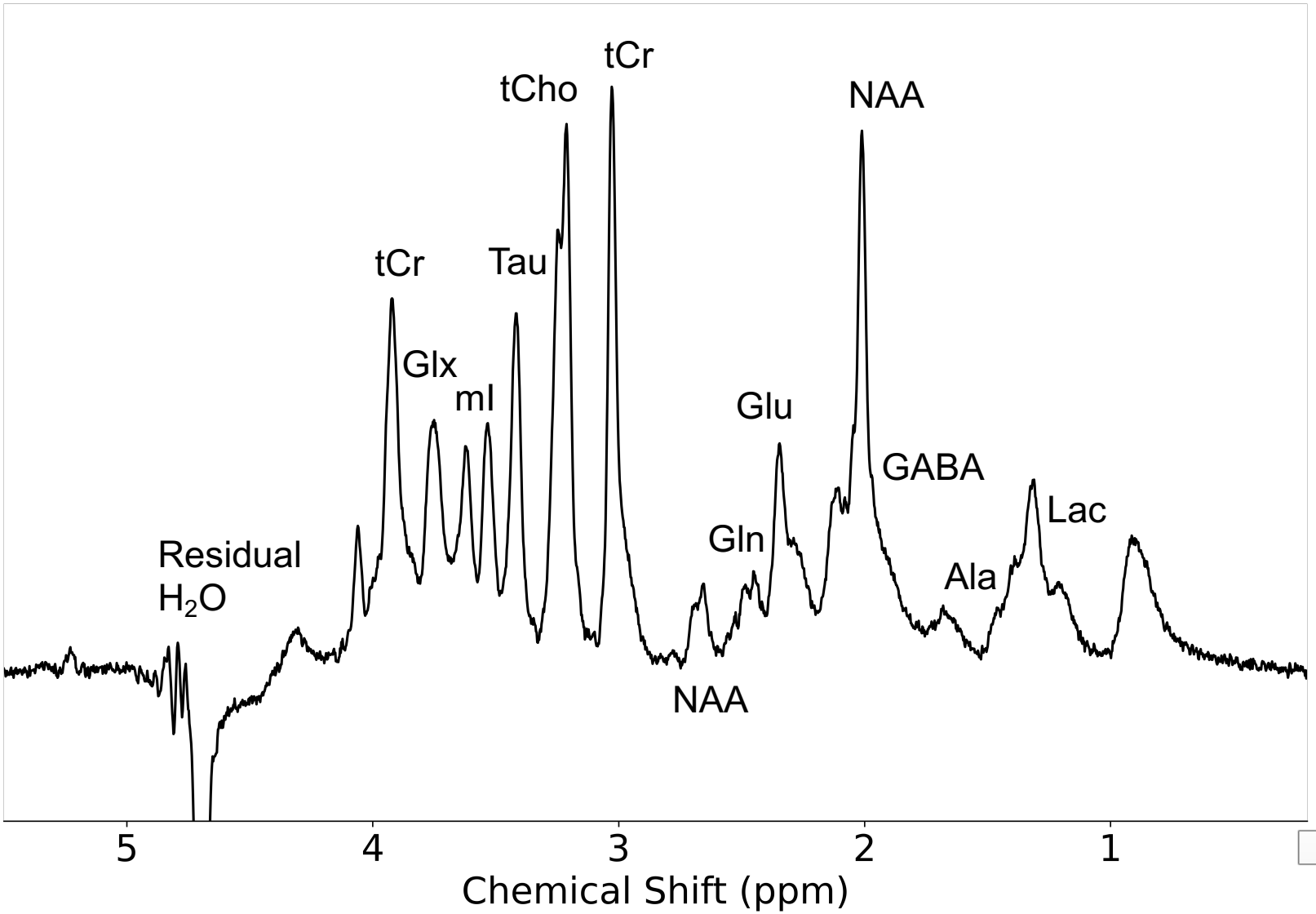
✓ “Macromolecules”: amino acid residues & peptides

x Solids, proteins, bound substrates.

x Low concentration (<1 mM)



The in vivo spectrum



Metabolites

***N*-acetylaspartate (NAA)**
- **Present only in neurons (not glia)**
- **Biomarker for neuronal integrity**

Lactate (Lac)
- **Indicates anaerobic glycolysis**
- **Complex, dynamic metabolism.**
- **Tricky to monitor by MRS**

Total creatine (tCr: Cr + PCr)
- **Energy buffering**
- **Often a static reference, except in metabolic disorders**

Myo-inositol (mIns)
- **(Disputed) marker for gliosis**
- **Varied physiological uses and variations in pathology.**

Total Choline (tCho: PCho + GPC)
- **Marker of cellular proliferation, membrane turnover, inflammation.**

Glutamate (Glu) + GABA
- **Primary neurotransmitters**

Glutathione (GSH)
- **Oxidative stress in astrocytes**

See

1) Rae CD. A Guide to the Metabolic Pathways and Function of Metabolites Observed in Human Brain 1H Magnetic Resonance Spectra. Neurochem Res 2014;39:1–36

2) De Graaf RA. In Vivo NMR Spectroscopy: Principles and Techniques. Chapter 2

Equipment

GRE
FLAIR
DWI
SWI
T1w

PRESS
STEAM
sLASER
CSI

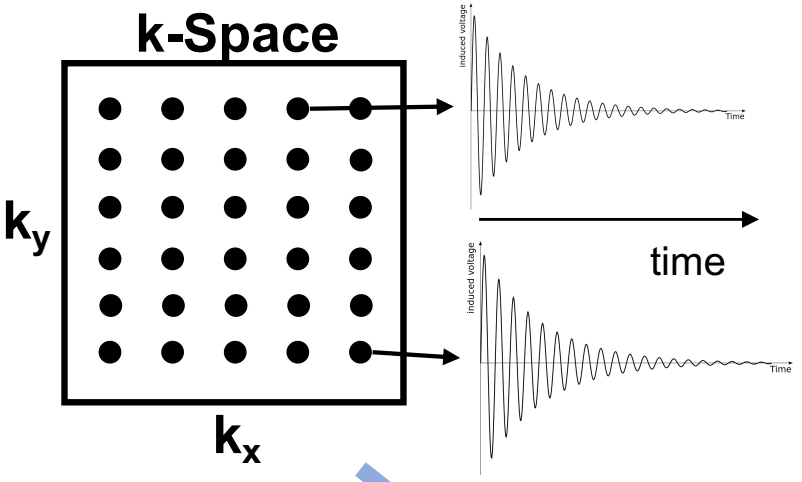
✓ **Same scanner**

✓ **Same coil hardware**

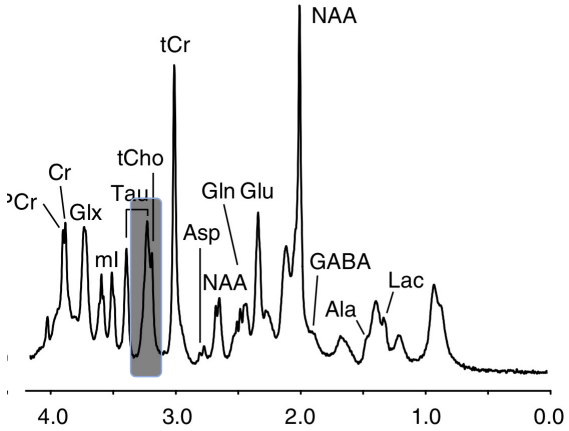
✗ **Different sequences**

✗ **Additional training**

Spectroscopy pulse sequences

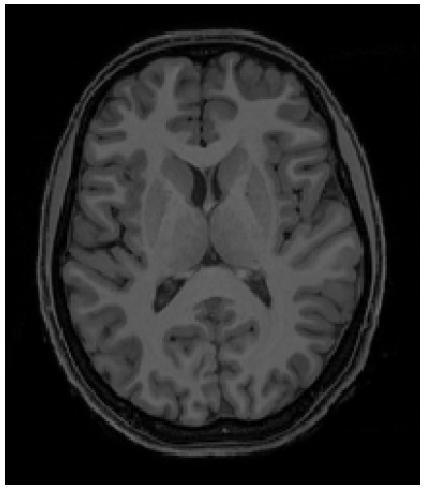


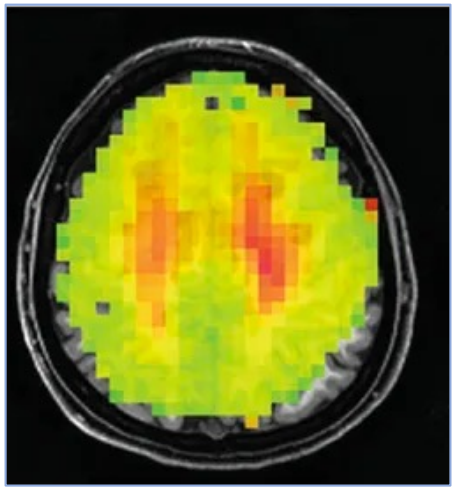
Fourier Transform



+

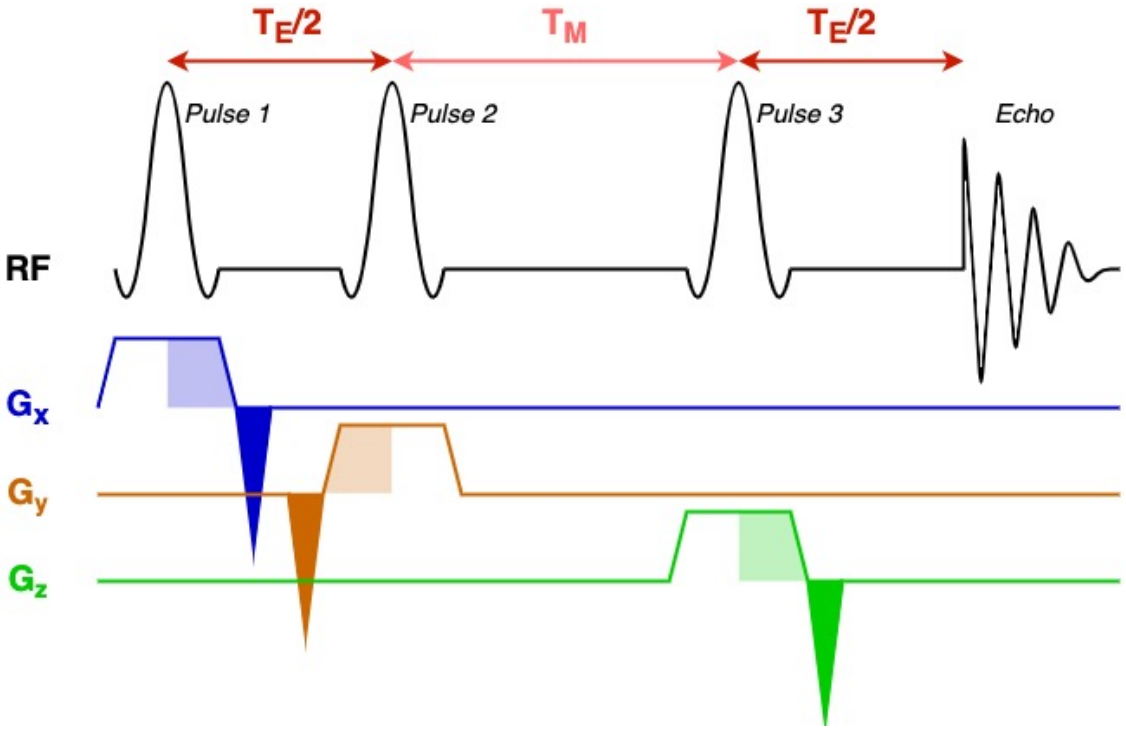
Fourier Transform

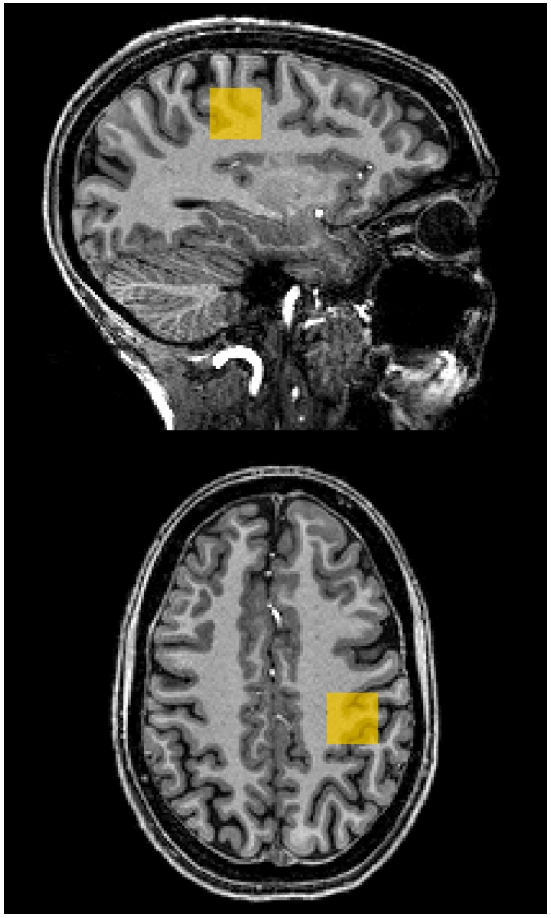




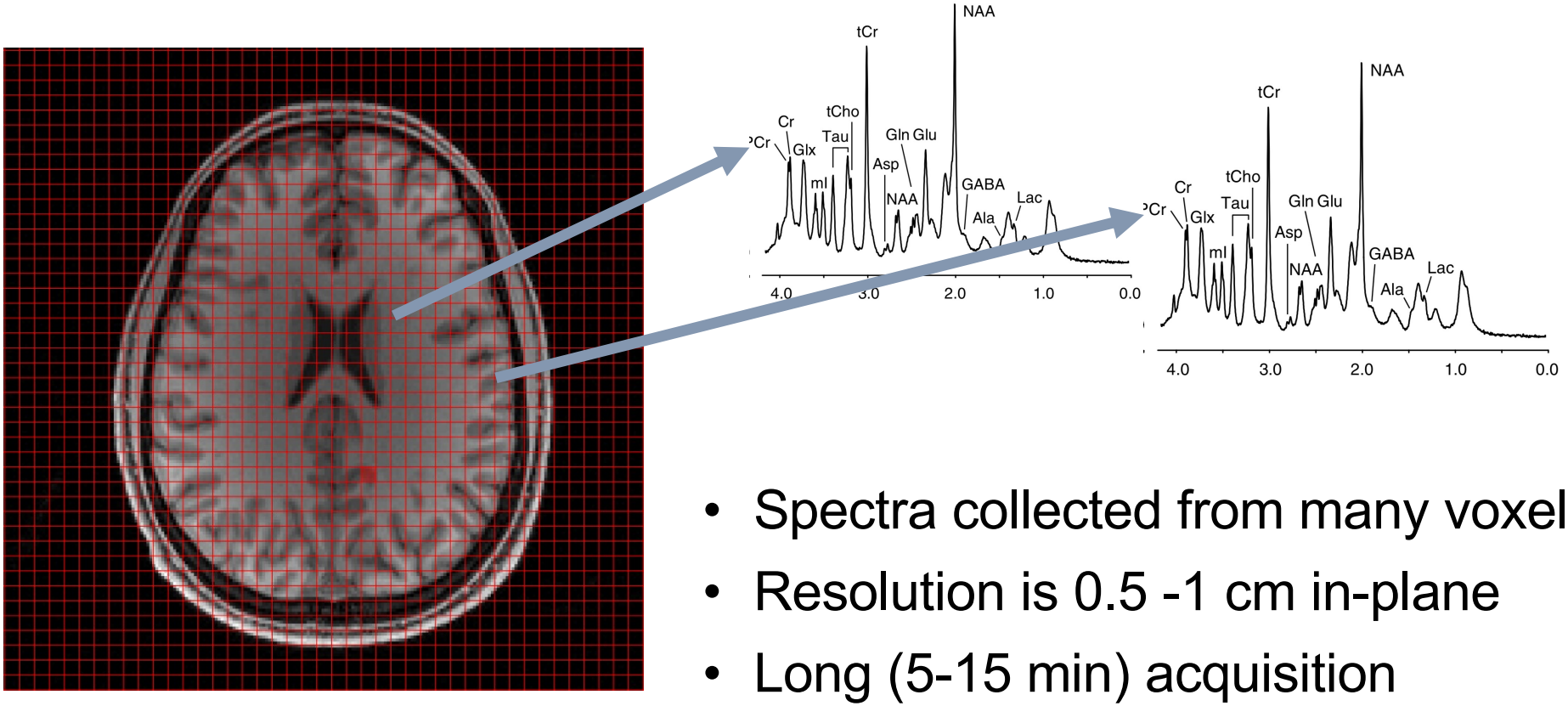
Single Voxel Spectroscopy (SVS)

- Single spectrum acquired from one volume
- 2-3 cm isotropic size, ~5 min acquisition
- Examples: PRESS, **STEAM**, Semi-LASER
- Three intersecting slice selective pulses.





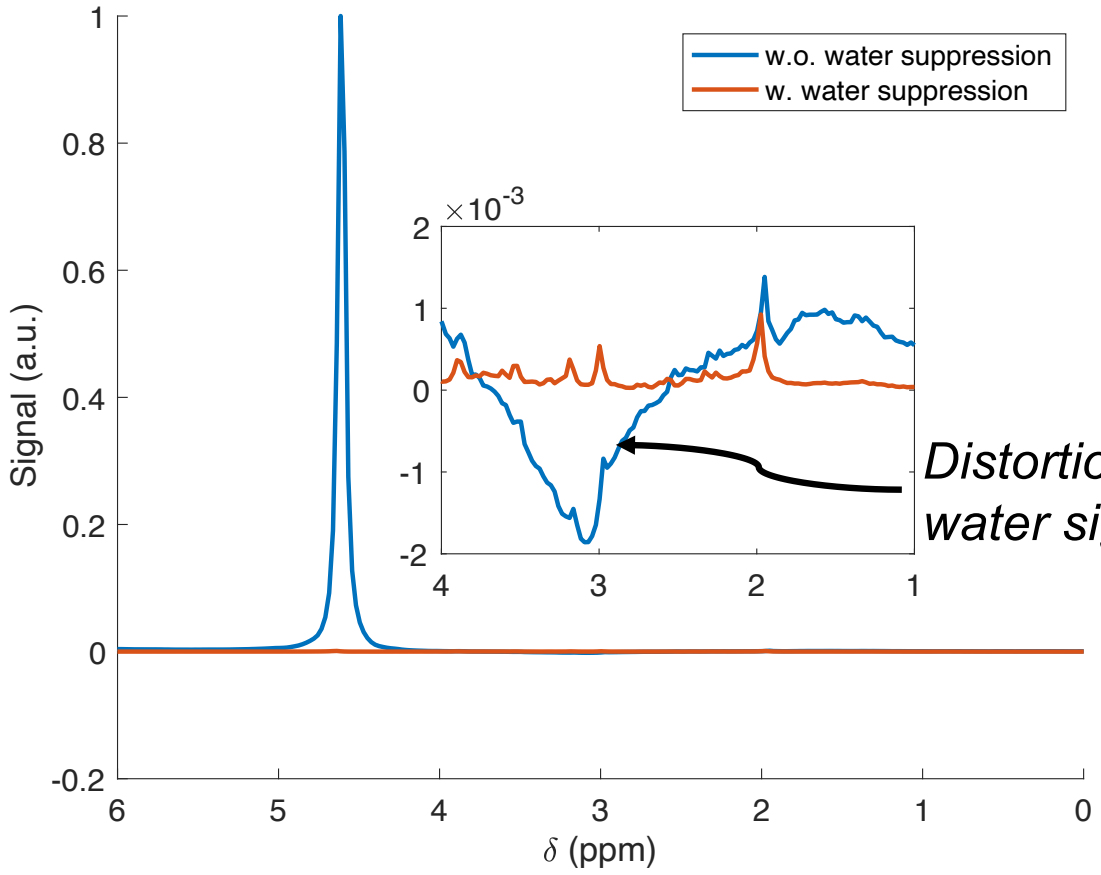
MR Spectroscopic Imaging (MRSI)



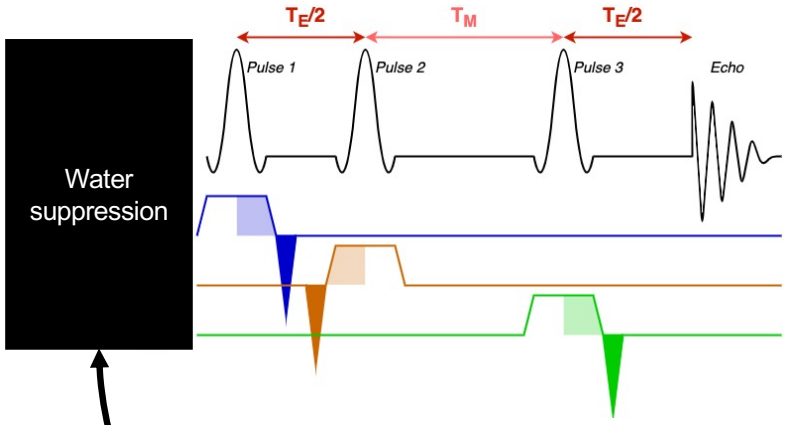
- Spectra collected from many voxels
- Resolution is 0.5 -1 cm in-plane
- Long (5-15 min) acquisition
- Examples: CSI, EPSI, CRT

Water suppression

- Water signal >> metabolite signal
- Selective suppression used to remove water
- Reduces baseline distortion

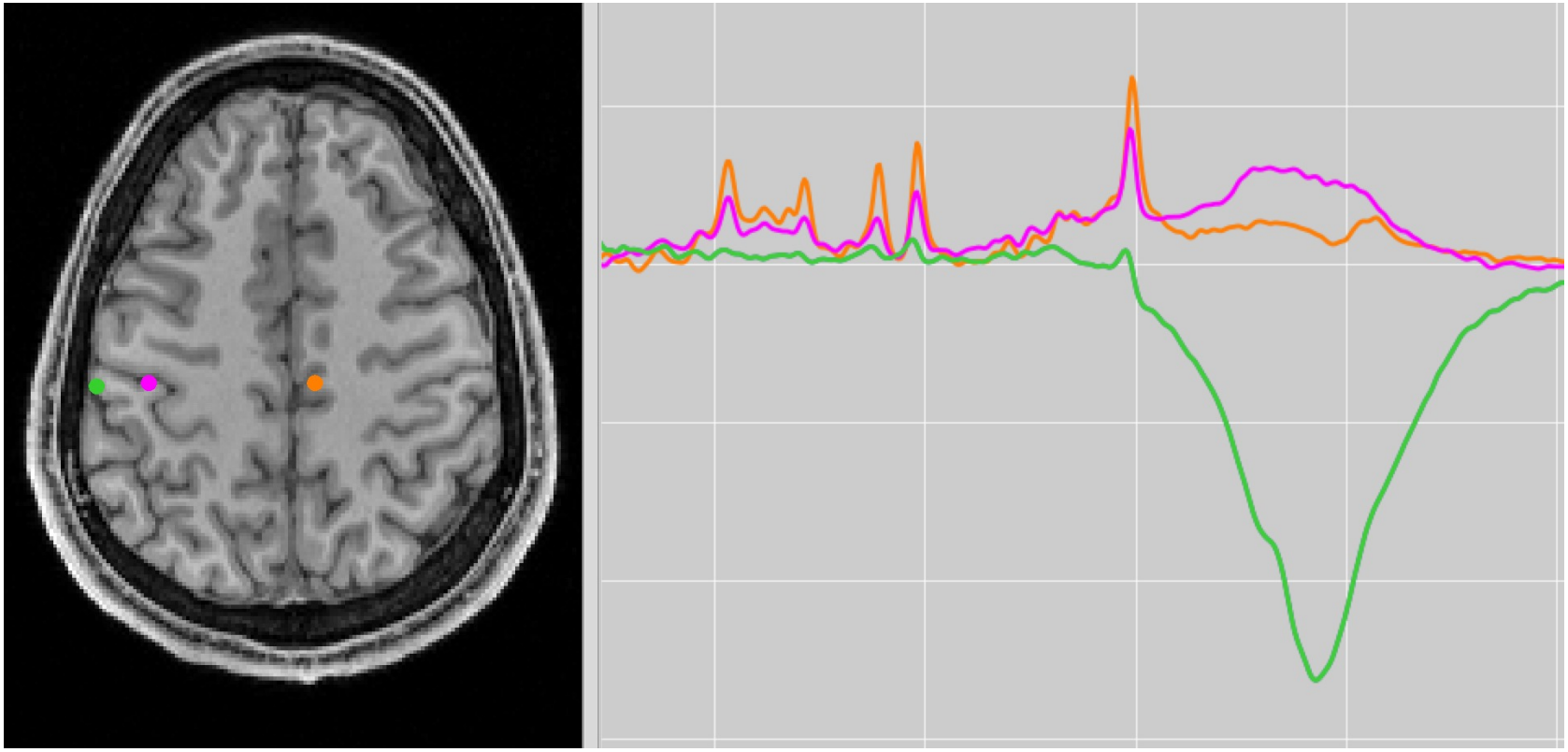


Distortion from water signal



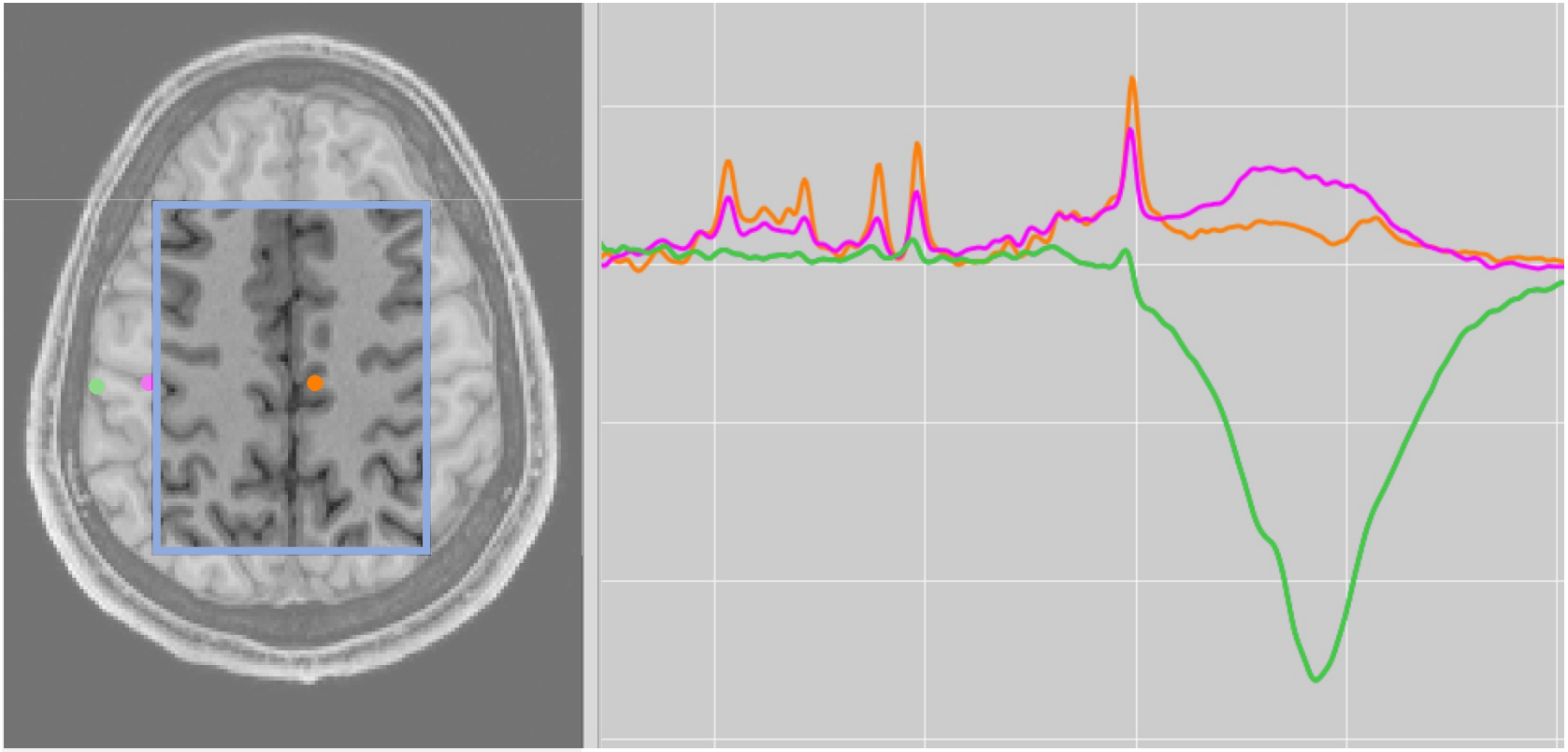
Water suppression module placed before SVS sequence

Outer volume suppression



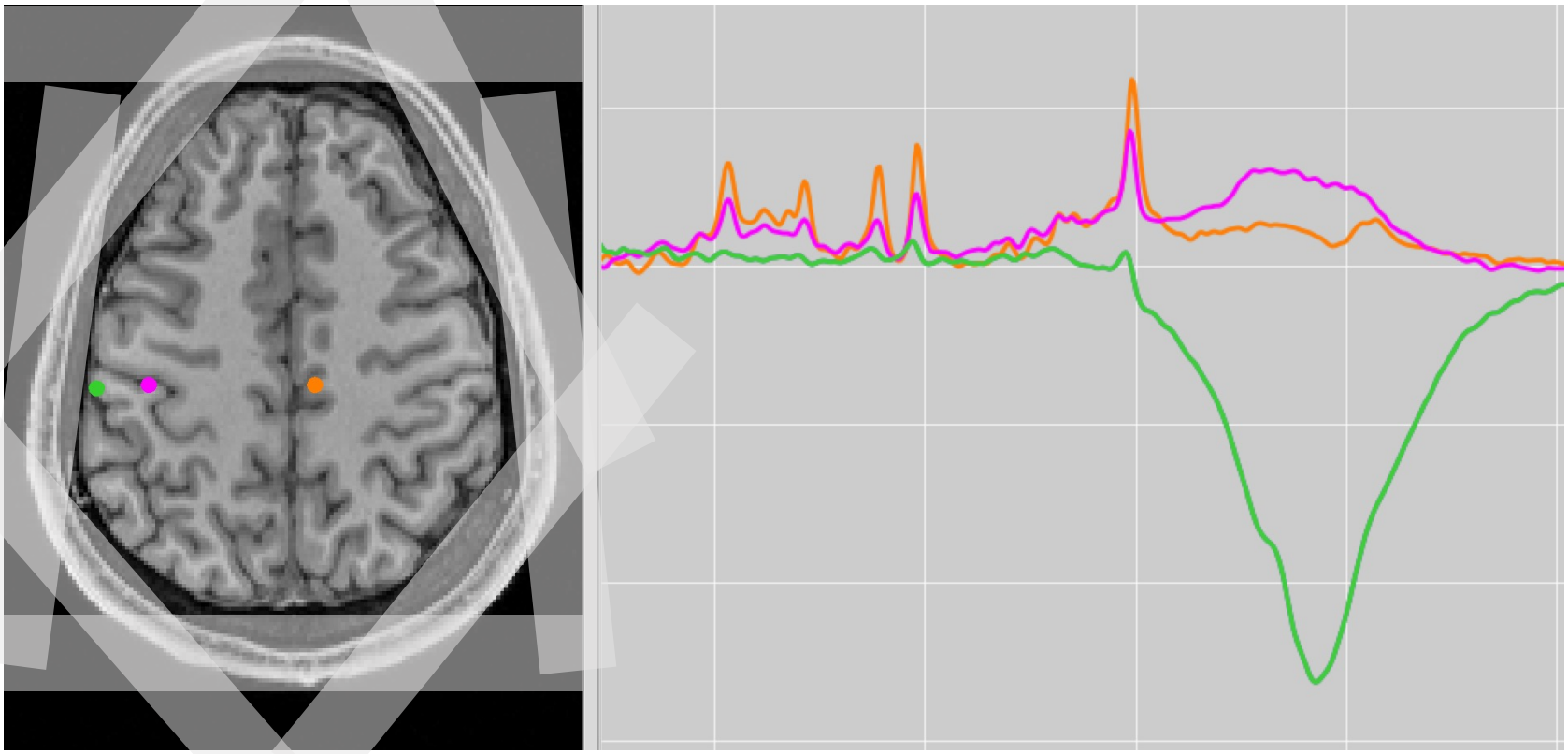
High concentration lipids present in dura and skull can distort spectra near the edge of measured volume.

Outer volume suppression



First approach – Use SVS localisation to only excite signal from brain tissue.

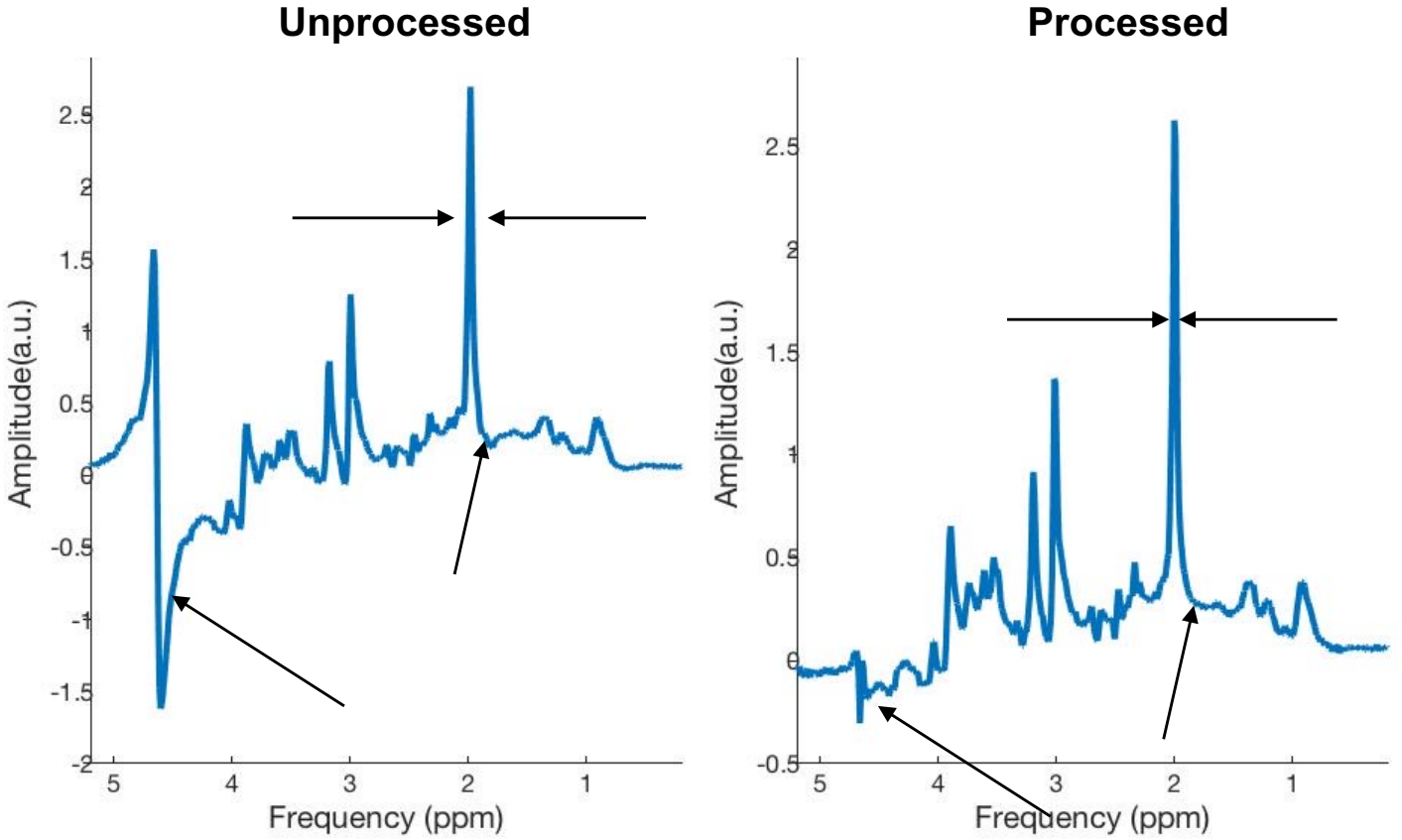
Outer volume suppression



Second approach – Use saturation bands to suppress signal from outside brain.

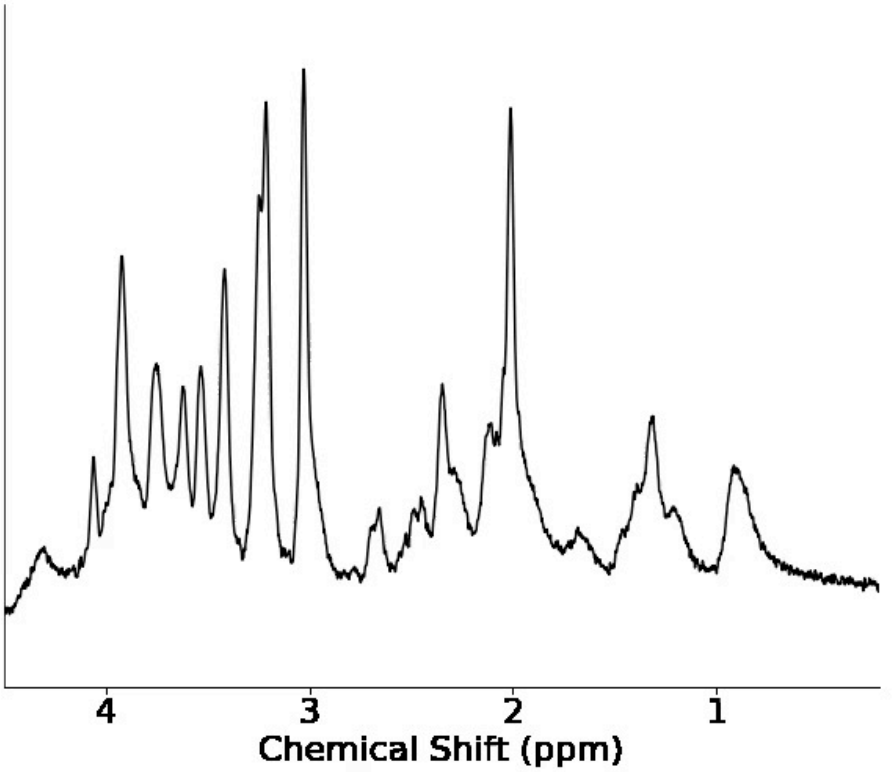
Analysis: Preprocessing

1. Coil combination
2. Frequency & phase correction
3. Eddy current correction
4. Residual water removal

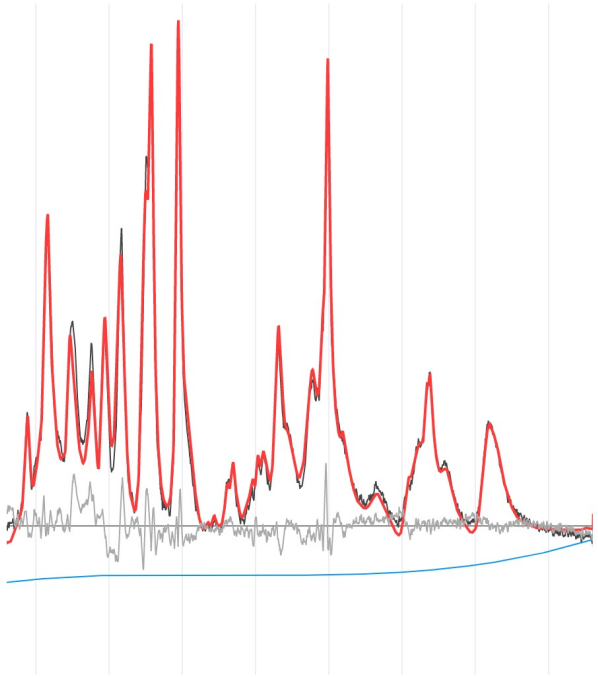


More on pre-processing in the second lecture.

Analysis: Fitting

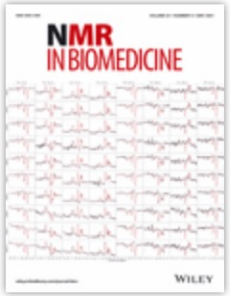


Metab	unscale	CRLB	%CRLB	/Cr+PC
Ace	0.04	0.007	20.1	0.14
Ala	0.04	0.004	8.1	0.17
Asp	0.09	0.008	8.2	0.36
Cho	0	0.001	999	0
Cr	0.13	0.006	4.1	0.52
GABA	0.03	0.006	21.4	0.11
GPC	0.04	0.004	8.5	0.17
GSH	0.07	0.003	3.7	0.27
Glc	0.14	0.004	3.1	0.55
Gln	0.11	0.005	4.6	0.41
Glu	0.25	0.005	1.9	0.96
Gly	0.11	0.008	6.9	0.43
Ins	0.21	0.004	1.8	0.8
Lac	0.12	0.003	2.8	0.48
MM_WT	0.39	0.011	2.9	1.52
NAA	0.18	0.003	1.5	0.7
NAAG	0.03	0.002	7.1	0.1
PCho	0.02	0.004	20.6	0.07
PCr	0.12	0.006	4.6	0.48
PE	0.07	0.007	9.6	0.27
Tau	0.28	0.004	1.3	1.11
sIns	0.02	0.007	37.5	0.07
Cr+PCr	0.26	0.003	1.1	1



More on fitting in the third lecture.

MRS Resources



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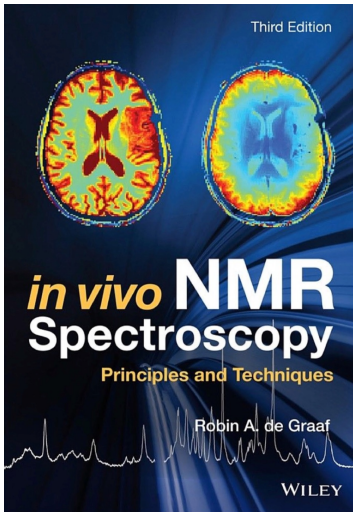
Special Issue: Advanced methodology for in vivo magnetic resonance spectroscopy

May 2021

Issue Edited by: **In-Young Choi, Roland Kreis**

NMR in Biomedicine special issue on MRS methods

Robin de Graaf
YouTube channel & book
https://www.youtube.com/c/BasicsOfInVivoNMR



MRSHub

Online community dedicated to MRS. Ask a question in the friendly forums!