MRS data acquisition and Raw Data Handling Instructions

M A Oghabian

Isotopes in *in-vivo MRS*

Resonance Condition

Larmor equation

$$\omega_0 = |\gamma| * B_0 \quad \text{or} \quad \nu_0 = \frac{|\gamma|}{2\pi} * B_0$$

	γ $[*10^7 \text{ rad s}^{-1}\text{T}^{-1}]$	1T [MHz]	1.5T [MHz]	3T [MHz]	7T [MHz]
^{1}H	26.75	42.6	63.9	127.7	298.0
^{31}P	10.84	17.3	25.9	51.8	120.8
^{13}C	6.73	10.7	16.1	32.1	75.0

Frequency / Chemical shift

absolute - in Hz (field dependent)

relative - in ppm or [δ]

$$\delta = 10^6 * \frac{\nu_{signal} - \nu_{standard}}{\nu_{standard}}$$

[δ] scale   or   [ppm] scale

In vitro: tetramethylsilane (CH3) ……... 0 ppm
In vivo: N-acetylaspartate (CH3)……... 2.01

Lactic acid
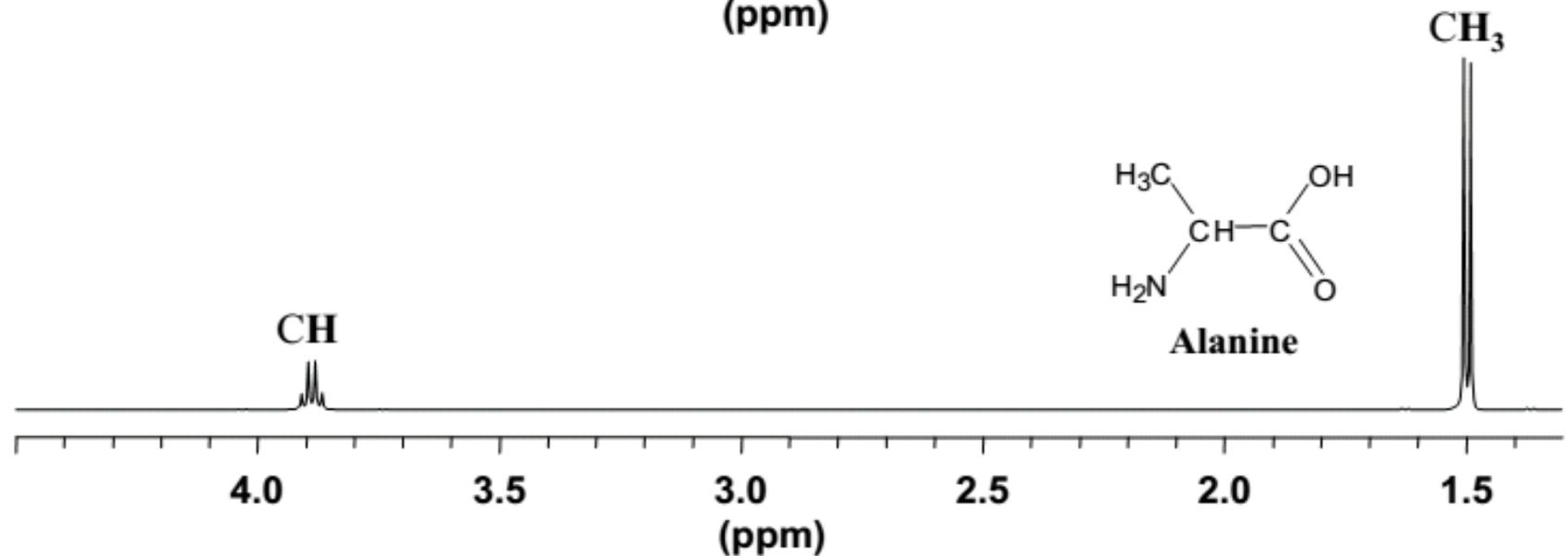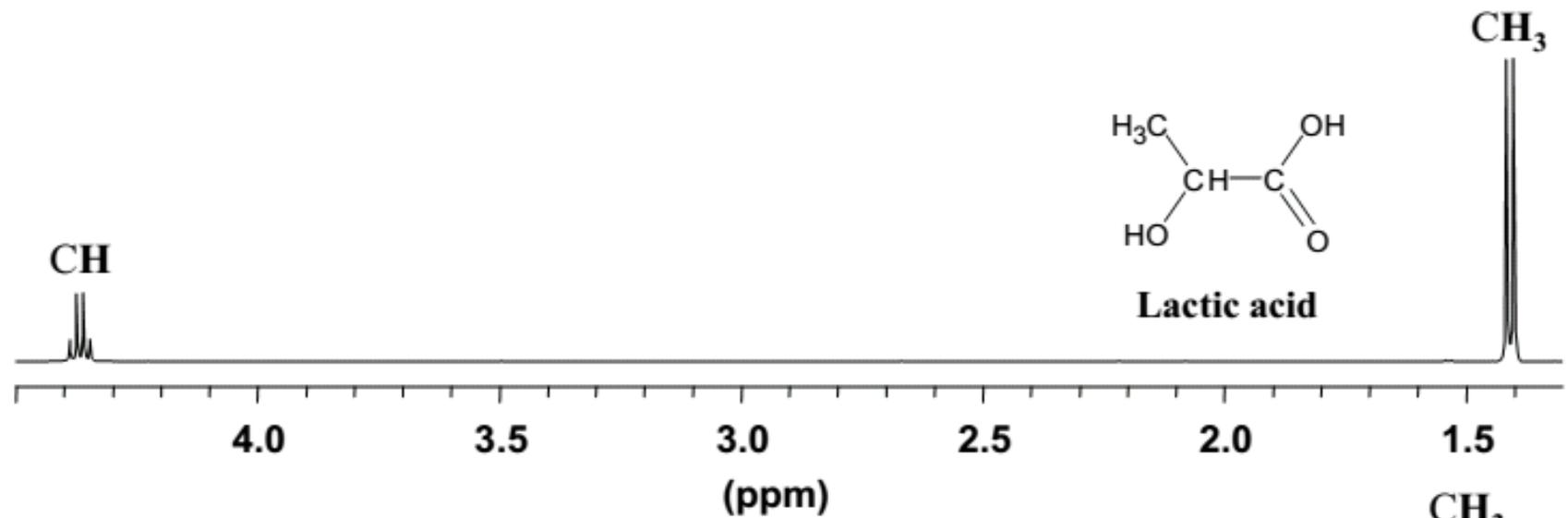
Alanine

two molecules that have a quite similar chemical structure are lactic acid and alanine. The only difference is that lactic acid has a hydroxyl group whereas alanine has an amino group

Spin-spin coupling

- In $_1$H-NMR, signals arising from one or more equivalent protons are often split into two or more components due to interaction between neighbouring protons (which may have equal probability of being in a parallel or an antiparallel spin state Some rules:
  1. No splitting is caused between equivalent protons, e.g. the CH_3-group protons of lactic acid.
  2. A proton that is coupled to n equivalent protons gives rise to (n + 1) lines.

- For example CH_3-group protons coupled to the CH-group proton give rise to two lines (a doublet) with relative intensities of 1:1.

- The CH proton coupled to the equivalent CH_3 protons gives rise to four lines with relative intensities of 1:3:3:1.

- Since the hydroxyl proton in lactic acid exchanges rapidly with water protons, it does not couple to any of the protons.

MR Spectrum

Signal intensity
- number of nuclei in resonance

Chemical shift
- type of chemical structure

Half-width (~ $1/T_2^*$)

N-Acetylaspartate: $HO_2C-CH_2-CH-[(NH)-COCH_3]-CO_2H$
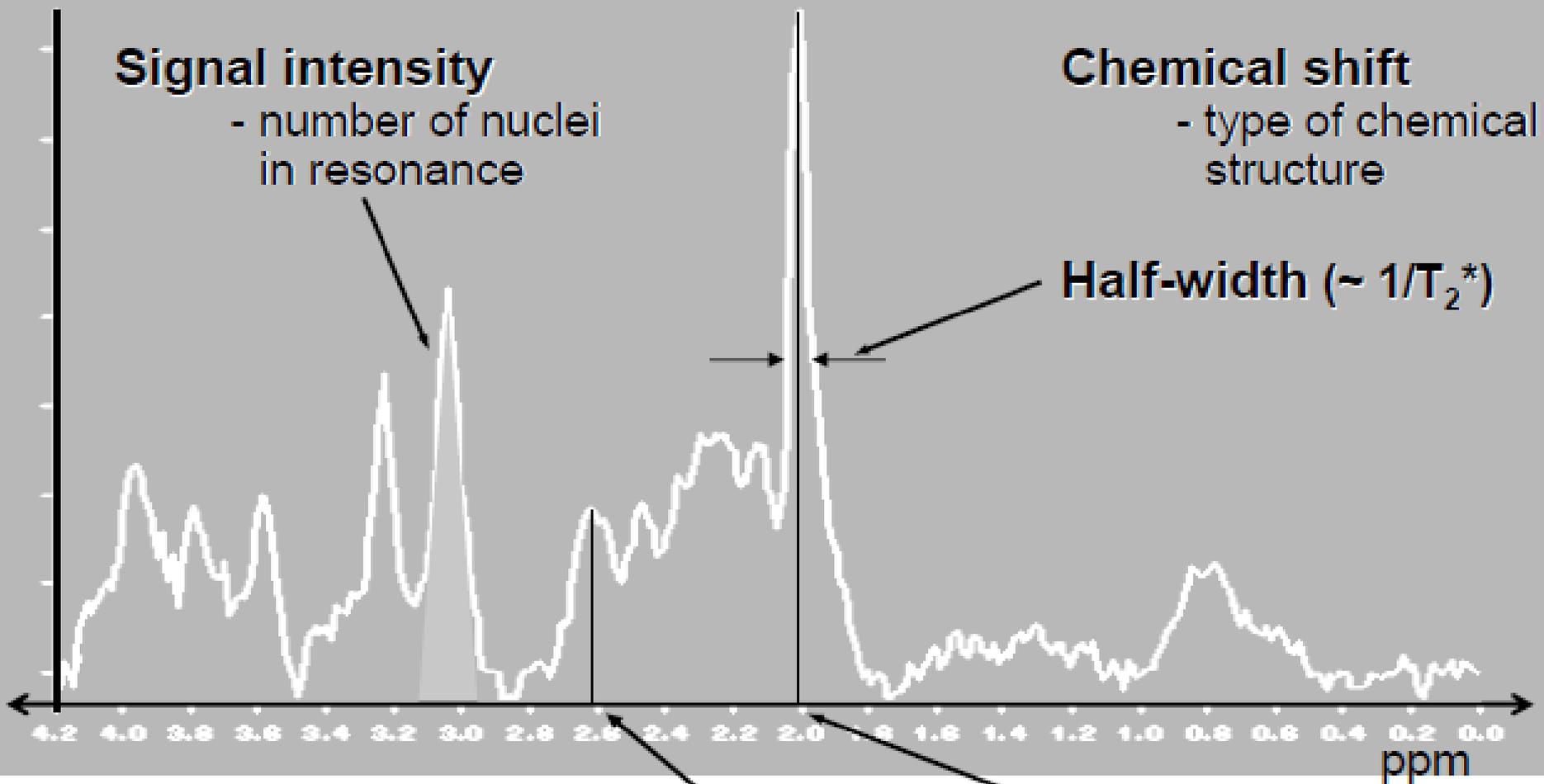
MR Spectrum

Signal multiplicity
Glu ~ 9 mM *vs.* NAA ~ 10 mM

Spin-spin coupling
- fine chemical structure

J = 7 Hz

TE=30 ms

TE=135 ms

Chemical Shift (ppm)

Lactate: $CH_3 - CH - COO^-$
                        |
                        OH
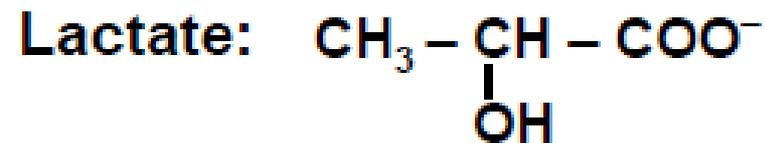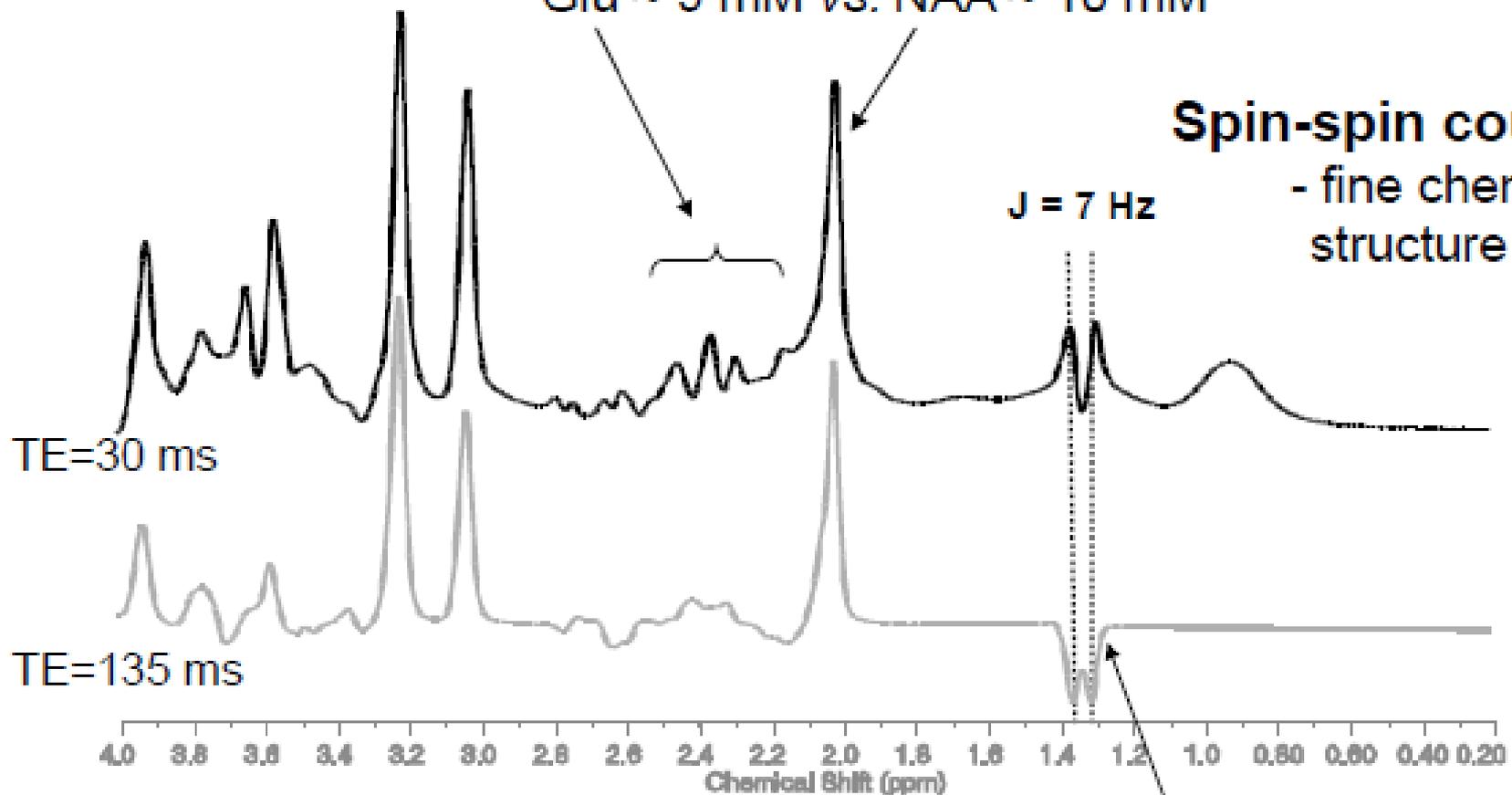
In vivo MR Spectroscopy

Representative MRS of a normal human brain @3T

Short TE vs Long TE

occipital GM PRESS spectra

TE 20
TE 30
TE 45

TE 67
TE 90
TE 135

TE 190
TE 270
TE 400

4 ppm   3   2   1   0
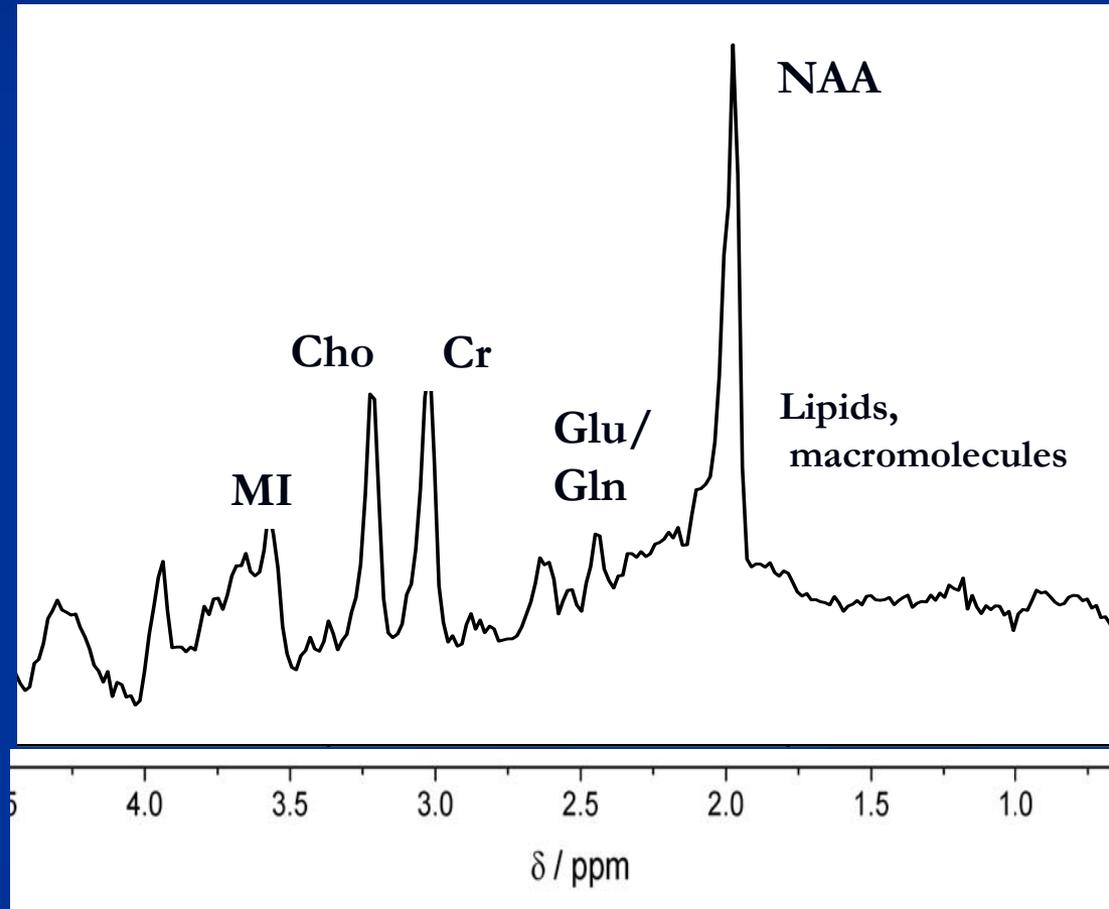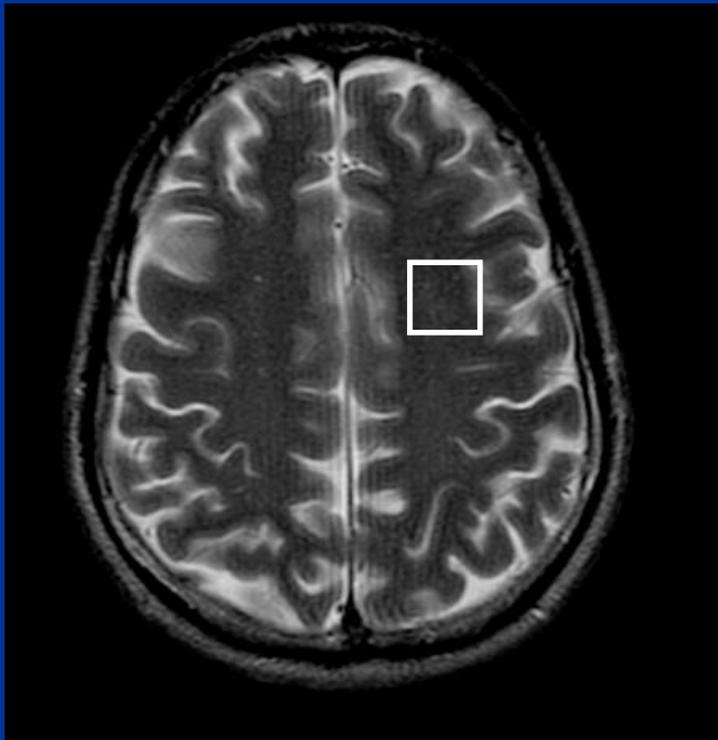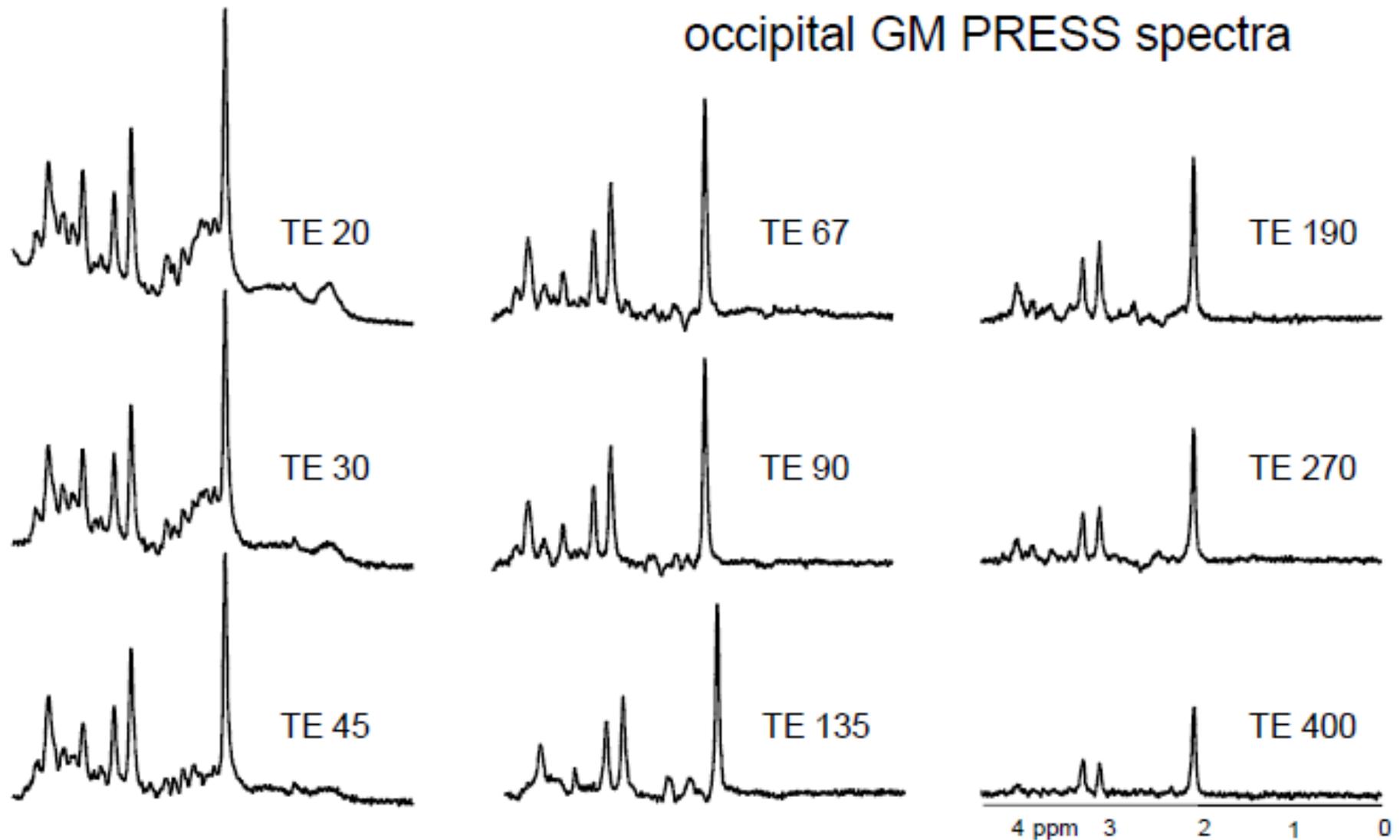
Advantages of higher magnetic field strength for MRS
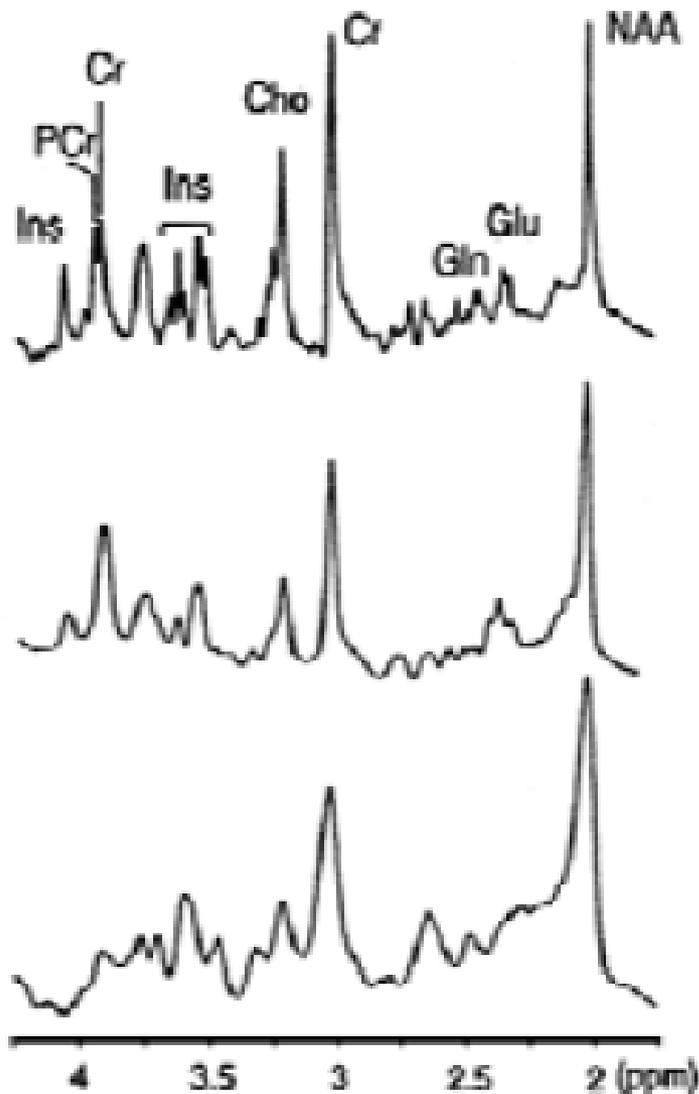
9.4 T : 1ml in dog brain

4.0 T : 27ml in human brain

1.5 T : 27ml in human brain

*Gruetter et al. J Magn Reson **135**, 260 (1998)*

What can be measured in brain?

- Water 40 M
- macromolecules
  - *(phospholipids, proteins, DNA, RNA)*
- metabolites (<2000 Da) 0.030 M
  - NAA, Creatine (Cr), Choline (Cho), Lipids
- true neurotransmitters 0.001 M
  - *(acetylcholine, norepinephrine, dopamine, serotonin)*

Metabolites in Proton MRS
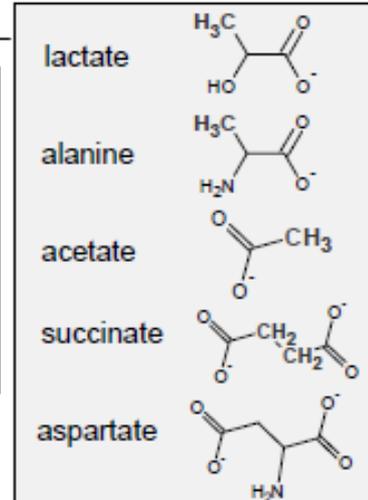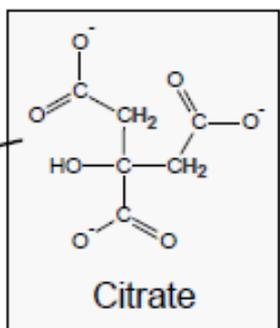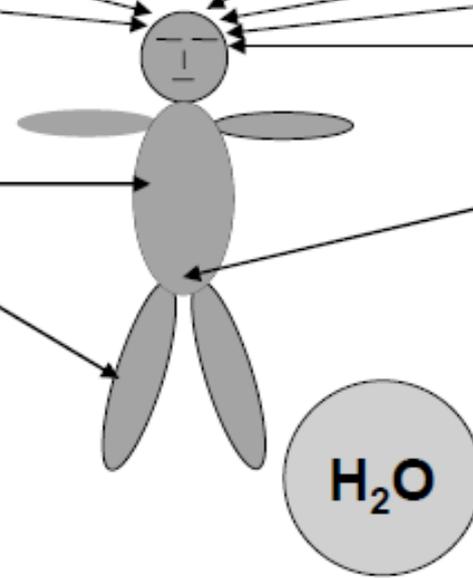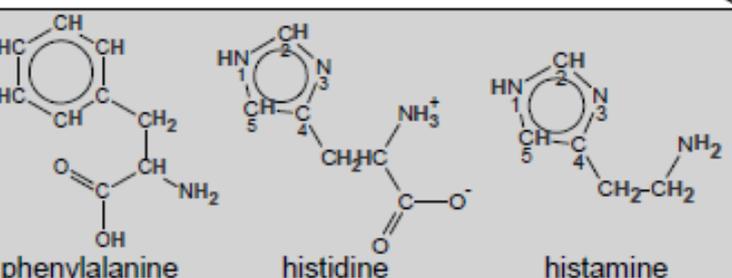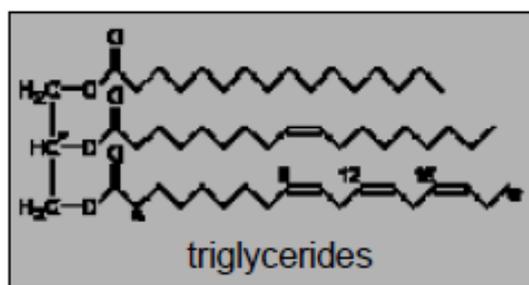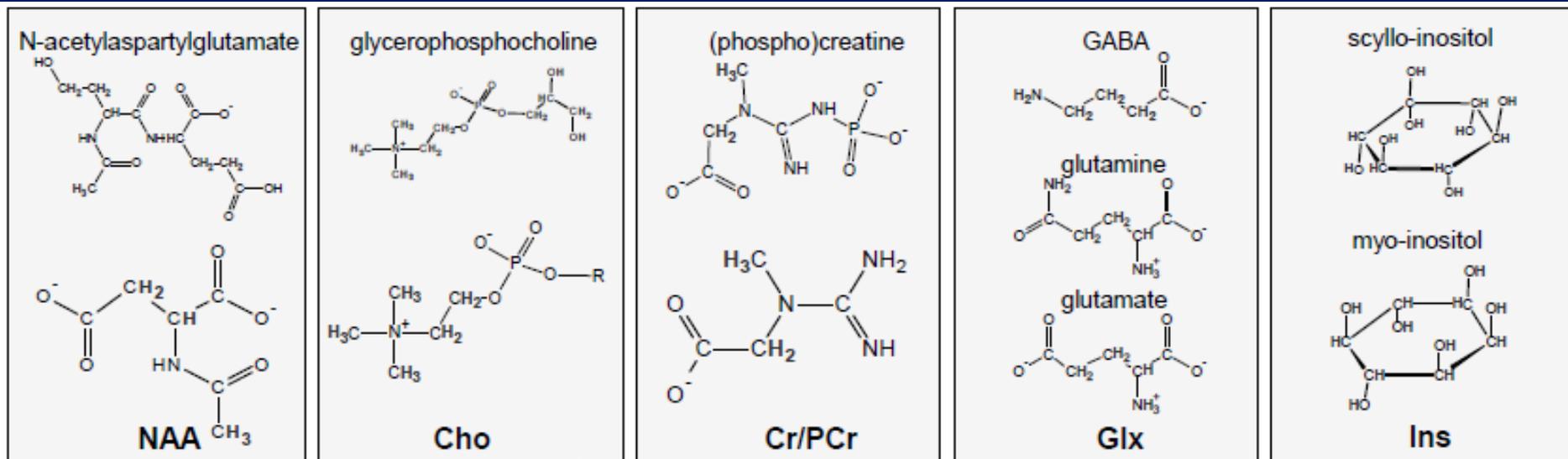
¹H NMR spectrum of the human brain at 7T
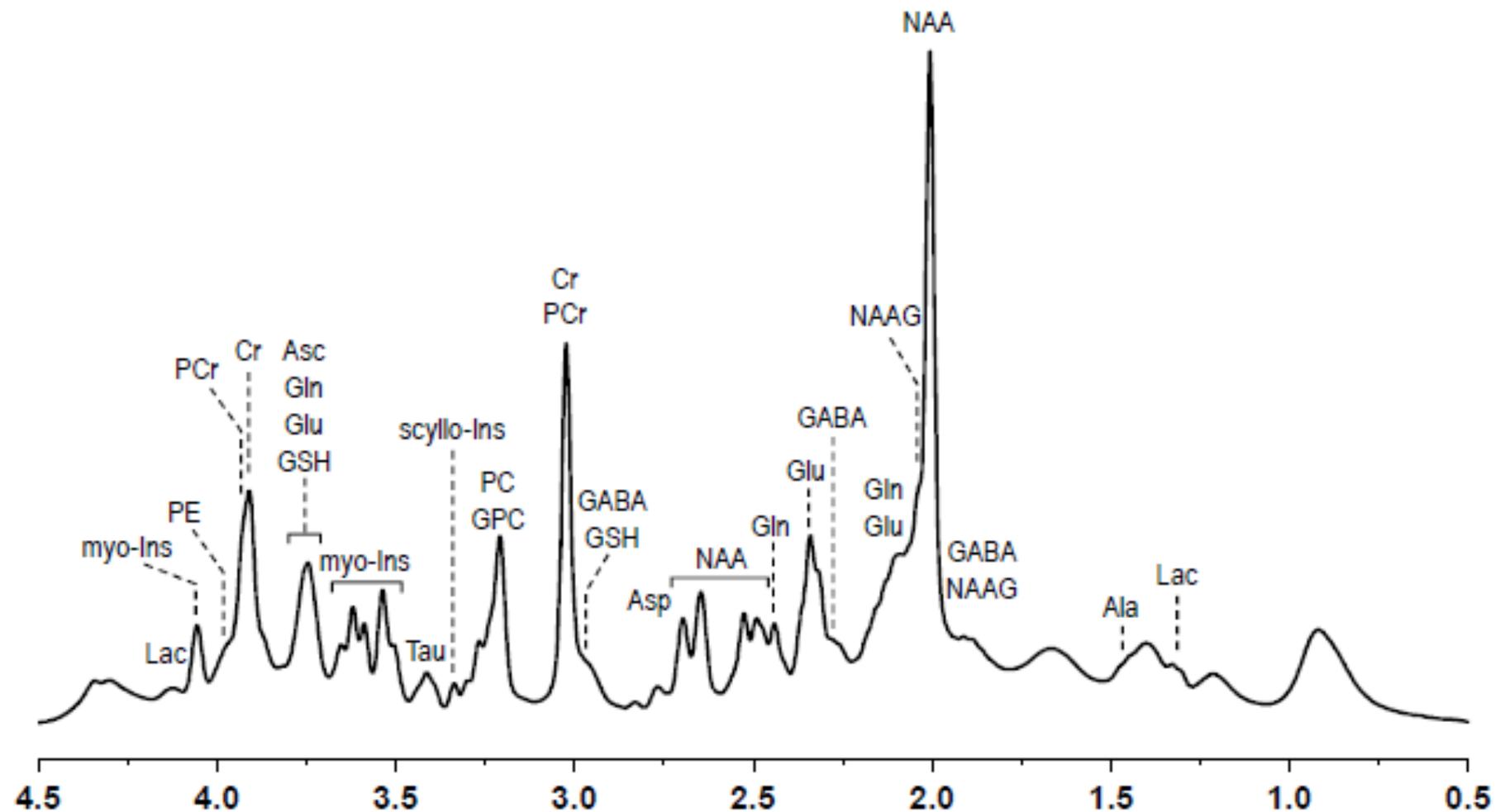
Proton MRS main metabolites:

- N-Acetyl Aspartate (NAA) at 2 ppm: Marker of neuronal density and viability

- Creatine (Cr) at 3 ppm: Energy metabolism, generation of ATP

- Choline (Cho) at 3.2 ppm: Pathological alterations in membrane turnover, increased in tumors

- Lipids (Lip) between 0.8 – 1.5 ppm: Breakdown of tissue, elevated in brain tumors - lipids indicate necrosis
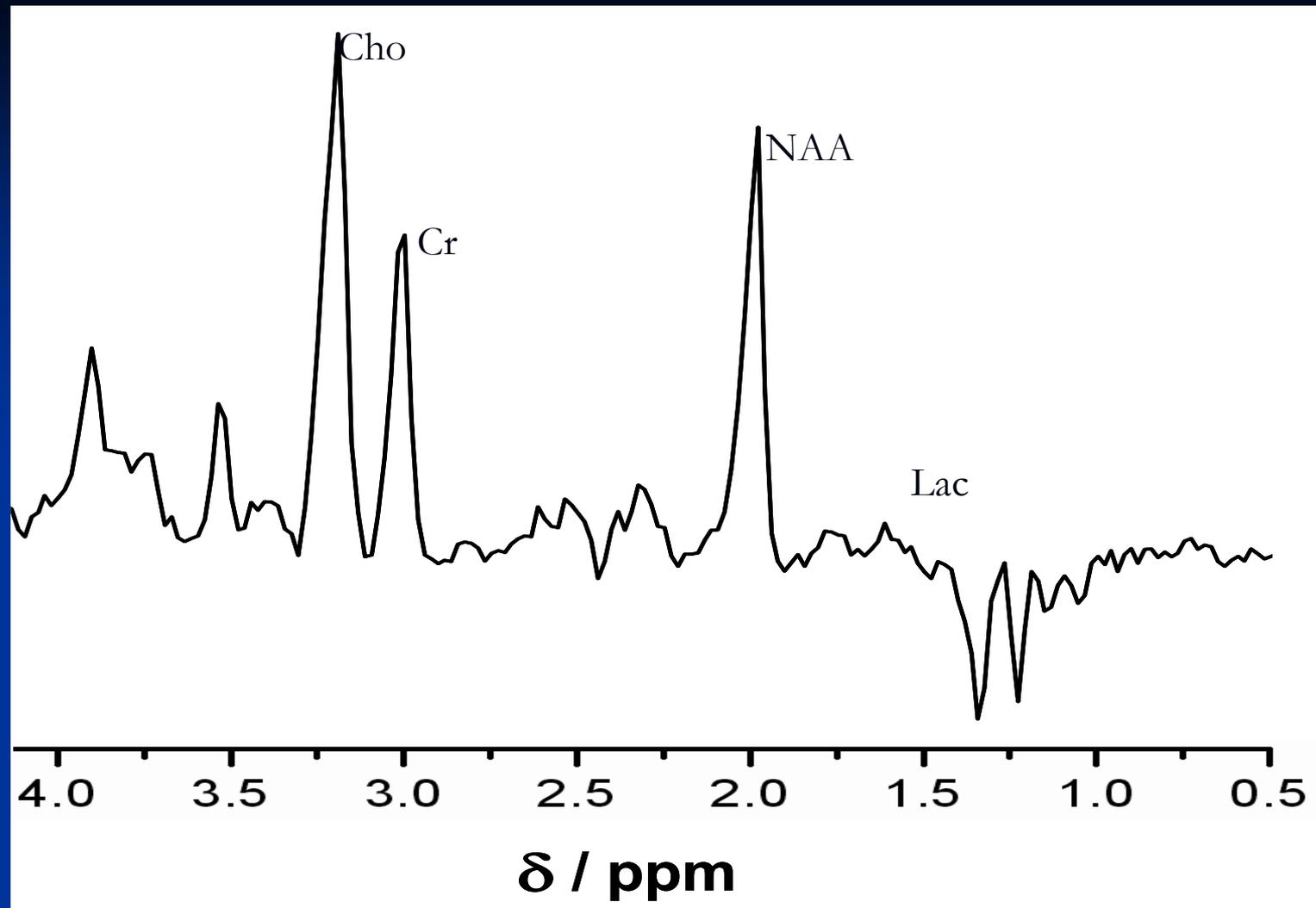
- Lactate (Lac) at 1.3 ppm, inverted at 144ms: produced by an anaerobic metabolism, found in tumor containing zones of necrosis

The Sequence

- Single Voxel Spectroscopy (SVS-PRESS & STEAM)

- 3D chemical shift imaging using a Point-resolved spectroscopy (PRESS) excitation pulse sequence.

- 3D Volumetric Spectroscopy

MRS pulse sequence property

- MRS signal is acquired **_without a frequency-encoding gradient_**.

- Consequently, in contrast to MRI, MRS signal contains different frequencies correspond to the chemical shift and not to the spatial origin of the signal.

- In MRS signal after FT, the spectrum, represents information about the chemical

- structure of the

- MRS signal is sampled either as an echo or as a free induction decay (FID).

basic MR imaging pulse sequence

RF — Excitation

G_z — Slice selection

G_y — Phase encoding

G_x — Frequency encoding

Signal acquisition

Time
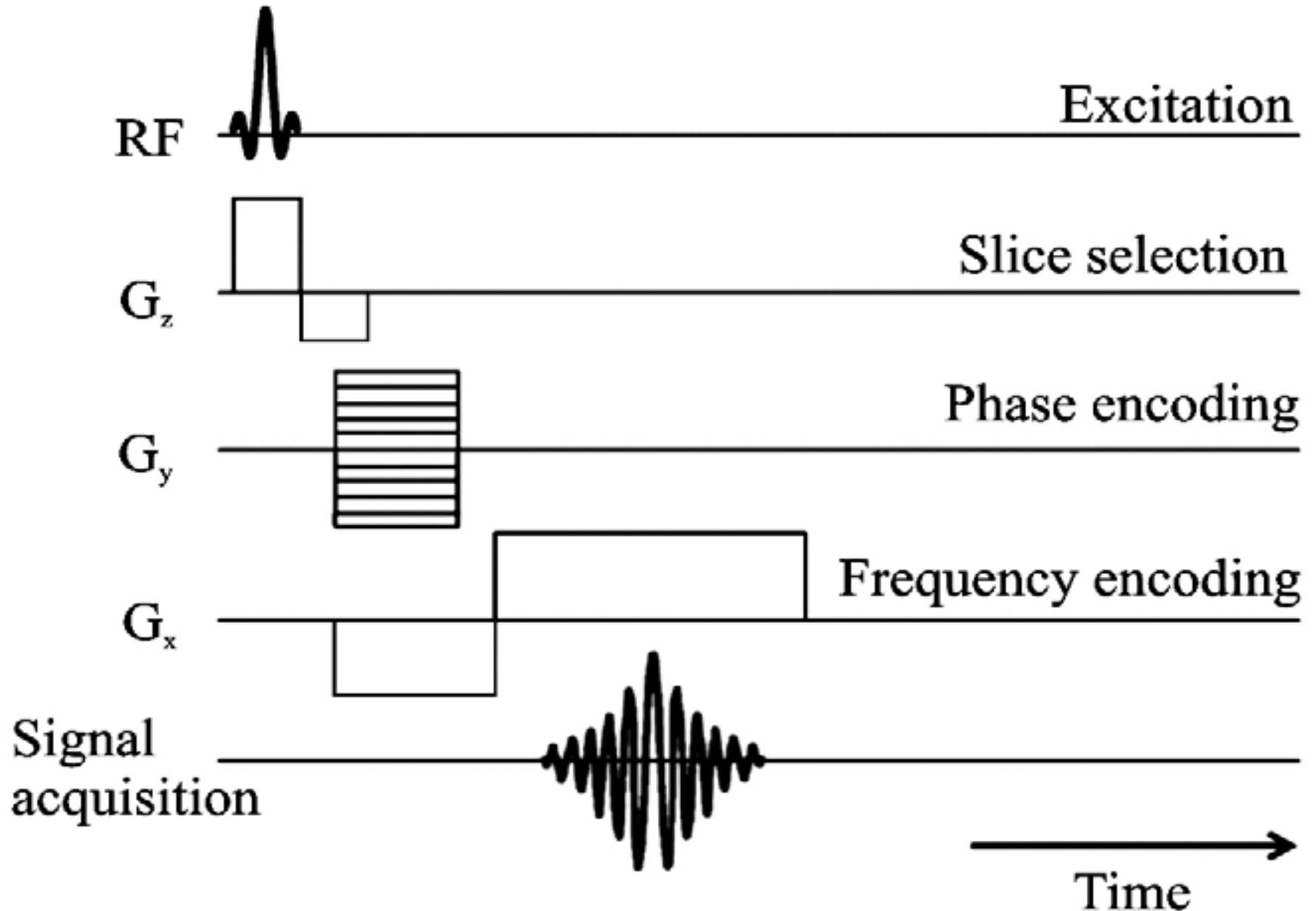
Single Voxel Spectroscopy (SVS-PRESS)

Timing diagram for a Point Resolved spectroscopy with one CHESS (CHEmical-Shift-Selective) pulse for water suppression. A PRESS sequence has three slice-selective RF pulses with the form of 90°-t1-180°-(t21t3)-180°-t4-SE

Single Voxel Spectroscopy (SVS-STEAM)
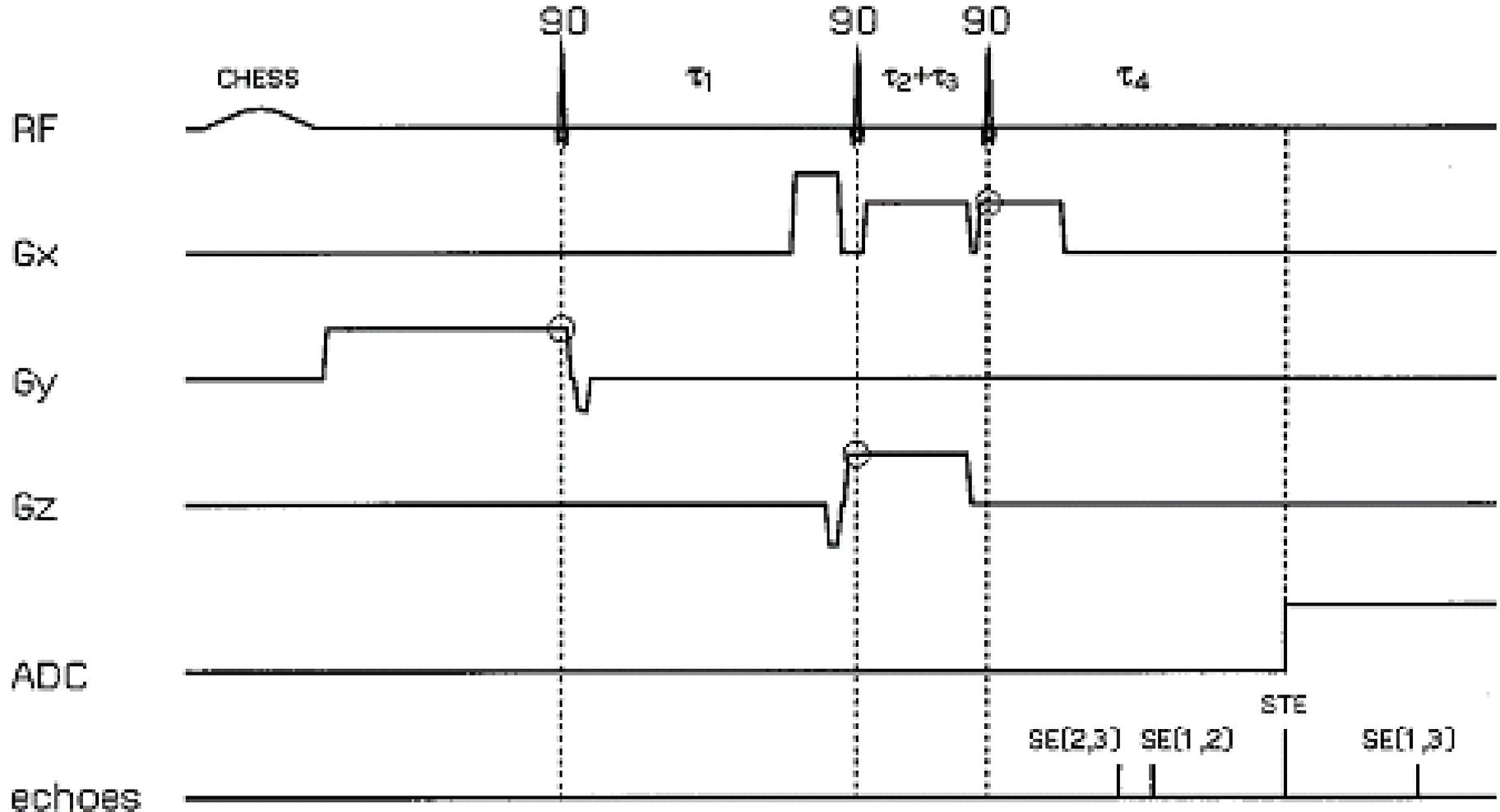
Timing diagram for a **Stimulated echo acquisition mode (STEAM).** Which has 3 slice-selective RF pulses with form of 90°-t1-90°-(t21t3)-90°-t4-STE with one CHESS pulse

2D spectroscopic imaging pulse sequences

(a)
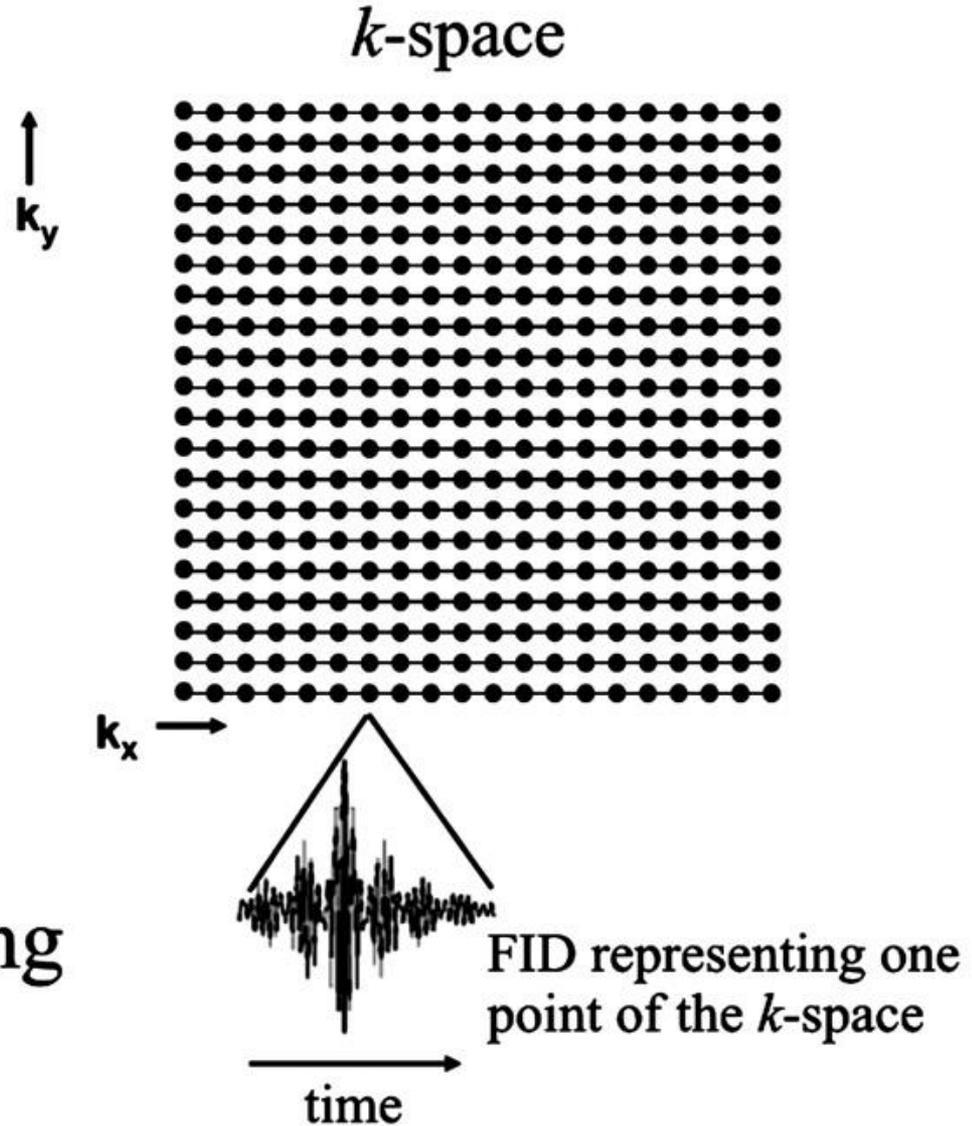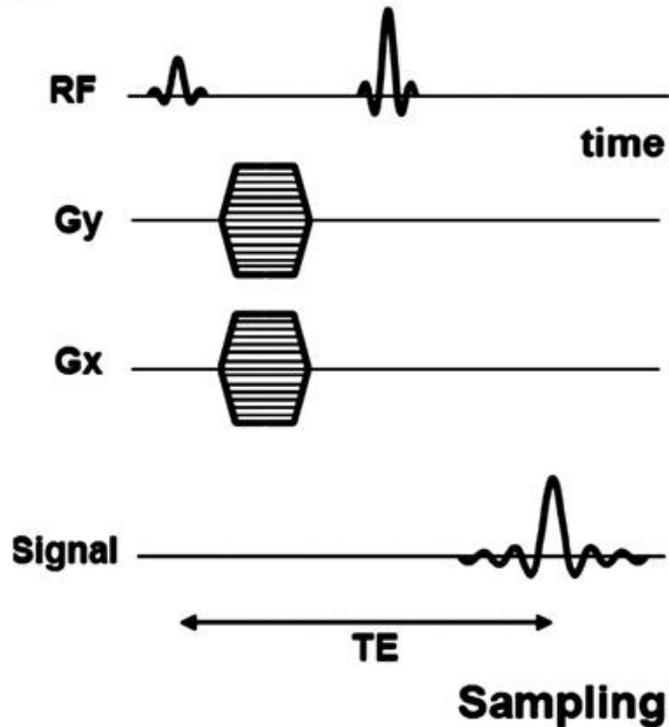
RF

Gy

Gx

Signal

time

TE

Sampling

2D Spectroscopic imaging

k-space

k_y

k_x

FID representing one point of the k-space

time

The slice selection gradients and additional gradients (spoilers) for the elimination of spurious coherences are not shown. two orthogonal phase-encoding gradients are applied,

3D spectroscopic imaging pulse sequences
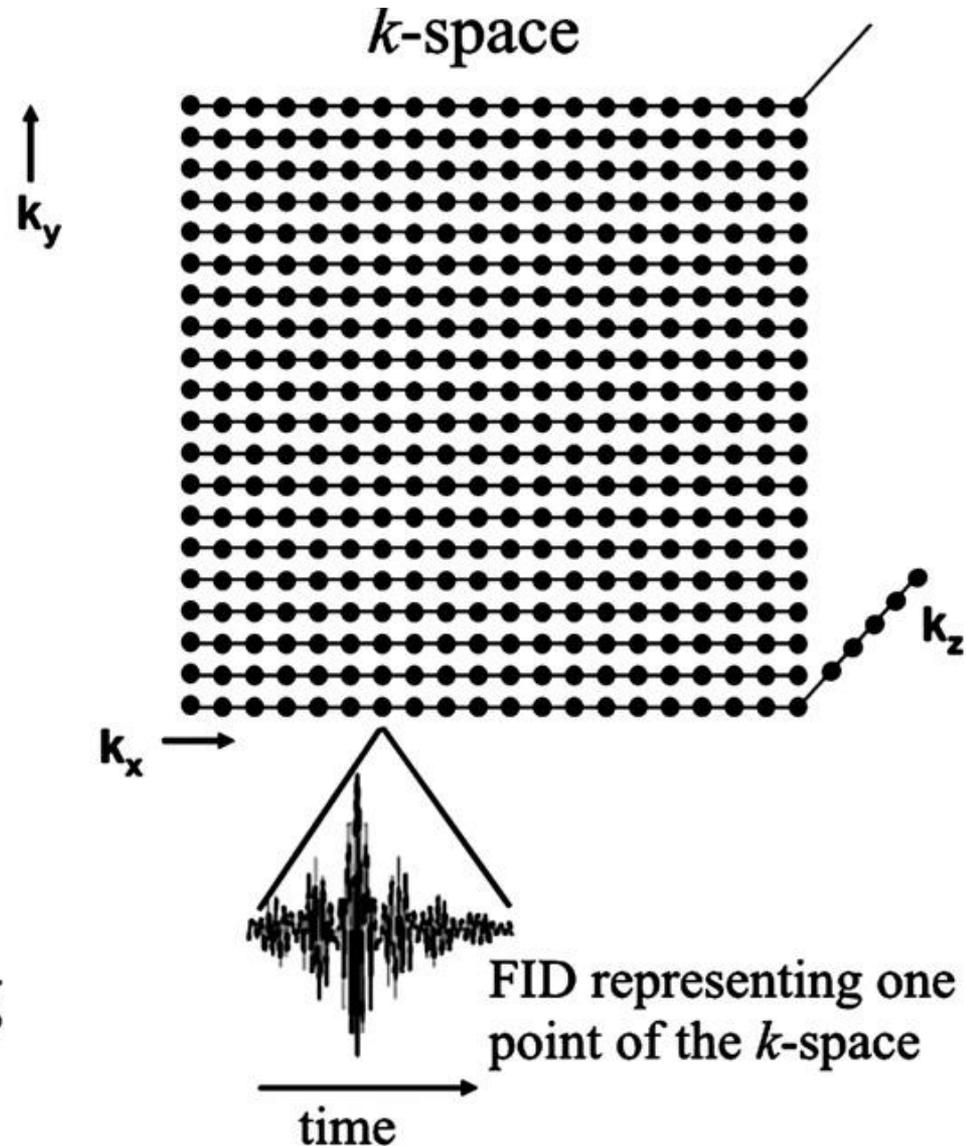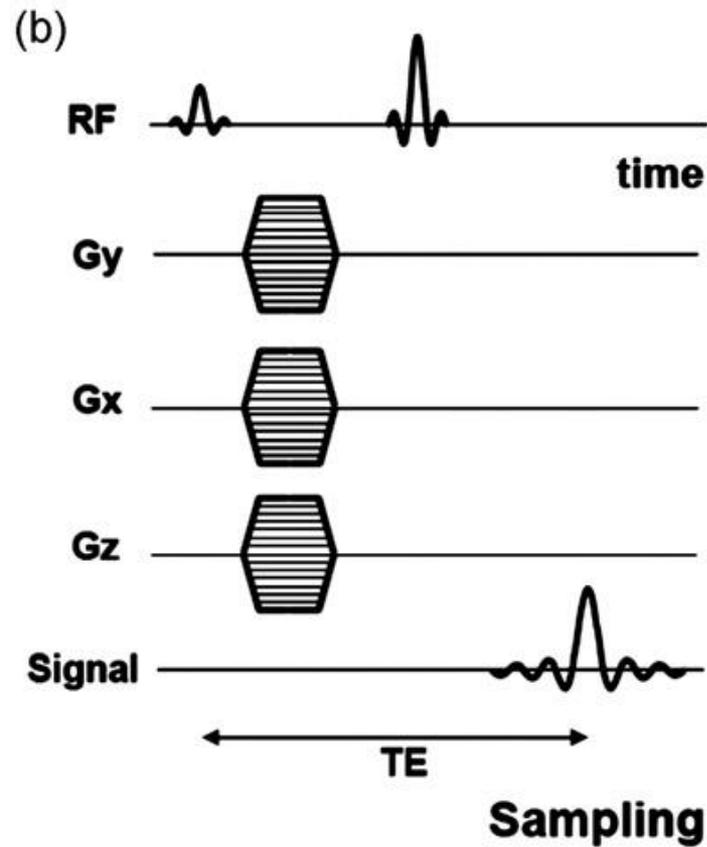
(b)

RF

time

Gy

Gx

Gz

Signal

TE

Sampling

3D Spectroscopic imaging

k-space

k_y

k_x

k_z

FID representing one point of the *k*-space

time

The slice selection gradients and additional gradients (spoilers) for the elimination of spurious coherences are not shown. Three orthogonal phase-encoding gradients are applied,

- In 2D SI, the size of the grid corresponds to the field of view (FOV)

- The number of voxels depends on the number

- of phase-encoding steps along the corresponding direction.

Point spread function (PSF)

- Non-rectangular profile of RF pulses in SVS cause contamination of closely neighboring areas.

- In CSI, a finite number of phase-encoding steps are used. Therefore, due to the properties of FT, during data reconstruction, the signal of the voxel is contaminated with signals from other voxels, based on the weight from PSF.

- In fact, the signal in a particular voxel after FT corresponds to the convolution of spatially continuous time domain signal and the PSF Voxel "bleeding", (ringing artifact effect in MRI)

- Typical shape of PSF for 1D CSI with 16 phase-encoding steps and FOV= 160 mm.
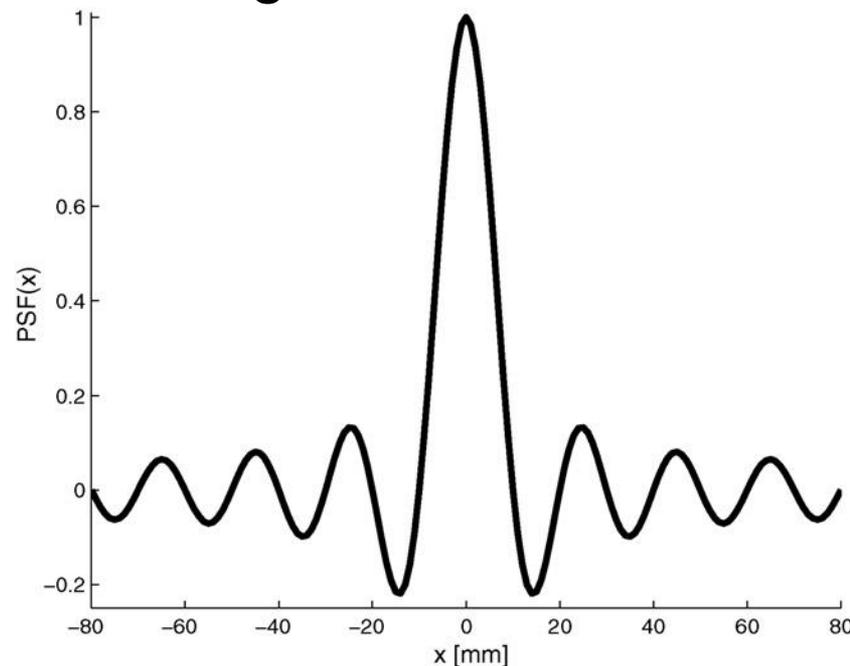
Point spread function (PSF) in CSI
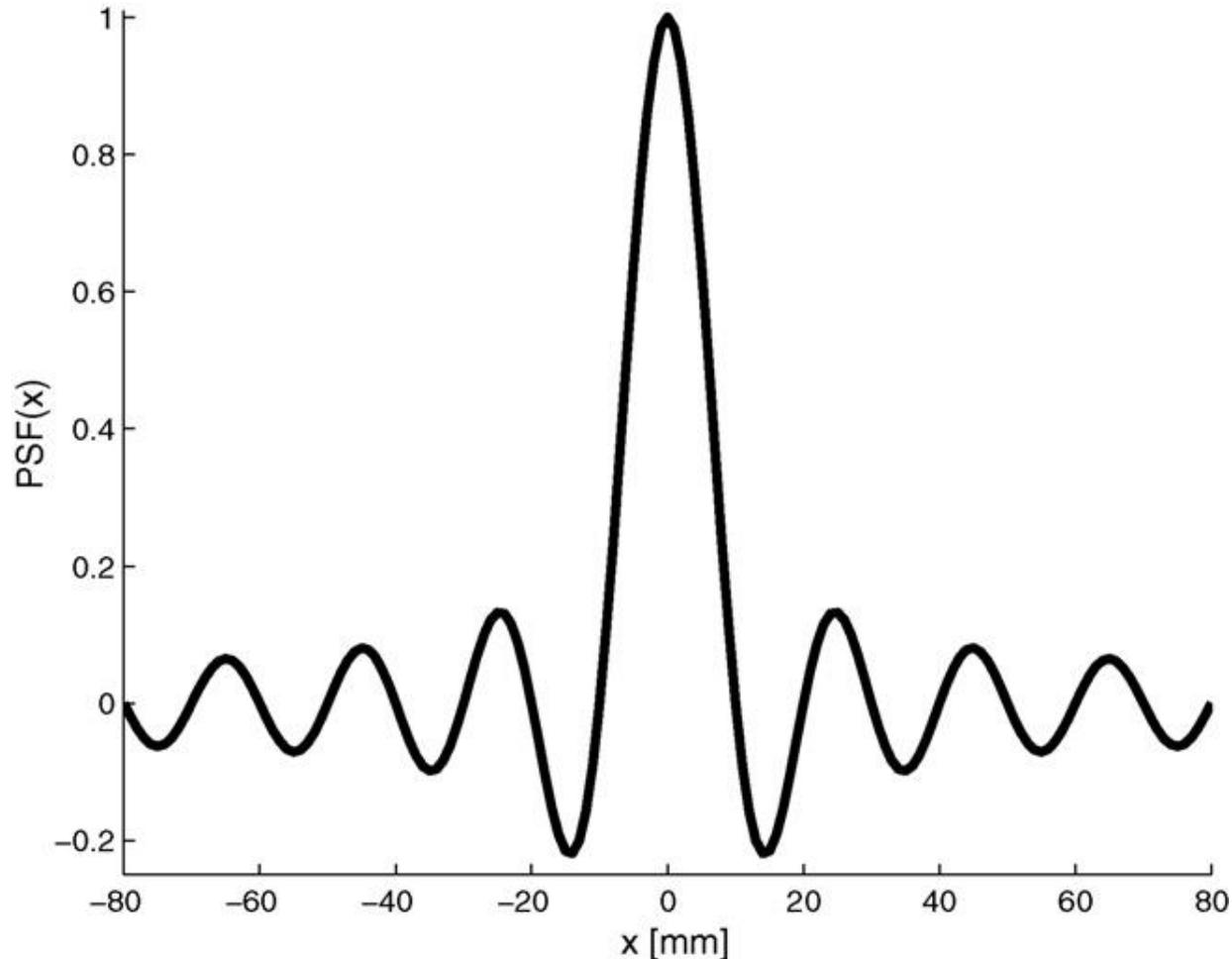
- With a decreasing number of phase-encoding steps, the shape of the main lobe broadens and the side lobes become higher.
- Because the lipid signal from the subcutaneous regions is about a 1000 times greater than the metabolites, its contribution should be avoided using eg; "Outer Volume Suppression"

spatial resolution

- Nominal spatial resolution *D, is defined in imaging:*

$$D \equiv \text{FOV}/N$$

- The effective spatial resolution D' is directly related to PSF shape, k-space filtering, and possible non-rectangular sampling of k-space.

Suppression of unwanted signals

- ## *Volume pre-selected CSI*

- Incorporate the volume selection protocol (PRESS or STEAM) used in SVS into a CSI sequence.

- This volume selection is achieved by a combination of 3 orthogonal slice-selective excitations (VOI), in addition to two-phase-encoding gradients for data sampling (FOV)

- Due to imperfections in the pulse profiles, areas outside the selected VOI are also partially excited and contribute to the measured signal. Therefore, the FOV should always be larger than the VOI in the center of grid.

- ## *Outer volume suppression*

Phase encoding direction

Phase encoding direction

Nominal spatial resolution

SI FOV
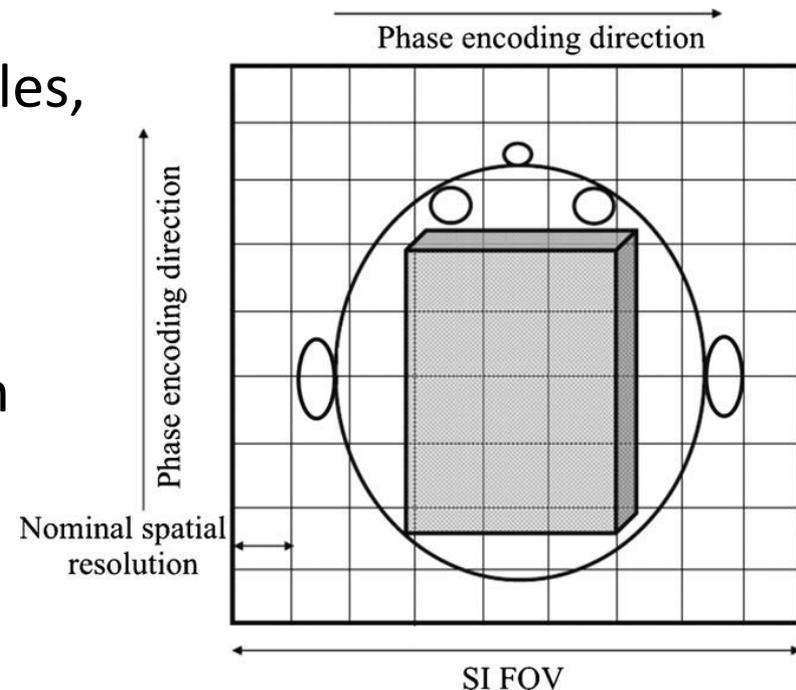
Optimal Voxel Placement

ROI will be placed at center of enhancing tumor covering lesion & normal brain as much as possible but excluding subcutaneous fat and sinuses.
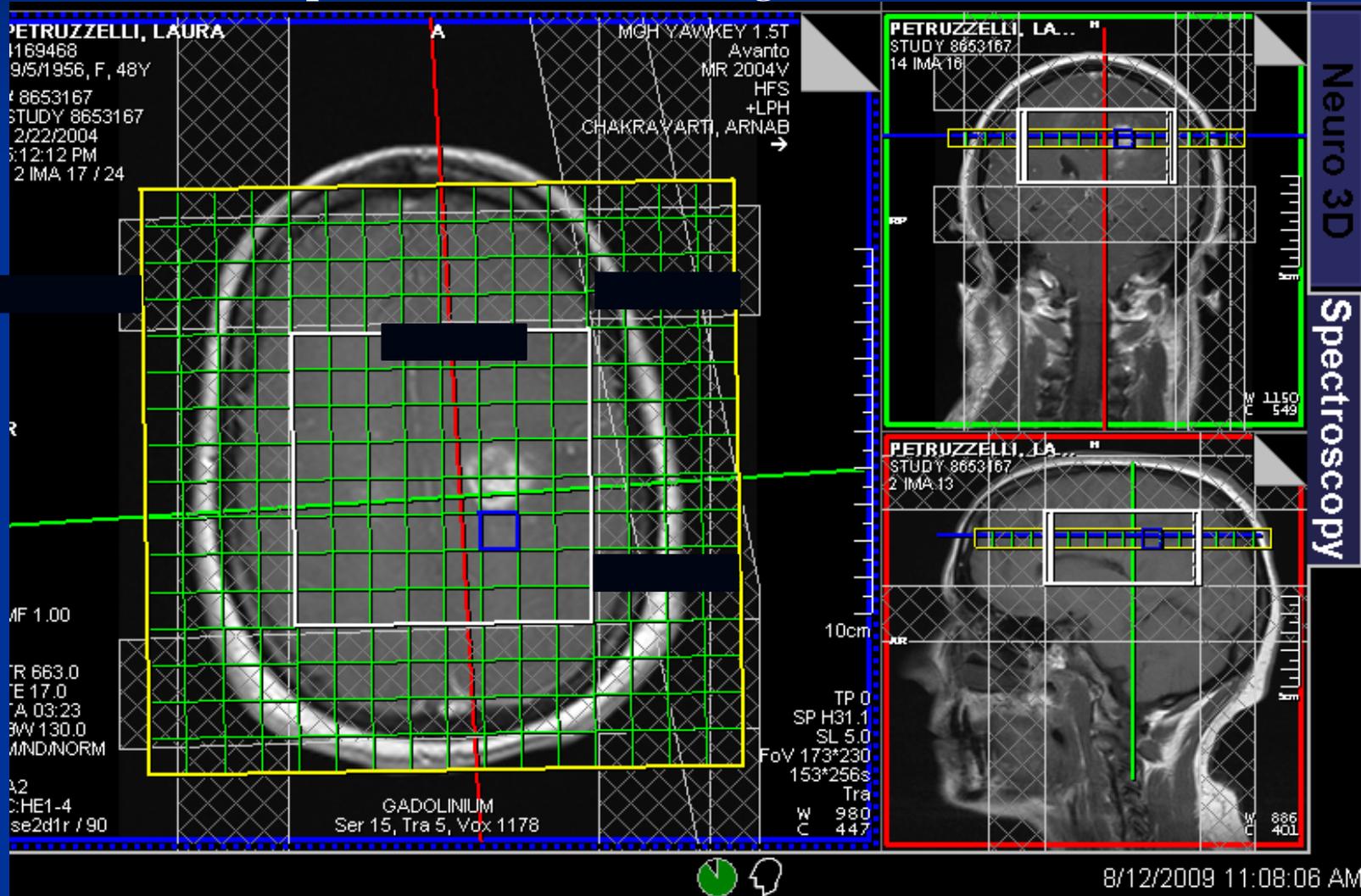
3D MRSI Parameters

- TE 144 ms, TR 1140 ms,

- FOV > 160 mm^2,

- Phase encoding arrays 12 x 12 x 8

- Numbers of Acquisitions: 1

- Spatial zero-filling to 16 x 16 x 8 phase encoding arrays will result in an individual voxel size of 1 x 1 x 1 cm^3.

- Approximate imaging time: ~6 min utilizing elliptical k-space sampling k-space sampling

- Manual shimming is recommended before the acquisition to obtain the best magnetic field homogeneity.

Shimming

- "Shimming" = adjusting the magnetic field to make it more homogeneous

- 1.5T: Signal line width or full width at half maximum (FWHM): <15 Hz for 3D MRSI

- 3 T: FWHM < 25 Hz for 3D MRSI
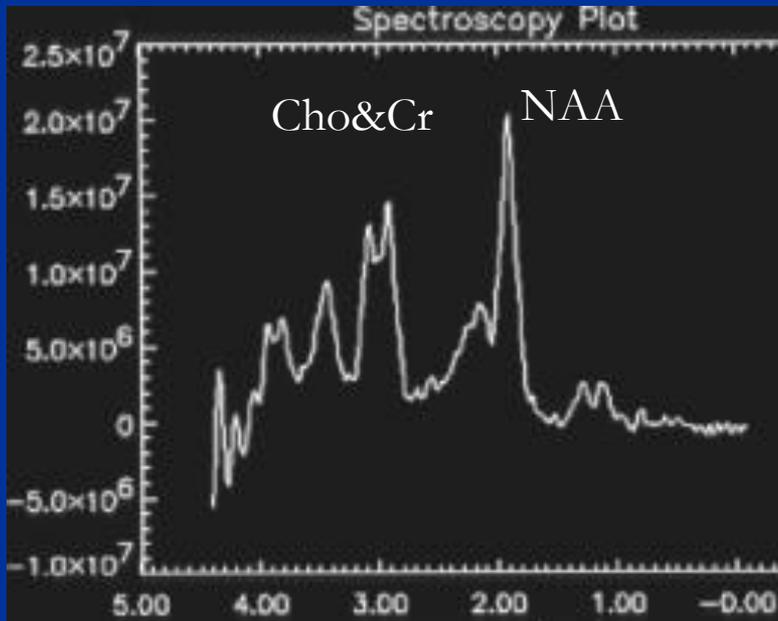
- Suboptimal shimming
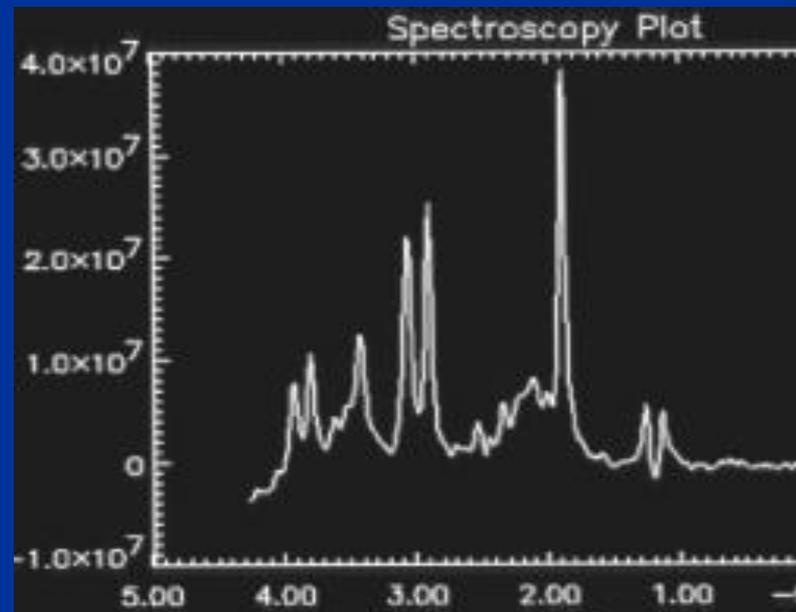
- Better signal separation, thus better quantification of metabolites
- Better water suppression

Saturation Bands

■ Click SAT and place up to 10 SAT bands around the voxel to suppress signals from lipid/fat
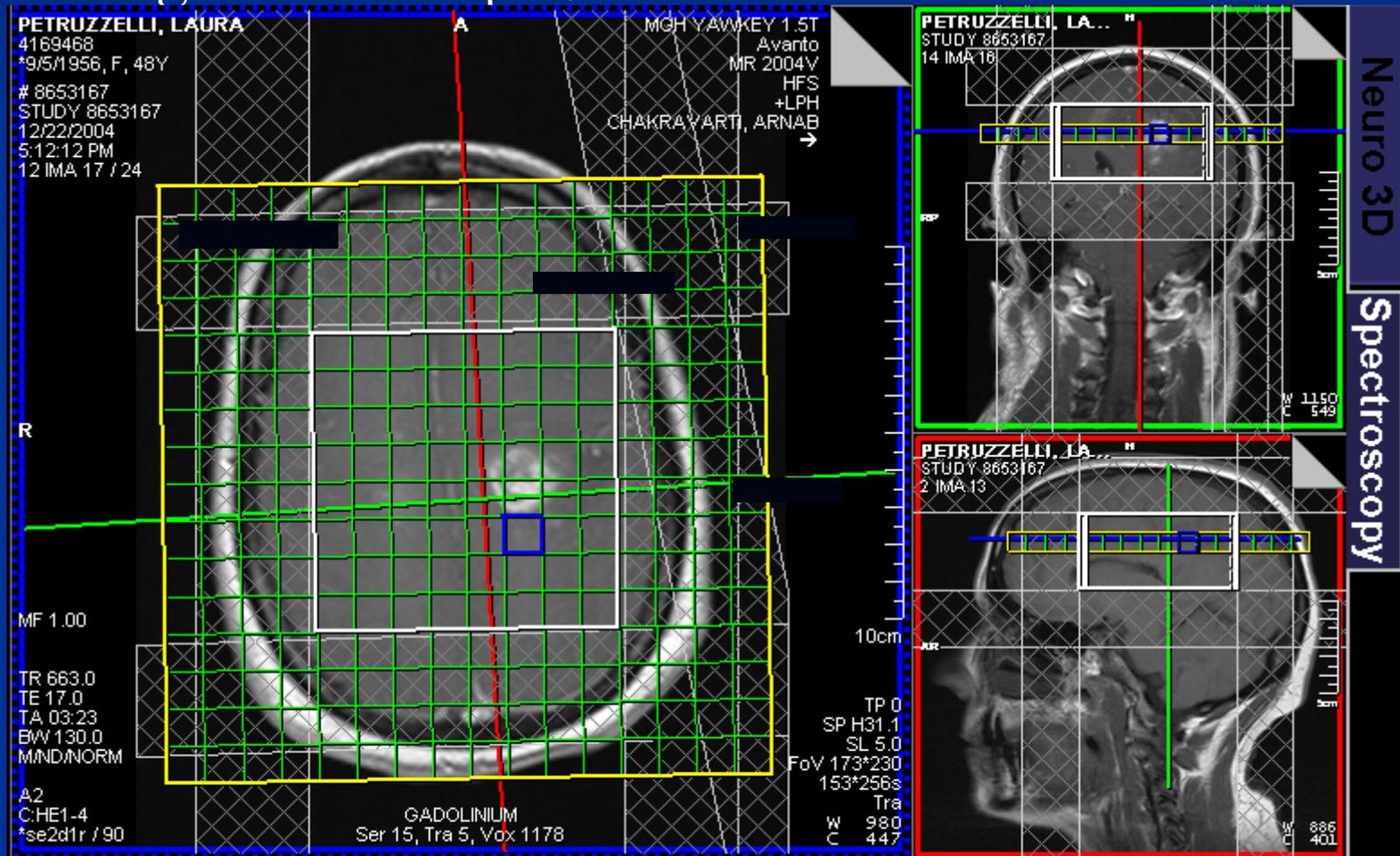
Saving the Data in .rda format

Select the raw data for the spectroscopy, either double click it or use the drop down menu to send the data to post processing "spectroscopy"

Under 3D CSI Selection:
Choose Plane number
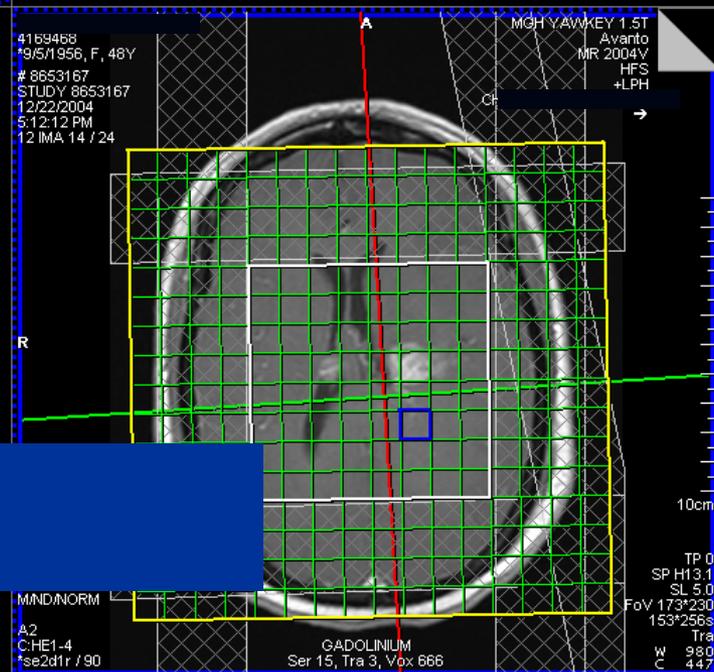
Pitfalls from acquisition problems

- Chemical shift artifact
    - ROI shift
    - Improper quantitation reference
    - Asymmetry of contralateral side
    - Peak disappearance
    - Inefficient Editing
- Voxel profile
- B1 miscalibration
- Motion

Causes of Distortions in MRS spectrum
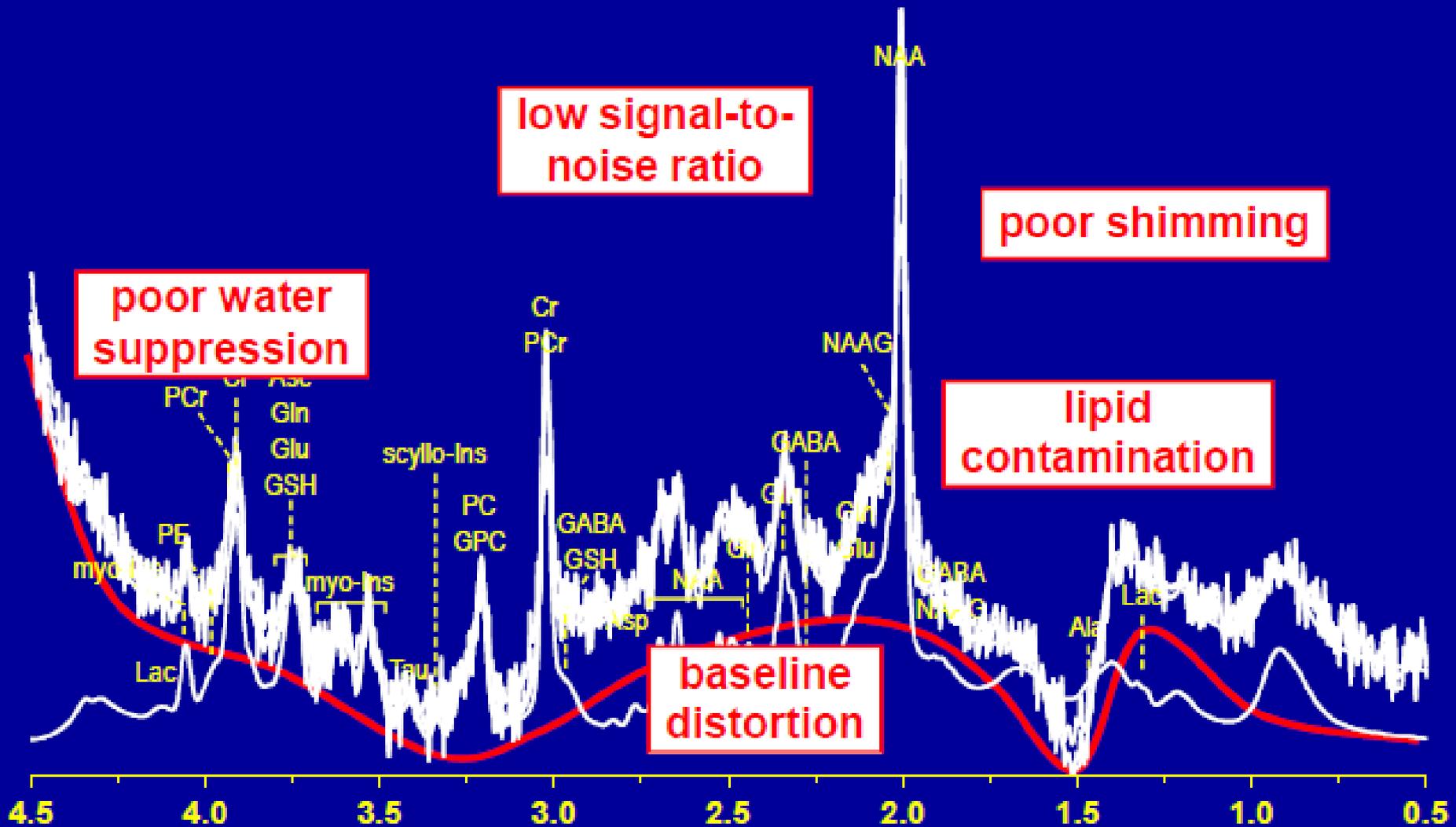
Spectroscopic frequency difference due to J-coupling or chemical shift, is misinterpreted with gradient-based encoding as spatial shift, in MRSI
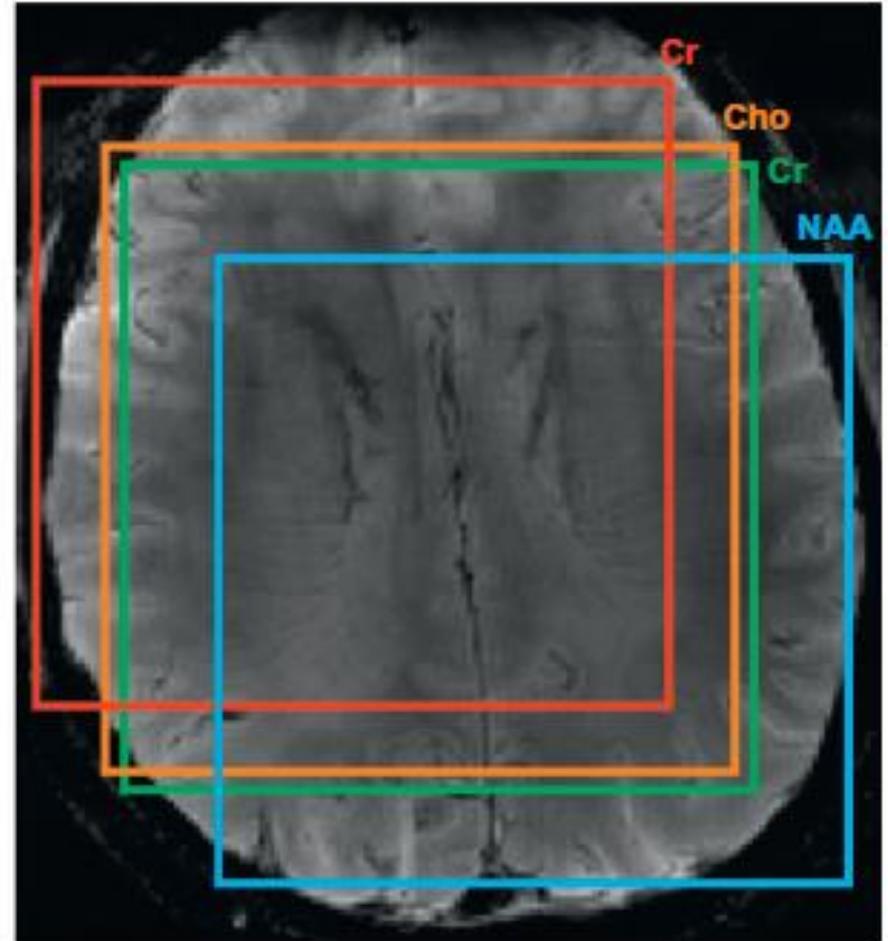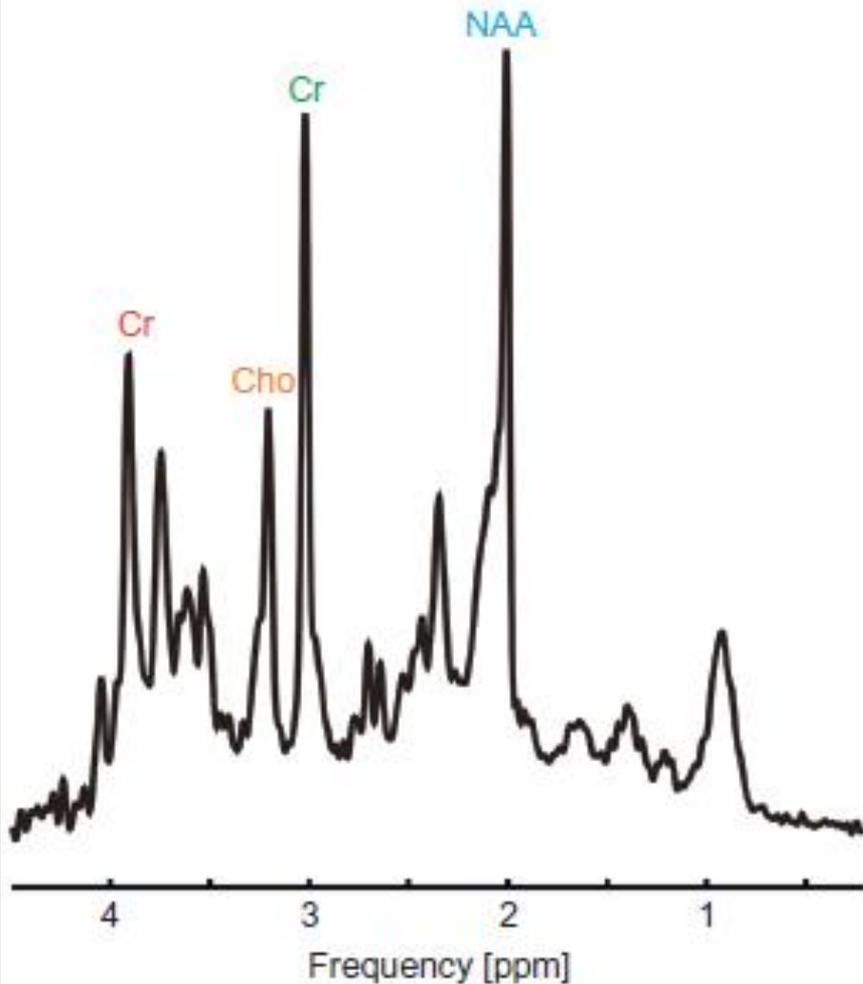
Outer Volume Lipids
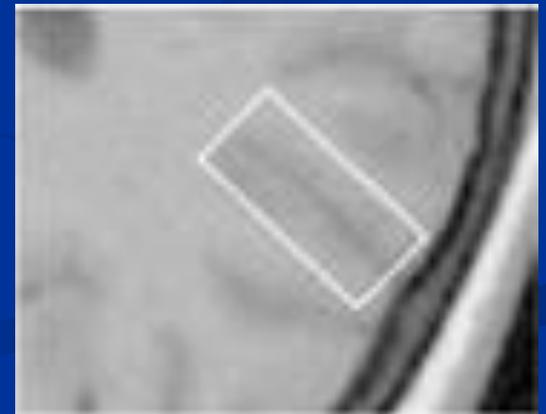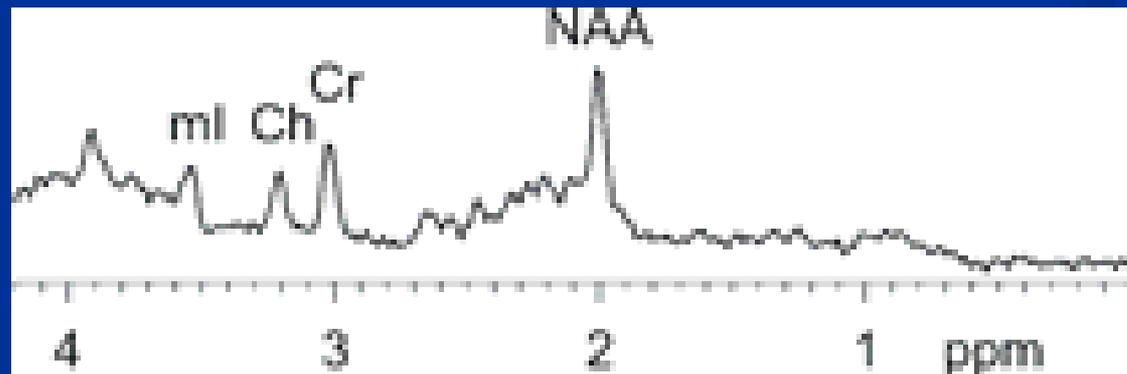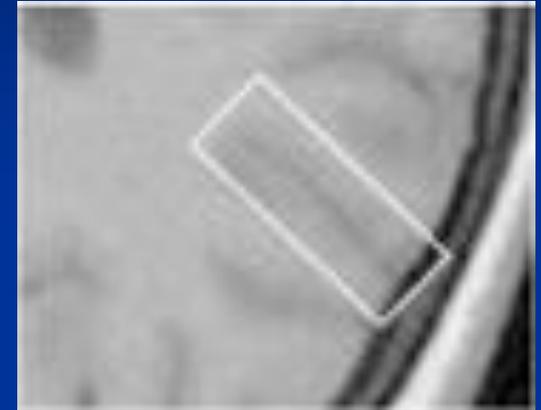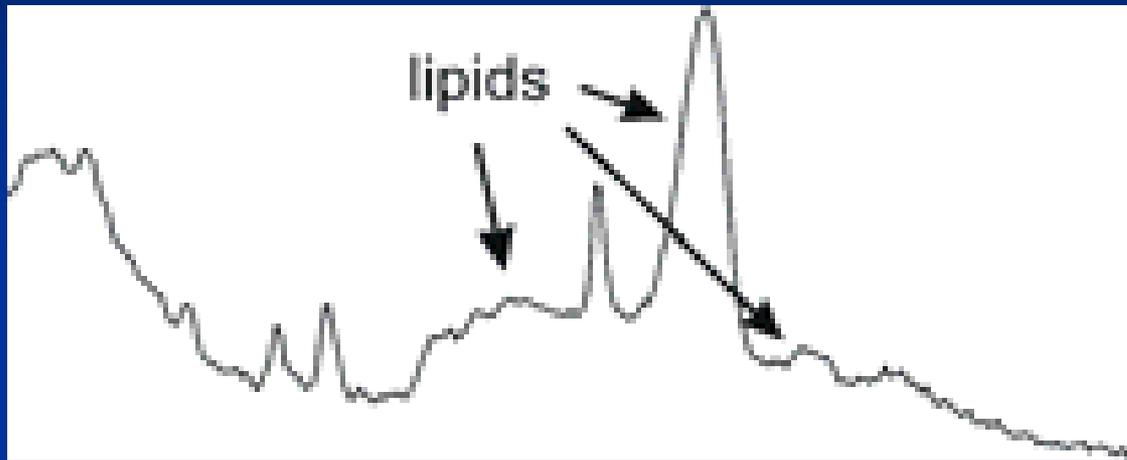
Sources of Artifacts and Noise

- Gross Motion:
  - wrong location
  - broadening of peaks
- Physiologic Motion:
- Out of volume signals
- Eddy currents
- Lineshape
- Baseline
- Phase
- Sidebands
- ROI shape
- "Ghost" (spurious echoes)

- Water suppression
- Chemical shift artifact
- Lipid contamination
- DC-offset
- RF leakage
- Nonlinear amplification
- Frequency drift
- Receiver gain
- Misassignments
- Wrong fitting model