Appendix 7

In Vivo Spectra and Assignments for Some Tissues and Disease States

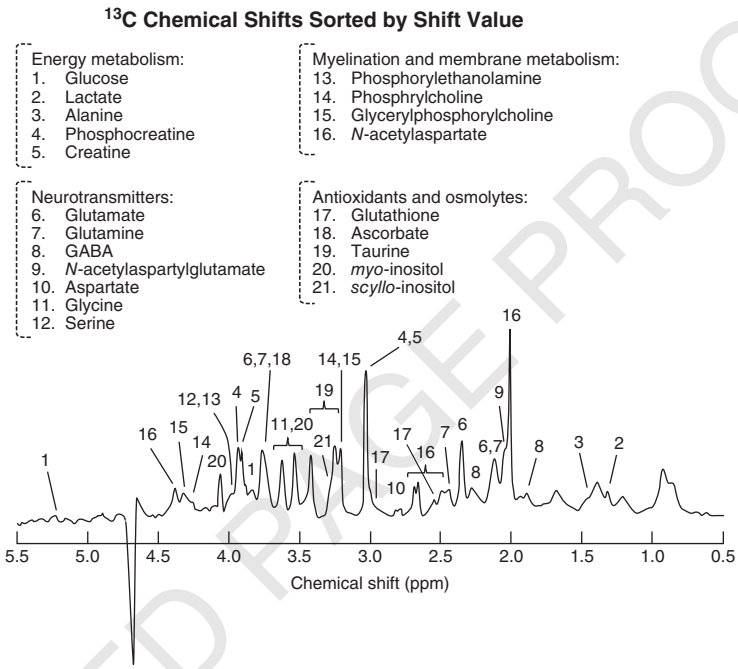

Figure 1. Compounds detected in the brain with in vivo ^{1}H NMR spectroscopy. The **s**pectrum was acquired from the rat hippocampus at 14.1 T using SPin ECho full Intensity Acquired Localized (SPECIAL) spectroscopy.[1] Reprinted from NeuroImage, **61**, J.M.N. Duarte, L. Hongxia, V. Mlynárik and R. Gruetter, The neurochemical profile quantified by in vivo ^{1}H NMR spectroscopy, 342. © 2012, with permission from Elsevier

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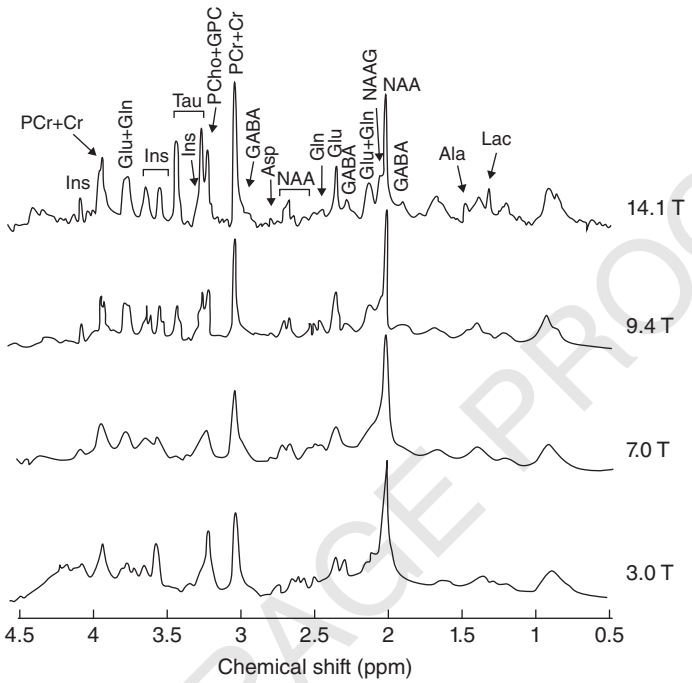

Figure 2. Localized ^{1}H NMR spectra acquired with SPECIAL spectroscopy at different magnetic fields. Spectra at 3.0 and 7.0 T were acquired from cortical regions of the human brain. Spectra at 9.4 and 14.1 T are from the hippocampus of the rat and mouse, respectively. Metabolites in the spectra are assigned as follows: myo-inositol (Ins), phosphocreatine (PCr), creatine (Cr), glutamate (Glu), glutamine (Gln), taurine (Tau), glycerophosphorylcholine (GPC) phosphorylcholine (PCho), γ-aminobutyrate (GABA), aspartate (Asp), *N*-acetylaspartate (NAA), *N*-acetylaspartylglutamate (NAAG), alanine (Ala), and lactate (Lac).[1] Reprinted from NeuroImage, **61**, J.M.N. Duarte, L. Hongxia, V. Mlynárik and R. Gruetter, The neurochemical profile quantified by in vivo ^{1}H NMR spectroscopy, 342. © 2012, with permission from Elsevier

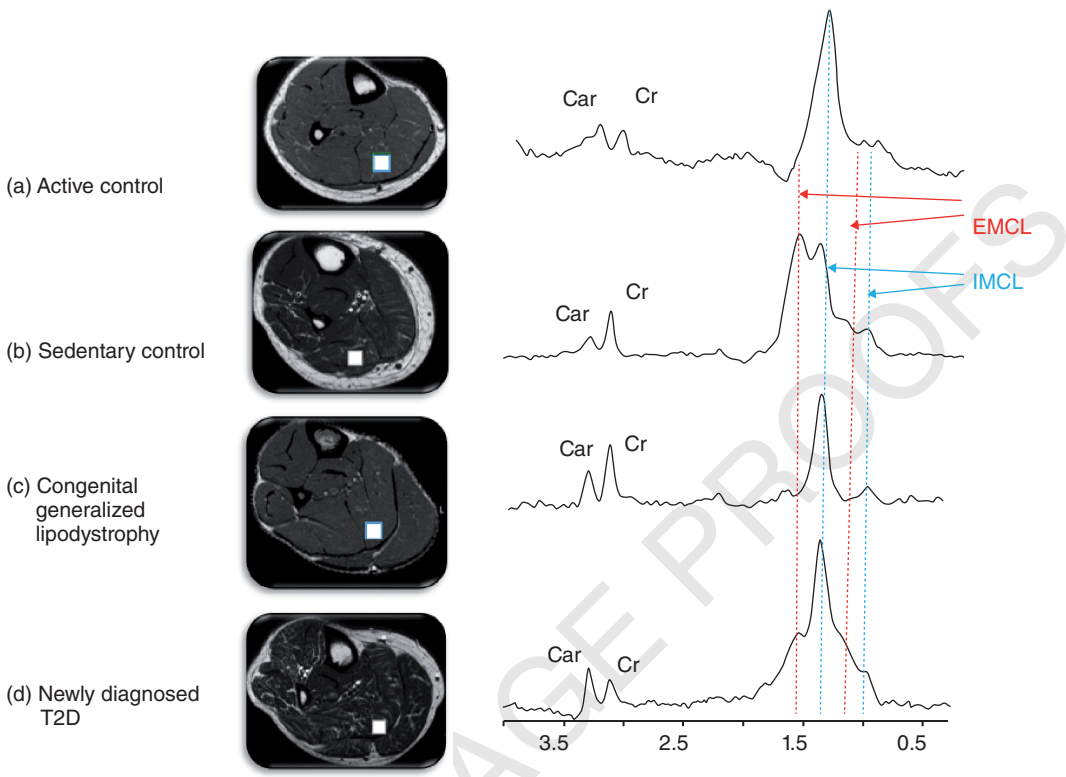

Figure 3. Localized ^{1}H MRS in skeletal muscle. High-resolution axial images of calf muscle at left were used for selection of a volume of interest (VOI), 10 × 10 × 10 mm in the soleus (white rectangle). Fat appears bright, muscles gray, and bones black. Blood flowing into vessels appears bright and blood flowing out of vessels appears dark. Calves of control subjects (a and b) and a type 2 diabetes (T2D) patient (d) have a layer of a subcutaneous adipose tissue and white fatty spots between muscle fibers. A lipodystrophic, adipose fat deficient patient (c) had no adipose fat. Therefore no signals from subcutaneous adipose tissue or fat deposits between muscle fibers are present on the image from his calf. A localized ^{1}H NMR spectrum from the VOI was collected without water suppression. It contained a strong signal from tissue water at 4.8 ppm (not shown). The ^{1}H spectra at right show intense lipid signals between 0 and 2 ppm and signals from muscle metabolites between 2 and 4 ppm are shown. The hallmark of ^{1}H MRS in skeletal muscle is the presence of resonances from fat droplets that reside within myocytes (intramyocellular lipids, IMCL), in addition to lipid resonances from fat cells between muscle fibers (extramyocellular lipids, EMCL). This is best demonstrated in spectrum (b) from a healthy, sedentary control. Here Cr, denotes total creatine including PCr and Car denotes carnitine. Imaging and spectroscopy were performed at 1.5 T using a Gyroscan NT whole body system (Philips Medical Systems). Image courtesy of Lidia S. Szczepaniak, Cedars-Sinai Medical Center, Los Angeles

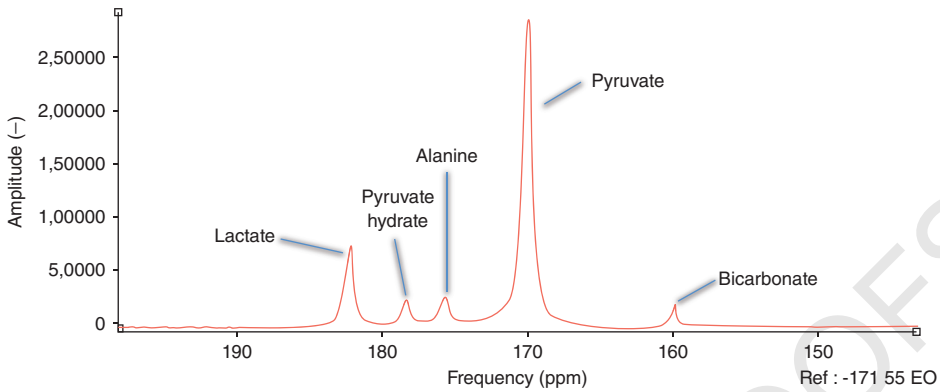

Figure 4. In vivo ^{13}C rat heart spectrum following injection of hyperpolarized pyruvate. The spectrum is the summation of 30 s worth of data acquired with a repetition period, TR = 1 s and a flip angle of 10°. The coil was a 2-cm butterfly coil placed directly over the heart and the spectra were cardiac gated to end-diastole. Image courtesy of Damian Tyler, Oxford University

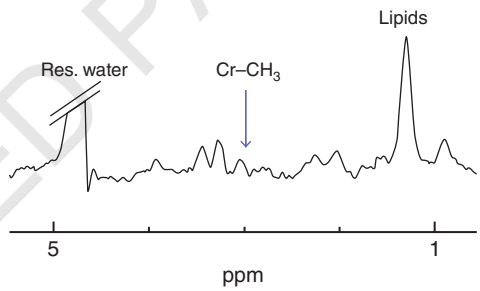

Figure 5. Single voxel ^{1}H spectrum (double-triggered point resolved spectroscopy, PRESS, spin echo time, TE/TR = 10/2000 ms, 2 µl) obtained from the septum of a mouse heart in vivo. Image courtesy of Jürgen Schneider, Oxford University

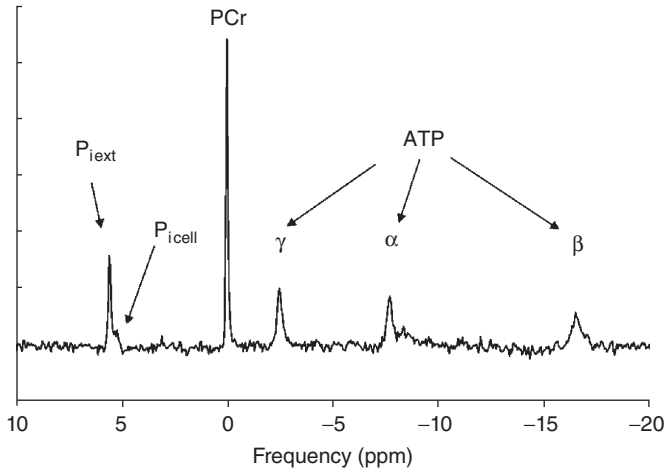

Figure 6. ^{31}P NMR spectrum from an isolated, beating mouse heart, acquired in an 11.7 T magnet in 20 min with a TR of 10 s and 60 μs pulse (ATP, adenosine triphosphate; $P_{i\ cell}$, intracellular inorganic phosphate; and $P_{i\ ext}$, inorganic phosphate in buffer surrounding the heart). Image courtesy of Mark Cole, Oxford University

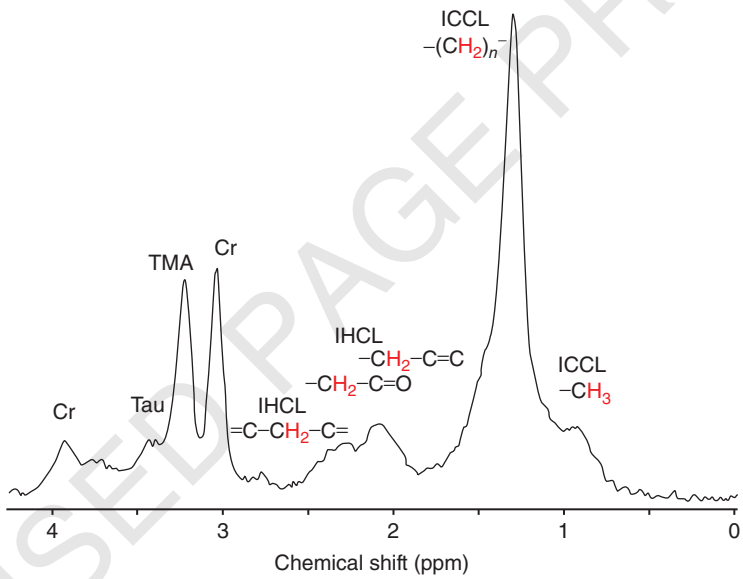

Figure 7. ^{1}H NMR spectrum of human heart tissue. This spectrum, obtained at 3 T (on a Siemens Verio system), is an average of 18 individual spectra from five subjects as part of a study on repeatability of cardiac ^{1}H MRS and potential diurnal variations of intracardiomyocellular lipids (ICCL).[2] A region of interest of 5 cm^3 was localized in the cardiac septum using double-triggered PRESS localization and a prospective acquisition correction scheme (PACE) for respiratory triggering at end-expiration and ECG triggering to synchronize PRESS localization to mid-systole (TE = 35 ms; TR of 2.5–6 s depending on the respiratory rate; 4 times 8 scans per spectrum with water presaturation). Various proton groups of ICCL with contributing protons are indicated in red. (TMA: trimethylammonium group protons; Cr: methyl and methylene protons of creatine and PCr, methylene protons partially suppressed by water presaturation. Image courtesy of Roland Kreis, Bern University

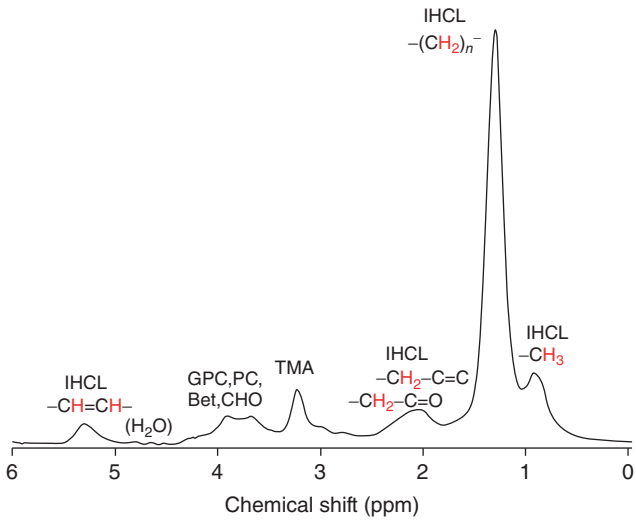

Figure 8. ^{1}H spectrum of human liver obtained at 3T (on a Siemens Trio system). This spectrum is an average of 28 individual spectra from eight subjects as part of a study on the effects of coffee consumption upon short-term fructose-induced liver insulin resistance and intrahepatocellular lipids (IHCL).[3] A region of interest of 19 cm^3 was localized in the liver evading = avoiding large vessels using PRESS localization combined with PACE (TE = 30 ms; TR = 2.5 to 6 s depending on the respiratory rate; 32 scans per spectrum, water presaturation). Various proton groups of IHCL with contributing protons are indicated in red. (GPC: glycerophosphoryl choline, non-TMA protons; PC: phosphoryl choline, non-TMA protons; Bet: betaine, non-TMA protons; CHO: carbohydrates like glucose, myo-inositol and potentially a fraction of glycogen; H_2O: position of residual water, which had been removed in postprocessing using Hankel–Lanczos singular value decomposition). Image courtesy of Roland Kreis, Bern University

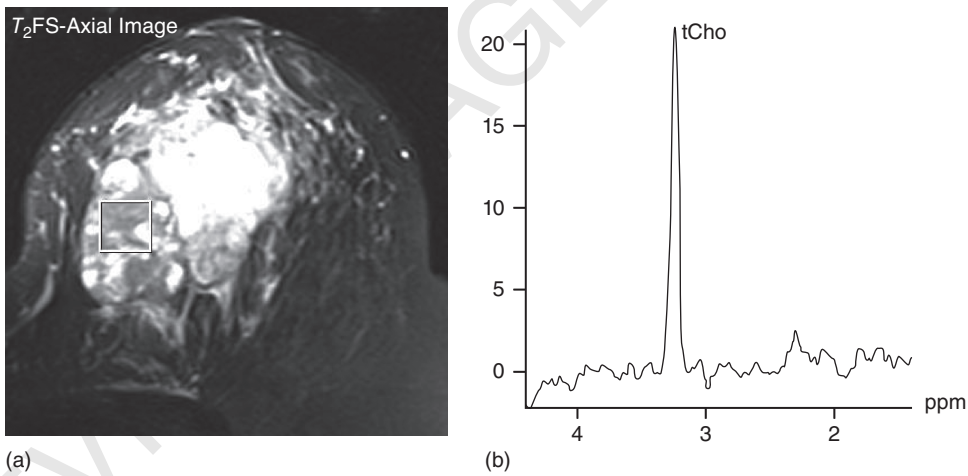

Figure 9. (a): Spin-spin relaxation (T_2)-weighted fat-saturated axial image acquired from a 45-year old women suffering with metaplastic breast carcinoma (MRI parameters: TR/TE = 6270/102 ms; slice thickness 3 mm with no gap; and matrix size = 512 x 440) showing the voxel (15 × 15 × 15 mm^3) location from a malignant tumor. (b) the corresponding ^{1}H spectrum showing the total choline (tCho) peak; acquired using PRESS (TR = 1500 ms; TE = 100 ms; number of sequence averages, NSA = 128; spectral width =1000 Hz; vector size = 1024 with a total acquisition time of 3.18 min). Image courtesy of N. R. Jagannathan, All India Institute of Medical Sciences, Delhi.

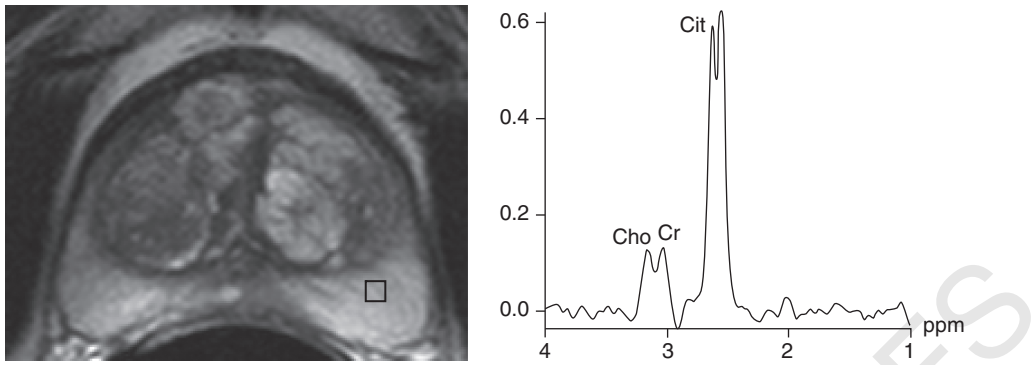

Figure 10. (a): T_2-weighted axial image of a normal prostate acquired on a 1.5 T MRI system (Sonata, Siemens, Germany) using an endorectal coil (MRI parameters were: TR = 5000 ms; TE = 107 ms, slice thickness = 5.0 mm. (B) In vivo ^{1}H spectrum acquired from the voxel shown in (A) in the peripheral zone (□). The acquisition employed a PRESS-localized three-dimensional magnetic resonance spectroscopic imaging (3D MRSI) sequence with a TR of 650 ms, TE of 120 ms and with a voxel size of 5mm x 5mm x 5mm (Cit: citrate; Cr: total creatine). Image courtesy of N. R. Jagannathan, All India Institute of Medical Sciences, Delhi.

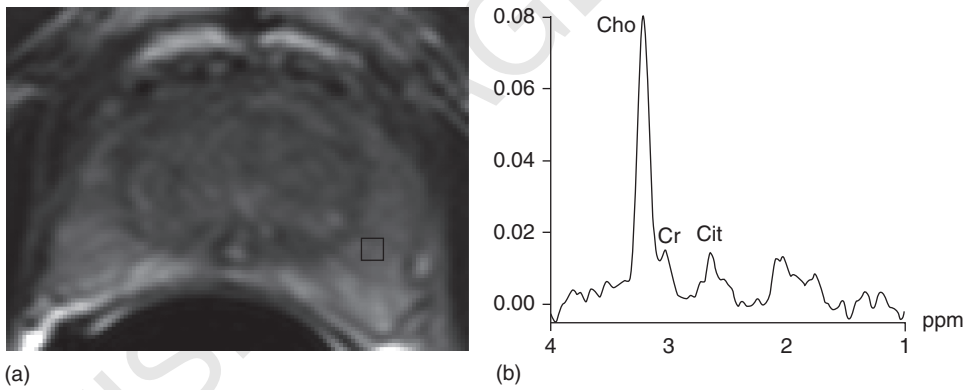

Figure 11. (a) T_2-weighted axial image of malignant prostate of a patient (prostate specific antigen, PSA = 7.8 ng/ml) acquired at 1.5 T MRI system (Sonata, Siemens, Germany) using an endorectal coil (MRI parameters TR = 3400 ms; TE = 93 ms with a slice thickness of 4.0 mm). (b) In vivo ^{1}H MR spectrum acquired from a voxel from the peripheral zone of prostate shown in (A). The acquisition was carried out using a PRESS localized 3D MRSI sequence with a TR of1300 ms and a TE of 120 ms. The voxel size used was 4mm x 6mm x 5mm (Cit: citrate; Cr: total creatine). Image courtesy of N. R. Jagannathan, All India Institute of Medical Sciences, Delhi.

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1. J. M. N. Duarte, L. Hongxia, V. Mlynárik, and R. Gruetter, *NeuroImage*, 2012, **61**, 342.
2. M. Ith, C. Stettler, J. Xu, C. Boesch, and R. Kreis, *NMR Biomed.*, 2014, **27**, 1285.
3. V. Lecoultre, G. Carrel, L. Egli, C. Binnert, A. Boss, E. L. MacMillan, R. Kreis, C. Boesch, C. Darimont, and L. Tappy, *Am. J. Clin. Nutr.*, 2014, **99**, 268.