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The Fast Spiral-SelMQC Technique for *In Vivo* MR Spectroscopic Imaging of Polyunsaturated Fatty Acids (PUFA) in Human Breast Tissue[‡]

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Abstract

The Selective Multiple-Quantum Coherence Transfer (Sel-MQC) method has been applied to image polyunsaturated fatty acids (PUFA) distributions in human breast tissues *in vivo* for cancer detection, with complete suppression of the unwanted lipid and water signals in a single scan. The Cartesian k-space mapping of PUFA *in vivo* using the Sel-MQC CSI technique, however, requires excessive MR scan time. In this article, we report a fast Spiral-SelMQC sequence employing a rapid spiral k-space sampling scheme. The Spiral-SelMQC images of PUFA distribution in human breast were acquired using two-interleaved spirals on a 3T GE Signa MRI scanner. Approximately 160-fold reduction of acquisition time was observed as compared to the corresponding Sel-MQC CSI method with an equivalent number of scans, permitting acquisition of high-resolution PUFA images in minutes. The reconstructed Spiral-SelMQC PUFA images of human breast tissues achieved a sub-millimeter resolution of 0.54×0.54 or $0.63 \times 0.63 \text{ mm}^2/\text{pixel}$ for FOV = 14 or 16cm, respectively. The Spiral-SelMQC parameters for PUFA detection were optimized in 2D Sel-MQC experiments to suppress monounsaturated fatty acids (MUFA) and other lipid signals. The fast *in vivo* Spiral-SelMQC imaging method will be applied to study human breast cancer and other human diseases in extracranial organs.

Keywords

fast MRSI; human breast cancer; PUFA; metabolite imaging

INTRODUCTION

The Selective Multiple-Quantum Coherence Transfer (Sel-MQC) methods were originally developed for *in vivo* detection of lactate in mammary tumor models, achieving complete suppression of lipid and water in a single scan (1). Several versions of Sel-MQC sequences have been published to achieve simultaneous detection of multiple metabolites (2,3). Sel-

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MQC methods have been applied to detect antineoplastic agents *in vivo* in tumor tissues (4). Multi-slice Sel-MQC methods have been developed for three-dimensional mapping of metabolites using the Hadamard Matrix approach (5–7). In addition, effective volume-localization of metabolite signals using Sel-MQC techniques was demonstrated by employing the spectral-volume selective 1331 pulses (8) and digitally optimized spatial-spectral RF pulses (9). Quantification of tissue metabolite concentrations may be achieved in part using T_1 - and T_2 -SelMQC sequences to determine the relaxation times of metabolite signals *in vivo* (10). An interesting application of the Sel-MQC methods is detection of glucose *in vivo* in diabetic animals (11) as well as Gamma-Amino Butyric Acid (GABA) and glutamate *in vitro* in brain tissue extracts (12). Recently, Sel-MQC technique has been applied to observe the spatial distributions of polyunsaturated fatty acids (PUFA) in human breast tissues (13). PUFA distribution patterns are sensitive to abnormal human breast tissue changes and malignant transformations (13). In animal tumor models, PUFA appear to be a potential biomarker of tumor progression (14,15) and may be used to monitor therapeutic responses (16–18). *In vivo* Sel-MQC metabolite imaging may be applied for early diagnosis of human breast cancer (19) and other extracranial cancers (20).

Single-scan two-dimensional Sel-MQC CSI mapping of metabolites and PUFA requires relatively long acquisition time (at least 10min for single-scan data acquisition) to image a sagittal slice of human breast tissue (13). The slow rate of the Cartesian k-space mapping in a Sel-MQC CSI experiment limits the spatial and temporal resolution of PUFA and metabolite imaging of human tissues *in vivo*. Rapid k-space mapping techniques may accelerate Sel-MQC data sampling rate. In this project, 2D spiral x- and y-gradients were employed to trace a spiral wave-form in the (k_x, k_y) -plane during the acquisition period replacing the discrete k_x and k_y in Cartesian mappings (21). Spiral-MRI has been implemented for fast cardiac imaging (22), time resolved MRA (23), and fMRI (24). Spectroscopic imaging with spiral-based k-space trajectories using spin-echo techniques was developed by Adalsteinsson *et. al.* to map brain metabolite distributions (25,26). In Spiral-SelMQC, pure PUFA signal was obtained by multiple-quantum editing and subsequently imaged by applying orthogonal gradient fields to define a spiral trajectory in k-space. A gridding algorithm was applied to resample the non-uniformly spaced data points in the plane of a k_z -slice onto a Cartesian grid. PUFA images were obtained by a two-dimensional Fast Fourier Transformation (FFT) of the re-gridded k-space. Since pure PUFA signal was used for spiral imaging with a complete suppression of water and unwanted lipid signals by Sel-MQC editing, it was unnecessary to sample data points along the t -axis to resolve NMR resonances. Compared to the corresponding Sel-MQC CSI experiment with an equivalent number of scans, the fast *in vivo* Spiral-SelMQC method reduced the PUFA imaging time by approximately 160-fold. Reconstructed PUFA images from human breast tissues were obtained with sub-millimeter resolutions using Spiral-SelMQC technique.

METHODS

A. Sel-MQC editing

The Spiral-SelMQC sequence consists of two parts – (a) Sel-MQC spectroscopic editing (1) to obtain uncontaminated PUFA or Monounsaturated Fatty Acids (MUFA) signal and (b) spiral k-space mapping of the PUFA signal (Fig. 1). Sel-MQC editing gives a pure PUFA (or MUFA) signal at 5.4ppm and suppresses water and unwanted lipid signals (1,13). Specifically, the olefinic methylene protons at 5.4ppm ($-\text{CH}=\text{CH}-$) in both PUFA and MUFA (15,27) are excited by the first slice-selective 90° pulse, and the allylic methylene protons of PUFA ($=\text{CH}-\text{CH}_2-\text{CH}=\text{}$) at 2.8ppm or MUFA ($-\text{CH}_2-\text{CH}_2-\text{CH}=\text{}$) at 2.2ppm are selectively excited by the second frequency-selective 90° pulse (Fig. 1). During the preparation time period τ after the slice-selective 90° pulse, the AX_2 spin system evolves according to the Hamiltonian containing chemical shift and J-coupling terms, $H = \omega_1 I_{1z} +$

$\omega_2 I_{2z} + 2\pi J_{12} I_{1z} I_{2z}$, where I_{1z} , I_{2z} are the z-angular momentum and ω_I and ω_2 are the chemical shifts of spin A and X, respectively, and J_{12} is the spin-spin coupling constant. The two-spin state is produced under the influence of the J-coupling Hamiltonian term to give the spin density matrix, $\rho = I_{1x} \cos(\pi J_{12}\tau) + I_{1y} I_{2z} \sin(\pi J_{12}\tau)$, where I_{1x} and I_{1y} are the x- and y-angular momentum of spin A and X, respectively. When $\tau = 1/2J_{12}$, I_{1x} evolves into the anti-phase magnetization $I_{1y} I_{2z}$. The second 90° pulse creates Zero-Quantum (ZQ) coherence, $I_1^+ I_2^-$, and Double-Quantum (DQ) coherence, $I_1^+ I_2^+$. Higher multiple-quantum coherences (MQC) are also present in lesser quantities (1). In contrast, magnetizations from water at 4.7ppm and lipid protons at 1.3ppm stay in single-quantum (SQ) state, which is dephased by MQ-selection gradients, $g_1:g_2:g_3 = 0:1:-2$. The frequency-selective 180° pulse applied at 5.4 ppm interchanges ZQ and DQ coherences during the MQ-evolution time delay, t_I , between the second and the last 90° pulses. The last 90° pulse converts the ZQ and DQ coherences into an anti-phase single-quantum (SQ) magnetization. In the detection period, the anti-phase magnetization evolves under the J-coupling Hamiltonian term into an in-phase magnetization to form a MQ-coherence transfer echo at $\tau' = (1/2J_{12})-t_I$ (1). The remaining magnetization is dephased by crusher gradients (G_{crs}) after data acquisition. A pair of spiral readout gradients (G_x , G_y) starting at the center of the MQ-coherence transfer echo of PUFA is applied to achieve rapid 2D k-space mapping in the selected slice. A t_1 -crusher gradient (g_1) and a pair of t_e -crusher gradients (g_{cr}) are also applied to spoil the unwanted multiple-quantum coherences and transverse magnetization created by imperfect RF pulses.

B. Spiral trajectory

Spiral trajectory generation occurs in three stages: (a) constant density spiral mapping in the center of k-space followed by (b) variable density spiral mapping in the slew rate limited case, and finally (c) variable density spiral mapping in the amplitude limited case. This sophisticated trajectory was designed to reduce spiral imaging (29) and motion artifacts (30).

a. Slew rate limited case—The Glover's constant density spiral trajectory (28),

$$k_c(\tau) = k_{max} \tau e^{i\omega_k \tau}, \tau \in [0, 1] \quad [1.1]$$

was used in our Spiral-SelMQC experiments to sample the k-space center with a constant sampling density, where k_{max} is the radius of the k-space coverage. $|k_c(0)|=0$ at the center of k-space when $\tau=0$, and $|k_c(1)|=k_{max}$ when $\tau=1$. For the slew rate limited case (28),

$$\tau(t) = \frac{\frac{1}{2}\beta t^2}{\omega_k \left(\frac{1}{q} + \frac{\beta t}{2\alpha} \right)}, \quad [1.2]$$

where $\alpha = \left(\frac{9}{4} \frac{s_m}{k_{max} \omega_k^2} \right)^{1/3}$, $\beta = \frac{s_m \gamma}{k_{max}}$, s_m is the maximum slew rate, and γ is the gyromagnetic ratio. The constant, $q=0.2$, controls the behavior of $\tau(t)$ when t is small. The gradient waveform $g(t)$ as a function of time is given by:

$$g(t) = \frac{k'(t)}{\gamma} = \frac{k'(\tau) \cdot \tau'(t)}{\gamma}. \quad [1.3]$$

As the formula of $k_c(\tau)$ implies, the radial distance $|k_c(\tau)| = k_{max}\tau$ is proportional to the angular distance $\theta = \omega\tau$ so that the distance between neighboring spiral lines is constant. In Spiral-SelMQC experiments for PUFA imaging, the spiral k-space density was set to 1.3 times the nominal density ($\Delta k' = 1.3\Delta k$, $\Delta k = 1/\text{FOV}$). As the trajectories reach a certain point in k-space ($\sim 25\% k_{max}$), the algorithm switched to a variable density trajectory in k-space given by:

$$k_r(\tau) = k_{max} f(\tau) e^{i\omega\tau}, f(\tau) = a\tau^2 + b\tau + c, \quad [1.4]$$

where $\tau \in [0,1]$ and a , b , and c can be solved using boundary conditions including the two trajectory switching points. In this way, the k-space center was oversampled and the sampling density gradually decreases toward outer k-space. At the end of the trajectories, the sampling density was about 0.7 times the nominal density.

C. Experimentals

MRI/MRSI experiments were conducted on a GE Signa LX 3T whole-body MRI scanner (version VH3) operated at the ^1H resonant frequency of 127.7MHz. The scanner was equipped with actively shielded gradients in all three directions (maximum gradient strength = $4.0 \times 10^{-2}\text{T/m}$). The Spiral-SelMQC sequence was implemented to selectively detect the olefinic methylene protons of PUFA at 5.4ppm, which were J-coupled with the allylic methylene protons of the unsaturated acyl chain at 2.8ppm. All RF pulses were 1-lobe 90° and 180° sinc pulses with pulse width of 11.7ms to achieve narrow-band frequency excitation. RF transmission frequency was centered on the intense lipid peak at 1.3ppm. This defined the offset excitation frequencies of the individual RF pulses and the receiver frequency (Fig. 1). In Spiral-SelMQC, the receiver frequency was set to 5.4ppm for PUFA imaging. The first slice-selective 90° pulse and the 180° pulse were applied at 5.4ppm with the other two 90° pulses at 2.8ppm. The Multiple-Quantum (MQ) evolution time (t_1) between the second and third 90° pulses was 33ms. The MQ-evolution period was surrounded by two t_e -crusher gradients ($g_{cr} = 0.3 \times 10^{-2}\text{T/m}$). Spiral gradient waveforms were generated in real time with a two-shot interleaved spiral implemented to acquire the spectroscopic images of PUFA in breast tissues. The T_1 relaxation delay $\text{TR} = 2\text{s}$. Total data points per spiral leaf were 2048 for a bandwidth of 125 kHz. FOV in different experiments varied from 12 to 20 cm. The acquired spiral data in k-space was gridded to a corresponding 2D data matrix ranging from 12×12 to 20×20 in size, and then interpolated onto a 256×256 Cartesian matrix. In the re-gridding process, the value at each trajectory point is radially-weighted and transferred to the neighboring points toward the center of k-space on the Cartesian grid (red region) (Fig. 1b). Thus, each Cartesian grid point may accumulate re-gridding values from several neighboring spiral segments (green region) (Fig. 1b). PUFA images were obtained by 2D Fourier transformation of the re-gridded Cartesian Matrix. Reconstructed spiral PUFA images of the human breast had a resolution of 0.54×0.54 or $0.63 \times 0.63\text{mm}^2/\text{pixel}$ for $\text{FOV} = 14$ or 16cm .

In each Spiral-SelMQC experiment, a one-dimensional (1D) Sel-MQC spectrum was acquired in the absence of the spiral imaging gradients (Fig. 1). Two-dimensional (2D) Sel-MQC experiments (1) were carried out to optimize the pulse sequence parameters for selective detection of a pure PUFA signal without contaminations from MUFA, water, or other unwanted lipid signals. In the 2D Sel-MQC experiment, the multiple-quantum evolution time, t_1 , between the second and the last 90° pulses was incremented by 0.5ms from 24ms to 56ms. Each FID was acquired with 2048 data points. The 2D Sel-MQC data matrix was subsequently converted into the frequency-domain spectrum by 2D FFT, giving separated cross peaks of PUFA at (2.8ppm, 5.4ppm) and MUFA (2.2ppm, 5.4ppm) away

from residue water or other lipid peaks (Fig. 2). Multiple-quantum selection gradients with an amplitude of $g_2=g_3=2.0 \times 10^{-2}$ T/m and durations $\delta_2: \delta_3 = 3\text{ms}:6\text{ms}$ were applied in opposite directions. The t_1 -crusher gradient of amplitude $g_1 = -3 \times 10^{-4}$ T/m and duration $\delta_1 = 3\text{ms}$ was applied between the second 90° pulse and the 180° pulse. The amplitude and duration of the pair of t_e -crushers (g_{cr}) were 3×10^{-3} T/m and 6ms, respectively. By shifting the RF frequency offsets of the two 90° pulses on the lipid allylic methylene protons at 2.8ppm, the 2D Sel-MQC sequence can be optimized to detect pure PUFA or MUFA (Fig. 2), which was demonstrated with a phantom of soybean oil (PUFA: MUFA = 3:1). The two-scan 2D Sel-MQC experiment took ~4min.

A three compartment phantom was constructed to demonstrate the Spiral-SelMQC imaging method using pure soybean oil, canola oil, and olive oil with the PUFA concentrations at a ratio of 4.5:2:1. Two inner tubes, each 3cm in diameter, were filled with soybean oil and olive oil and placed in a large beaker of canola oil. Thus, the outer phantom chamber had an intermediate concentration of PUFA. For comparison, two additional images of this phantom were also acquired using gradient echo (GRE) and spin echo (SE) sequences. In both GRE and SE experiments, matrix size = 256×256 , NEX = 1, FOV = 14cm. In the GRE experiment, the echo time TE = 3.7ms, RF pulse flip angle = 30° , TR = 20ms, and scan time = 5.3s. In the SE experiment, TE = 30ms, TR = 2s, and scan time = 4.3min.

Five healthy female volunteer subjects were recruited to demonstrate the feasibility of the Spiral-SelMQC method. Each woman was positioned prone (head first) in the GE 3T magnet, and her tested breast placed inside the transmit/receive breast coil constructed in-house (32). Three-dimensional anatomical structure of the breast was imaged using a fast SE or fast GRE sequence. PUFA was then mapped from one or two 1cm sagittal breast tissue slices using the Spiral-SelMQC sequence with optimized parameters from the 2D Sel-MQC experiments. The number of scans (NEX) in various Spiral-SelMQC experiments was set between 16 and 128 with a corresponding total scan time ranging from 1 to 8 min. The corresponding single-scan Spiral-SelMQC imaging of PUFA was only 4s. This is about a 160-fold scan time reduction as compared to the Sel-MQC CSI experiment using an equivalent number of scans. The PUFA images were processed using Matlab 6.5 (MathWorks). Each Spiral-SelMQC map of PUFA was subsequently superimposed to the corresponding anatomical GRE or SE image acquired from the same breast tissue slice. All procedures for human subject investigation were approved by the Institutional Review Board (IRB) at the University of Pittsburgh.

RESULTS

A. Phantom studies

a. Optimization of PUFA detection with 2D Sel-MQC—A 2D Sel-MQC sequence was employed to optimize the sequence parameters for PUFA selection. To minimize the RF “bleeding” excitation outside the specified excitation bands, the offset frequencies of the two 90° pulses at 2.8ppm were adjusted independently in the 2D Sel-MQC experiment for exclusive PUFA observation without contamination from MUFA or *vice versa* (Fig. 2). When the excitation frequency of the second 90° pulse was decreased by 140Hz, the offset frequency of the last 90° pulse was shifted by -140Hz , 0Hz (on resonance), and $+140\text{Hz}$ (Fig. 2a, b, c). The pure MUFA cross peak at (5.4ppm, 2.2ppm) emerged with the offset combination (-140Hz , -140Hz) when the residual lipid peaks were reduced to minimum (Fig. 2c). Similarly, when the second 90° pulse was increased by 140Hz, the last 90° pulse was shifted by -140Hz , 0Hz , and $+140\text{Hz}$ (Fig. 2d,e,f). The J -coupled spin pair of PUFA (5.4ppm, 2.8ppm) was selected in the 2D Sel-MQC experiments as the signals from other resonances were minimized with the offset frequencies (-140Hz , $+140\text{Hz}$). The number of data points from each FID was 2048 in the first dimension, with 64 increments in the second

dimension. NEX = 2, TR = 2s. The data was acquired from a 2cm coronal slice of the soybean oil phantom.

b. Spiral-SelMQC imaging—A three compartment phantom containing soybean oil, canola oil, and olive oil with a PUFA concentration ratio of 4.5:2:1 was used to demonstrate the Spiral-SelMQC sequence. Data was acquired from a 1cm coronal slice of the phantom (Fig. 3a). FOV = 14cm. Two spiral interleaves with 2048 data points each were applied to map k-space. NEX = 16, TR = 2s, and scan time = 1 min. The Spiral-SelMQC image gave a distinctive PUFA contrast among the three phantom compartments, signal intensity reflecting the different PUFA concentrations. In contrast, the GRE (Fig. 3b) and SE (Fig. 3c) images from the same slice presented minimum or no difference in signal intensities in the three different phantom compartments.

B. *In vivo* studies using healthy human volunteer subjects

a. 1D Sel-MQC PUFA spectra of human breast tissue—Since residual magnetizations from signals other than PUFA can contaminate the images obtained by a Spiral-SelMQC experiment, it is crucial to optimize the performance of water and lipid suppression in the 1D and 2D Sel-MQC experiments before imaging human subjects. Pure PUFA signal at 5.4ppm was acquired from a 1cm breast tissue slice of each subject in the 1D Sel-MQC experiments (16K data points). Two typical 1D Sel-MQC spectra from a 43-year-old and a 40-year-old woman are presented as examples (Fig. 4). Water and other lipid signals including the intensive lipid resonance at 1.3ppm and MUFA at 2.2ppm were completely suppressed. Again, the offsets of the second and last 90° pulses on 2.8ppm were optimized for PUFA detection in a 2D Sel-MQC experiment. The cross peak of PUFA at (5.4ppm, 2.8ppm) or MUFA at (5.4ppm, 2.2ppm) was observed dominating the 2D-SelMQC spectra from human breast tissues at the same optimal offset frequencies as in the phantom experiments (data not shown). The MQ-evolution time t_1 = 33ms, NEX = 8, and TR = 2s.

b. Spiral-SelMQC imaging of human breast tissues—*In vivo* Spiral-SelMQC imaging of PUFA distributions of healthy human breast tissues was carried out using five female volunteer subjects. PUFA images were obtained from one or two 1cm sagittal slices of the selected breast of each subject, with 2048 data acquisition points per spiral interleaf. TR = 2s. The re-constructed 256×256 high-resolution PUFA images (Fig. 5, green images) were superimposed on the corresponding fast GRE anatomical images (Fig. 5, red background) acquired from the same tissue slices. The center of the PUFA echo (the MQ-coherence transfer echo) was ~25ms away from the starting point of the spiral image acquisition, corresponding to the center of k-space. Four PUFA images from three volunteer subjects are displayed as examples (Fig. 5). (i) PUFA images were obtained from a center breast tissue slice and an off-center slice of a 43-year-old subject (Fig. 5a&b). FOV = 14cm, NEX = 64, scan time = 4.3min. (ii) The PUFA distribution was mapped in breast tissue from an off-center slice of a 40-year-old healthy woman (Fig. 5c) using the following Spiral-SelMQC parameters: FOV = 16cm, NEX = 128, and scan time = 8.5min. (iii) Similarly, PUFA distribution was imaged from the breast tissue of a 31-year-old woman (Fig. 5d). FOV = 14cm, NEX = 128, and scan time = 8.5min. In the GRE experiments, matrix size = 256×256, NEX = 1, TE = 3.7 ms, and TR = 20ms. PUFA signals in these individuals mostly originated from the fatty tissues, although PUFA signals were also detected in other regions throughout the women's breast tissues (Fig. 6a) (13,21).

DISCUSSION

The combination of the Sel-MQC spectral editing and spiral readout gradients for fast *in vivo* spectroscopic imaging has been demonstrated by Spiral-SelMQC experiments for

PUFA detection in human breast tissues. Spiral k-space mapping has the advantage of starting data acquisition from the center of k-space, which defines the main features of the image (in low resolution). Sel-MQC spectral editing pulses and coherence selection gradients produced a multiple-quantum coherence transfer echo exclusively from PUFA magnetization, with complete suppression of MUFA, water, and unwanted lipid signals. Since only one resonance peak (e.g., PUFA) was selected for signal acquisition and spectroscopic imaging, fast SelMQC imaging would not encounter signal cancellations due to destructive interferences of multiple metabolite signals in different phases. Spiral-SelMQC technique may be applied to detect metabolites or antineoplastic agents one at a time in a clinically feasible time frame. Because sampling along the time axis was unnecessary to resolve multiple metabolite signals in PUFA imaging, the length of the spiral readout was not determined by the spectral width. Consequently, the parameters of the spiral readout such as resolution, the number of interleaves, and oversampling factors can be selected to enhance image quality without consideration of resolving multiple spectral peaks in the frequency domain. The length of the spiral readout was determined only by the relaxation rate of the PUFA or the metabolite signal for detection. In addition, the Spiral-SelMQC sequence did not require any spatial saturation pulses or CHESS pulses for water suppression (33). Thus, RF absorption resulting from the four RF pulses in Sel-MQC was minimal as compared to other MRSI methods. For TR = 2s, the active scan time of the Spiral-SelMQC sequence was less than 200ms. Therefore, the Specific Absorption Rate (SAR) of this sequence was adequate for human PUFA imaging *in vivo*.

As observed in the PUFA images from a 1 cm breast tissue slice of a 25-year-old woman carrying a silicone implant, residual signals from water or lipid resonances may generate artifacts to obscure the image interpretations (Fig. 6a). We have performed computer analysis to evaluate possible Spiral-SelMQC artifacts produced from residual lipid signals at 1.3ppm (the most intensive lipid peak) in the PUFA imaging of human breast tissues. We found that the residual lipid peak at 1.3ppm (up to 20%) would not severely distort PUFA images due to the off-resonance effect in spiral imaging. In addition, the computer simulations as described in this section indicated that two spiral interleaves were optimal for Spiral-SelMQC imaging of PUFA in human breast.

a. Number of Spiral Interleaves

Spiral sampling requirements can be mathematically satisfied with any given number of spiral interleaves. To evaluate how well small structures can be resolved with different numbers of interleaves in Spiral-SelMQC, computer simulations were performed to image a disc having an 8cm diameter and three small holes (diameter = 1cm) (Fig. 6b). Spacing between the neighboring small holes was 1cm. An analytical function in k-space can be used to simulate the disc or a hole as follows:

$$F_{2D}[circ(r)] = \frac{J_1(2\pi\rho)}{\rho} \equiv jinc(\rho), \rho = \sqrt{k_x^2 + k_y^2}, r = \sqrt{x^2 + y^2}, \quad [2.1]$$

where $circ(r)=1$, when $r = (x^2 + y^2)^{1/2} \leq 1$, and $circ(r)=0$, otherwise. k_x and k_y are coordinates in k-space and ρ is the radius in k-space. J_1 is a Bessel function of the first kind,

$$J_\alpha(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m+\alpha+1)} \left(\frac{x}{2}\right)^{2m+\alpha}, \text{ where } \alpha = 1 \text{ and } \Gamma(z) \text{ is the Gamma function, and } F_{2D} \text{ signifies a 2D Fourier transformation.}$$

A set of k-space trajectories was generated for evaluation with the following imaging parameters: FOV=16, matrix size = 32×32, and the oversampling factor was 1.2 at the center

of k-space. The trajectories differed in the number of interleaves (nl) and the lengths of the trajectories (δt). Four different spiral trajectories ($nl = 1, 2, 12$, and 64 and $\delta t = 3230, 1610, 404$, and 252 , respectively) are analyzed as illustrations. Mathematically, each spiral trajectory contains nl arrays of k-space coordinates (k_x, k_y). Experimentally, the k-space points in a spiral trajectory were generated linearly in the time domain at a rate of $4\mu\text{s}/\text{pts}$. Assuming $T_2^* = 8\text{ms}$ for PUFA in human breast tissues, the estimated k-space data points are

$$s_{nl}(i) = \sum_p \text{jinc}_p(k_x(i), k_y(i)) \cdot \exp\left(\frac{-i\delta t}{T_2^*}\right) + N(SNR_u \cdot \sqrt{NEX_{nl}}), \quad [2.2]$$

where the normalized SNR is defined by

$$SNR_u = \frac{\langle s(t) \rangle}{\sqrt{\langle s(t) - \bar{s} \rangle^2 \cdot \sqrt{NEX}}} \quad [2.3]$$

as a function of the mean of signal $\bar{s} = \langle s(t) \rangle$, the standard deviation (STD) $= \sqrt{\langle s(t) - \bar{s} \rangle^2}$ and number of scans (NEX). Summation of *jinc* functions represents the target image (Fig. 6b). Each disc or circular hole in the image is represented by a *jinc* function distinguished by an index p in Eq. 2.2. The *jinc* functions are weighted, scaled and phase shifted in k-space to represent different amplitudes, sizes, and locations in image space. The added White Gaussian Noise, N , represents a Gaussian noise source with amplitude controlled by SNR that increases with NEX (Eq. 2.3). NEX, on the other hand, is determined by nl . For example, when $nl=1$ and NEX is chosen to be 64, the total number of acquisition points is 64. When $nl=2$, the total number of acquisition is fixed at 64 and $NEX = 32$. When $nl=32$, each spiral interleaf is only repeated twice ($NEX = 2$). The value of SNR_u is set as 1.13.

The k-space data of the targeted image was simulated using 12 sets of spiral trajectories (data not shown), and the same spiral reconstruction program was used to construct the final images as in the Spiral-SelMQC experiments. Four examples are plotted in Fig. 7 as simulations resulting from the four corresponding trajectories of spiral interleave numbers 1, 2, 12, and 64. The one-shot spiral image lost the high resolution information to resolve the three dots of 1 cm in diameter due to the long spiral readout (Fig. 7a). Significant resolution improvement from $nl=1$ to $nl=2$ was observed when the spiral readout length was cut in half (Fig. 7b). Three dots of 1cm in diameter with 1cm spacing were resolved when $nl = 2$, as is the case when $nl = 12$ (Fig. 7c) and $nl = 64$ (Fig. 7d). Based on the computer simulation results, there is no significant advantage to an imaging resolution with $nl=12$ or $nl=64$ over $nl=2$. In the Spiral-SelMQC experiment, we chose $nl=2$ for PUFA imaging in human breast tissues.

b. Off-resonance artifacts

In Spiral-SelMQC experiments, the major potential contamination source for the PUFA imaging artifacts is the possible residual lipid peak at 1.3 ppm (offset frequency = 530 Hz). Computer simulations were carried out in typical experimental conditions at 3T to estimate the artifacts generated in a Spiral-SelMQC image of PUFA at 5.4 ppm. In an MRI Cartesian mapping of k-space, an off-resonance signal source would result in a spatially shifted image (e.g., chemical shift artifact). The direction of the spatial shift is determined by the readout gradient direction in an imaging experiment (i.e., the linear frequency-encoding direction in k-space mapping). In spiral imaging, however, the off-resonance source would produce

artifacts of image blurring. To illustrate this, we simulated a contaminated spiral image of a circular disc object represented by $\text{circ}(r)$ in the image space, where the image intensity is 1 within radius r and 0 outside r . The 2D Fourier Transform of the function $\text{circ}(r)$ in k-space gives $jinc(\rho)$ as described in Eq. 2.1, where $J_1(2\pi\rho)$ is a Bessel function of the first kind, and

$\rho = \sqrt{k_x^2 + k_y^2}$ is the radius of the k-space. The k-space sampling values can be generated analytically according to Eq. 2.1 with k-space coordinates (k_x, k_y) . When these k-space samples were acquired on resonance, the result of the analytical formula simulated the k-space value correctly (Fig. 8a). It should be noted that the spectral noise and spin relaxations were neglected in the simulation. When the data were acquired off-resonance, the signal would be modulated by a phase factor $e^{-i2\pi\Delta f t}$ as a function of the offset frequency Δf , where t is the sampling time in k-space. In spiral imaging, t is proportional to the length of the spiral path traveled from the k-space center along the trajectory. During the image reconstruction process, each data point along a spiral trajectory was re-gridded onto a Cartesian matrix (Fig. 1b), which was subsequently Fourier transformed to form the final image in Cartesian coordinates.

When a spiral image was generated as an off-resonance source in image space, the phase factor $e^{-i2\pi\Delta f t}$ that modulates the k-space signal was carried over to the Cartesian locations through the re-gridding process. The final value at a Cartesian data point combined contributions from several nearby spiral segments with different phases. Consequently, image intensity was reduced due to destructive superimpositions of signals from different spiral segments. For comparison, spiral images were simulated from the same disc with off-resonances of 0Hz, 530Hz, and 1060Hz. The on-resonance image correctly displayed the shape of the disc (Fig. 8a). In the off-resonance images, the disc “smeared out” over a larger region, with increasingly reduced signal intensity in the disc region as the off-set frequency value increased from 530Hz (Fig. 8b) to 1060Hz (Fig. 8c). Thus, the off-resonance 1.3ppm lipid peak as an imaging contamination source to the on-resonance PUFA image in Spiral-SELMQC would not cause severe artifacts in PUFA mapping.

To demonstrate this effect, the circular disc having an 8cm diameter was used again with a normalized signal intensity of 1.0 (Fig. 6b). In the lower right corner, there were three small discs with diameters of 1cm and signal intensities of -0.5 . An additional circular signal source of intensity 0.2 (diameter = 1.5cm) (Fig. 8) was inserted as a contamination signal source into the upper left corner of the 8cm disc. FOV = 16cm. If the contamination signal was set on-resonance, the acquired image gave a “bump” at the correct location of the contamination source (Fig. 9a). The one-dimensional projection profile of the contaminated image correctly reflected the increased image intensity of $\sim 20\%$ at the location of the contamination source. On the other hand, if the signal source of this disc was set +530Hz off-resonant from the center frequency, the contamination signal source appeared to “smear out” with greatly reduced signal intensity (Fig. 9b). This suggests that when 5.4ppm PUFA is set as the center frequency for spiral imaging, less than 20% contamination from the residual lipid signal at 1.3ppm would not severely affect PUFA imaging features in Spiral-SELMQC experiments at 3T. This reduction of the contamination signal is proportional to the off-resonance frequency. The further away the contamination signal is from the center frequency, the greater the “smearing” effect. Thus, for PUFA imaging at the higher magnetic field (e.g., 7T), more artifact reduction would be observed from the residual lipid resonance at 1.3ppm. Of course, the off-resonance contamination signals would contribute to the spiral imaging noise.

CONCLUSION

A fast Sel-MQC sequence with a spiral k-space sampling scheme was demonstrated to selectively detect PUFA or MUFA signals in tissues containing high fat concentration. Spiral-SelMQC maps of PUFA distributions in human breast tissues were obtained *in vivo* with approximately 160-fold imaging time reduction compared to Sel-MQC CSI experiment with an equivalent number of scans (13). Thus, fast Sel-MQC spectroscopic imaging techniques may be applied for time-resolved acquisitions to study metabolic processes in human breast cancer or other human diseases in extracranial organs. Spiral-SelMQC parameters can be optimized using 2D Sel-MQC techniques to suppress MUFA and other unwanted lipid and water signals. Metabolites with coupled spins (e.g., lactate) or antineoplastic agents may be imaged similarly within a clinical time limit. The effective Sel-MQC selection of PUFA, MUFA, or metabolite signals depends on their chemical shift differences at high field MRI systems (>2.1T). We are currently developing multiple-quantum spin editing methods that can be applied to 1.5T MRI scanners used in most hospitals. Other fast data acquisition techniques may also be employed—e.g., echo-planar methods (34,35) may be applied to detect multiple metabolites simultaneously in the Sel-MQC methods. On modern MRI scanners equipped with multiple coil array devices, SENSE (36,37), SMASH (38), and GRAPPA (39) or other parallel imaging techniques may be employed in Sel-MQC spectroscopic imaging to further improve spatial and temporal resolution of PUFA and metabolite mapping in human breast tissues (40) or other extracranial organs with complete suppression of unwanted lipid and water signals.

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Fig. 1.

(a) A pulse sequence diagram of the Spiral-SelMQC spectroscopic imaging method. The first 90° slice-selective pulse excites all proton resonances in the entire spectrum. The second and the last 90° frequency-selective pulses excite the allylic methylene protons of PUFA ($=CH-CH_2-CH=$) at 2.8ppm or MUFA ($=CH-CH_2-CH_2-$) at 2.2ppm. The second 90° pulse converts the anti-phase magnetization into the MQC and the last 90° pulse converts the MQC into the anti-phase SQ transition to form an MQ-coherence transfer echo for PUFA or MUFA detection at 5.4ppm, respectively. The 180° frequency-selective pulse excites the PUFA olefinic methylene protons ($-CH=CH-$) at 5.4ppm and interchanges the DQ and ZQ coherence transfer pathways. In the two-dimensional Sel-MQC experiment without application of the spiral gradients, the MQ-evolution period, t_1 , between the second and the last 90° pulses is incremented to generate discrete sampling points in the second frequency dimension. (b) A schematic diagram to illustrate the Spiral-SelMQC re-gridding process in image reconstruction. The value at each spiral trajectory point is radially-weighted and transferred to the neighboring points toward the center of k-space on the Cartesian grid (red region). Each Cartesian grid point accumulates the re-gridding values from several neighboring spiral segments (green region).

Fig. 2.

A series of 2D Sel-MQC spectra from a soybean oil phantom (PUFA: MUFA = 3:1) to demonstrate the experimental optimization procedures for selective MUFA (a, b, c) or PUFA detection (d, e, f). The offsets from the nominal excitation frequencies of the second and last 90° pulses were gradually changed as labeled on the horizontal axes of the 2D spectra. Data was acquired from a 2cm coronal slice of the soybean oil phantom with 2048 sampling points in the first dimension and 64 increments in the second dimension. NEX = 2, TR = 2s, and total experimental time was 256s. The residual unwanted signals diminished as the two 90° pulses reached optimal offset frequencies (-140Hz , -140Hz) for MUFA detection (c) or ($+140\text{Hz}$, -140Hz) for PUFA detection (f).

Fig. 3.

Spiral-SelMQC, gradient echo and spin echo images acquired from a three-compartment phantom containing soybean oil, canola oil, and olive oil with a PUFA ratio of 4.5: 2: 1, respectively. (a) The Spiral-Sel-MQC experiment detected the different PUFA concentrations in the three phantom compartments. FOV = 14cm, NEX = 16, and TR = 2s, and the total scan time = 64s. Two spiral interleaves were used in the spiral trajectory for k-space mapping, with 2048 data points acquired in each spiral interleaf. (b) The Gradient Echo image did not reflect the PUFA concentration in the three phantom compartments, but provided a slight proton image contrast mostly due to small differences in proton relaxation times of the different oils. FOV = 14cm, slice thickness = 1cm, matrix size = 256×256, TR = 20ms, NEX= 1, TE = 3.7ms, RF pulse flip angle = 30°, and scan time = 5.3s. (c) The spin echo image gave no image contrast among the three phantom compartments. Matrix size = 256×256, FOV = 14cm, slice thickness = 1cm, NEX =1, TE = 30ms, TR = 2s, and scan time = 4.3min.

Fig. 4.
In vivo 1D Sel-MQC spectra of the PUFA signals from 1cm sagittal breast tissue slices of (a) a 43-year-old and (b) a 40-year-old healthy woman. NEX = 8, the number of data points acquired was 16,384, TR = 2s. Residual MUFA or other unwanted lipid and water signals were not detected.

Fig. 5.

In vivo Spiral-SelMQC PUFA images (green) from healthy female volunteers overlaid on the corresponding GRE anatomical breast images (red) from the same sagittal slices (1 cm). The PUFA images from (a) a center and (b) an off-center breast tissue slice of a 43-year-old subject. The Spiral-SelMQC parameters were: FOV = 14cm, TR = 2s, NEX = 64, and scan time = 4.3min. The parameters in the fast GRE experiment were: RF pulse flip angle = 30° , matrix size = 256×256 , NEX = 1, FOV = 14cm, TE = 3.7ms, and TR = 20ms. (c) An off-center breast imaging slice of a 40-year-old healthy volunteer. The Spiral-SelMQC parameters: FOV = 16cm, NEX = 128, and scan time = 8.5min. The fast GRE image from the same breast tissue slice was obtained using the same FOV, NEX = 1, RF flip angle = 30°

and matrix size = 256×256 . TE = 3.6ms, and TR = 20ms. (d) The PUFA mapping from a 1cm off-center breast tissue slice of a healthy 31-year-old woman. In the Spiral-SelMQC experiment, FOV = 14cm, NEX = 128, and scan time = 8.5min. In the fast GRE experiment, matrix size = 256×256 , NEX = 1, FOV = 14cm, TE = 3.7ms, and TR = 20ms.

Fig. 6.

(a) The Spiral-SelMQC image of PUFA (red) from a 1cm center breast slice of a 25-year-old healthy subject carrying a silicone implant was superimposed on the background (grey) fast GRE image from the same breast tissue slice. The GRE parameters were: matrix size = 256×256 , FOV = 20cm, RF flip angle = 30° , TE = 3.5ms, TR = 34ms, and scan time = 8.9s. The Spiral-SelMQC parameters: FOV = 14cm, NEX = 32, TR = 2s, 2048 data points were acquired in each of the two spiral interleaves. The total scan time is 2.2min. The routine PUFA-scanning Spiral-SelMQC parameters did not completely suppress the water signal from the silicone implant and produced spiral artifacts (arrow). (b) An 8cm disc with three 1cm holes as a target image to evaluate spiral imaging resolution and artifacts in computer simulations. The neighboring small holes were separated by 1cm.

Fig. 7.

The four simulated spiral images using the four spiral trajectories with (a) 1, (b) 2, (c) 12, and (d) 64 spiral interleaves and $T_2^* = 8\text{ms}$. (a) The single-shot spiral image lost the high-resolution information and did not resolve the small holes. The images simulated using (b) 2, (c) 12 and (d) 64 interleaves have an improved resolution of the small holes. The presence of the mild Gibbs ringing artifacts (the small bright edge around the circles) indicates that the image resolution of 32×32 was too low to resolve the sharp edges of the circular patterns.

Fig. 8.

The computer simulations to evaluate the off-resonance effects in Spiral-SelMQC imaging of PUFA spatial distributions. The simulated spiral images from the same circular disc acquired with 3 different off-resonance values: (a) The on-resonance disc gave a correct image matching the original object. (b) When off-resonant frequency $\Delta f = 530\text{Hz}$, the intensity of the disc smeared out over a larger imaging region than the original object. (c) When $\Delta f = 1060\text{Hz}$, the simulated image contained ringing artifacts to cover a much larger region than the real object with reduced signal intensity.

Fig. 9.

The computer simulation of offset artifacts in Spiral-SelMQC imaging of PUFA from assumed 20% residual signal of the 1.3ppm lipid peak with an offset frequency $\Delta f = 530\text{Hz}$ at 3T. The simulated spiral images from an 8cm disc contained a contamination source in the upper left corner at different offset frequency, Δf . (a) The signal intensity profile was obtained along the dash line across the on-resonance contamination source ($\Delta f = 0\text{Hz}$) in the simulated spiral image. When $\Delta f = 0\text{Hz}$, the spiral image contains a bright artifact with increased signal level at the position of the contamination source. (b) If the contamination source had an off-resonance frequency $\Delta f = 530\text{Hz}$, however, the image intensity profile obtained along the dash line across the same contamination source in the spiral image presented much reduced artifact contribution due to the off-resonance smearing effect in spiral imaging. Thus, the residual 1.3ppm lipid peak represented by the object at $\Delta f = 530\text{Hz}$ did not cause severe distortions of the PUFA images represented by the 8cm disc.