High Field Parahydrogen Induced Polarization of Succinate and Phospholactate

Supplementary Information

1. ^{1}H PASADENA Spectra of Succinate and the ^{13}C Isotope Effect

Experimental and theoretical PASADENA spectra of SUC were compared to estimate the difference in Larmor frequency Δ_{CS}. After hydrogenation, a single 45° ^{1}H excitation was applied and the ^{1}H NMR signal was recorded (no decoupling during hydrogenation; Equations 2,3, and 7 in the main text). The experimental spectrum was acquired on an NMR spectrometer (Avance 3 HD 300 MHz, Bruker, Germany) using a dual-channel ^{1}H/broad band probe head (5mm PA BBO 300S1 BBF-H-D-05-Z) at a magnetic field of 7 T. The experimental spectra was compared to simulated spectra with and without the ^{13}C isotope effect including singlet-triplet mixing (Figure S1). When an isotope effect with Δ_{CS} = 4 Hz was considered, a better match was found.

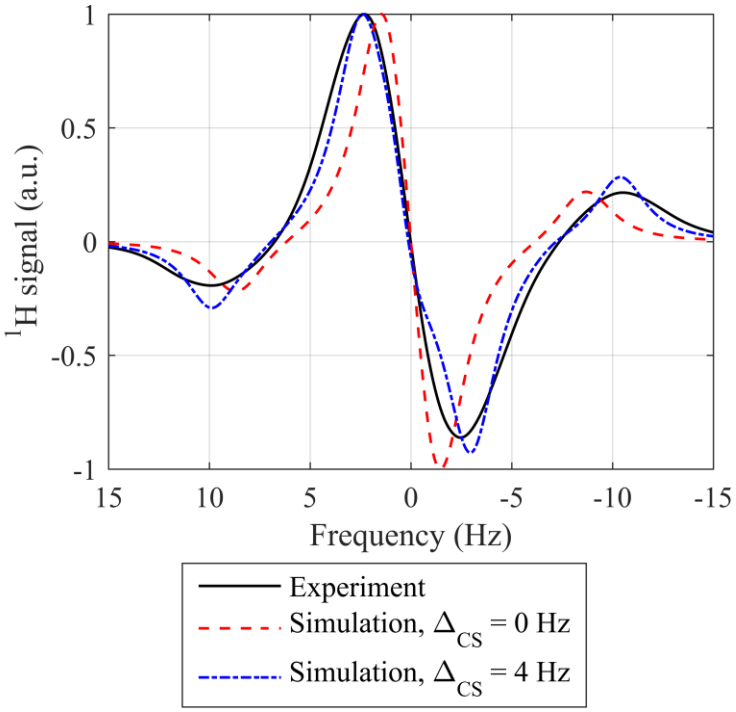

Figure S1: ***Centered Experimental and theoretical PASADENA spectra of SUC.*** *The ^{1}H signal was acquired after hydrogenation with pH_2 and a single 45° ^{1}H excitation (black). The experimental spectrum was compared to simulated PASADENA spectra neglecting (red line) or considering the isotope effect (blue line).*

2. Quantification of the PEP to PLAC Conversion by NMR Spectroscopy

After a hyperpolarization experiment with PEP/PLAC on the MRI system, a ^{13}C NMR spectrum (900 averages, 45° excitation, and 30 s repetition time) was acquired in thermal equilibrium of the same sample (Figure S2). The signal intensities of the PEP and PLAC resonances at 171 ppm and 181 ppm, respectively, were compared and a 63 % conversion from PEP to PLAC was found.

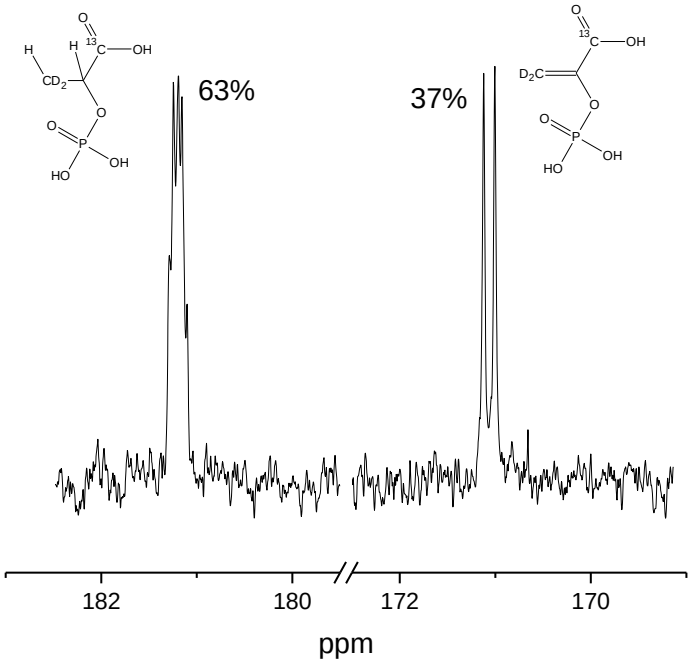

*Figure S2: **^{13}C NMR spectrum of the PEP/PLAC sample after a hyperpolarization experiment.** The signal intensities of the PLAC resonance at 181 ppm and PEP resonance at 171 were compared.*

3. ***Measurements of the Relaxation Times of PLAC***

The ^{13}C T_1 relaxation times of PEP and PLAC were measured in an inversion recovery experiment (8 averages, 50 s repetition time, and ^{1}H decoupling). The T_1 relaxation times read (62 ± 10) s for PEP and (31.0 ± 1.0) s for PLAC (Figure S3). The T_2 relaxation time was determined as (1.6 ± 0.5) s in a CPMG experiment (1 ms refocusing).

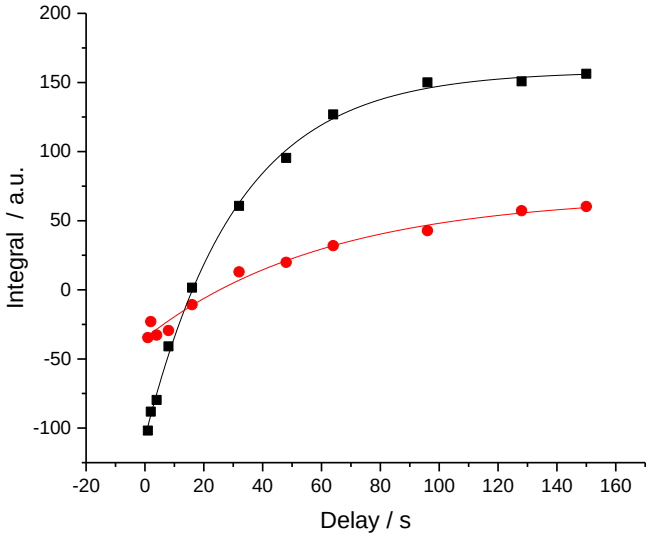

Figure S3: ***Inversion recovery experiment to determine the ^{13}C T_1 relaxation times of PEP and PLAC.*** *The relaxation times were quantified to (62 ± 10) s for PEP (red line) and (31.0 ± 1.0) s for PLAC (black line).*

The ^{1}H T_1 relaxation times of both PLAC-protons were determined by an inversion recovery experiment (8 averages, 15 s repetition time, and ^{2}H decoupling). The values read (6.8 ± 0.4) s and (5.5 ± 0.7) s (Figure S4). The T2 relaxation time of the methyl proton was measured as (3.5 ± 0.2) s in a CPMG experiment (20 ms refocusing).

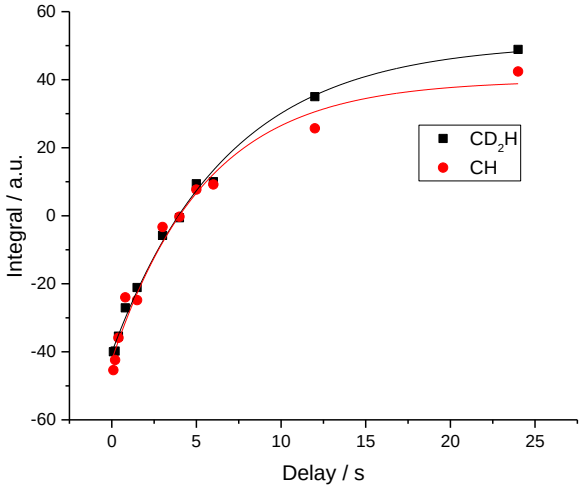

Figure S4: ***Inversion recovery experiment to determine the ^{1}H T_1 relaxation times of the PLAC-protons.***