**INTRODUCTION**

Random translational motion, diffusion, is the main form of transport in biological and chemical systems. Diffusion measurements are used to study intermolecular interactions, binding and self-association. NMR Diffusion measurements are conducted using a variety of spin-echo sequences. Precise measurements are critical for an accurate analysis of molecular interactions.

$J$-coupling occurs between nuclei due to magnetic interactions and is present in almost all molecules, especially complex biological molecules. Signals are split depending on the number of spins interacting and the strength of the interaction. Homonuclear $J$-couplings cause undesirable distortion of signals in diffusion measurements due to the mixture of in-phase and anti-phase magnetisation created during spin-echo.

The purpose of this project is to construct a pulse sequence for diffusion measurements that is less sensitive to $J$-coupling distortions than other currently available pulses.

**THEORY**

1. Trim pulses are used in a TOCSY (total correlation spectroscopy) experiment to remove anti-phase magnetisation. Adding the spin-lock trim pulse to a spin-echo sequence could lead to a reduction in anti-phase magnetisation in the spectrum.

2. Composite radio-frequency (RF) pulses have previously been used to compensate for errors in RF pulses and magnetic fields. A $180^\circ_x$ pulse is replaced by a group of 3 pulses $90^\circ_x-180^\circ_y-90^\circ_x$, with minimum delay in between pulses, whereby the $180^\circ_y$ pulse minimises errors. This type of RF pulses can be used as templates for creating $J$-compensated sequences, which may produce less anti-phase magnetisation in a spin-echo sequence.

2-Propanol has been chosen to illustrate the relationship between the time given for diffusion and distortions in the spectra. The spectrum with its simple well spaced peaks and $J$-constant of approximately 6.2 Hz is an ideal molecule to determine any reductions on distortions by different pulse sequences.

**RESULTS**

![Fig 1: Spin-echo sequence with spin lock component ($\Psi$) added](image1)

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![Fig 2: Water fall plot of 2-Propanol after spin-echo with varying values of $J$ (from 0 to 1/4J), (a) with spin lock (p17 = 2.4 ms and p10 = 7.04 dB) and (b) without spin lock (p17 = 0 and p10 = 0) (a)](image2)

Fig 2: Water fall plot of 2-Propanol after spin-echo with varying values of $J$ (from 0 to 1/4J), (a) with spin lock (p17 = 2.4 ms and p10 = 7.04 dB) and (b) without spin lock (p17 = 0 and p10 = 0)

![Fig 3: Pulsed gradient spin-echo (PGSE) sequence with added spin-lock component ($\Psi$)](image3)

Fig 3: Pulsed gradient spin-echo (PGSE) sequence with added spin-lock component ($\Psi$)

![Fig 4: Diffusion measurement of 2-Propanol at $\tau = 1/4J$, (a) with spin lock (p17 = 2.4 ms and p10 = 7.04 dB) and (b) without spin lock (p17 = 0 and p10 = 0)](image4)

Fig 4: Diffusion measurement of 2-Propanol at $\tau = 1/4J$, (a) with spin lock (p17 = 2.4 ms and p10 = 7.04 dB) and (b) without spin lock (p17 = 0 and p10 = 0)

**DISCUSSION**

The spectra in Fig. 2(b) shows a great amount of reduction in anti-phase magnetisation compared to Fig. 2(a) which used the same pulse sequence but with both spinlock component set to 0. The peaks either become positive or negative with almost no anti-phase. 1/2$J$ which shows the most anti-phase is severely reduced in magnitude but becomes almost entirely positive.

Calculating the diffusion measurement of 2-propanol using the spectrum in Fig. 4(b) is far easier than using Fig. 4(a) which had no spin-lock. There is almost no anti-phase magnetisation in Fig. 4(b) though both were given the same diffusion time.

**CONCLUSION**

A $J$-compensated sequence is still under development. However, the spin lock method already shows a lot of promise. Adding a spin-lock component to an existing PGSE sequence shows a considerable reduction of distortions in diffusion measurements.

**ACKNOWLEDGEMENTS**

The financial support of the NSW State Government BioFirst award is gratefully acknowledged. The author would also like to thank “The Price is Right” NMR group.

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