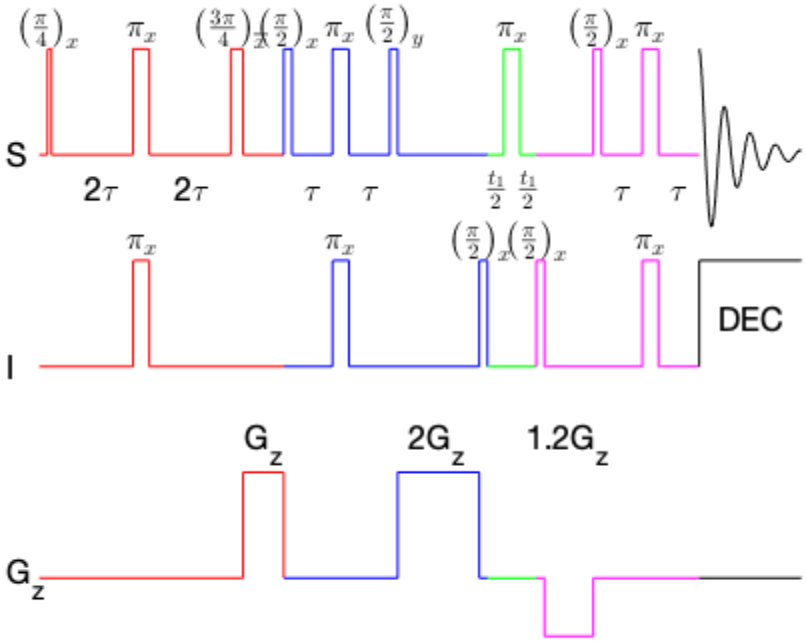
February 2022 NMR Topic of the Month: The HSQC Pulse Sequence



For what does the acronym HSQC stand?

HSQC = Heteronuclear Single Quantum Correlation

What is the role of the HSQC sequence?

The HSQC is a cornerstone of characterization by NMR. The resulting 2D spectrum is a map of which S spins are coupled to which I spins. There are many variations of this sequence, as it is easily adapted to answer specific connectivity questions.

How does the HSQC work?

The HSQC is a poster-child for building block sequences. The red part of the above pulse sequence diagram is an optional TANGO (see last month's topic), it varies only in the phase of the last (red) S pulse and with the gradient thereafter. The change in phase puts the desired magnetization (selected with $\tau = 1/|4J|$) back along $\hat{z}$, and the gradient pulse removes all other magnetizations. The blue part of the above pulse sequence diagram is an INEPT (see the topic from two months ago), where the last (blue) I pulse follows a gradient pulse. Preempting the final I pulse in an INEPT leaves the magnetization along $\hat{z}$, then the gradient pulse removes all other magnetizations, and then the INEPT is completed. The green part of the above pulse sequence diagram is a spin echo on the S spins with variable duration (t_1), this is how the indirect dimension is collected. Keep in mind, the magnetization of interest is on the I spins during this t_1 time, so the indirect dimension will have I spin information. The magenta part of the above pulse sequence is a refocused reverse INEPT. This building block moves the magnetization from the I spins back onto the S spins for detection (proof left to reader). Finally, the magnetization is detected on the S spin channel with I spin decoupling, so the direct dimension (t_2) will have S spin information.

References

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2. R.R. Ernst, G. Bodenhausen, and A. Wokaun, *Principles of Nuclear Magnetic Resonance in One and Two Dimensions [Chapter 8.5]*, Oxford Science Publications, New York (1987).
3. J. Cavanagh, W.J. Fairbrother, A.G. Palmer III, and N.J. Skelton, *Protein NMR Spectroscopy. Principles and Practice [Chapter 7]*, Academic Press, San Diego (1996).