CALIFORNIA STATE SCIENCE FAIR
2011 PROJECT SUMMARY

Name(s)

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Project Number

31517

Project Title

A Theoretical Study to Increase Molecular Specificity in Nuclear Magnetic Resonance Spectra

Abstract

Objectives/Goals

The purpose of this theoretical research is to study ways to increase the molecular specificity in Nuclear Magnetic Resonance (NMR) spectra, thus providing earlier detection of life-threatening diseases, such as cystic fibrosis and COPD.

Methods/Materials

Using an exponential function modeling spin-lattice relaxation time T1 (Mz(t)=[Mz(t)-M(Infinity)]*e^(-t/T1)), it is graphically shown that T1 does not vary with changes in the strength (Mz) or angle of the magnetic pulse applied in NMR. Various values of Mz and the angle of the pulse were plugged into the function. The resulting functions were graphed, yielding graphs of Mz(t) vs. t, where t is the elapsed time after the pulse is applied.

Wilson et al. proposed a new method of Dynamic Nuclear Polarization (DNP), which minimizes the amount of hyperpolarization lost, and thus increases the molecular specificity of the NMR spectrum. In their research, C13-acetic anhydride is hyperpolarized, and then mixed with 5 amino acid derivatives, hyperpolarizing them also. Wilson et al. state that C13-acetic anhydride is a good substrate to use in their method since it has a long T1 and can react rapidly with many amines. A long T1 is beneficial since it decreases the amount of polarization lost, and thus increases the molecular specificity of the NMR spectrum. In this study, C-13-glycine is proposed as a better alternative to C13-acetic anhydride.

Results

It is observed graphically that T1 does not vary with changes in Mz and the angle of the magnetic pulse. C-13-glycine is proposed as a better alternative to C13-acetic anhydride since it has a longer T1, meaning that it would provide even greater molecular specificity in an NMR spectrum. Furthermore, C13-glycine can also react rapidly with many amines.

Conclusions/Discussion

The fact that T1 does not vary with strength and angle of the magnetic pulse applied shows that it does not vary with changes in the external conditions, but rather varies with changes in the internal physical characteristics of the sample. This justifies that C13-glycine and C13-acetic anhydride can have different T1 values. C13-glycine is a better alternative to C13-acetic anhydride since it has a longer T1 and can also react rapidly with many amines. Therefore, C13-glycine, when used in NMR, would increase the molecular specificity of an NMR spectrum even more.

Summary Statement

In this theoretical study, I propose a compound that provides greater molecular specificity in NMR spectra, allowing for earlier detection of life-threatening diseases such as cystic fibrosis and Chronic Obstructive Pulmonary Disease.

Help Received

My faculty mentor at school advised me on some of the technical aspects of my study.