Acquisition of Multidimensional NMR Spectra in a Single Scan

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Overview

Multidimensional nuclear magnetic resonance (NMR) is used nowadays in many applications (e.g., discovering new pharmaceutical drugs, characterization of new catalysts, and investigation of the structure and dynamics of proteins). One drawback of this technique is that multidimensional NMR requires relatively long measurement times associated with hundreds or thousands of scans, in contrast to one-dimensional spectroscopic methods. Therefore, rapidliy changing chemical systems and in vivo clinical measurements such as magnetic resonance imaging (MRI) are not suited for this technique. The current technology allows the acquisition of multidimensional NMR scans using a single continuous scan, thereby shortening the time needed to acquire high-quality MRI images. This technique could be applied to existing NMR/MRI devices.

The Need

NMR and MRI are costly devices due to their inner superconductive magnet. Along with their high cost, the long acquisition time needed for high-resolution spectra/images made these instruments the bottleneck for structure solving and in-vivo diagnostics (for multidimensional NMR and MRI, respectively). Shortening the time needed for each measurement will enable higher measurement capacities with better resolution.

The Solution

While regular multidimensional NMR acquisition is based on many experiments which are being conducted in different scans one by one, in this technique, all the experiments are performed in parallel in the same scan. This method allows obtaining high-resolution multidimensional NMR spectra after a single scan[i].

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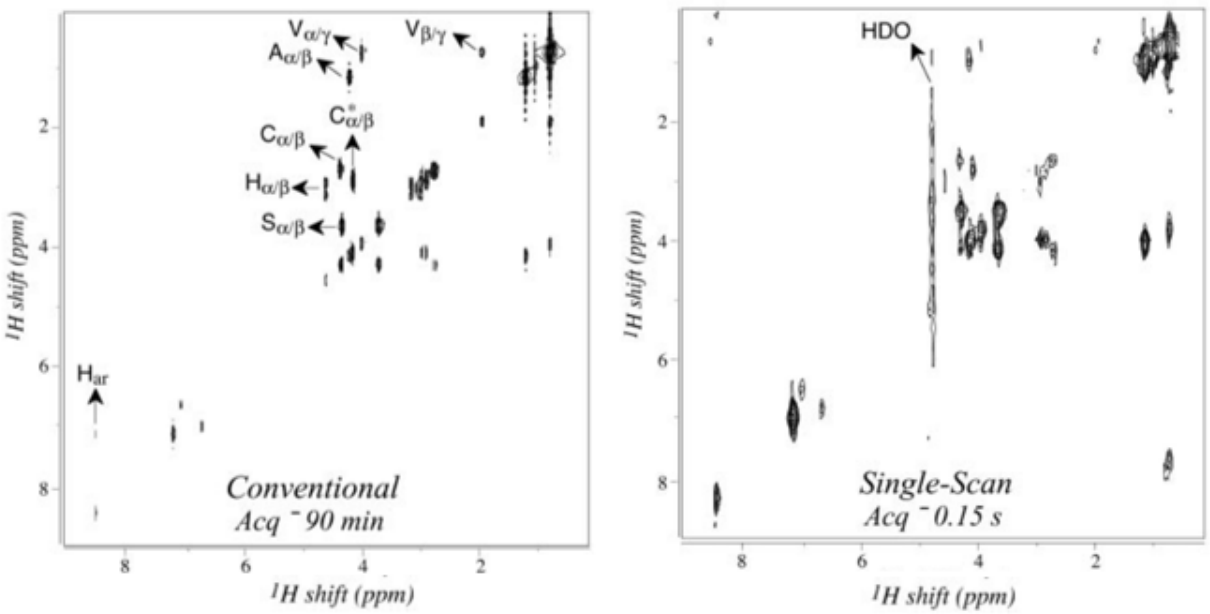

2D H¹ NMR (TOCSY) spectras of hexapeptide: Conventional protocol (left), Single-Scan protocol (Right)

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[i] L. Frydman, T. Scherf and A. Lupulescu, Proceedings of the National Academy of Sciences Dec 2002, 99 (25) 15858-15862; DOI: 10.1073/pnas.252644399

Technology Essence

This technology â€œslices upâ€ the molecular sample into numerous thin layers and then simultaneously performs all the measurements required on every one of these slices. The protocol then integrates these measurements according to their precise location, generating an image of a full multidimensional spectrum from the entire sample.

Applications and Advantages

Applications

- In vivo diagnostics
- High-throughput proteomics/metabonomics
- NMR of unstable chemical systems
- Metabolic dynamics
- High-resolution NMR in tabletop systems
- Extensions to non-MR spectroscopies

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Advantages

- Can shorten the acquisition time of any multidimensional spectroscopy experiment by orders of magnitude
- Compatible with the majority of multidimensional pulse sequences
- Can be implemented using conventional NMR and MRI hardware

[1] L. Frydman, T. Scherf and A. Lupulescu, Proceedings of the National Academy of Sciences Dec **2002**, 99 (25) 15858-15862; DOI: 10.1073/pnas.252644399

Patent Status

USA Granted: 6,873,153 USA Granted: 7,271,588 USA Granted: 7,944,206 USA Granted: 10,794,980