Absolute Minimal Sampling of Homonuclear 2D NMR TOCSY Spectra for High-Throughput Applications of Complex Mixtures

Technology #37865

A technique to increase the processing speed of data collection without losing accuracy

The Need

Modern applications of 2D NMR spectroscopy for diagnostic screening, metabolomics, quality control, and other high-throughput applications are limited by the time-consuming sampling requirements. 2D Total Correlation Spectroscopy (TOCSY) provides unique spin connectivity information for the analysis of a large number of compounds in complex mixtures, but standard methods typically require more than 100 t1-increments for an accurate spectral reconstruction, rendering these experiments ineffective for high-throughput applications. A system or technique is needed to improve the process for high throughput applications.

The Technology

Dr. Rafael Bruschweiler and his research team at The Ohio State University have developed a novel process that uses as few as 16 t1-points of a complex metabolite mixture to accurately find spectral reconstruction of TOCSY spectra. The proposed method uses absolute minimal sampling (AMS). The collected data via direct fitting of resonance frequencies and amplitudes during the time domain. The technique results in a 16-fold speed-up over standard 2D Fourier transform, which is essential for high through applications.

Commercial Applications

- Food processing
- Clinical work
- General research

Benefits/Advantages

- Faster than other 2D NMR methods
- More accurate
- Can sample a wider range of molecules

Inventors

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