Center for Eukaryotic Structural Genomics

Technology Dissemination Report

CESG Tech Report No.	012
Title	HIFI-C (High-Resolution Iterative Frequency Identification of Couplings)
Research Unit	NMR
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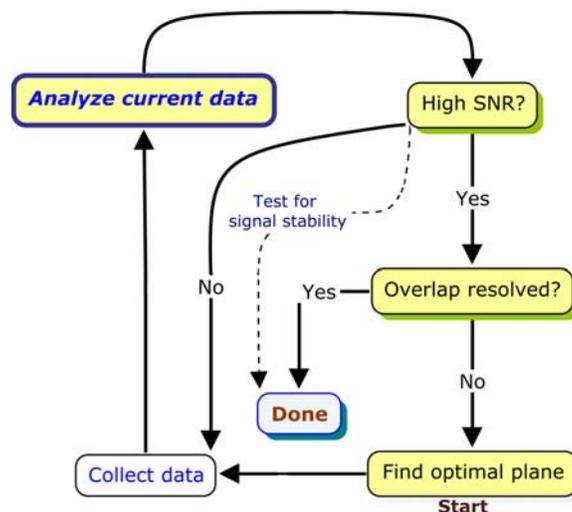
Summary

HIFI-C is a novel method for the robust, rapid, and reliable determination of J couplings in multi-dimensional NMR coupling data, including small couplings from larger proteins [1]. HIFI-C is an extension of the adaptive and intelligent data collection approach introduced earlier in HIFI-NMR. HIFI-C collects one or more optimally tilted two-dimensional (2D) planes of a 3D experiment, identifies peaks, and determines couplings with high resolution and precision. The HIFI-C approach offers vital features that advance the goal of rapid and robust collection of NMR coupling data. (1) Tilted plane residual dipolar couplings (RDC) data are collected adaptively in order to offer an intelligent trade off between data collection time and accuracy. (2) Data from independent planes can provide a statistical measure of reliability for each measured coupling. (3) Fast data collection enables measurements in cases where sample stability is a limiting factor (for example in the presence of an orienting medium required for residual dipolar coupling measurements). (4) For samples that are stable, or in experiments involving relatively stronger couplings, robust data collection enables more reliable determinations of couplings in shorter time, particularly for larger biomolecules. The new approach has shown excellent quantitative agreement with values determined independently by the conventional 3D quantitative J NMR method (in cases where sample stability in oriented media permitted these measurements), but with a factor of 2–5 in time savings. The statistical measure of reliability, measuring the quality of each RDC value, offers valuable adjunct information even in cases where modest time savings may be realized.

Publication:

[1]   Cornilescu, G., Bahrami, A., Tonelli, M., Markley, J.L., and Eghbalnia, H.R. (2007). HIFI-C: a robust and fast method for determining NMR couplings from adaptive 3D to 2D projections. *J Biomol NMR* 38(4):341-51.

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