Center for Eukaryotic Structural Genomics

Technology Dissemination Report

CESG Tech Report No.	011
Title	HIFI-NMR (High-Resolution Iterative Frequency Identification for NMR)
Research Unit	NMR Spectroscopy
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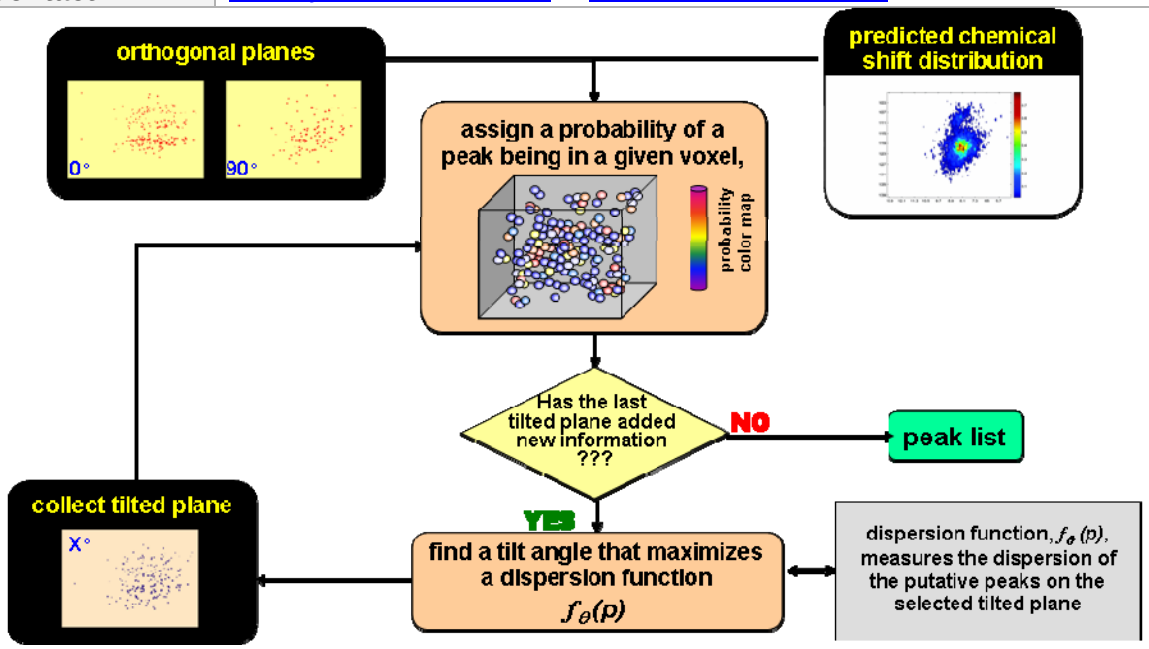

Summary

HIFI-NMR is a rapid method for collecting data from a series of three-dimensional NMR experiments and determining the positions of peaks so as to develop a probabilistic peak list [1]. HIFI-NMR uses the tilted-plane reduced dimensionality approach to data collection developed by E. Kupce and R. Freeman, but without spectral reconstruction. The pioneering features of HIFI-NMR are that tilted planes are collected adaptively, one at a time, with an on-board algorithm choosing the angle of the next plane to be collected and determining in advance whether or not to collect these data on the basis of an estimation of the impact the new data would have on the evolving model of spectral peak locations in three dimensions. If collection of an additional plane is predicted not to improve the model, the software terminates the current NMR experiment and starts a new one. When data from all NMR experiments have been collected, the software provides peak lists for each experiment (chemical shifts in each dimension and probability measures for peak detection and shift accuracies). One output format option is NMR-STAR for direct deposition into BMRB. The progress of HIFI-NMR can be monitored from the spectrometer console, or data collection can be launched and followed from a remote computer. HIFI-NMR is being exported to other NMR laboratories, but currently is available only for Varian spectrometers.

Publication:

[1] Eghbalnia, H.R., Bahrami, A., Tonelli, M., Hallenga, K., and Markley, J.L. (2005) High-resolution iterative frequency identification for NMR as a general strategy for multidimensional data collection. *J Am Chem Soc* 127(36):12528-36.

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