

Reconstructing 3D Data from 2D Planes

There are a variety of methods to shorten the experimental time of nD experiments commonly used in Bio-NMR. One of those is projection spectroscopy (also known as reduced dimensionality) where higher dimensional spectra are projected onto 2D planes at a given projection angle.

TopSpin 3.5 has a new FnTYPE, which automatically expands a given pulse program so that it becomes suitable for projection spectroscopy. The requested projection angle is directly set in the eda interface.

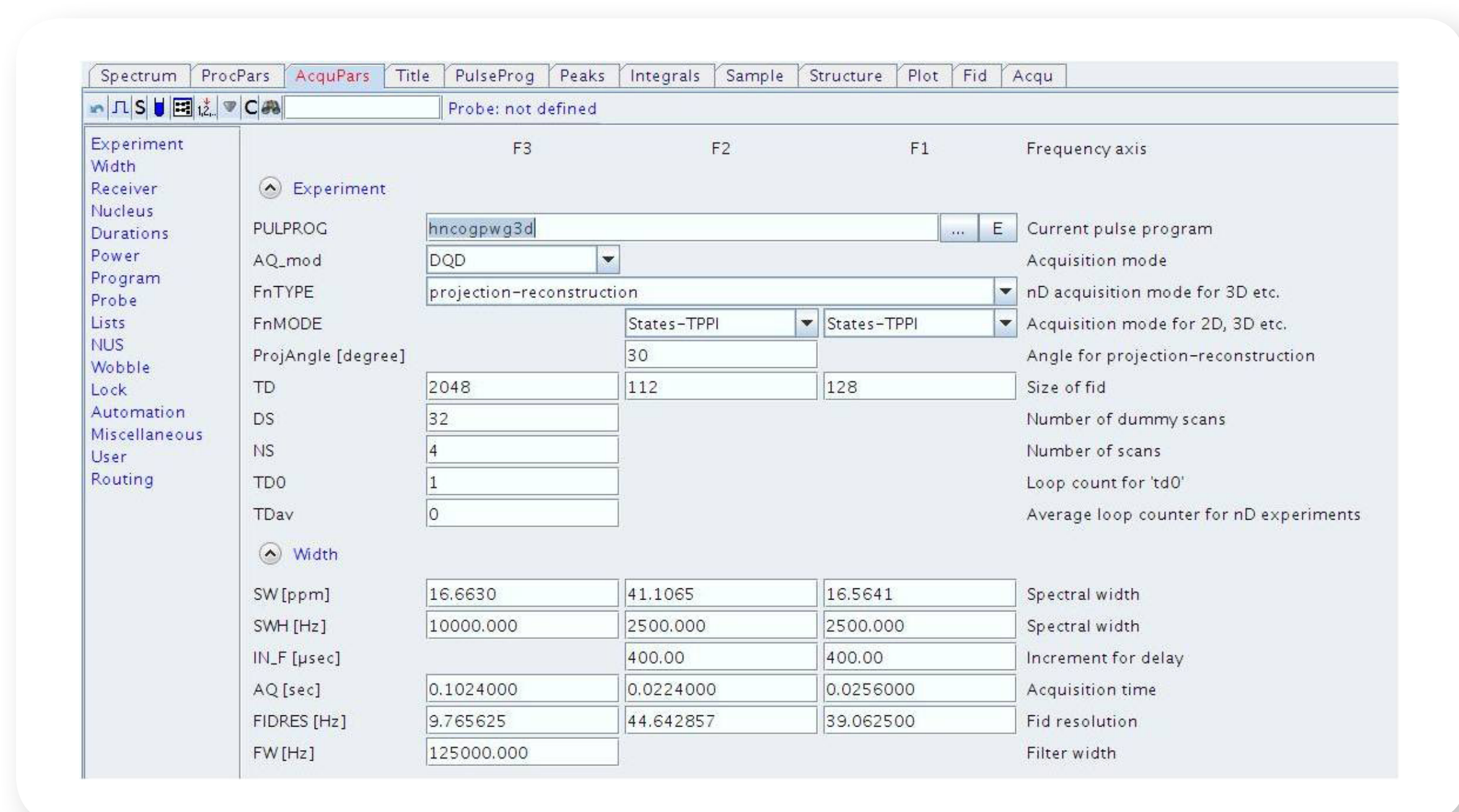


Fig. 1 eda interface showing the new parameters FnTYPE and ProjAngle.

The data is preprocessed to obtain spectra that correspond to projection angles of +/- alpha.

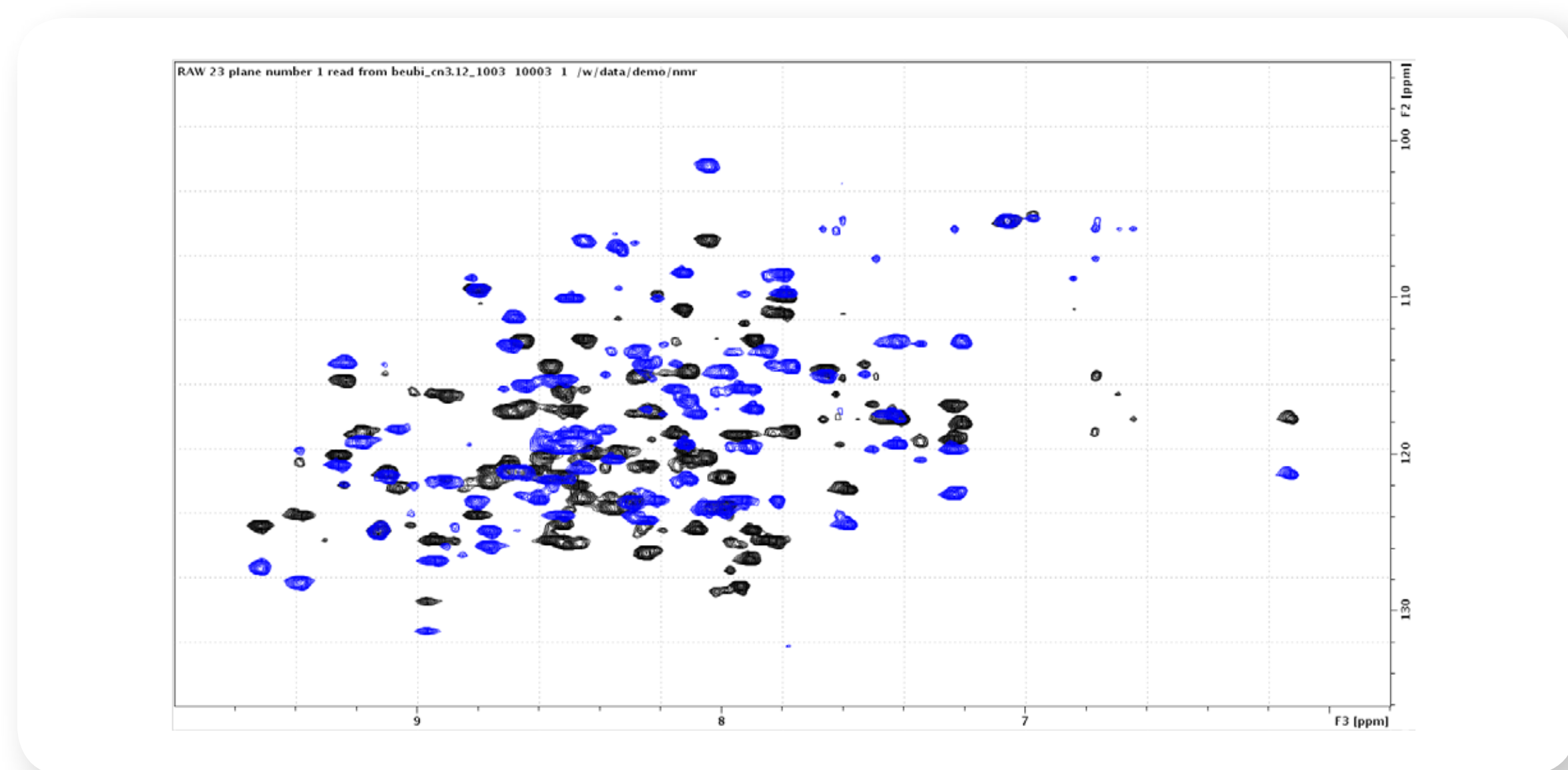


Fig. 2 2D spectra of a HNCO experiment corresponding to a projection angle of +30° (black) and -30° (blue).

There are several ways to utilize the data, from the evaluation of peak lists (as done in APSY) to the actual reconstruction of the spectra.

From the projections the possible peak positions are calculated (Fig. 3a and 3b for 0° and 90° respectively). Using projections at 0°, 90°, 30°, 45° and 60° allows the reconstruction of the correct spectrum. The overall acquisition time was 1h55m (a spectrum with 64*56*1k complex points acquired traditionally would take 22h16m).

The reconstruction allows for opposite signs of cross peaks as well as peaks where the position is shifted in a TPPI like manner to make better use of the available space.

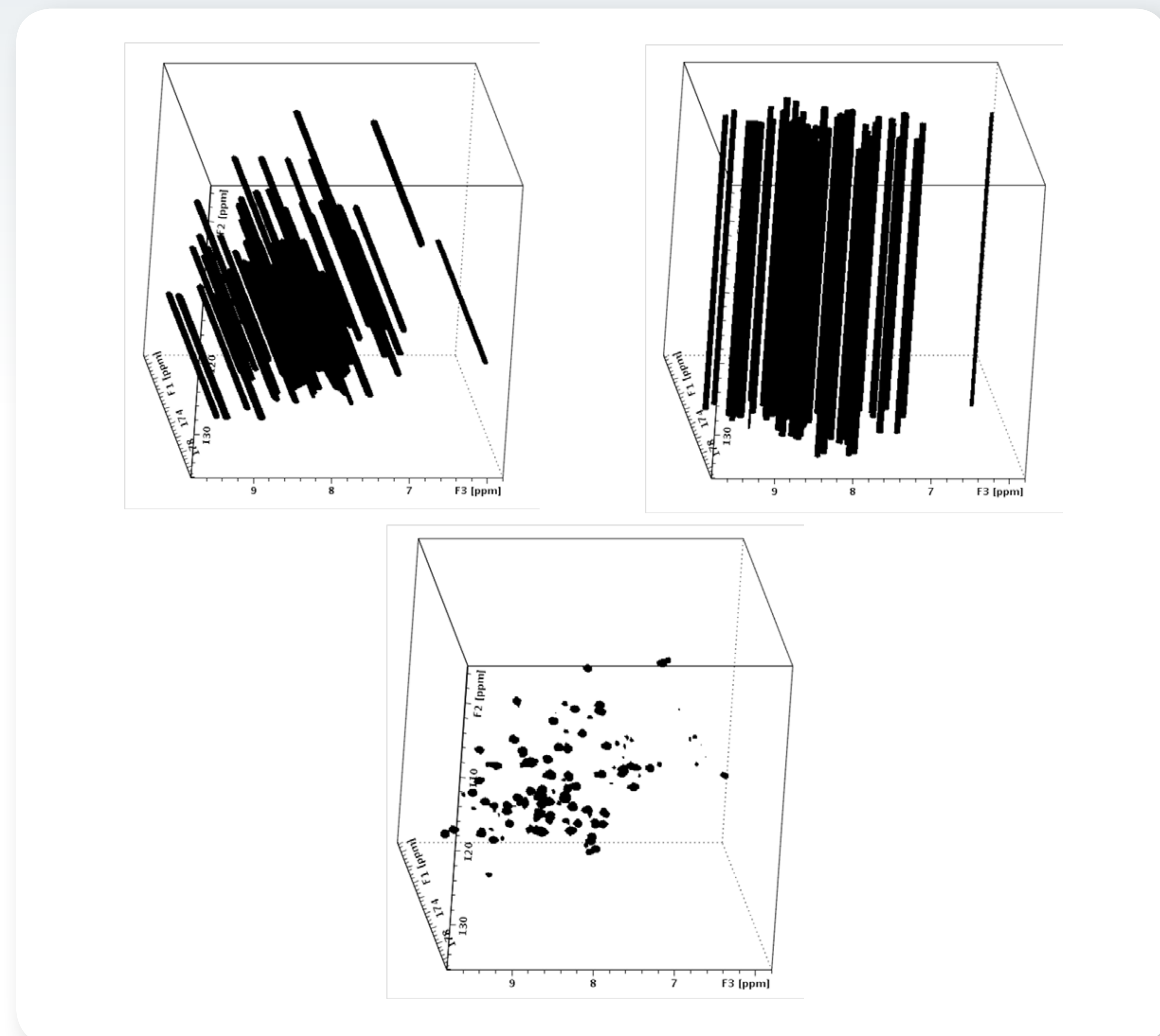


Fig. 3 a and b (top) possible peak position from a 0° and 90° projection c) final reconstructed 3D HNCO.

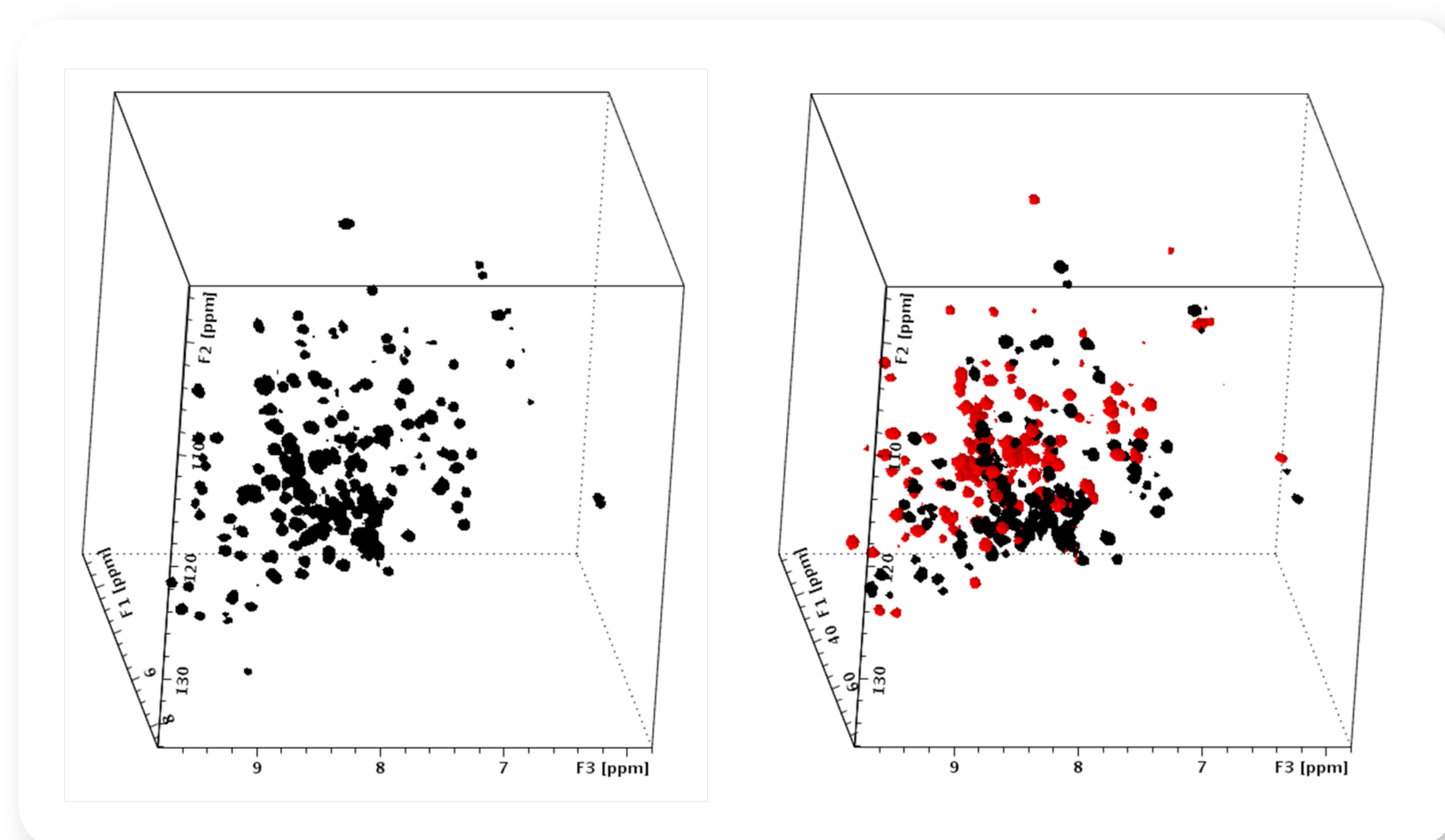


Fig. 4 reconstructed HNCaCb and HbHaCONH 3D.

" I am fascinated by the rapid progress in the theory and applications of novel signal acquisition and processing techniques that push boundaries of the dimensionality and resolution of the NMR spectra and permit real-time investigation of biological processes with atomic resolution. A combination of high field magnets of 1 GHz and higher offered by Bruker and the non-uniform sampling techniques greatly enhances our capability to tackle challenging biomedical problems, including characterization of large protein machines and intrinsically disordered proteins. I have no doubts we are witnessing the most striking development in this field!"

- Prof. Vladislav Orekhov, University of Gothenburg

Summary

- TopSpin 3.5 enables fully integrated acquisition of NUS and projection spectroscopy data for any appropriate experiment.

