HC(C) hd-TROSY-ECOSY processing
Projection of the 3D matrix along F3

• Data are processed using standard FT procedure in F1 and F3 dimension. Linear prediction is then used to double the number of time-domain points in the F2 dimension. Use macro "diag.com" to optimize this processing step before making the projection. Signal in the (F2,F3) plane appears as an extensively folded diagonal. Use diag.tcl script to check if this 3D matrix is correctly processed: signal should appear on the red lines.

 • Apply an F2-dependent frequency shift in the F3 dimension, such that the diagonal signals are now positioned vertically, using the macro lines.com. Use the lines.tcl script to check if this 3D matrix is correctly processed: signal should appear on the red lines.

• Vertical bands from the shifted spectrum are transposed and reassembled horizontally to construct an unfolded spectrum in the F2 dimension, using slide.com.

• Projection along F3 onto the F2 dimension: Use the output 3D matrix from slide.com macro to optimize in the F3 dimension the width of the central band containing the signal that need to be extracted. Extraction of signal, application of a sine-bell appodization window before projection along F3, is realized using the xyz1.com macro. The resulting 2D matrix : test001.dat, will then be located in the ft directory.

References :

Boisbouvier, J., Bryce, D., O'Neil-Cabello, E., Nikonowicz, E. & Bax A. "Resolutionoptimized NMR measurement of 1DCH, 1DCC and 2DCH residual dipolar couplings in nucleic acids bases." J. Biomol. NMR, 30, pp287-301 (2004).

Boisbouvier, J. , Delaglio, F. & Bax A. "Direct observation of dipolar couplings between distant protons in weakly aligned nucleic acids" Proc. Natl. Acad. Sci. USA, 11, 11333-11338 (2003).