COVARIANCE PROCESSING OF 3D AND 4D NOESY DATA

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Introduction

Covariance NMR [1] is a technique which, either following or *in lieu of* a Fourier Transform of a multi-dimensional NMR spectrum, allows for the indirect dimension to achieve the same nominal resolution and spectral width as the direct dimension. A matrix square root operation or, alternatively, the use of a singular value decomposition in implementation of the covariance transformation, suppresses spectral artifacts, as has been demonstrated in the analysis of 2D TOCSY spectra [2]. Simulations of 4D NOESY data, which account for finite resolution and line-widths while representing the data as easy to analyze square matrices, demonstrate that the covariance transform, followed by a matrix square root operation, enhances resolution and suppresses artifacts. Comparisons between regular and Covariance processed NOESY data for ubiquitin indicate that Covariance NMR indeed provides for significant resolution enhancement when applied to 4D NOESY data.

Experimental

4D NOESY data, as well as other NMR spectra to verify ubiquitin resonance assignments, were collected on the 800 MHz Bruker magnet with a cryogenically cooled probe at the NHMFL facility.

Results and Discussion

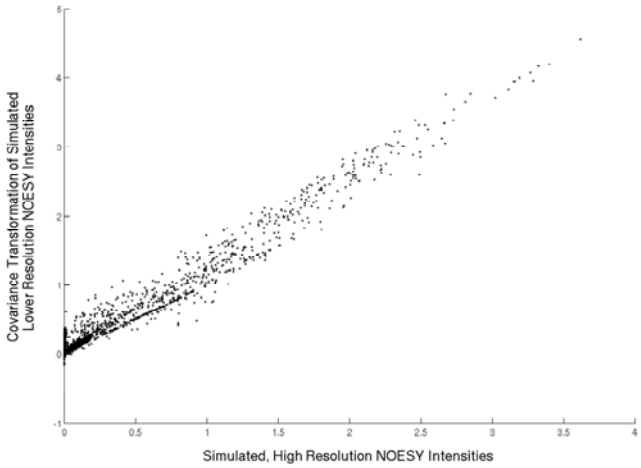

Figure 1: Covariance transformed data, simulated with resolution typical for a 4D dataset, compared to a simulated dataset at the resolution covariance NMR attempts to recover: the high linear correlation demonstrates that covariance NMR provides resolution enhancement without inducing artifacts

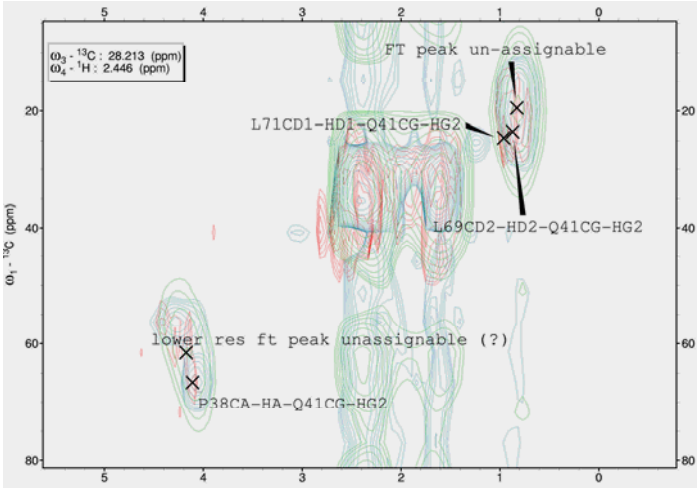

Figure 2: Overlay of a higher resolution 4D NOESY of ubiquitin (blue), a lower resolution 4D NOESY of ubiquitin (green) and the covariance transform of the lower resolution dataset (red): note the covariance result resolves peaks not even resolved in the full resolution 4D NOESY.

Acknowledgements

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References

[1] Brüschweiler, R., *et al*. Journal of Chemical Physics, **120**, 5253-5260 (2004).
[2] Trbovic, N., *et al.* Journal of Magnetic Resonance. **171**, 277-283 (2004).