Developing new NMR pulse programs for IDP assignment

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IDPs have significantly lower signal dispersion in NMR spectra compared to folded proteins. Due to the presence of heavily crowded spectral regions, the necessary assignment step of IDPs is made difficult. On the other hand, the better transverse relaxation properties of IDPs and the structural similarities of the same types of amino acids in their sequences gives the opportunity to use selective amino acid edited experiments. In this poster we present the development of new pulse programs based on the earlier "MUSIC" ones [1]. In order to increase resolution in the indirect dimension and allow the use of the time saving NUS method, we changed the sampling of the nitrogen chemical shift evolution time to a semi-constant time scheme. For better sensitivity and resolution for large IDPs and their complexes in high magnetic fields we made TROSY variants of the pulse programs. The new pulse programs were tested on a large IDP in complex with a folded protein: chikungunya nsP3 HVD with BIN1 and a folded protein: BR domain of PsrP and compared their performance.

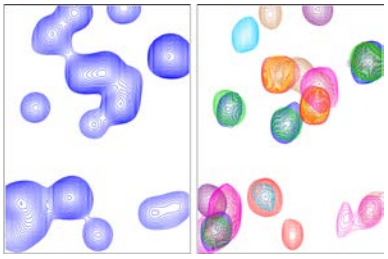

Figure 1. HSQC fragment of the large IDP: chikungunya nsP3 HVD (left) vs a combination of some modified MUSIC type spectra (each in its own color) (right).

[1] M. Schubert al. *Journal of Biomolecular NMR* **2005,** *31* (2), 115–127.