MS13-05 | Dealing with Modulated Macromolecular Structures With Translational Non-Crystallographic Symmetry

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Translational non-crystallographic symmetry (tNCS) is a pathology of protein crystals in which multiple copies of a molecular assembly are found in similar orientations. This causes an overall modulation with systematically strong and weak intensities, affecting structure determination and refinement. Addressing this pathology is less developed in macromolecules than in chemical crystallography, as severe cases preclude solution altogether.

Modulation gives rise to strong peaks in the Patterson function. In commensurate modulation, peaks are located at simple fractions of the vectors of the reciprocal lattice whereas in incommensurate modulation peaks occupy positions that do not represent a simple fraction.

In order to take into account the statistical effects of these modulations, the Patterson map can be used to determine the translation relating the copies. Then any small rotational differences in their orientations, and the size of random coordinate differences caused by conformational differences can be refined against a likelihood function to account for the effects of tNCS [1,2].

In the present project we deal with the determination from the experimental data of the parameters describing the tNCS before a structure is solved and in order to aid structure solution. For this purpose a database containing a representative PDB [3] subset with nearly 80000 protein structures has been characterized and used to train a decision algorithm.

[1] Read RJ *et al*. (2013). Acta Cryst. D69, 176-183
[2] Sliwiak J *et al*. (2013). Acta Cryst. D69, 176-183
[3] Burley SK *et al.* (2019) Nucleic Acids Research 47: D464–D474.