

MS23-P08 | NOVEL APPROACH TO STRUCTURE DETERMINATION OF COMPLEX PROTEIN SYSTEM HYP-1/ANS

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Newly discovered modulated crystal structure in organic systems, and still uncommon, require a deeper investigation. No exact and detailed solution of such systems has not been done up-to-date. One possibility is to use an approximation of commensurate modulation which enables constructing a supercell, extending to the case, where translational symmetry (periodicity) is recovered, and simplify the analysis. An assumption of commensurateness of the modulation is, however, questionable and rather unverifiable. The goal of our project is to use a novel, original statistical method of structural modeling which enables a refinement based on the average unit cell with (commensurate or incommensurate) modulation without unclear assumption of commensurateness and supercell approach. Our model system is a pathogenesis-related protein (Hyp-1) complex with fluorescent probe 8-anilino-1-naphthalene sulfonate (ANS) which is a unique example of macromolecular system with modulated crystal structure. Previous studies have shown that Hyp-1/ANS complexes are tetartohedral twinned and crystallized in an asymmetric unit cell containing repetitive motif of four protein molecules arranged with 7-fold noncrystallographic repetition along c axis of the C2 space group. This commensurate structure modulation demands description of structure in highly expanded unit cell with 28 unique protein molecules inside. The Hyp-1/ANS structure was solved by molecular replacement and refined using maximum-likelihood targets with reliability factor R_{free} of 27%. Our approach involves development of the original software, re-integration of raw data and multidimensional analysis used to build the structure model and perform the refinement for significant improvement of results.