Oral Contributions

[MS29] Getting more from your electron density

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[MS29 - 01] About the first VLD (Vive La Difference) applications.

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The VLD (*Vive La Difference*) phasing algorithm is based on the properties of the difference Fourier synthesis ρq = ρ ¬ρp whose new coefficients have been obtained by using the joint probability distribution function P (E, Ep, Eq) and by taking into account both errors in the model and in the measurements [1]. Methods based on its modifications play an important role in combination with electron density modification approaches to improve phase estimates from a given structure model. The ab initio VLD algorithm allows the recovery of the correct structure starting from a random model working in the correct space group without the explicit use of structure invariants and semi-invariants [2],[3]. To improve the efficiency of the algorithm, we modified the initial approach by integrating it with *RELAX* procedure [4],[5] to translate molecular fragments correctly oriented but incorrectly located [6]. The new procedure has been implemented in SIR2011[7], the latest release of the package SIR, and it has been checked on a large set of small-medium size structures and on proteins, provided the data have atomic resolution. The VLD algorithm was also combined with the hybrid Fourier syntheses: they show properties that are intermediate between those of the observed syntheses and those of the difference syntheses. The new coefficients for the hybrid Fourier syntheses have been obtained from the study of the joint probability distributions functions P (F, Fp, FQ) where FQ is the structure factor corresponding to the ideal hybrid Fourier synthesis ρQ = τρ -ωρp , where τ and ω are any pair of real numbers [8]. The combination of the VLD algorithm with the hybrid Fourier synthesis for ab initio phasing shows that the original VLD algorithm is only one of several variants all with relevant phasing capacity[9]. The last application of the VLD algorithm is its integration in a Molecular Replacement pipeline for automatic protein crystal structure solution: in the preceding cases VLD was never used for non ab initio phasing, where some phase information is available but data resolution is usually very far from 1Å [10]. The preliminary results are very encouranging.

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