

SAD / MAD techniques in “il Milione”

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Keywords: SAD, MAD, Anomalous Scatterers

SAD and MAD techniques play an important role in the crystal structure solution of macromolecules.

A new theoretical approach, applying the method of joint probability distribution has been recently proposed ([1] [2] Burla *et al.* 2002, 2003) to estimate the amplitudes of the structure factors of the anomalously scattering substructure given the experimental diffraction moduli. Its advantage is that the estimates can simultaneously exploit the anomalous and the dispersive differences from several wavelength data.

An automatic procedure has been devised which performs the structural determination of the substructure both in SAD and MAD cases. The procedure is able to select the most informative wavelength combination and determine the best limit for data.

The procedure has been tested on a large set of SAD and MAD data and has been introduced in the Direct Methods Program SIR2004, which will be distributed as part of the package “il Milione”. This new package is able to solve crystal structures in the following cases: a) *ab initio*, for small, medium and for protein structures; b) SIR-MIR, SIRAS-MIRAS, SAD-MAD cases for proteins; c) powder data.

[1] Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacobazzo, C., Polidori, G. & Siliqi, D. (2002). *Acta Cryst.* **D58**, 928-935

[2] Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacobazzo, C., & Polidori, G. (2003). *Acta Cryst.* **D59**, 662-669