IL MILIONE: A Complete Package for a global Phasing, from Powders to Proteins

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IL MILIONE is a multipurpose compact, user friendly, efficient package for the global phasing of the crystal structures. The following tasks can be accomplished:

a) phasing and refining powder data. The program EXPO2004 [1] has been incorporated;

b) ab initio crystal structure solution of small, medium and macromolecules. The program SIR2004 [2] has been incorporated. Structures can be solved both by Patterson and Direct Methods (resolution up to 1.4-1.5Å, up to 2000 atoms in the asymmetric unit)

c) a new molecular replacement routine has been incorporated;

d) SAD-MAD, SIR-MIR, SIRAS-MIRAS cases can be faced. The new method provides quite simple and effective formulas both for locating heavy-atom/anomalous-scatterer substructures, and for phasing reflections ([3], [4]).

The program is highly automatic and suitable for high throughput crystallographic. Results of numerous applications will be shown.

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Keywords: structure determination, crystallografic software, protein crystallography structures