SIR2004: New Features for *ab-initio* Crystal Structure Solution

Benedetta Carrozzini[a], Maria C. Burla[b], Rocco Caliandro[a], Mercedes Camalli[c], Giovanni L. Cascarano[a], Liberato De Caro[a], Carmelo Giacovazzo[a], Giampiero Polidori[b], Riccardo Spagna[c], *[a]IC-CNR, Bari, Italy. [b]Dipartimento di Scienze della Terra, Perugia University. [c]IC-CNR, Rome Section, Italy.* E-mail: benedetta.carrozzini@ic.cnr.it

SIR2004 [1], the evolution of the SIR2002 program [2], is devoted to the *ab initio* solution of crystal structures by direct methods. Several new features implemented in SIR2004 make this program more efficient: it is able to solve both small/medium size structures as well as macromolecules (up to 2000 atoms in the asymmetric unit at atomic resolution data). The new algorithms succeed also in solving several protein structures with data resolution up to 1.4-1.5 Å, providing interpretable electron density maps.

According to circumstances, the SIR2004 phasing process may apply tangent procedures and/or Patterson methods. The new phasing strategy is also based on: a) an optimal use of the figures of merit, one of which may be successfully applied in the early stages of the phasing process; b) the use of the protein envelope in the direct space refinement.

A powerful graphic interface makes friendly the user interaction with the program. SIR2004 can run on any PC or WorkStation (Operating systems: Windows 9x/2000/Me/NT/XP; Linux, Unix).

[1] Burla M.C., CaliandroR., Camalli M., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., Polidori G., Spagna R., *J. Appl. Cryst*., 2005, **38.** [2] Burla M.C., Camalli M., Carrozzini B., Cascarano G.L., Giacovazzo C., Polidori G., Spagna R., *J. Appl. Cryst*., 2003, **36**, 1103.

Keywords: computer programs, *ab-initio* structure determination, macromolecular crystallography