Phasing at Resolution higher than the Experimental one

Rocco Caliandro, Benedetta Carrozzini, Giovanni L. Cascarano, Liberato De Caro, Carmelo Giacovazzo, Dritan Siliqi, *IC-CNR, Bari, Italy*. E-mail: rocco.caliandro@ic.cnr.it

We have developed a novel procedure which, combined with classical electron density modification (EDM) techniques, is able to:

a) extrapolate moduli and phases of non-measured reflections with resolution lower or higher than the experimental one;

b) actively use such moduli and phases in typical situations met in macromolecular crystallography:

1) *ab initio* phasing: data resolution (RES_{obs}) in the interval 1.5-1.0Å, an approximated electron density available (e.g., after the application of *EDM* procedures) with mean phase error (MPE_{obs}) in the range (25°, 60°);

2) *SAD-MAD*, *SIR-MIR*, *SIRAS-MIRAS* phases: RES_{obs} in the interval 2.8-1.5Å, an approximated electron density available with MPE_{obs} in the range (40°, 65°);

3) *ab initio* phasing, RES_{obs} in the interval 1.5-1.0Å, no phase information available.

Our results [1,2] indicate that in case 3 extrapolation can make difference between success and failure. In cases 1 and 2 the extrapolation procedure is able to reduce the mean phase error of the measured reflections, provides sensible estimates (in modulus and phase) for additional reflections behind and beyond RES_{obs}, and increases the interpretability of the final electron density map.

[1] Caliandro R., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., *Acta Cryst.,* 2005, D, *in press*. [2] Caliandro R., Carrozzini B., Cascarano G.L., De Caro L., Giacovazzo C., *Acta Cryst.,* 2005, D, *submitted*.

Keywords: macromolecular crystallography, extrapolated reflections, resolution