Phasing with Iodine and an X-ray Home Source

Frederico Moraes Ferreira[a], Ricardo Aparicio[a], Guillermo Hernández-Mendonza[b], Mário L. Calcagno[b], Glaucius Oliva[a], [a]*Instituto de Física de São Carlos, USP, Cx.P.369, 13560, São Carlos, SP, Brazil.* [b]*DB-FM, UNAM, México.* E-mail: oliva@if.sc.usp.br

The goal of the present work is focused on the phasing strategy employed to elucidate the crystal structure of the protein N-acetylglucosamine-6 phosphate (GlcNAc6P) deacetylase from *E. coli* [1]. GlcNAc6P deacetylase is an enzyme of the amino sugar catabolism pathway, catalyzing the conversion of the GlcNAc6P in to GlcN6P. The crystal structure was phased by SIRAS using low resolution (2,9Å) iodine anomalous scattering. Native crystals[1] were soaked in a cryo-solution consisting of 1.2 M NaH_2PO_4 and 0.7 M NaI for 10 min. A high redundancy dataset (694° angular sector) was collected on a rotating anode at 100K, resulting in 1,676,880 observed and 21,619 independent reflections. Seventeen iodine sites of partial occupation (1.0-0.3) were found with SHELXD and the output correlation coefficients between the observed and calculated SFs differences were 34.73% (all) and 18.93% (weak data). Phase calculation was carried out with the program SOLVE. Phase extension to 2Å resolution, based on a native data set collected at a synchrotron source [1], and succeeding density modification steps were performed with program RESOLVE. An initial hybrid model was built by merging residues traced in different runs and sub cycles of ARP/WARP model building. Some insights on the refined structure will be presented.

[1] Ferreira F. M., *et al., Acta Cryst.,* **D56**, 670.

Keywords: phasing, SIRAS, GlcNAc6P deacetylase