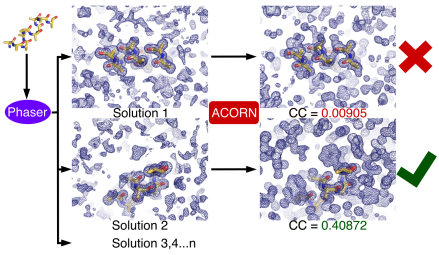

Figure 1. The Fragon process. The correct solution can be selected based on the correlation coefficient (CC) after density modification.

Keywords: Molecular replacement, Phasing, Fragments, Fragon

MS4-O4 BORGES_MATRIX: a tool to generate models for ab initio phasing and for structure interpretation.

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ARCIMBOLDO_LITE [1] is a pipeline that combines the search of small fragments, like alpha helices, with PHASER [2], and density modification and autotracing with SHELXE [3]. Even though the model constitutes only a small percentage of the total scattering, the method has proven to be successful for high resolution cases (better than 2.1 Å). In order to correctly locate and extend the input search model it is required that its main chain matches very accurately the one of the final structure. This assumption is generally correct for helices but it does not hold true for composite secondary structure elements. Thus, exploiting the idea that there are common building blocks (such as three beta strands in a sheet, or two small parallel helices) common to unrelated protein structures, we developed BORGES [4], a tool to extract and use libraries of small local folds for phasing. Other bioinformatic tools are also available to search for similar structural occurrences of a fold [5,6], but they tend to retrieve continuous domains, and give a relatively general view of the fold. Our new program BORGES_MATRIX implements a detailed description, based on discrete distributions of characteristic vectors to entail the local conformation of the main chain and to geometrically compare extracted models with a search template. Our method also extracts folds formed through crystallographic and non crystallographic symmetry, and does not require sequence information to retrieve similar occurrences. Recently, a library of three antiparallel strands was used to solve the structure of a viral all beta structure of 130 aa diffracting to 1.55 Å presenting a novel fold [7]. Beyond phasing, the program contributed to the understanding of the structural environment of the binding site by extracting and comparing similar occurrences of the local geometrical conformation.

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