

New in the ARCIMBOLDO toolbox for phasing with small fragments

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ARCIMBOLDO (1) combines the search of small and accurate fragments with PHASER (2), with their expansion to a full structure solution through density modification and autotracing with SHELXE (3). Fragments can be as small and general as a single ideal polyaniline helix, libraries of tertiary structure local folds such as beta sheets, or even fragments extracted from a distant homolog. These three approaches are accessible through our programs ARCIMBOLDO_LITE, ARCIMBOLDO_BORGES, and ARCIMBOLDO_SHREDDER. Our recent implementations include strategies tailored to deal with challenging cases, tackling lower resolution, larger size, data pathologies or the ambiguity in the crystal contents. This communication will focus on the latest developments in our group, illustrated through examples of their application to previously unknown structures.

Coiled coil structures required to develop new features in order to tackle their inherent phasing difficulties. PHASER's new packing constraints can now be used at the translation search, and automatic handling of the anisotropy and translational non crystallographic symmetry corrections have been included. Both helix directions are tested for all fragments in partial solutions to increase the search base at low resolution. Moreover, we now make use of a different autotracing algorithm from the SHELXE beta version.

ARCIMBOLDO_SHREDDER derives and improves model fragments starting from a distant homolog template, and implements new approaches to refine them in order to reduce the deviations within an overall correct fold. Finally, we also have the possibility of using phase combination of partial solutions in order to increase their information content of the starting map to be expanded into a full solution.

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Keywords: [Phasing, small fragments,](#)