MS01-1-3 Search for optimal phasing parameters with SHELIXIR
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P. Kolenko [1], J. Stránský [2], T. Koval [2], M. Malý [1], J. Dohnálek [2]
[1]Czech Technical University in Prague - Prague (Czech Republic), [2]Institute of Biotechnology CAS - Vestec near Prague (Czech Republic)

Abstract
Experimental phasing represents a minority of phasing procedures in macromolecular crystallography. Nevertheless, it is an inevitable option when no model suitable for the molecular replacement method is available or the diffraction limit of the crystal is too low for the ab initio methods.
Experimental phasing frequently requires data collection at non-standard wavelengths, special crystal treatment, or multiple combinations of both. Data collection at multiple wavelengths is time consuming, and a special crystal treatment usually represents a work with chemicals that burden the environment. Therefore, minimization of both time and consumption is the desired approach. In both cases, optimized phasing pipelines may help. Especially when difficult experimental phasing at synchrotron is performed.
SHELIXIR [1] is a simple and efficient tool for both routine and difficult experimental phase-problem solutions. It utilizes the *SHELX C*/*D*/*E* [2] program package. It works as a pipeline that links the processes together and provides the user with a comprehensive output in form of an HTML page. Beyond the standard protocols, *SHELIXIR* can screen through the following parameters: space groups, solvent content, and high- and low-resolution diffraction limit.
Parallelized screening for optimal solvent content minimizes the computational time. Moreover, it helps to find better experimental phases using the parameter that can significantly differ from the real solvent content (by more than 16%). In some cases, the screening played a crucial role in successful experimental phasing.

References
[1] P. Kolenko, J. Stransky, T. Koval, M. Maly, J. Dohnalek. (2021). *J. Appl. Cryst.*, **54**, 996-1005.
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Examples of screening procedures.