

SHELIXIR: fast and efficient phasing

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Version 2.0



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- Experimental phasing (EP) is used for the determination of novel crystal structures.
- EP requires optimization of the experiment (wavelength, lower dose, *etc.*).
- EP usually takes longer than simple native dataset collection.
- *Phasing is usually performed at home, not during the data collection?*
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-
- **The best indicator of data usefulness is ability to solve the structure!**
 - ***SHELIXIR* may help you to reduce your experimental time and find better phases.**



- Command-line tool for automation of experimental phasing using *SHELX C/D/E* package.
- Minimal software dependencies: *BASH*, *GNUplot*, *SHELX C/D/E*.
- Phasing methods: SAD, MAD, SIRAS, RIP
- Screening in multiple space groups.
- Screening for optimal solvent content parameter (parallelized).
- Screening for optimal high- and low-resolution limits.
- GUI is available.



shelixir_gui

SHELIXIR_GUI 1.0

Prefix

Working directory

Select phasing method

List of files:

```
PEAK /home/kolenko/demo/ger_e_peak.sca
INFL /home/kolenko/demo/ger_e_infl.sca
HREM /home/kolenko/demo/ger_e_hrem.sca
LREM /home/kolenko/demo/ger_e_lrem.sca
NAT /home/kolenko/demo/ger_e_nat.sca
```

Wavelength

Unit cell parameters

Space groups selection

Parameters for ShelxC

Element

Number of heavy atoms

Parameters for ShelxD

Number of trials

Resolution (e.g. 50 2.3)

No. of disulphides

Min. distance

Parameters for ShelxE

Set parameters

Parallelization of ShelxE

Available CPUs

View results in browser

Parameters of solvent screening

Use solvent screening

Minimal solvent content

Maximal solvent content

Step width

Parameters of high resolution screening

High resolution screening

Fixed low resolution

High resolution limits

Parameters of low resolution screening

Low resolution screening

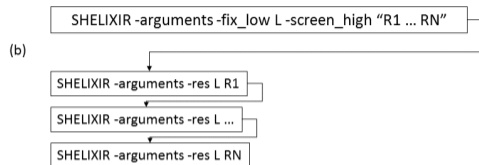
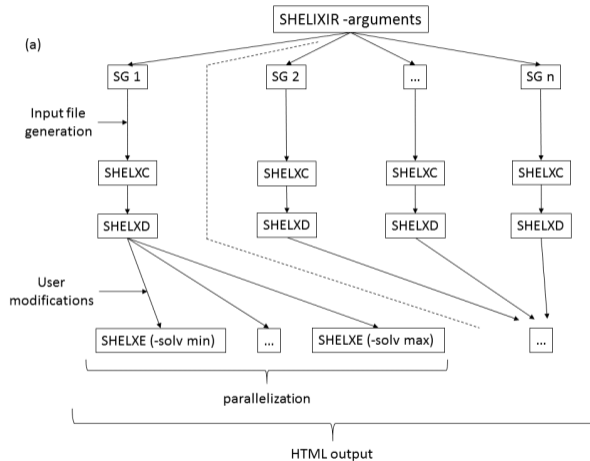
Fixed high resolution

Low resolution limits

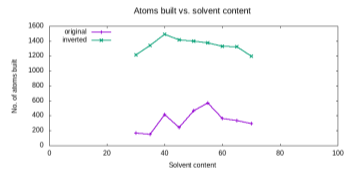
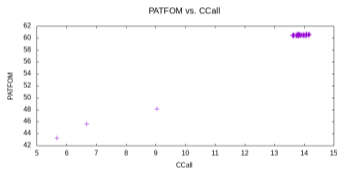
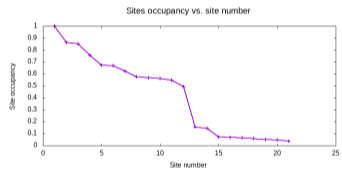
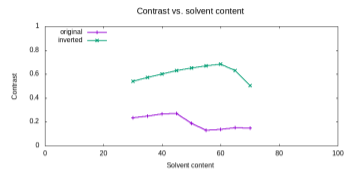
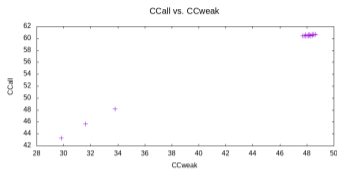
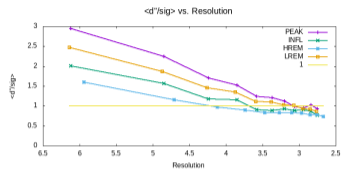
*Click multiple times during the resolution screening.



SHELIXIR workflow

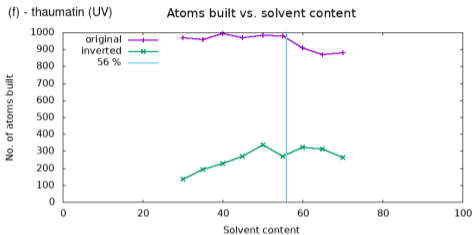
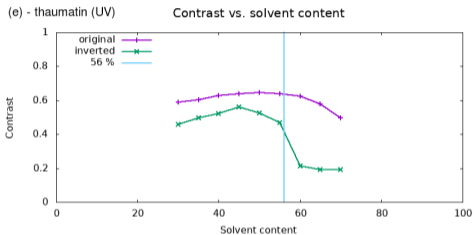


GerE: benchmarking data



Comparison with Sheldrick 2010:

No solvent content parameter screening - under 3 minutes. **SHELIXIR** using better hardware - **under 100 s!**

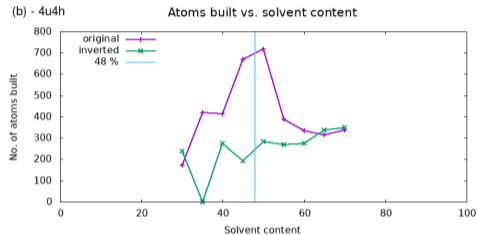
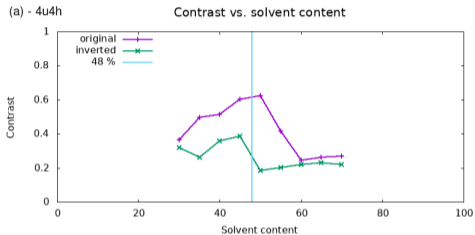


Solvent content screening

Widely used statistics, contrast, and connectivity are not optimal. Number of atoms built gives apparently better results and indicates better initial phases.



N-terminal domain of UL21

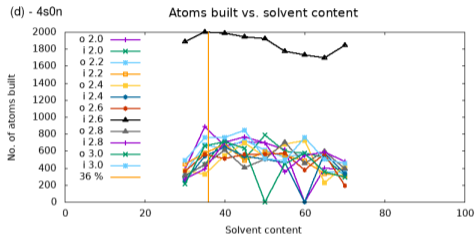
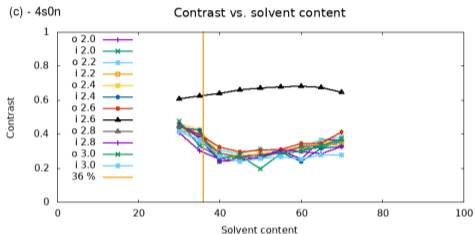


PDB id 4U4H: *autoPROC* tutorial

Solvent content parameter may play a crucial role in experimental phasing. Only 45% and 50% solvent content leads to successful phasing.



Helicase-like transcription factor



PDB id 4U4H: high resolution diffraction limit

Surprisingly, only one high resolution cutoff (2.6 Å) led to successful phasing out of range from 2.0 to 3.0 Å.



What can be done with *SHELIXIR*:

- Experimental time at the synchrotron is limited.
- High-performance CPU clusters are usually available at synchrotron beamlines.
- *SHELIXIR* may provide a fast, efficient, and sophisticated analysis of the “phasing power” of your crystal.
- Screening of multiple parameters with *SHELIXIR* is highly encouraged.
- Everything can be done in *SHELIXIR_GUI*.



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Things that cannot be done with *SHELIXIR*

- Improve your anomalous signal.
- Treat your crystal pathology.
- Prove your solution with refinement.

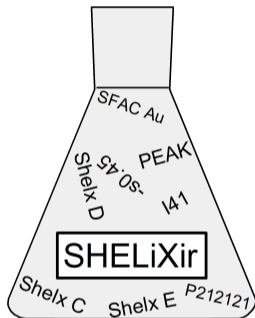
P. Kolenko, J. Stransky, T. Koval, M. Maly, J. Dohnalek. (2021). *SHELIXIR*: automation of experimental phasing procedures using *SHELXC/D/E*. *J. Appl. Cryst.*, **54**, 996-1005.



Acknowledgement

People who contributed

- Jan Stránský
- Martin Malý
- Tomáš Koval
- Jan Dohnálek



<http://kmlinux.fjfi.cvut.cz/~kolenpe1/shelixir/>

<http://kmlinux.fjfi.cvut.cz/~kolenpe1/shelixir/gui>