PROFEX

OPEN SOURCE XRD AND RIETVELD REFINEMENT

New features in Profex 4.1

April 2020, Nicola Döbelin

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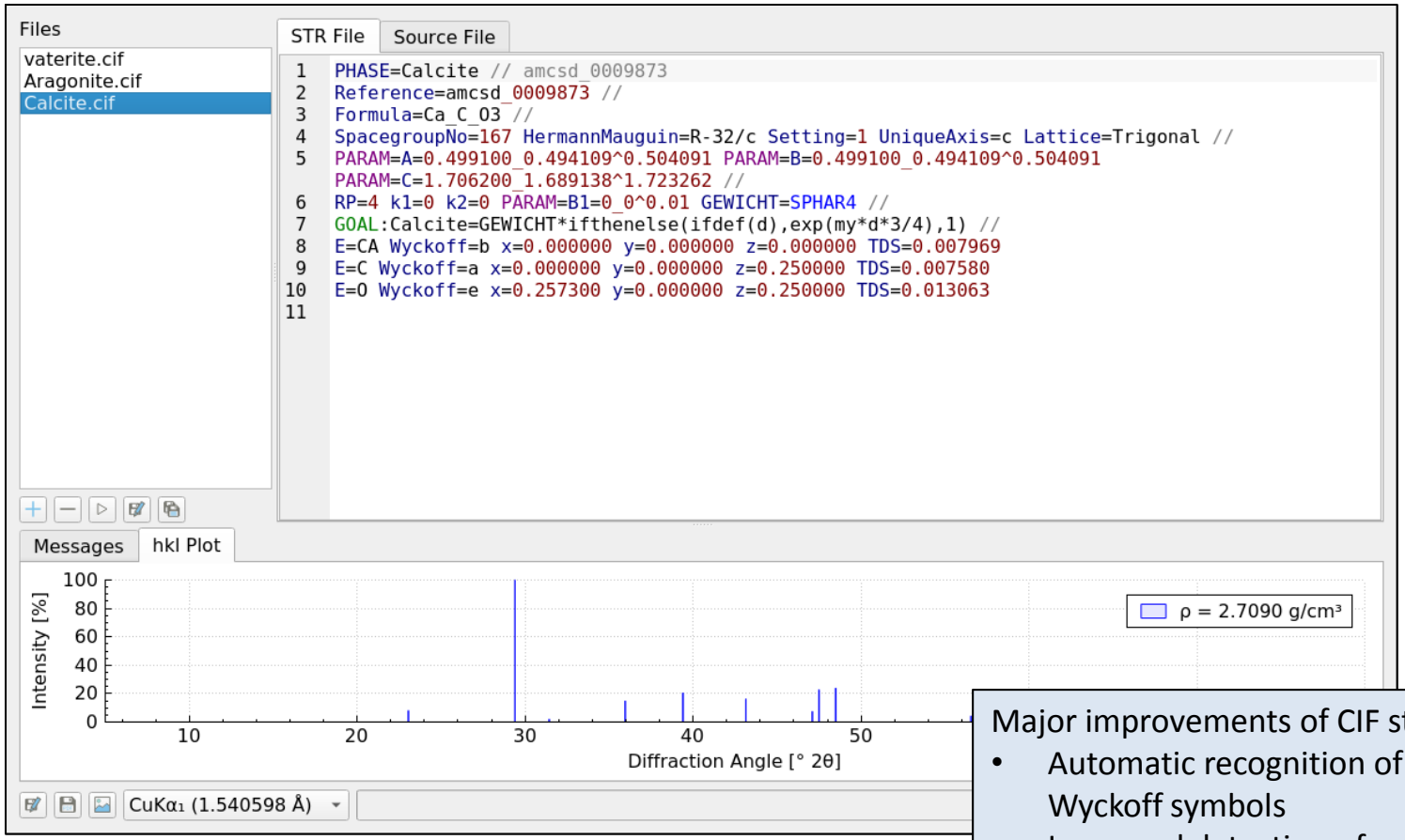

Major improvements of CIF structure import:

- Automatic recognition of missing Wyckoff symbols
- Improved detection of unit cell settings
- Automatically index new structure files

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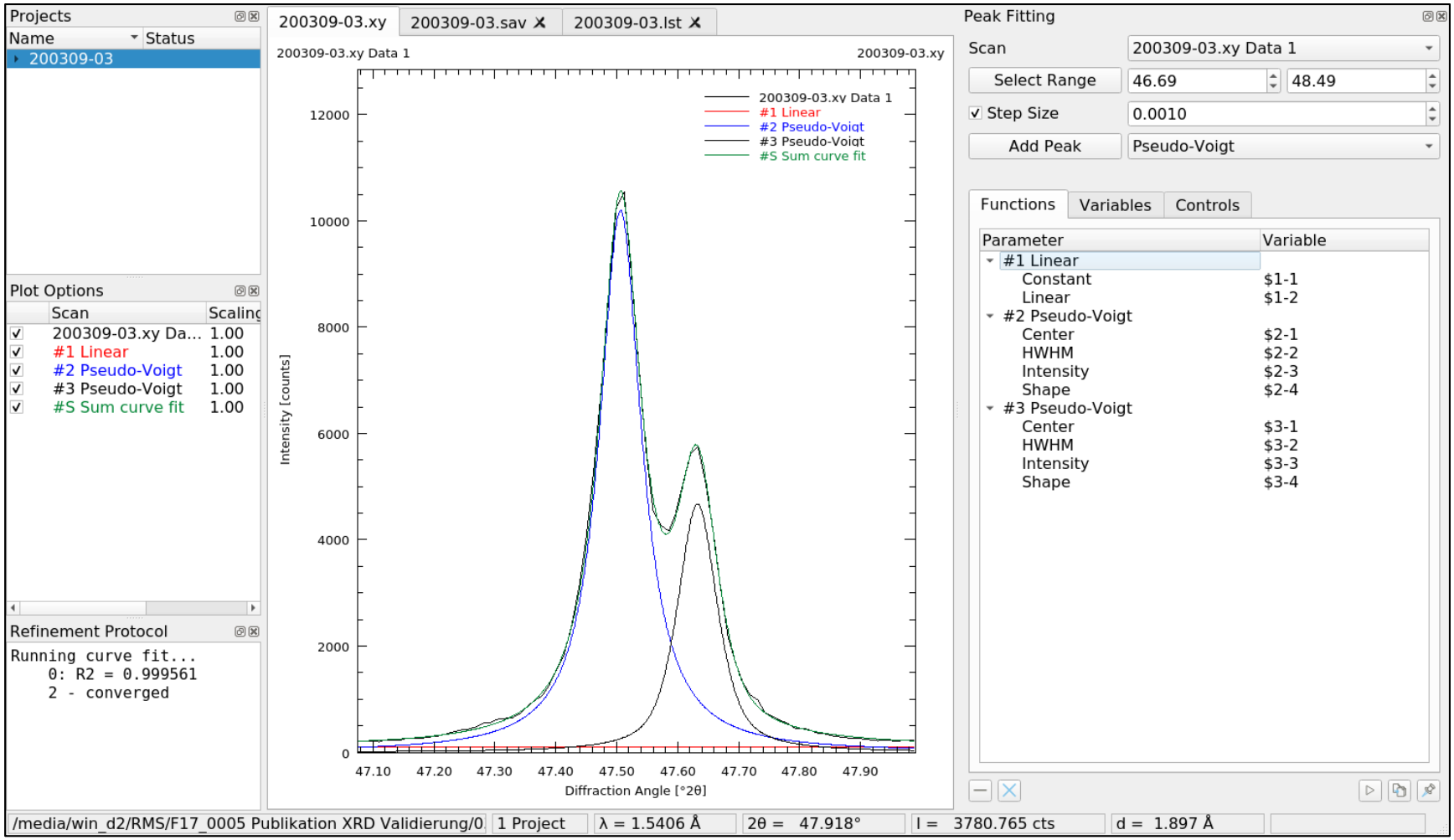
A new module for generic peak fitting:

- Gaussian, Lorentzian, Pseudo-Voigt, Pearson-VII peak functions
- Split functions for asymmetric peaks
- Polynomial background functions



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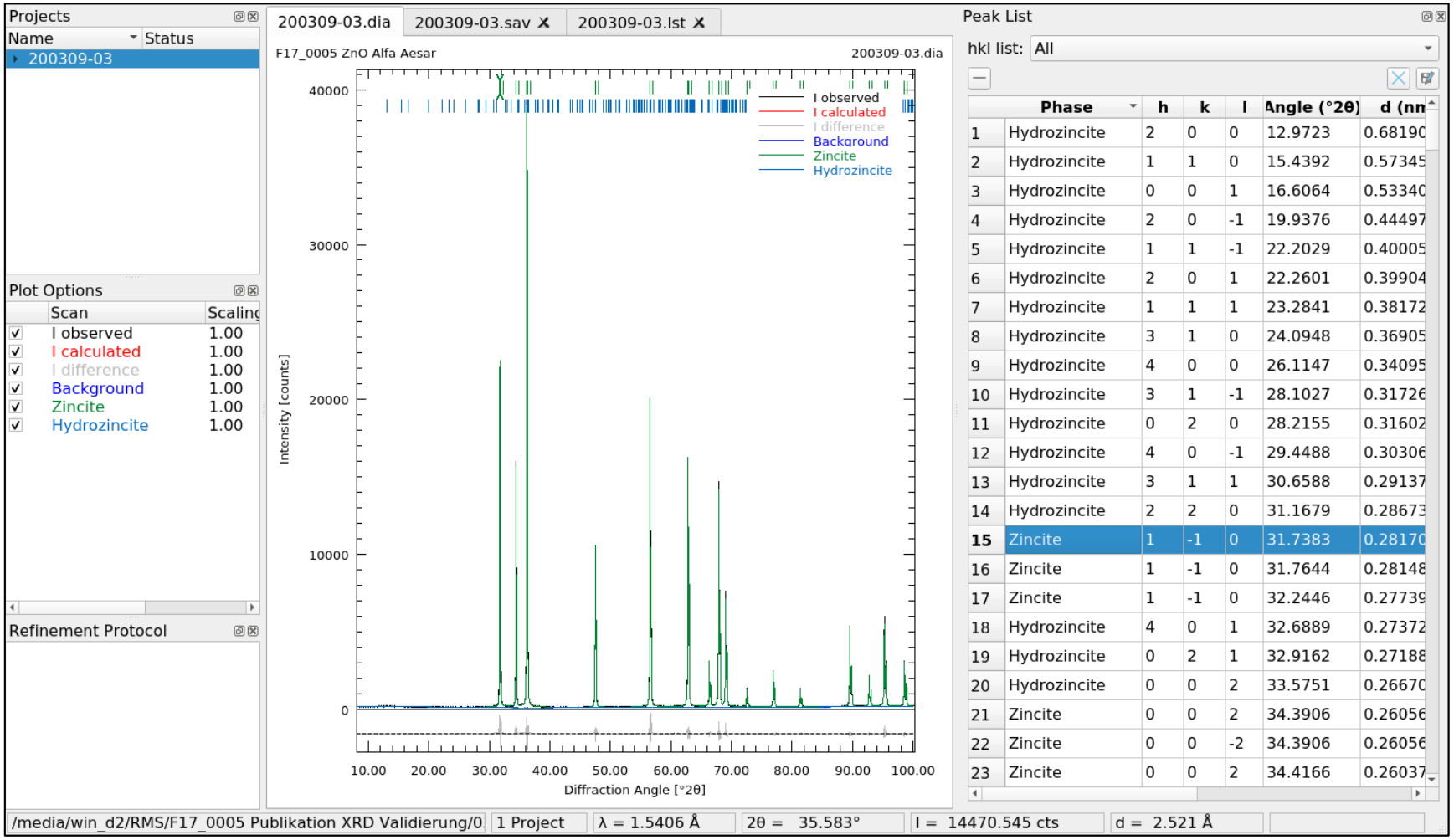
Peak list to analyze refined peak data (from BGMN *.par file)



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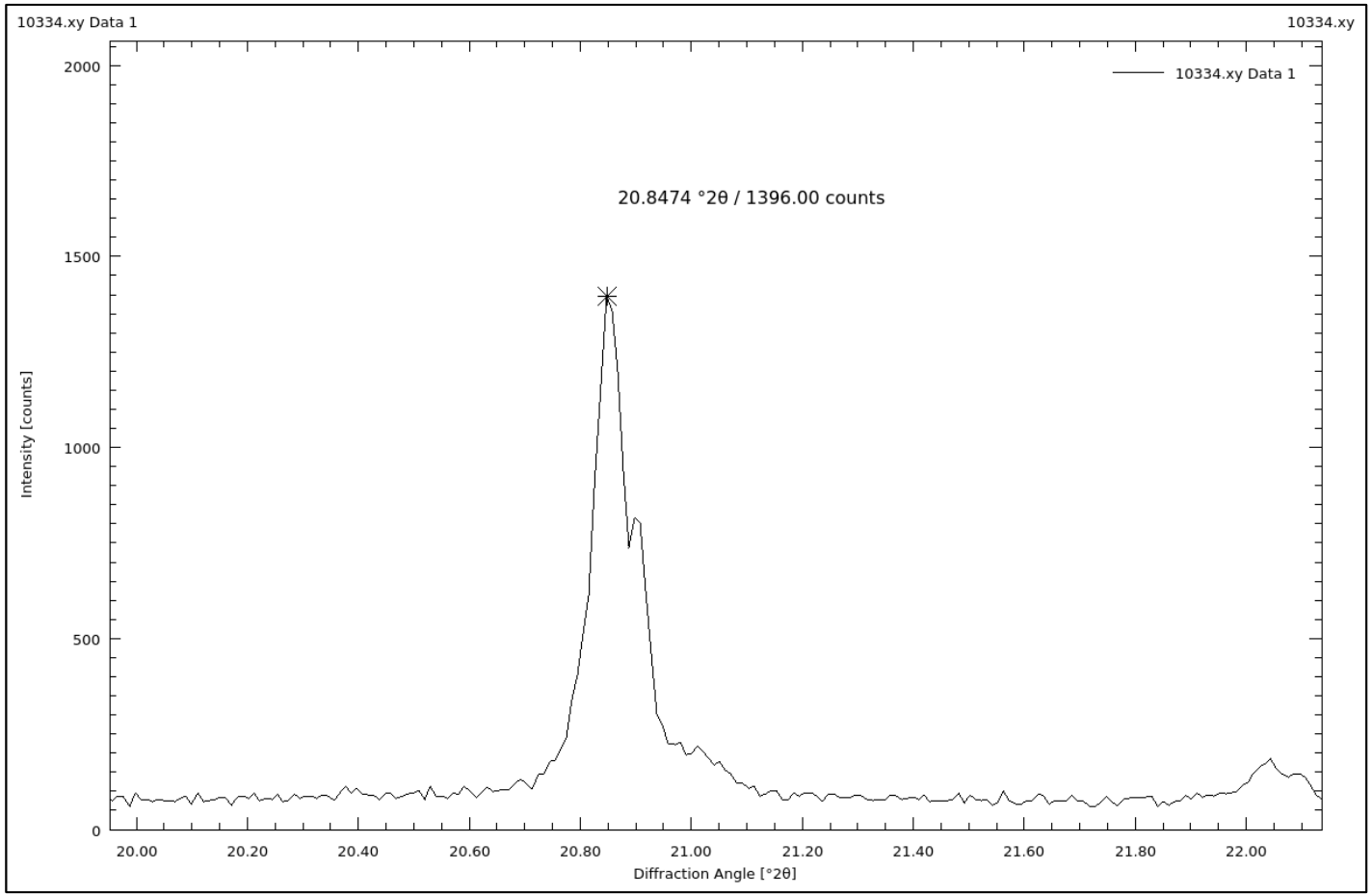
New „data inspection“ cursor („i“ key)



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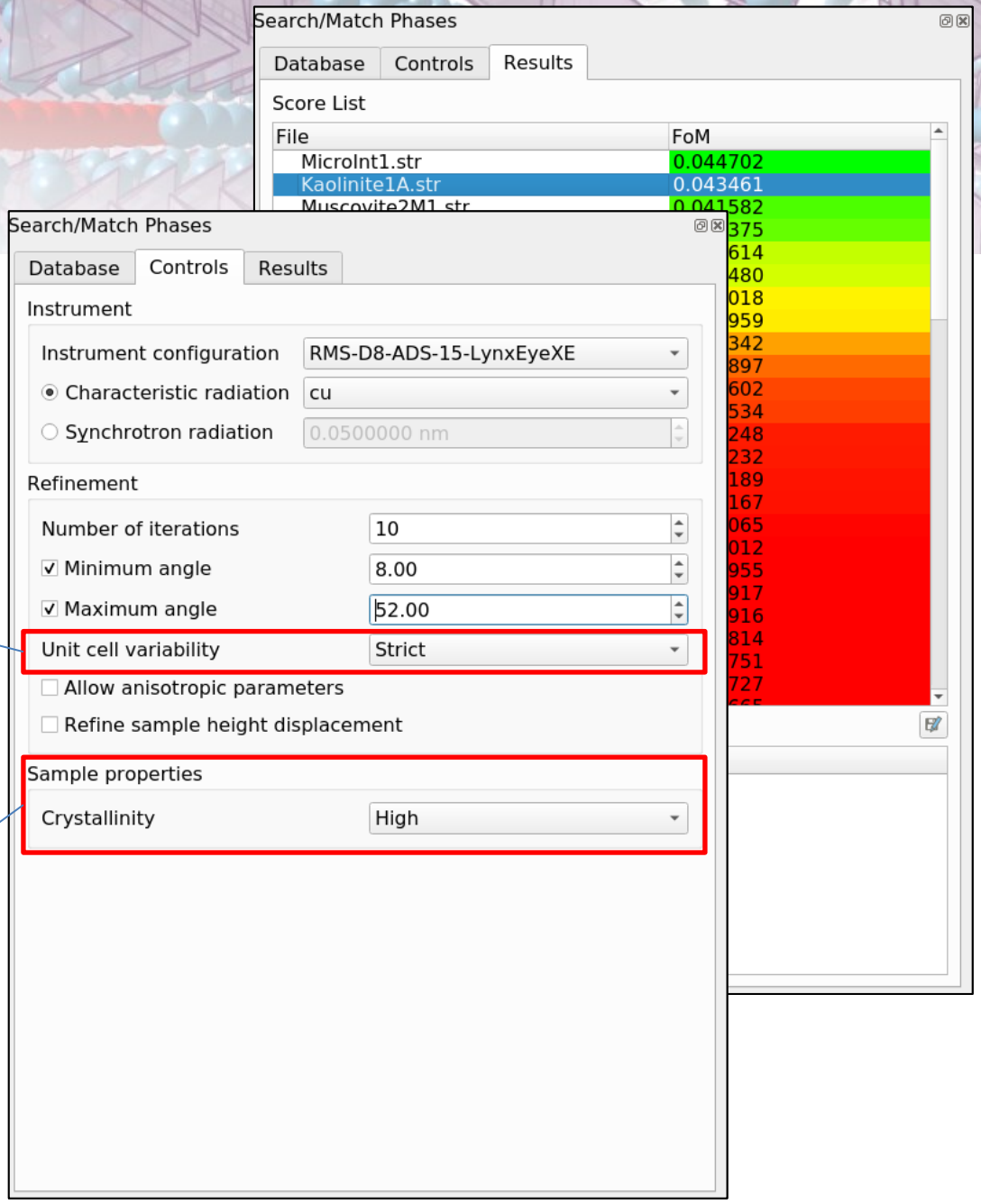
More options to improve phase matching (reduce false-positive phase matches)

Restrict unit cell variability

Restrict crystallinity for residual searches



+ many more improvements:

- Performance improvements of the user interface
- Support for Malvern/PANalytical XRDML v2.0 files
- Fixed wrong sorting of projects and wrong order of batch refinements
- Fixed wrong assignment of sample ID
- Fixed wrong calculation of chemical composition when goals are normalized to 100%
- Progress dialog for various „Apply to all projects“ functions
- Major internal code modernization

Bug image: http://www.thecomputeradvisor.net