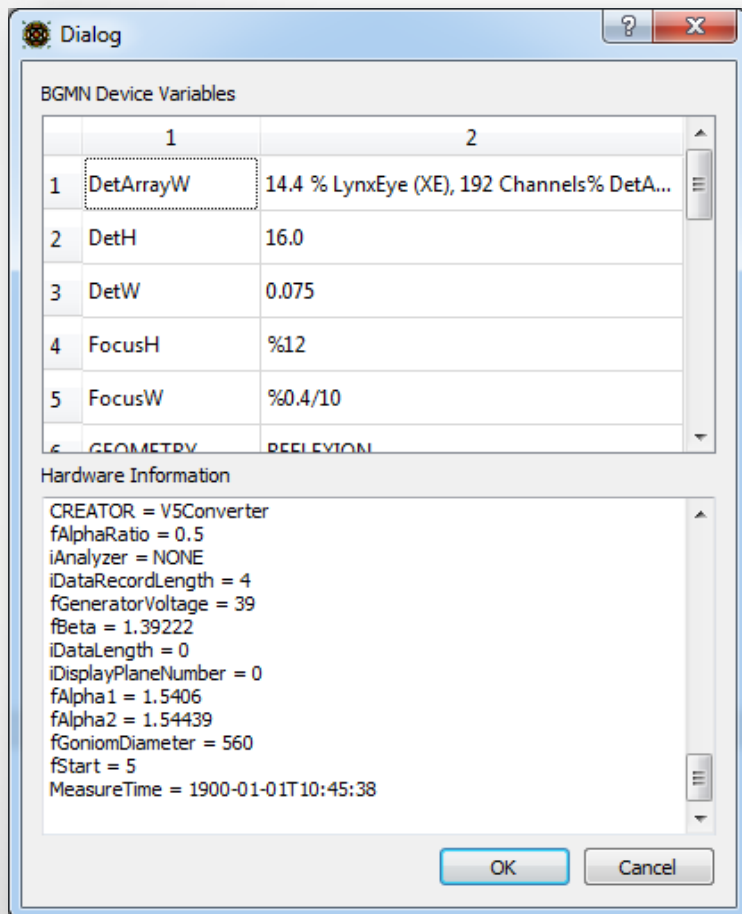


New Features in Profex 3.4

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Create Instrument Config Files from Raw Data



Instrument -> New Configuration:

Extracts Hardware Information from
raw data files (currently: Bruker V4, V5,
PANalytical XRDML)

(Work in progress)

Right Mouse Button: Add output files

The screenshot shows the Profex 3.5.0-alpha software interface. The main window displays a list of files in the 'Projects' pane and a text editor with the following content:

```
% Theoretical instrumental function
VERZERR=cubix-ads-15mm.geq
% Wavelength
LAMBDA=CU
% Polarization (CuKa with Graphite monochromator)
POL=sqr(cos(26.6*pi/180))
pi=2*acos(0)
% Phases
STRUC[1]=Hydroxylapatite.str
STRUC[2]=alphaTCP.str
FCFOUT[2]=alphaTCP.str
RESOUT[2]=alphaTCP.str
% Measured data
VAL[1]=1405221a.dia
% Minimum Angle
% WMIN=10
% Maximum Angle
% WMAX=60
% Result list
LIST=1405221a.lst
% Peak list
```

A right-click context menu is open over the 'STRUC[2]=alphaTCP.str' line. The menu items are:

- Undo
- Redo (Ctrl+Y)
- Cut (Ctrl+X)
- Copy
- Paste (Ctrl+V)
- Delete
- Select All (Ctrl+A)
- Open file
- Add STRUCOUT file
- Add SimpleSTRUCOUT file
- Add RESOUT file
- Add FCFOUT file
- Add PDBOUT file

The 'Add STRUCOUT file' through 'Add PDBOUT file' options are highlighted with a red box. Below the menu, a table shows refinement results:

Parameter / Goal	Value	ESD
alphaTCP	0.8011	0.0028
alphaTCP/sum	0.1989	0.0028

At the bottom of the window, the status bar displays: Wavelength: 1.54183 Å, Angle: 0.000°, Intensity: 0.000 cts, d-Spacing: 0.000 Å, Line 9, Column 13.

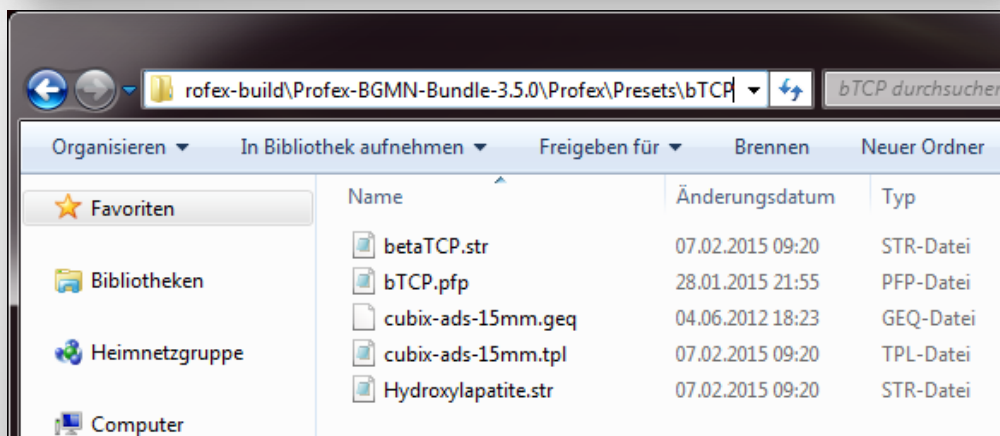
Refinement Presets

for common refinement scenarios

```
bTCP.pfp x
1 <preset name="bTCP">
2   <device>cubix-ads-15mm.geq</device>
3   <template>cubix-ads-15mm.tpl</template>
4   <structures>
5     <structure>betaTCP.str</structure>
6     <structure>Hydroxylapatite.str</structure>
7   </structures>
8 </preset>
9
```

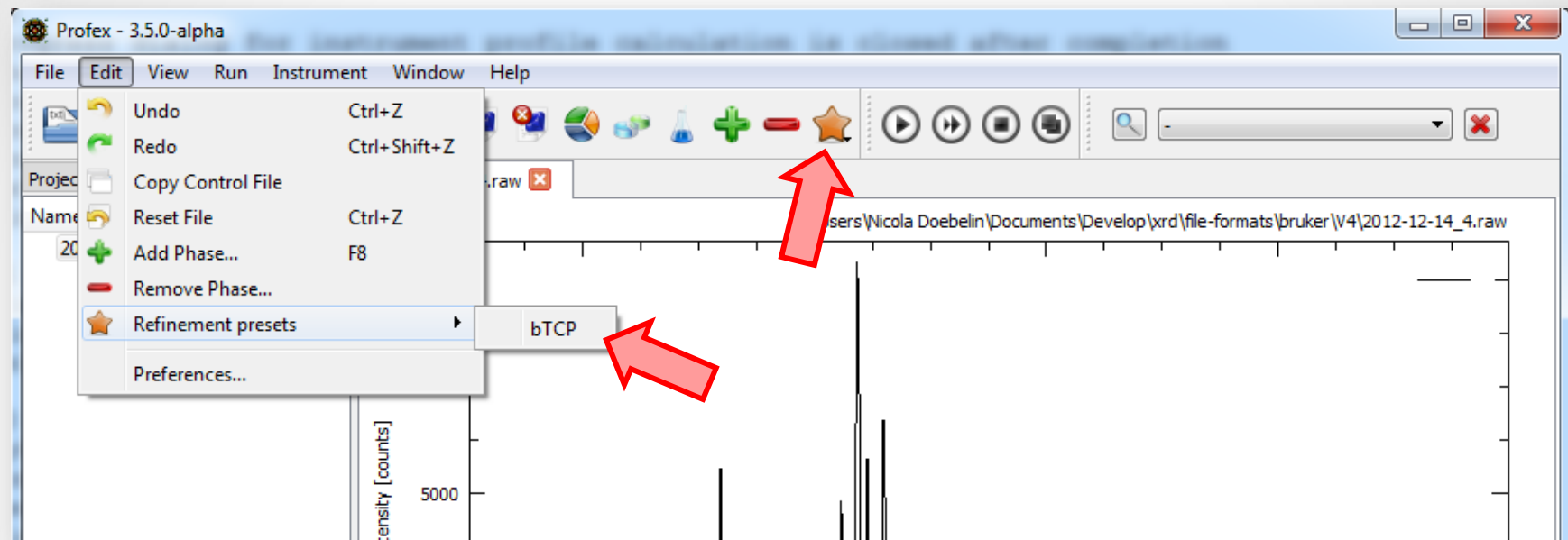
lengt Ln:9 Col:1 Sel:0|0 UNIX UTF-8 w/o BOM INS

Describe refinement scenarios
in a simple XML file



Store it in:
Profex-BGMN-Bundle-3.4.0\Profex\Presets
along with instrument and
structure files

Refinement Presets



Use only a few mouse clicks to apply and run the preset.

No selection of instrument configuration and phases required.