Instrument:
Data path:
Output path:

Sample	**Numor(s)/Files**						**Output workspace**
A 100 K	123456						
A 150 K	123460-123465	**REFERENCES**	MASKING	**CORRECTIONS**	NORMALIZATION	**OUTPUT**	
A 200 K	123468, 123470-123471						
A 300 K	123472:123480:2						

TOF

EPP default: Indicate that if nothing selected, EPP will be chosen from the fit of the 1st sample of the group.
I don't think that it is safe to let allow EPP to be determined individually for each numor (sample, bgr, vana, cadmium).

Elastic peak position	> Channel	(manual input of channel)
(exclusive menu)	> From file parameters	(manual selection of reference numor)
	> From fit	(manual selection of reference numor)
Flat background	> Non	(default)
(exclusive menu)	> From file	(manual selection of reference numor(s))

BS

Unmirror option	(default: 6) (selection)
(exclusive menu)	

If unmirror 5 or 6, make appear a box to select reference numor(s))

TOF & BS

Detectors masked: > Auto: If no EPP found or elastic peak intensity < Tolerance * median
(inclusive menu) > Auto: If background level too high
(default: nothing selected) > List of detectors

Tolerance: (input)
*Pb: How to determine if too high?

BS

*Use this window to determine what to do with min/max monitor and channels outside?

TOF

Detector efficiency: > None? *Option needed or can we decide to apply always?
> Apply (default) *1 or several equations

TOF & BS

Background subtraction > None
(exclusive menu) > None (but correct sample self-absorption)
> Use transmissions
> Compute self-shielding and absorption correction factors

If not None: **Background files:** (give numor or numors)

If 'use transmissions': **Sample transmission:** (manual input of value) *Possible to call a tool to help in calculating the transmissions (e.g. as DAVE)?
Background ('empty cell') transmission: (manual input of value)

$$I_S(2\theta, TOF) = \frac{1}{T_S T_B} \cdot \left[(S - C) - \frac{T_S T_B}{T_B} \cdot (B - C) \right] = \frac{(S - C)}{T_S T_B} - \frac{(B - C)}{T_B}$$

If Flat background (FB) used, the same FB will be subtracted to all the measurements (S, C, B), so it has no influence if the Cd (C) is used. If no Cd, then FB plays the same role as C.

If abscor (or self-absor): **Sample formula:** (input)
(Params needed by
PaalmanPings routines) **Sample mass density:** (input) *Add option to compute it from crystal cell?
Geometry: (select flat, cylinder or hollow cylinder)

If flat: **Sample thickness (cm)** (input)
Sample angle (deg) (input) *Help to show how the angle is defined

If flat + background: **Background (empty cell) formula:** (input)
Background (empty cell) mass density:
Can front thickness (cm) *This is Ok for an empty cell, but what if the background to subtract is e.g. a buffer? The most correct thing
Can back thickness (cm) would be to treat these as two separate measurements, correct them and then subtract one from the other!

If cylinder: **Sample radius (cm)** (input)
Beam height (cm) (input) *Need to check how the beam infos are used.
Beam width (cm) (input)
Step size (input) *This should be calculated automatically, without needing user input.

If cylinder + background: **Can formula:** (input)
Can mass density: (input)
Can thickness (cm) (input) *Or can outer radius?

If hollow cylinder: **Sample inner radius (cm)** (input)
Sample outer radius (cm) (input)
Beam height (cm) (input)

Beam width (cm) (input)
Step size (input)

If cylinder + background: **Can thickness (cm)** (input) *Or can outer radius?
Inner cylinder?
*Not in present algorithm, but standard cells are formed by 2 concentric cylinders. This needs to be taken into account in the calculation for the amount of 'empty cell' (would need to rewrite the algo, an alternative is to assume that the thickness of both cylinders is the same and multiply the value above by 2)

$$I_S(2\theta, TOF) = \frac{1}{A_{S,SB}(2\theta, E_i, E_f)} \cdot \left[(S - C) - \frac{A_{B,SB}(2\theta, E_i, E_f)}{A_{B,B}(2\theta, E_i, E_f)} \cdot (B - C) \right]$$

Cadmium: > None (default)
> Use Cd

If not None: **Cadmium files:** (give numor or numors)

TOF

Run normalization: > monitor (default) *better name?
(exclusive menu) > time

TOF & BS

Detector normalization: > none (default) *better name?
(exclusive menu) > vanadium
> other *perhaps give only V possibility, to simplify options below?

If vanadium or other: **Normalization files:** (give numor or numors)
Integration limits for EP: > full range
(exclusive menu) > auto *e.g. EP +/- 3*sigma?
> manual input

If vanadium: **DW correction for V:** > none
> yes *Select best choice for DW corrections. If no agreement, propose different formulas?

If V or other: **Background for normalization sample:** > none (default)

Assume same 'background' method as the one used
for the sample and defined in corrections > use sample background
> background files: (give numor or numors)

If transmission **Sample (V/other) transmiss** (input)
If not sample bgr: **Can transmission:** (input)

If absorption corr: **Sample formula:** (input) *Only if other
Sample mass density: (input) *Only if other
Geometry: (select flat, cylinder or hollow cylinder)

If flat: **Sample thickness (cm)** (input)
Sample angle (deg) (input)

If flat + other background: **Background (empty cell) formula:** (input)
Background (empty cell) mass density:
*This is Ok for an empty cell, but what if the background to subtract is e.g. a buffer? **Can front thickness (cm)**
The most correct thing would be to treat these as two separate measurements, **Can back thickness (cm)**

If cylinder: **Sample radius (cm)** (input)
Beam height (cm) (input)
Beam width (cm) (input)
Step size (input)

If cylinder + other backgrou **Can formula:** (input)
Can mass density: (input)
Can thickness (cm) (input)

If hollow cylinder: **Sample inner radius (cm)** (input)

Sample outer radius (cm) (input)
Beam height (cm) (input)
Beam width (cm) (input)
Step size (input)

If cylinder + other backgrou **Can thickness (cm)** (input)
Inner cylinder?

*Not in present algorithm, but standard cells are formed by 2 concentric cylinders.
This needs to be taken into account in the calculation for the amount of 'empty cell'
(would need to rewrite the algo, an alternative is to assume that the thickness
of both cylinders is the same and multiply the value above by 2)

Absolute units: > No (default)
> Yes

If Yes: **Ratio illuminated volumes sample/norm:** (input)
Sample formula *Only if not given in corrections (transmission)
Sample mass density *Only if not given in corrections (transmission)

TOF

Selection menu	> I(Q)	(possibility to give integration limits)
(inclusive menu)	> I(energy)	(possibility to give Q/detector limits)
	> I((Q,E)	
	> DOS	
	> Susceptibility?	
	> I(pixel,E)	

*Need to think of how to generate new outputs without running full reduction

BS

Selection menu	> I(Q)	(possibility to give integration limits)
(inclusive menu)	> I(energy)	(possibility to give Q/detector limits)
	> I((Q,E)	