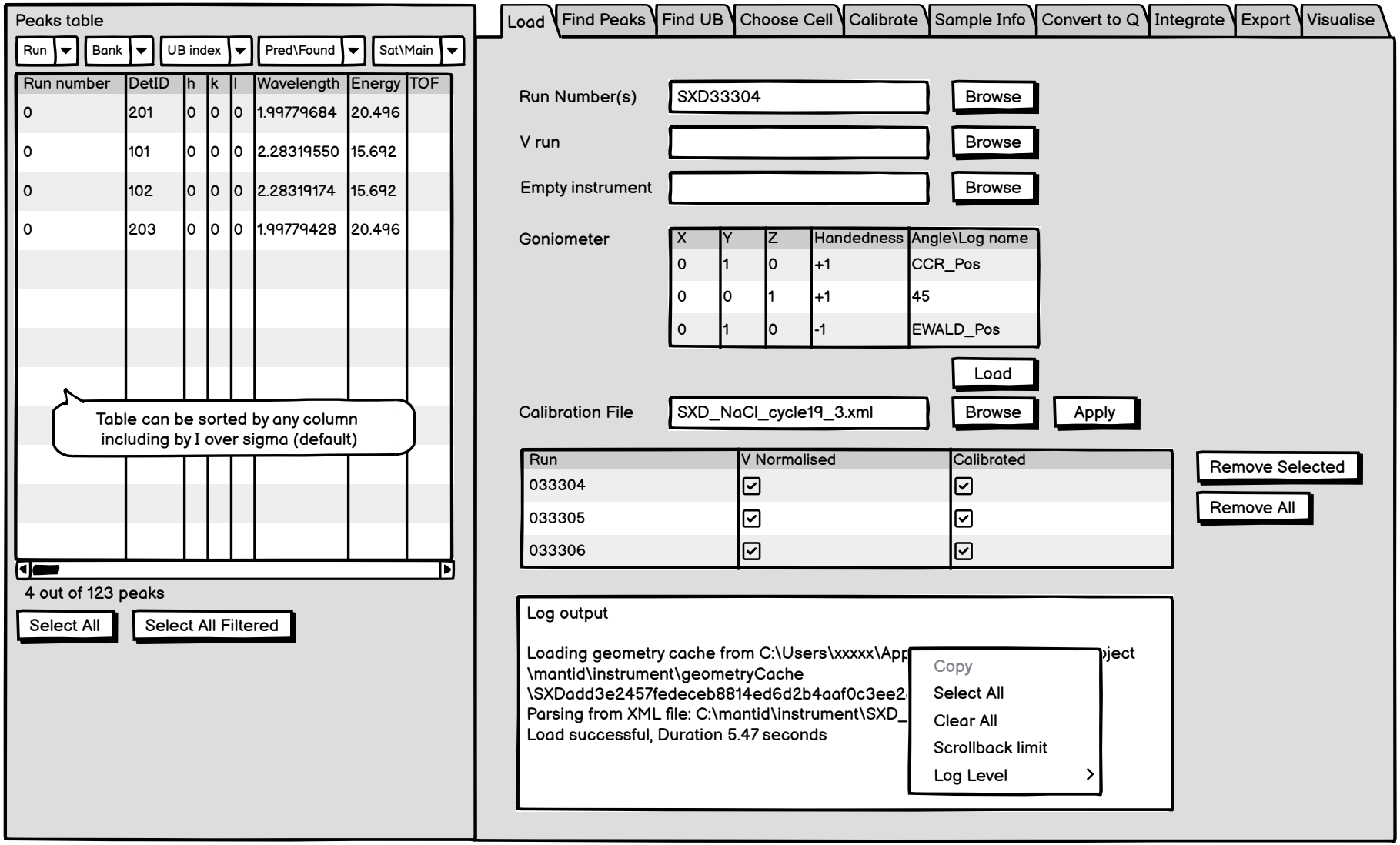


UI would need to remember the last used V run to avoid user having to respecify on each load

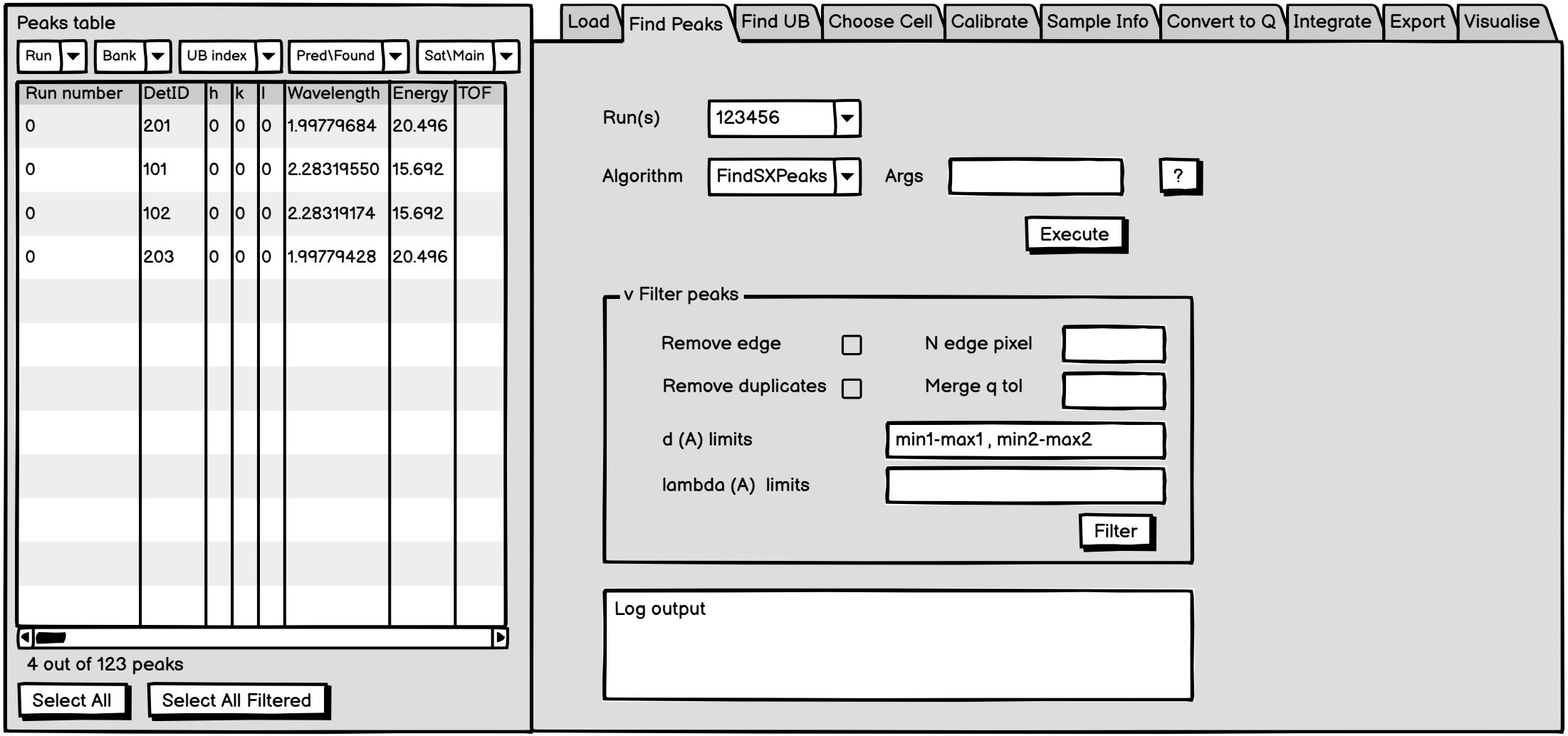
NormaliseByCurrent on Load as well

Goniometer log names remembers last ones used

calibration .xml file

Removing a run from the runs table deletes any associated peaks from the peaks table also

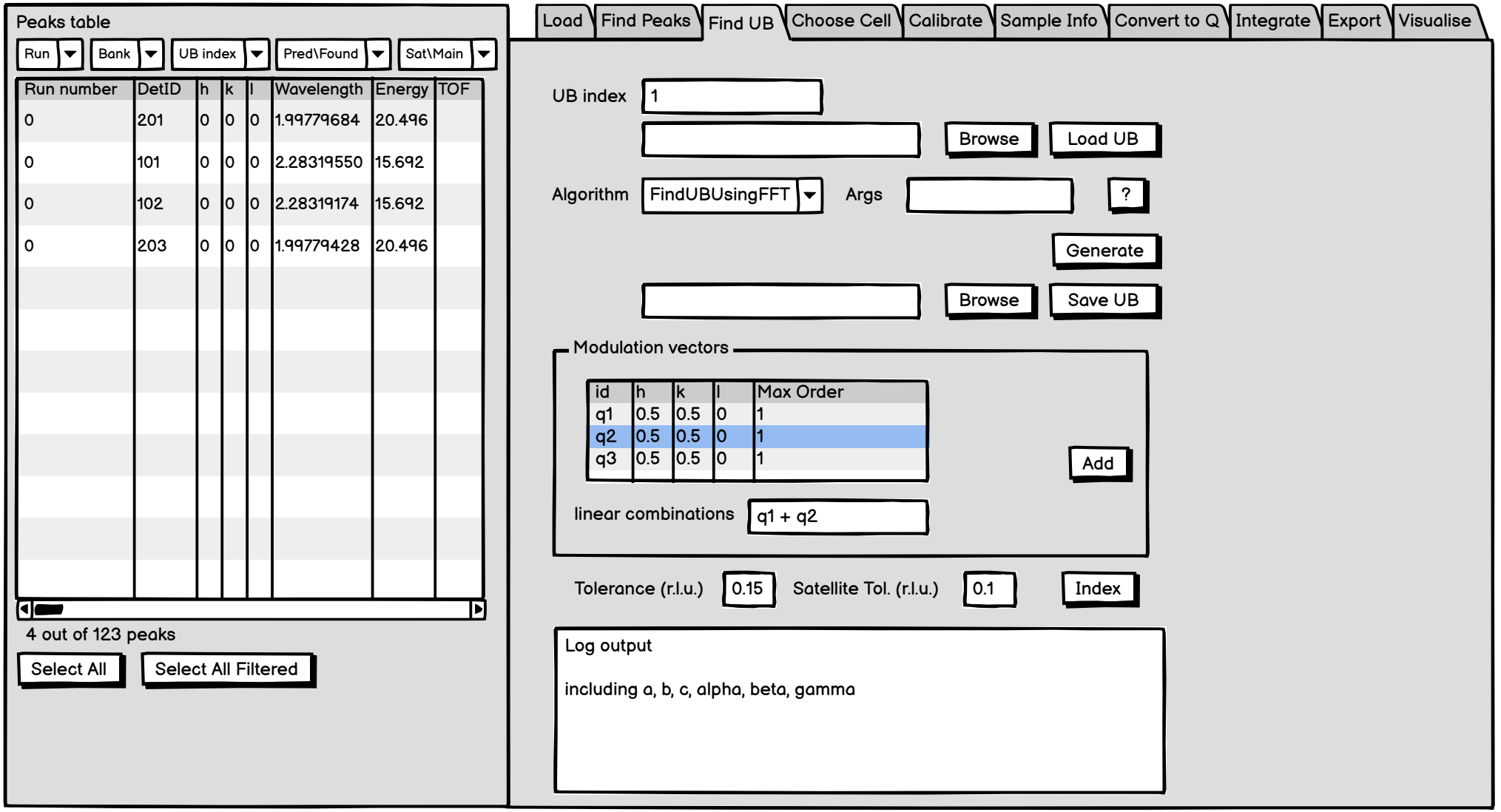
Each tab has a log output window showing output from processes initiated on that tab - so no need to go to master workbench message log



Args should be populated with the default value for all mandatory arguments

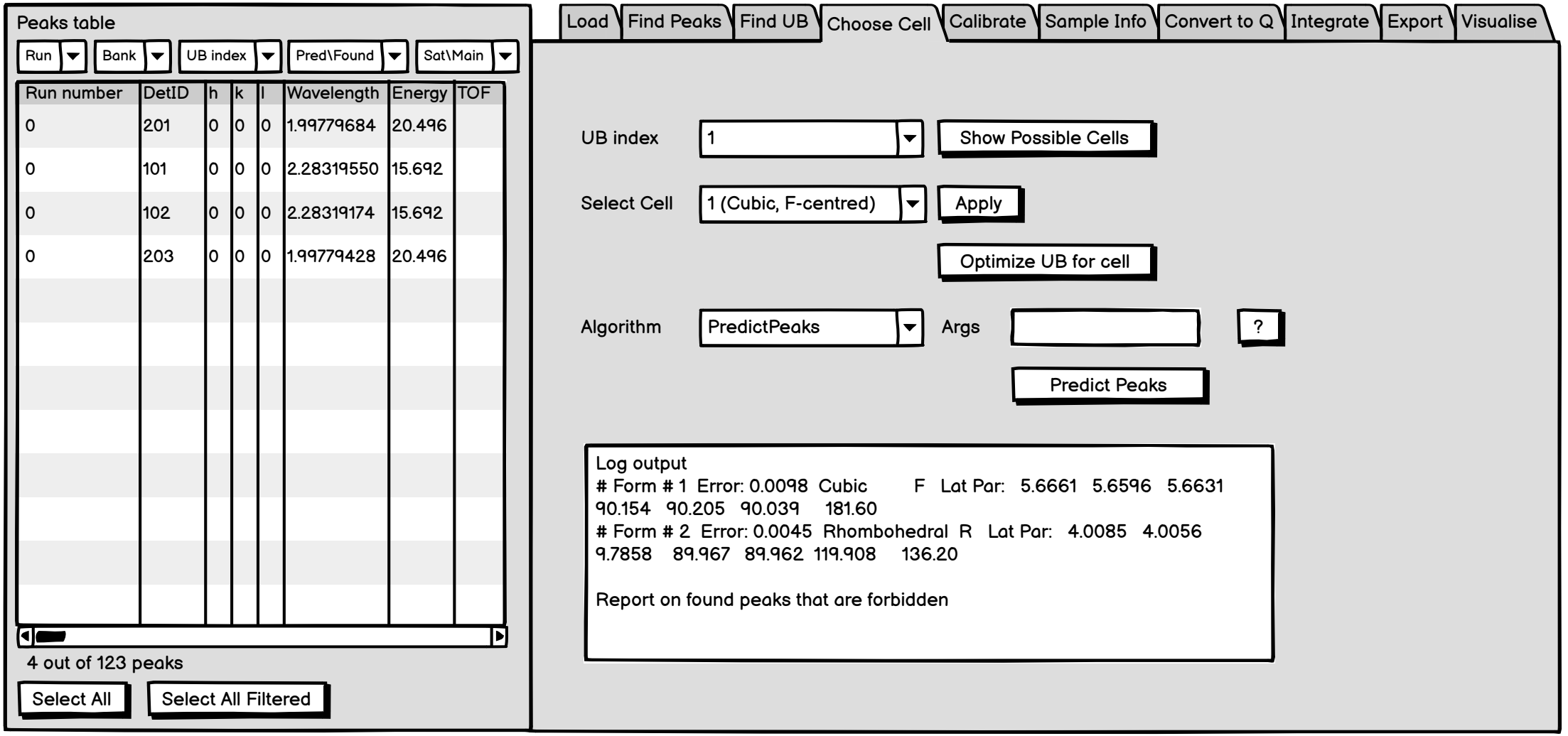
Populate peak markers on the instrument view (Visualise tab)
No slice viewer at this point

Peaks table gets populated



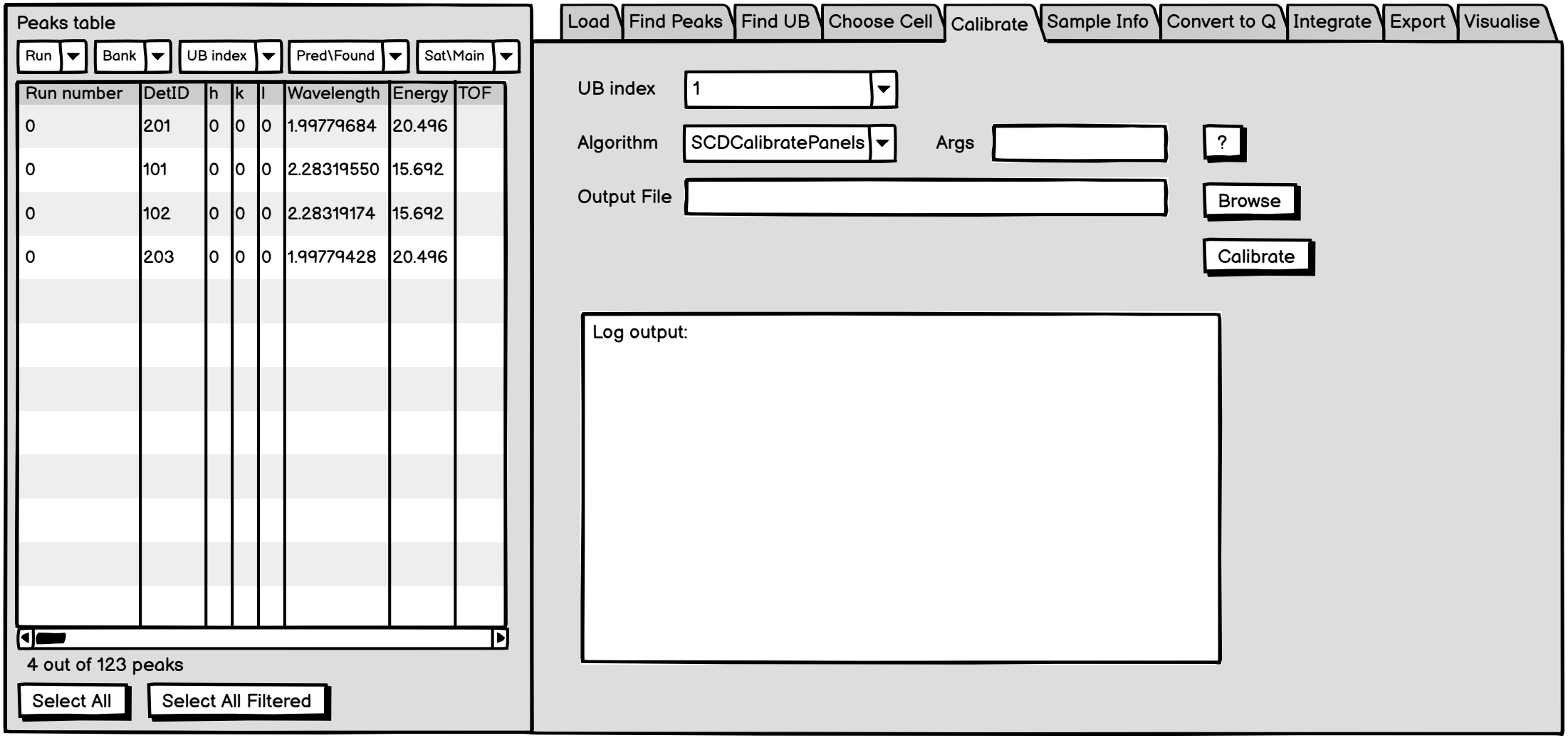
User selects subset of peaks displayed in peak table
User can load a UB from file or generate one
Behind the scenes Mantid has a temporary peaks workspace corresponding to filtered view of that the peaks table (corresponding to a UB index) - this could contains peaks from more than one run
When hit Execute, the calculated UB gets saved to a peaks workspace per UB index + the UB index will be populated against the relevant peaks in the table
"UB index" edit box auto populated with next ID when execute pressed (if blank). If user populated, an existing UB will be overwritten

Possible algorithms:
FindUBUsingFFT
FindUBUsingLatticeParameters



User blanks out UB index in the peaks table for systematically absent peaks
Apply - make new B matrix using best guess lattice parameters (might not be exactly cubic)
Optimize UB for cell - forces a=b=c (in this example)
Every UB index will have: a peaks workspace with found peaks + separate peaks workspace for predicted peaks
Apply to all button\option?

Possible extra - support way of supplying 3x3 transformation twinning matrix to generate related UBs corresponding to allowed domains

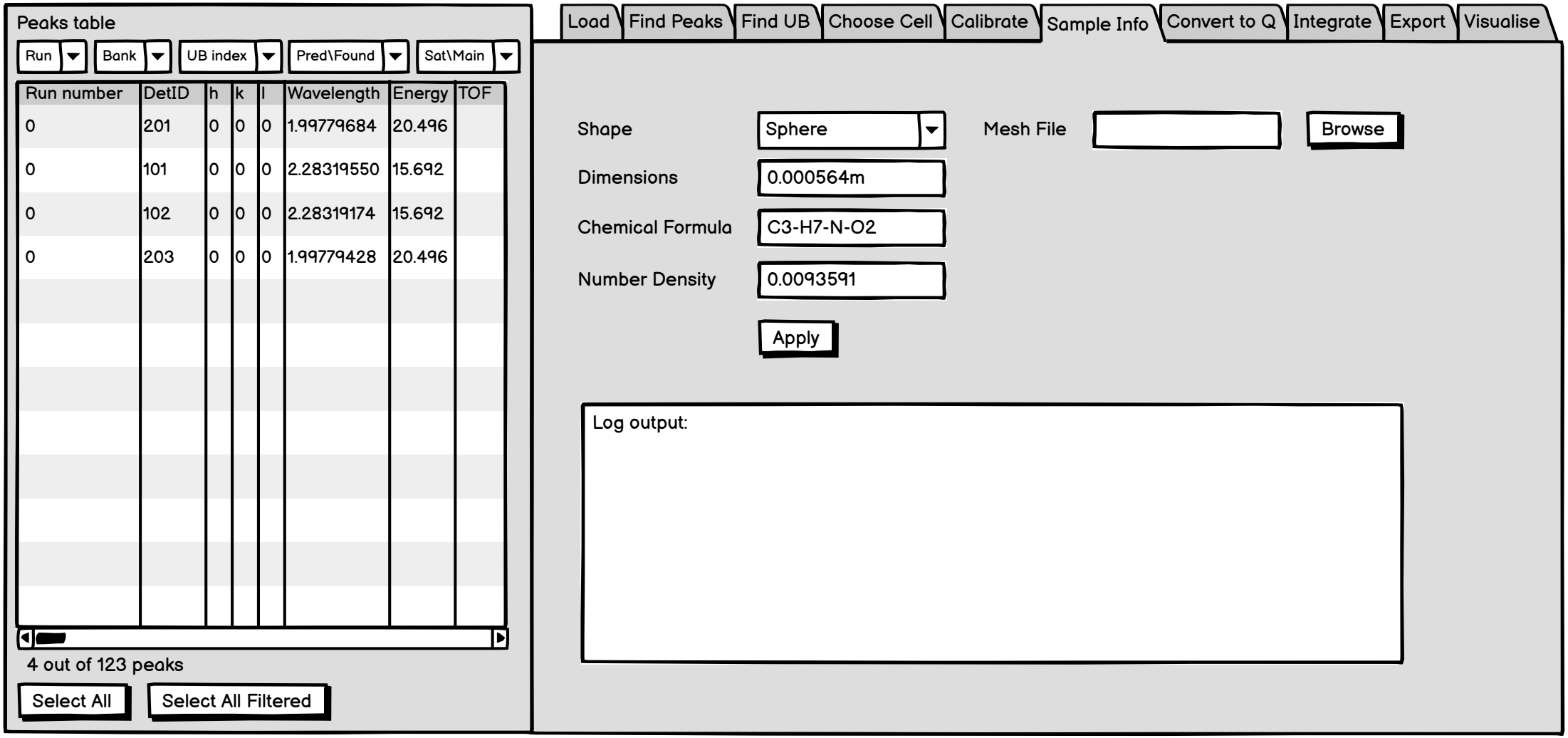


Args should be populated with the default value for all mandatory arguments

Choose either SCDCalibratePanels, OptimizeCrystalPlacement, OptimizeCrystalPlacementByRun algorithm

Successful calibration will update the calibration file input on the Load tab

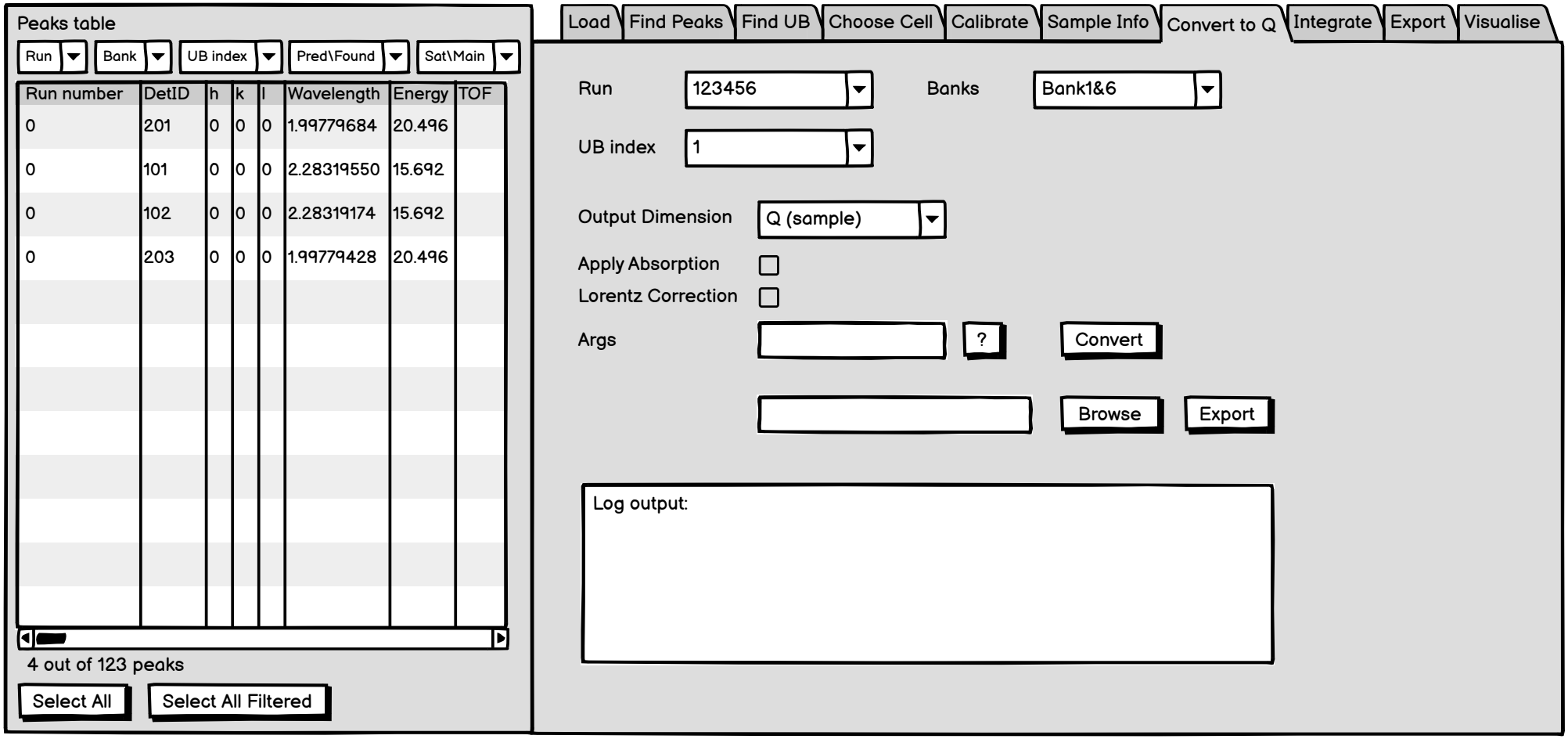
May visit this tab just for NaCl or could do it for every real sample



Run SetSample on all workspaces (all matrix and peaks workspaces)
Shape drop down has:
- Sphere
- Cylinder
- Mesh

If Mesh selected the Mesh File Browse box is enabled
Dimensions box will be shape specific eg radius only for sphere, radius, height, axis for cylinder etc
For mesh and maybe other shapes, need to supply initial orientation. May imply extra fields

Need to store the V sample details somewhere but won't vary for same instrument so put in settings somewhere?

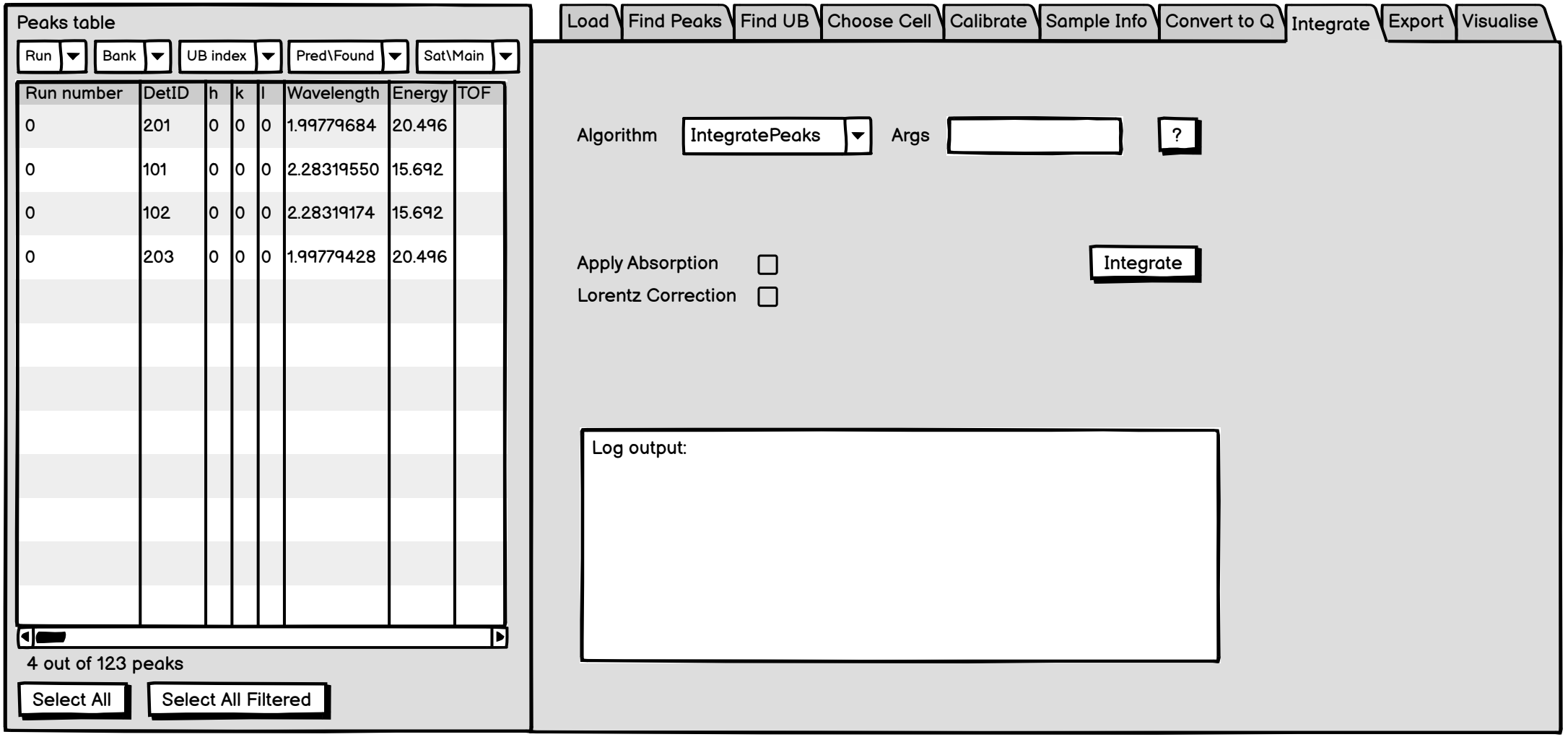


Users may select runs by multiselect run dropdown or specifying UB index
Only permit one selected UB index if output dimensions=HKL
Args should be populated with the default value for all mandatory arguments
Use algorithm: ConvertToDiffractionMDWorkspace
Slice viewer and 3D isosurface view activate (Visualise tab)

Output Dimensions:
- Q (sample)
- Q (lab)
- HKL

Possibly in future add k_f to possible output dimensions

May be more generic to allow bank selection via the instrument tree in instrument viewer rather than a bank drop down. Bank definition varies (level\type) across instruments



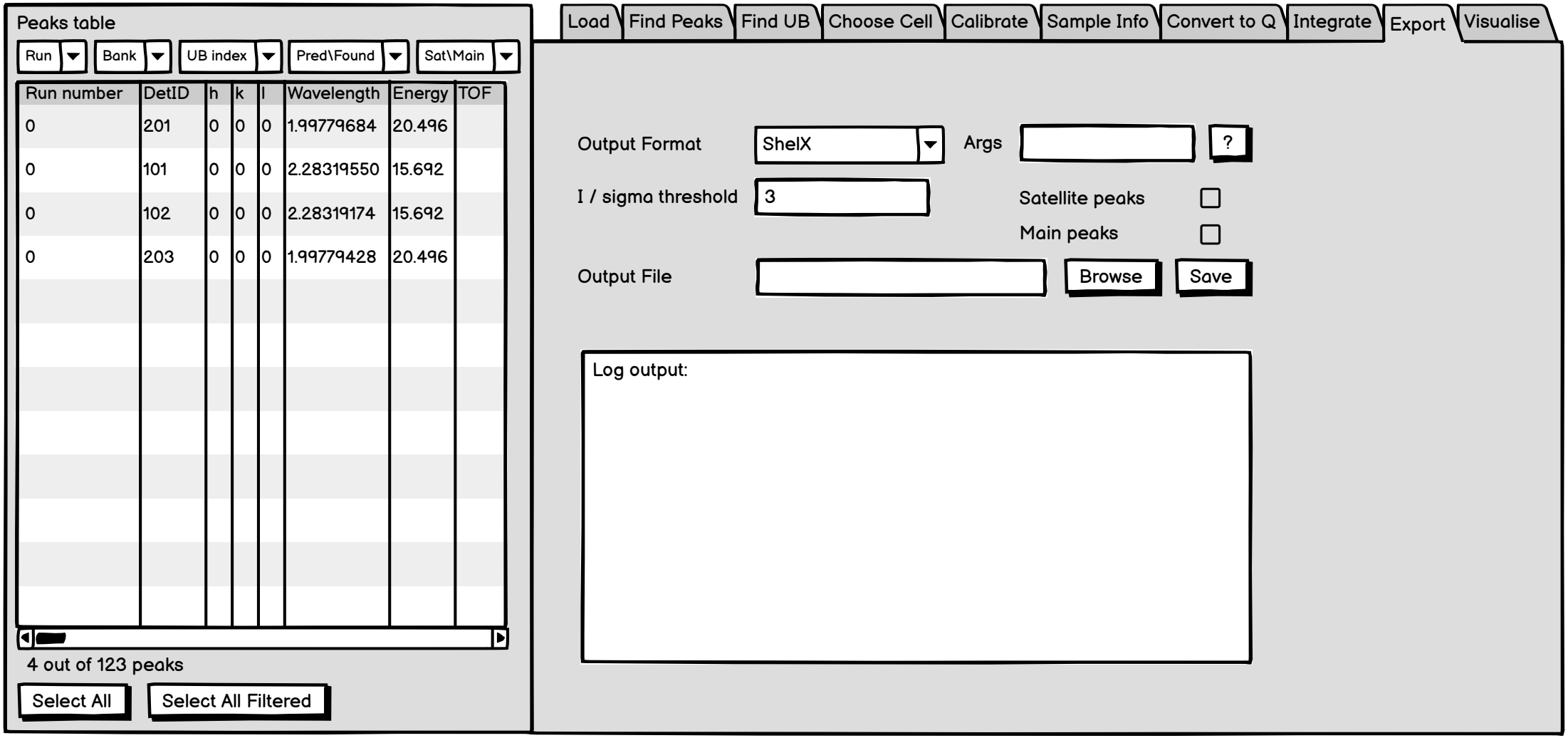
Available algorithms:
- Integrate in Detector space (IntegratePeaksSkew + perhaps others in future)
- Integrate in QLab (IntegratePeaksMD)
- Integrate in HKL (IntegratePeaksMDHKL)

Args should be populated with the default value for all mandatory arguments

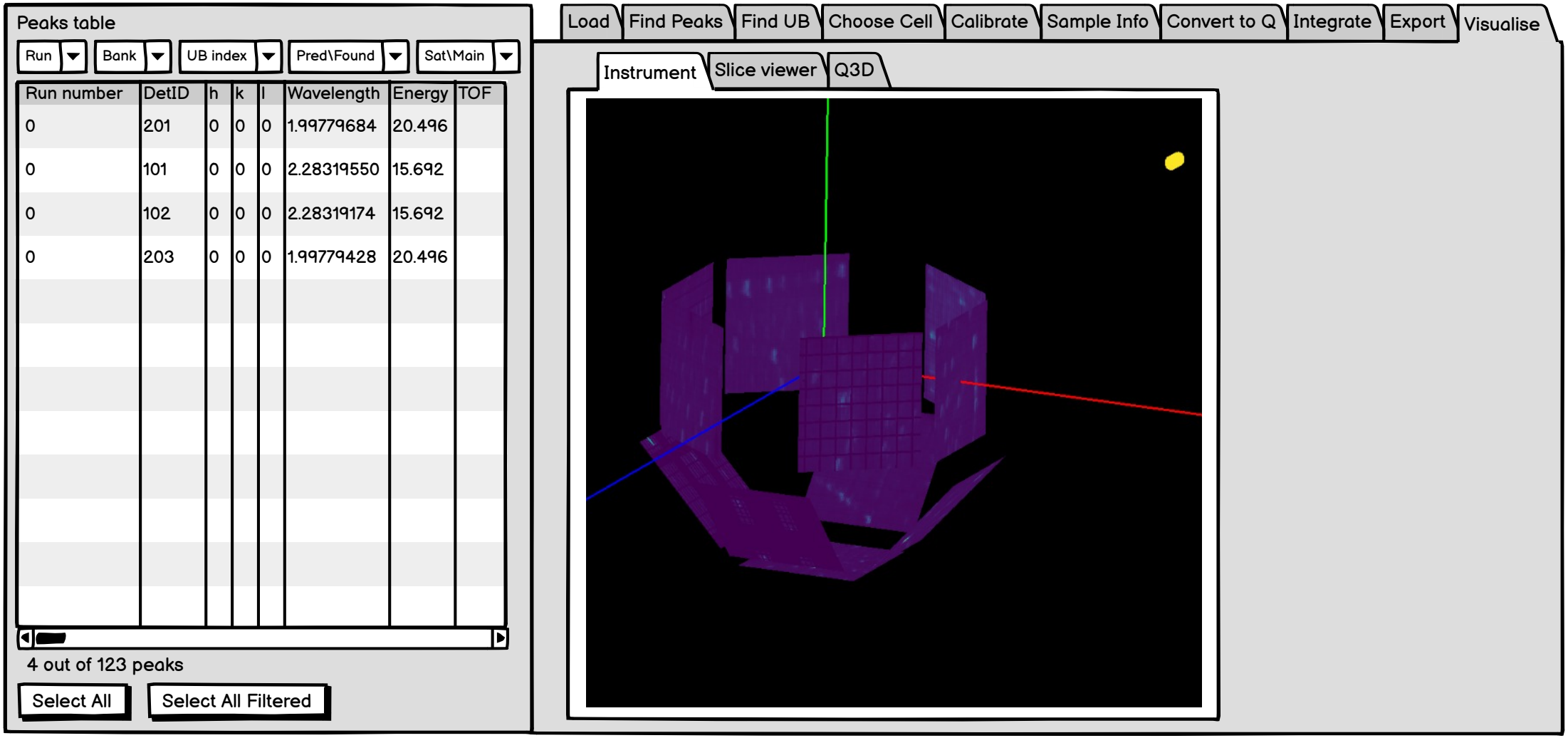
The set of peaks/runs that are to be integrated is driven by the peaks table on the left hand side. If the user selects peaks from more than one UB then the IntegrateHKL algorithm should be disabled

IntegratePeaksMD should be disabled if there isn't an MD workspace for every run that's been selected

Predicted\Found filter should never allow both to avoid integrating huge number of peaks



Runs SaveReflections
Support ShelX, Jana
Args should be populated with the default value for all mandatory arguments
Can add logic to autopopulate filename given runs selected



Will automatically overlay any peaks in the table on instrument.

Will zoom to selected peak on detector (and Q if present)

If more than one run in the table - will have drop-down box to select a specific run?

Probably want it to be possible to undock this so it can standalone as its own window