

New features, 2015-1 run

General

- ETA is displayed at the bottom of JBlulce while setting up a collect or raster task
- The 5-digit frame numbering is now in effect
- If the detector is busy or the software is not running, collect and raster will be disabled and further information is available by hovering over the start button
- The 120-sec countdown, if there is a problem with the detector software, is eliminated. The problem is now reported within 5-10 seconds

Sample tab

- No changes

Screening tab

- Crystal scoring and strategy calculations are now implemented for multiple attempts for the same sample

Raster tab

- View/Move modes have been added.
- Instead of right-clicking the video to select “view images”, view mode is automatically switched to during and after each raster
- In view mode, left-clicking a cell will show that cell in the table and load the corresponding diffraction image in the image viewer of the sample tab
- Diffraction image can also be viewed by selecting a cell from the results table
- User can control the Spotfinder options through the Spotfinder options window. A link in the window shows the documentation for these options
- Spotfinder can be re-run with changed parameters during or after the initial automatic processing
- The search field which was set up in the grid mode, can be offset by typing a number in the offset window
- The spreadsheet icon opens a spreadsheet version of the results table
- The diffraction image icon opens the sample tab peelout in viewer mode
- The keyboard icon opens a quick reference for Raster tab features
- New cell numbering and heat map schemes have been implemented and placed above the raster viewer
- When JBlulce is resized, the raster video will resize with it
- Video can be expanded vertically by moving the slider below it
- Runs can be hidden with the maximize button to add more area
- All SpotFinder output variables can be viewed by choosing the output tab below the video
- Sites can be created by right-clicking a cell in the video
- Sites created from the table, video, or hit selection don't overwrite each other
- When grid numbers are too close together, numbers are skipped to retain legibility
- Right-clicking a cell on the video provides the option to center that cell
- The site list is automatically hidden when it's empty, but can be shown by clicking the collapsed vertical header
- Typing a number in the table will go to that cell in the table. Hitting “Enter” after that will highlight the corresponding cell in the raster search field

- Columns can be added or removed by right-clicking the header
- Columns can be reorganized by dragging and dropping them

Collect tab

- Graphs of spot total, Bragg candidates and resolution estimate are shown in near-realtime below the image viewer
- Hovering in the graph shows information for a given frame, and frames can be loaded in the viewer by left clicking or dragging
- Click the legend items to show or hide the plots
- Click the downward triangle on the graph to hide it, and the upward triangle at the top of the image viewer to restore
- In vector mode, batch site selection (or deselection) is implemented. For example, user can select sites from “20 to 30”. Typing only one number (in the first cell) selects or deselects only that site
- In the vector mode, after entering a number of sites, choosing this option will calculate a step size to fill the defined vector
- If a collection task is set up with energy moves, a popup will ask to confirm the moves in the current and all subsequent data collection tabs
- Clicking the reset button above the viewer will center the image and reset the zoom
- When a collect run is in raster mode, a button “Add current site” will add the current position as a raster site
- Slowdowns related to working with thousands of frames are reduced
- The video tutorial and the help document in pdf format have been added in the Multi Crystal Strategy tab
- XPLAN strategy can be exported into a new collect run
- The “Merge datasets” has been renamed into “Combine datasets”
- Version of MOSFLM & BEST displayed in the strategy tab
- Help sub-tab added in the Strategy tab
- “Both” option has been added to the background data processing options and it is a default

Analysis tab

- The Help sub-tab has been added
- “Processed with” drop down menu has been added. Selecting the processing software will display the processing statistics from that software
- AIMLESS is now used for scaling instead of SCALA
- Processing with XSCALE is now added for better handling of inverse beam, vector with overlaps, and raster data

Other

- The video tutorial for data transfer with Globus is available on GMCA webpage