Torx® Quarterly Update   Q3 2023

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Torx Design and Analyze updates

Enhancements

Triage designs in the Data Table with multiparameter optimization

Torx Design now includes the MPO plot and score in the Data Table.

Use the properties plugin to configure parameters to include in the MPO plot based on your available properties.
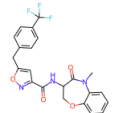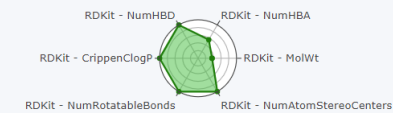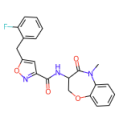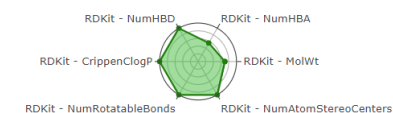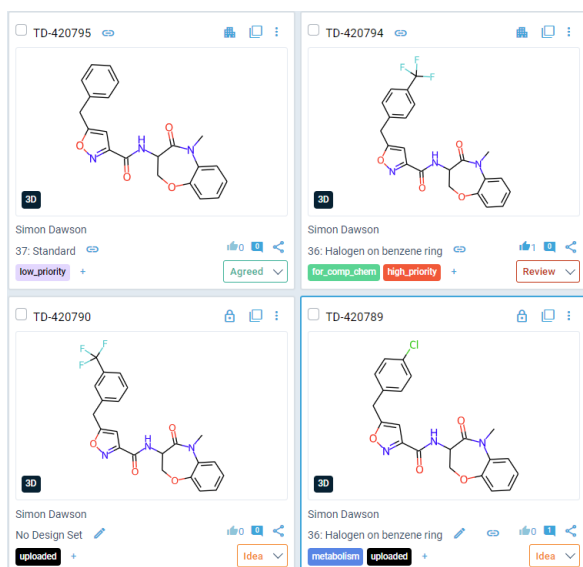

The MPO plot and score columns will then be updated in the Data Table, enabling more efficient triage and optimization of designs.

Categorize designs using labels

Tags have been renamed labels' in Torx Design, and you now have the option to add a color to each label to make them easier to differentiate in the Data Table and My Designs plugins. In this way you can easily draw attention to designs which are high priority, require a certain action to be taken, or which are members of a specific grouping.

Choose to download either 2D or 3D structures to SDF

When downloading molecules to SDF you now have a choice to include the 3D structures (if these are available) or default to just the 2D representation.
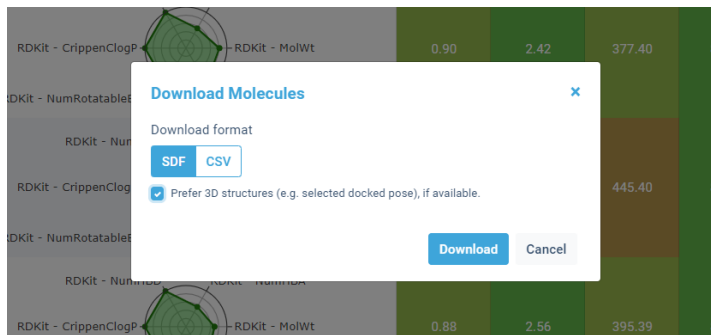
Data Table enhancements

Properties in the Data Table inherit properties color settings

Properties color settings are now made consistent across both the Properties and Data Table plugins. Simply define color function and values in the Properties plugin (or load global project settings) and the Data Table will adopt the same settings automatically.
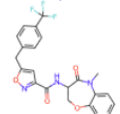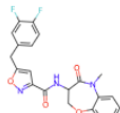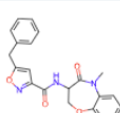

Group rows by any column

The row grouping feature has now been expanded to include any column in the data table, enabling you to categorize designs into groups based on any of the available data.

Sort by selected molecules

Easily bring selected molecules to the top of the Data Table by using the new sort function on the checkbox column.

Protein uploads

Uploading a protein structure with ligand still in the active site will now trigger a warning to the user in the Control Panel, avoiding confusion during docking experiments.

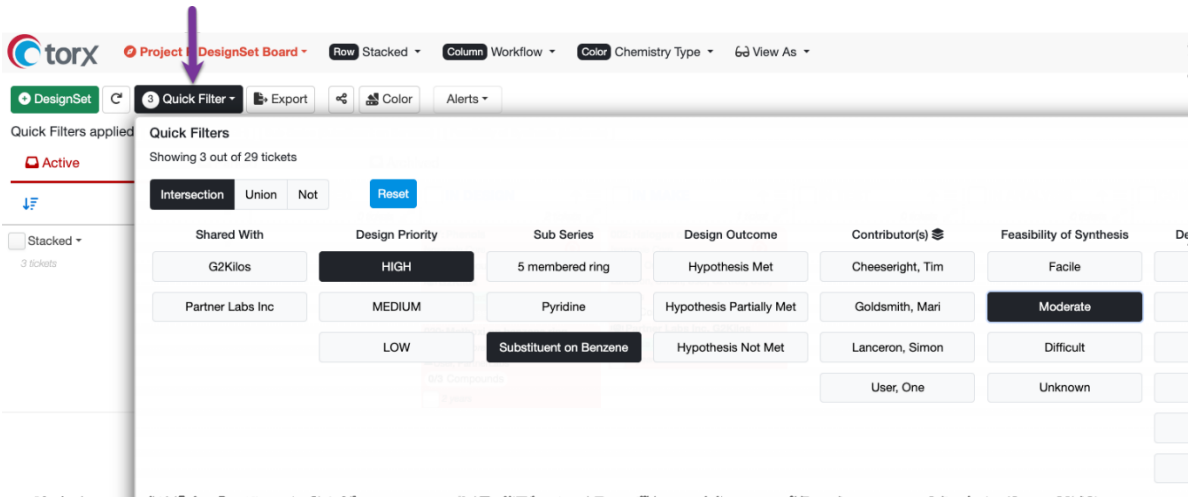# Bug fixes, performance and security

- We have fixed an issue where, after copying a molecule in the Data Table or My Designs plugins, the copied molecule is not selected.
- Various minor security patches and performance enhancements have also been implemented.

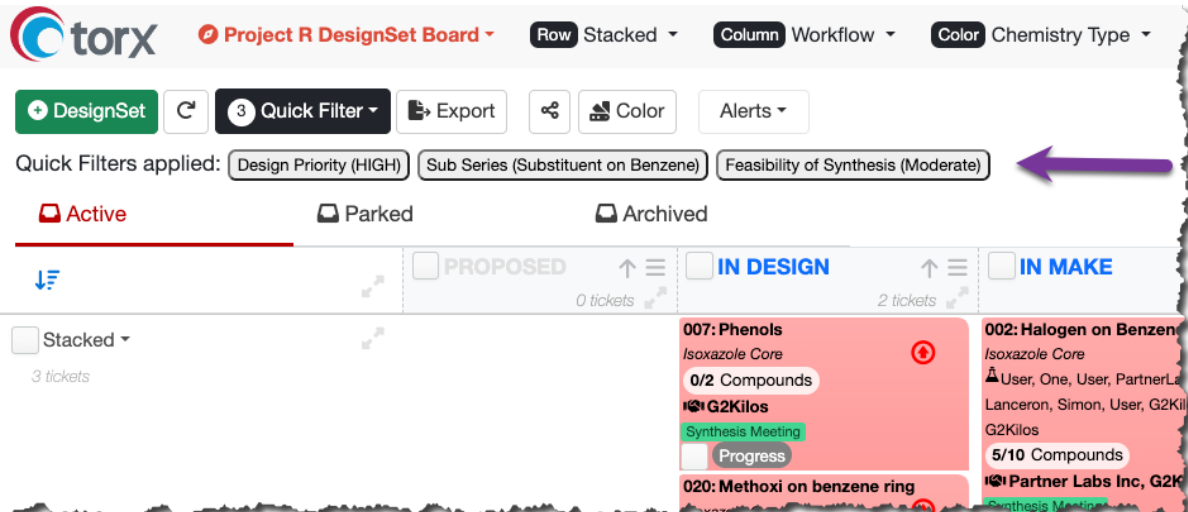# Torx Make and Test updates

Enhancements

Quick Filters

We have introduced the concept of Quick Filters, enabling easier filtering of the tracking boards for the desired view of the data. Clicking on the 'Quick Filter' button shows the available filters. The tracking board tickets can be filtered using 'Intersection' (default), 'Union' or 'Not' operators.

Once selected and the Quick Filter dialog is closed then the filters applied are shown above the tracking board. You can remove any of the filters by clicking on the individual filter.
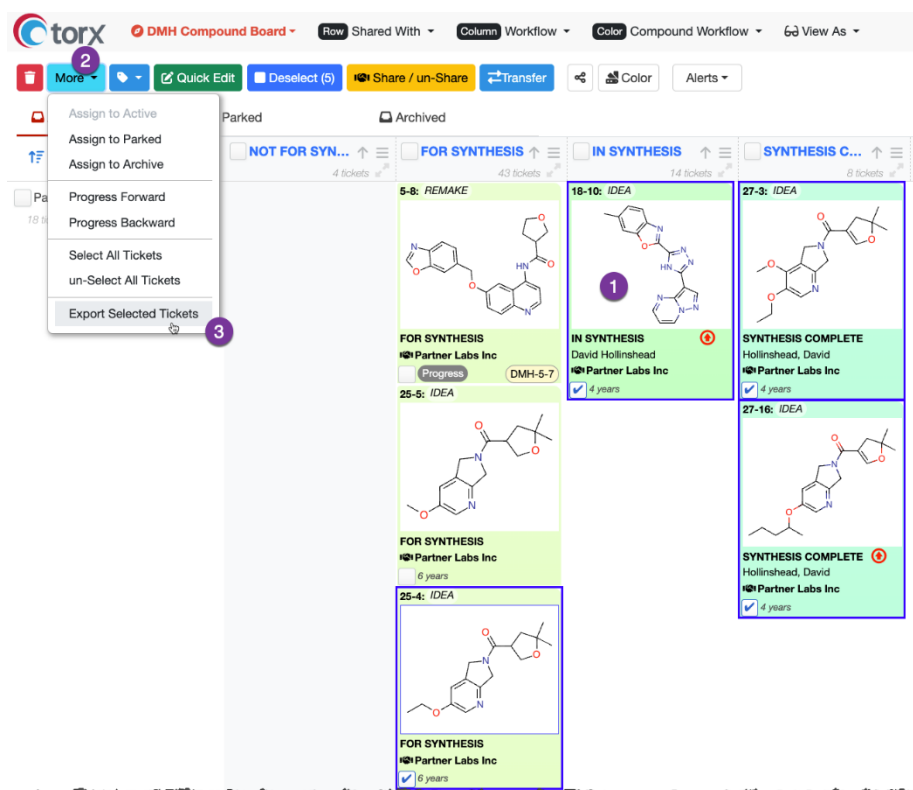
Ticket selection and export enhancements

You can now select tickets on either the tracking boards or the spreadsheet and then choose to export only those selected tickets by:

1. Selecting one or more tickets
2. Clicking the 'More' dropdown menu
3. Clicking on the 'Export Selected Tickets' option

This takes you to the standard export page where you can choose to export as CSV, SDF, or SMILES as appropriate.
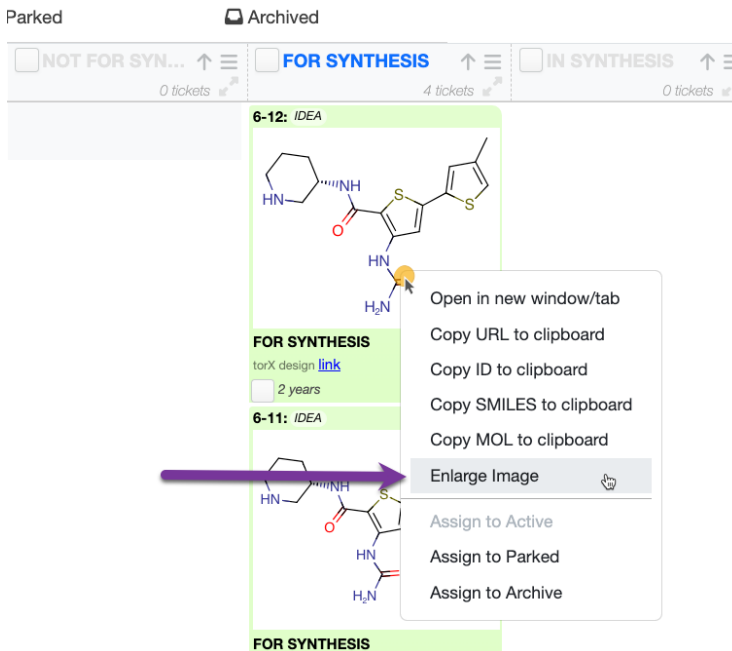
Compound tickets: Enlarge Image

Often chemical images as depicted on the tracking board can be difficult to inspect. This can be made worse in meetings.

There is now the ability to enlarge the image by **right-clicking** on the compound ticket and selecting '**Enlarge Image**' from the dropdown menu.
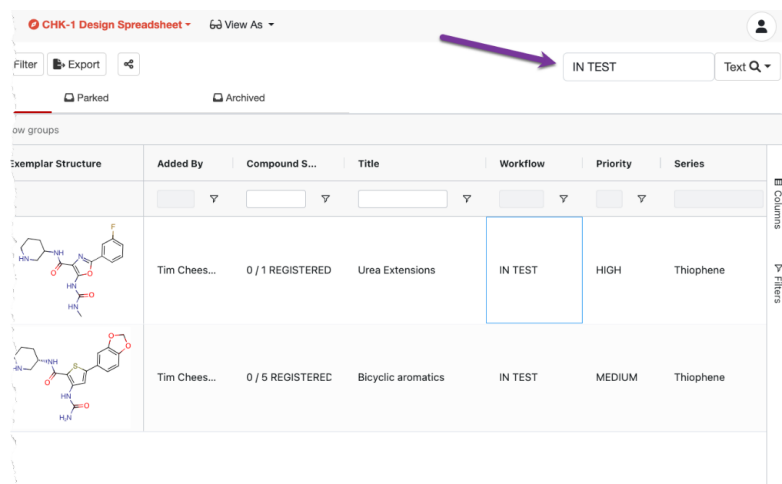
Spreadsheet Global Search
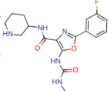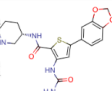
The spreadsheet view now has a global search feature similar to that of the tracking boards, enabling you to quickly filter across all fields in the spreadsheet.
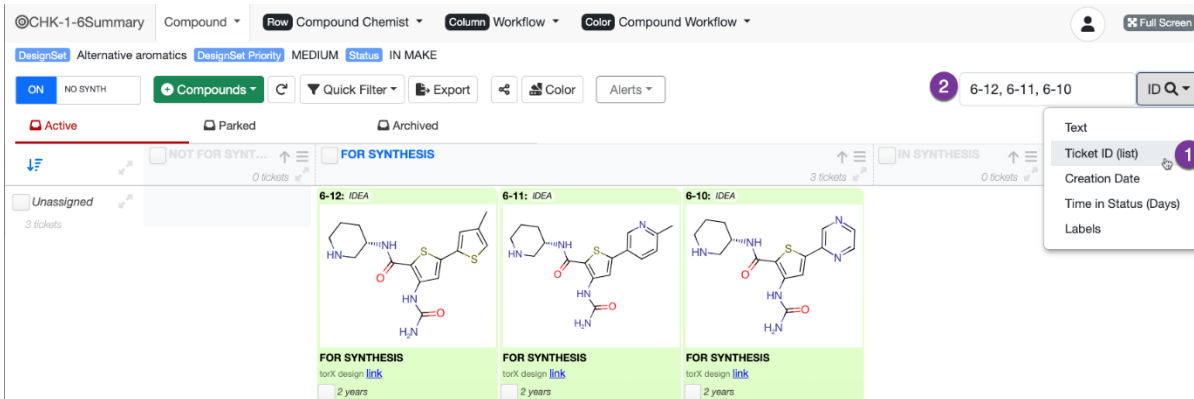
On the spreadsheet there is also now a Reset Spreadsheet button that appears if you have changed the spreadsheet default set-up, i.e., changing column order, grouping by, hiding columns. Clicking the button reverts the spreadsheet back to its original view.

Filtering by Ticket ID

Sometimes it's necessary to view several specific tickets at once. If you know the ticket IDs that you wish to view, you can now filter for these tickets on both the tracking board and the new spreadsheet Global Filter either from the 'Ticket ID (list)' option in the search dropdown (1) or by pasting a list of the IDs (comma or return separated) into the search field (2).
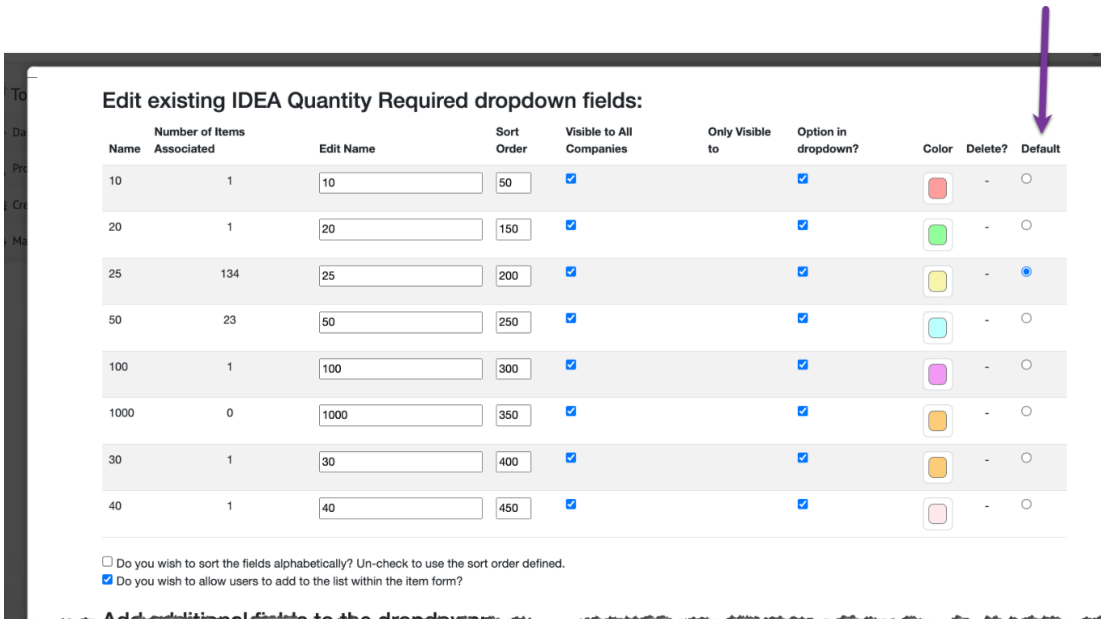

You can use either the full ID format (i.e., ABC1-12-3) or the shortened version (i.e. 12-3).

Project Admins can alter dropdown defaults

On occasions as a project progresses it may be necessary to alter the defaults for certain fields such as Amount or Purity Required. The project administrator can now go into the 'Edit Dropdown' admin section and choose to change the default (if set).
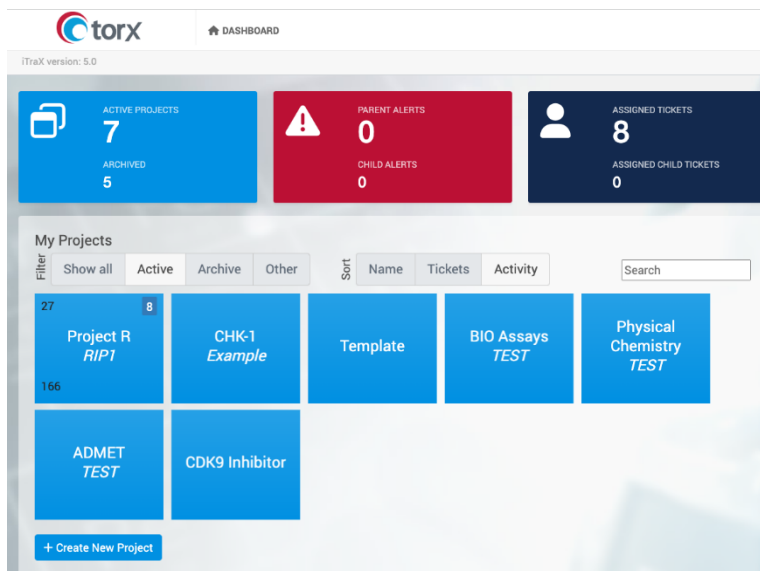
Enhancements to the main dashboard

The main Torx Make dashboard now has an updated color scheme and UI, and improved performance.
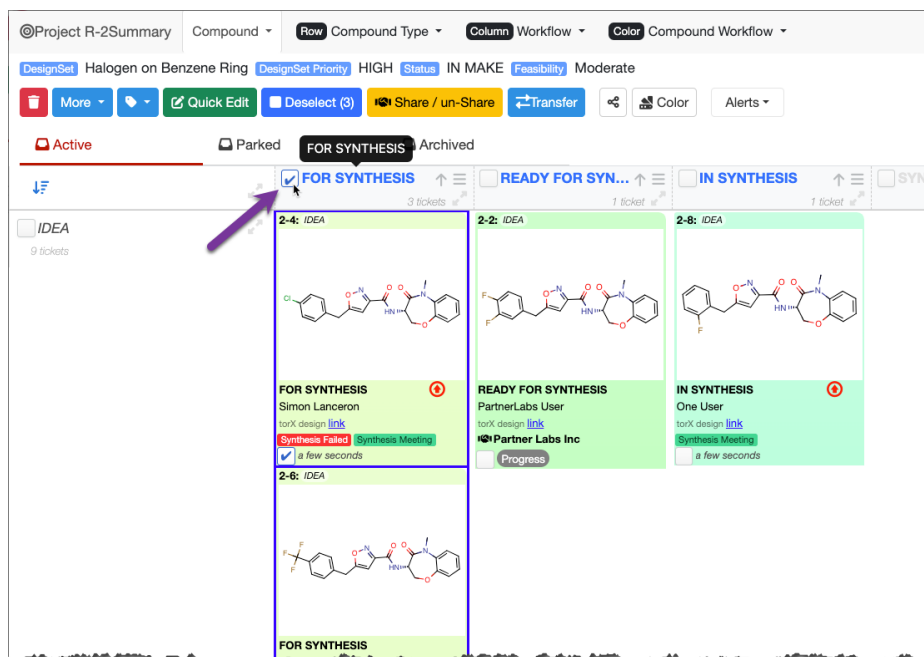
Document Drive supports uploads containing multiple files

You can now select multiple files and upload them in one action to the Document Drive.

Ticket column / row selection
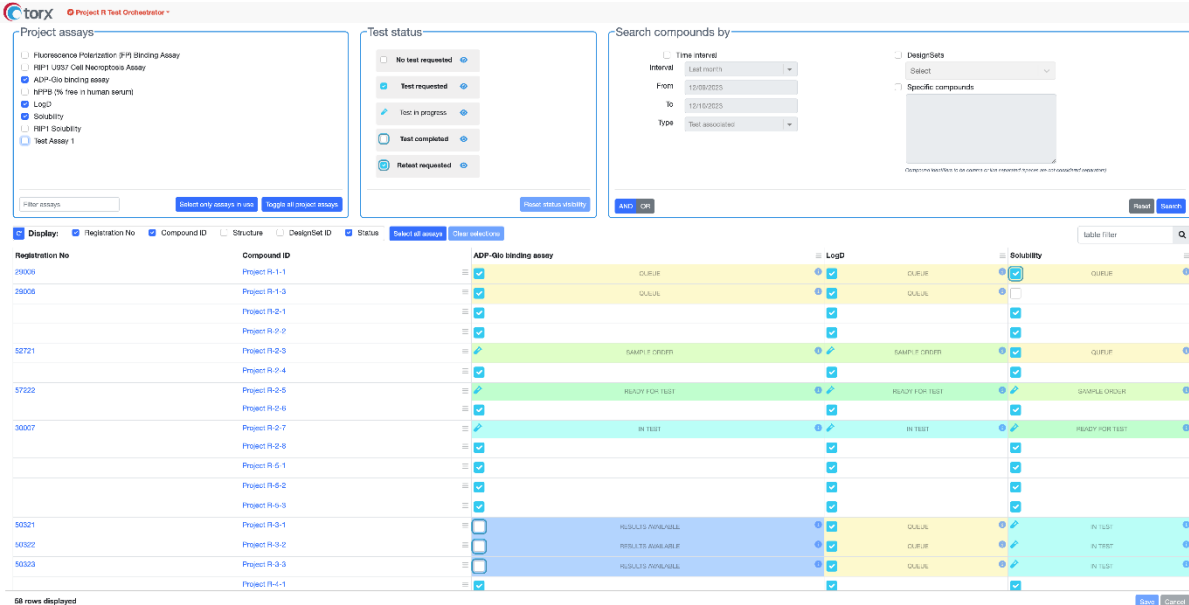
Tracking board tickets in a column or a row can now be easily selected by clicking on the checkbox(es) in the column header or row.

Torx Test Orchestrator

Torx Test now features the **Test Orchestrator**, a new interface for assignment of assays for creation of test requests at project, DesignSet and compound level. Using the Orchestrator, you can view an integrated display of chemical structure and assay information and easily search for associated compounds and test requests.

Further enhancements, bug fixes, performance, and security

- SDF upload now remembers previous mappings.

- All html tags are stripped when exporting.

- Users can now sort tickets within racking board cells by Date Created.

- Spreadsheet right click export now pads IDs with leading zeros: ABC-007-004

- Use of 'View As' in export view - board admins can download CSV, SDF files as a specific CRO user.

- Dragging and dropping into a column now has the drop area as the entire cell making it easier to drop tickets in the tracking board.

- Compound sharing with CROs in conjunction with dragging and dropping a DesignSet when using Row by Shared option.