Torx® Quarterly Update Q1 2024

Contents

Overview 2

Torx Design and Analyze updates 3

- Enhancements 3
  - Supporting multiple pose groups for each molecule 3
  - Data Table enhancements 3
  - Editable DesignSet summary 5
  - Enhancements to card-based plugins 5
  - Enhancements to bulk action toolbar 6
- UI changes, bug fixes, performance, and security 6

Torx Make and Test updates 7

- Enhancements 7
  - Pinned tickets can be bulk selected 7
  - Spreadsheet view enhancements 8
  - Torx Test Project and Orchestrator enhancements 8
- Bug fixes, performance, and security 10

Torx Software Limited,
New Cambridge House, Bassingbourn Road, Cambridgeshire, SG8 0SS, UK
Tel +44 (0)1223 858890 www.torx-software-group.com

Registered in England & Wales No. 12531791
VAT Registration No. GB 350 7034 28

Overview

With its rich 3D visualization environment, Torx enables users to collate 2D and 3D data about their molecule designs to make meaningful comparisons and drive decision making. In our latest release, it is now possible to view all pose groups for a molecule generated from the various docking and alignment experiments performed, and to compare poses from different groups.

Torx enables individual molecules to be grouped into DesignSets that target a specific issue or to address a specific hypothesis, and that rationale is captured in the DesignSet summary. This can now be edited directly from the Design module via the DesignSet summary plugin, making it easier for users to add contextual information on the fly as they design.

Torx enables users to combine capabilities and information in a variety of different views, optimized to the specific task they need to perform in the DMTA cycle. In the latest release we have made a range of enhancements to plugins in Torx Design, such as enabling Data Table columns to be archived, displaying the 2D structure of 3D reference molecules and improving plugin pagination, molecule selection and bulk molecule edit actions. We have also focused on these aspects in Torx Make, with enhancements to bulk selection of pinned tickets and improved spreadsheet filtering.

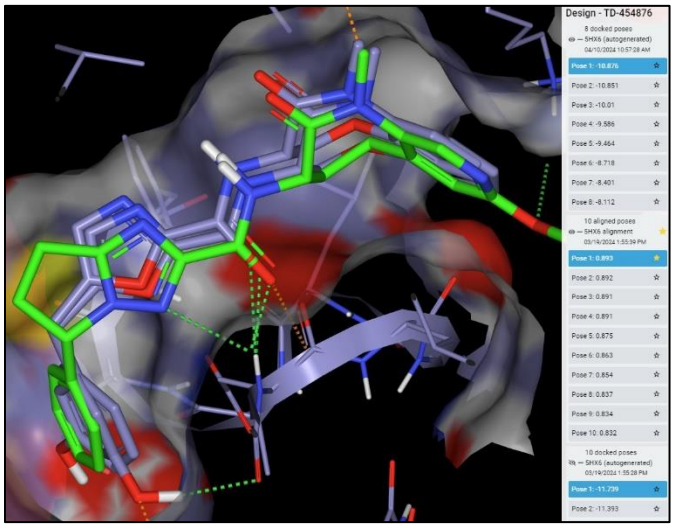
Torx Test links chemists with assay scientists, automating the submission of test requests and enabling effective assignment and management of assay work. In the latest release, we have made enhancements to the Test Management Table and improved support for requests at the compound batch level.

Torx Design and Analyze updates

Enhancements

Supporting multiple pose groups for each molecule

Torx Design features a completely user-configurable interface where plugins can be combined to compare and contrast 2D and 3D features on a single page. The Viewer plugin provides a rich 3D visualization environment and supports docking (including covalent docking) into one or more target binding sites or alignment to a reference molecule to aid triage of designs.



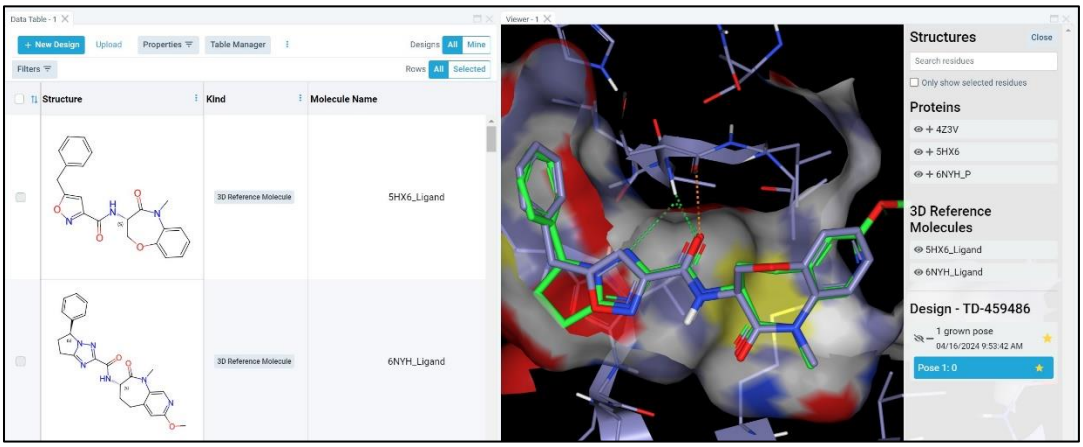
In the latest version, all pose groups associated to a molecule Design (e.g. generated through repeated docking or alignment experiments) are now listed in the Structures sidebar of the Viewer. Poses from different groups can be overlaid in the Viewer, and an enduring ‘favorite’ pose can be selected for each Design using the star icon, with the associated docking or alignment score for that pose referenced in the Data Table.

Data Table enhancements

The Torx Data Table plugin is an interactive spreadsheet that provides the main interface for users to collaborate on molecules contained in the project. It supports a wide range of filtering and grouping options, a calculation editor, a separate MPO plot and score for each molecule, and the ability to color numerical results according to a fitness function. In the latest release, we have added two major enhancements: visibility of 3D reference molecules and column archiving:

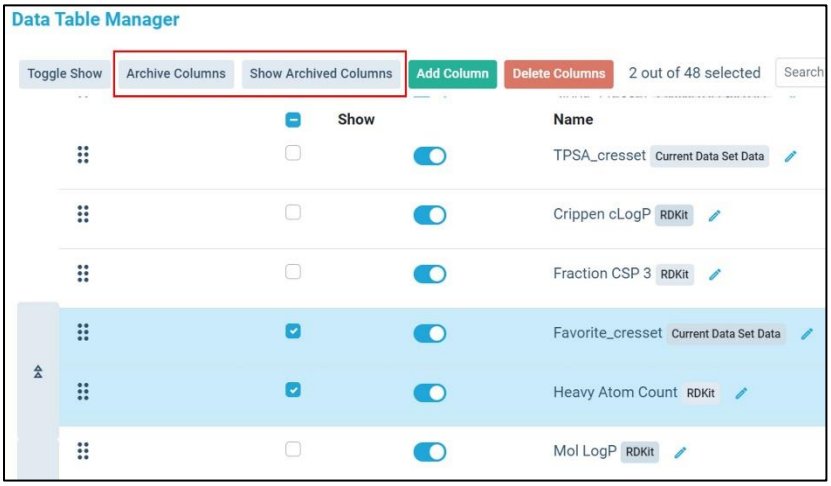
Visibility of 3D Reference molecules

Torx uses the concept of reference molecules in the 3D viewer for the purposes of docking and alignment experiments. Reference molecules that have been added to a project via the Control Panel are now visible as rows in the Data Table, enabling you to easily inspect their 2D structures and guide design work.



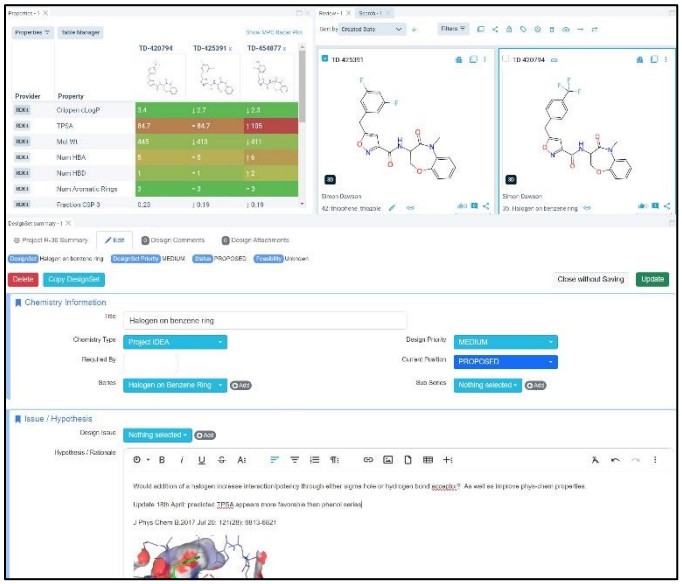
Column archiving

You can now archive Data Table columns via the Table Manager. Archiving a column removes it from display in the Data Table and places it into a dedicated archived section of the Table Manager. In this way, you can remove unwanted columns in the Data Table and reduce clutter in the Table Manager.



Editable DesignSet summary

In Torx, molecules are gathered together into DesignSets that are targeted against a specific issue or address a specific hypothesis. Similar to the workflow for individual molecules, DesignSets themselves can be tracked through the Design-Make-Test-Analyze cycle as hypotheses are tested and proven.

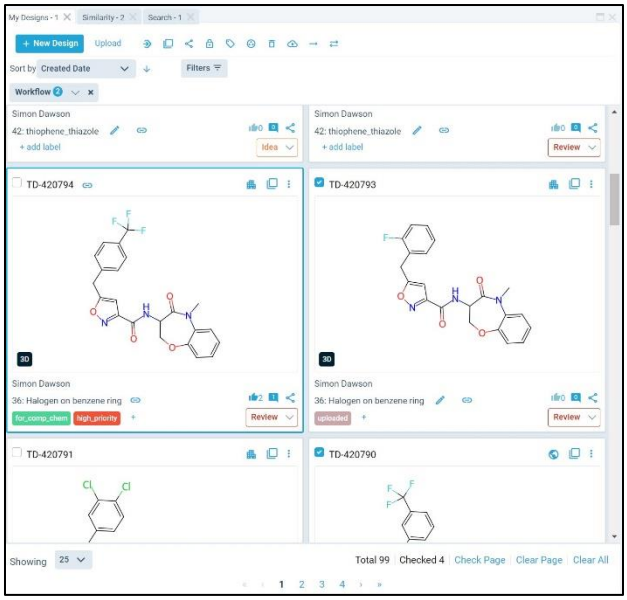


The DesignSet summary allows metadata related to the molecule grouping (e.g. hypothesis description, proposed synthetic route, literature references) to be compiled and tracked. The DesignSet plugin allows this information to be displayed seamlessly within the Torx Design canvas, enabling quick reference in scenarios such as team meetings.

In the latest version of Torx Design, you can edit the DesignSet summary directly from the plugin window, avoiding the need to navigate to another browser page.

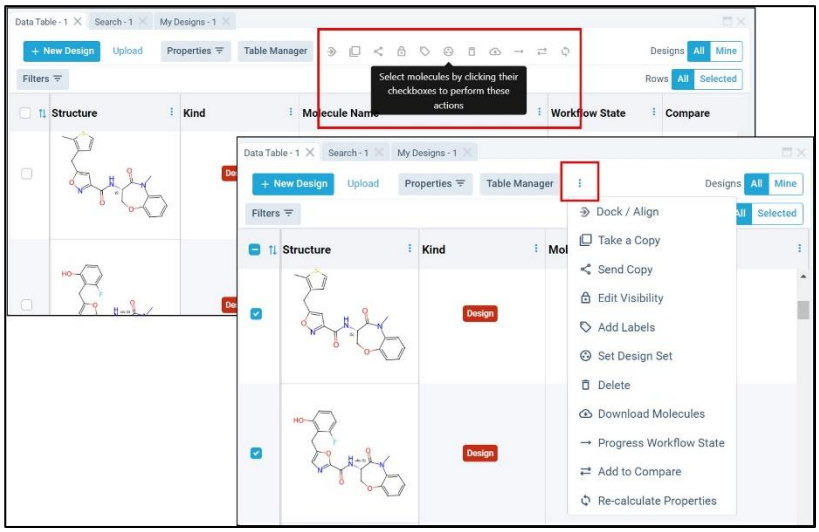
Enhancements to card-based plugins

Torx Design features a number of card-based plugins (e.g. My Designs, Search, Similarity) which show each 2D structure front and center, while also including key metadata associated to each molecule. In these plugins, the display is paginated, and in the latest release there is now a ‘Clear Page’ and ‘Clear All’ function on the footer allowing any checked molecules to be unchecked on the current page, or across all pages, respectively. Vertical scrolling behavior for these plugins has been adjusted to ensure the toolbar is always displayed in the plugin header.



Enhancements to bulk action toolbar

The Torx interface provides clear signposts to key functionality, much of which is present in multiple locations so that you can quickly perform key tasks.



One example of this is the bulk action toolbar, which enables you to perform actions on one or more Designs that you have selected via the checkboxes in either the Data Table or one of the various card-based plugins.

In response to user feedback, the bulk action toolbar is now permanently displayed in each of the relevant plugins, collapsing to a context menu icon (three vertical dots) as a plugin is made narrower.

UI changes, bug fixes, performance, and security

- The Viewer alignment and docking preset drop-down menu features vertical scrolling to better support where many alignment and docking presets have been created.
- We have improved the editing experience in ChemDraw when using the automatic save function.
- We have addressed issues where Data Set data was not appearing in the properties table, and grouping by structure for Data Set molecules was not working as expected in the Data Table.
- We have addressed an issue where 2D structures for macrocycles were not being represented as expected.
- We have improved checking behavior for Data Molecules when merged with Designs or where the Data Set is changed.
- We have addressed an issue where drag and drop column reordering in the Table Manager was not working as expected.

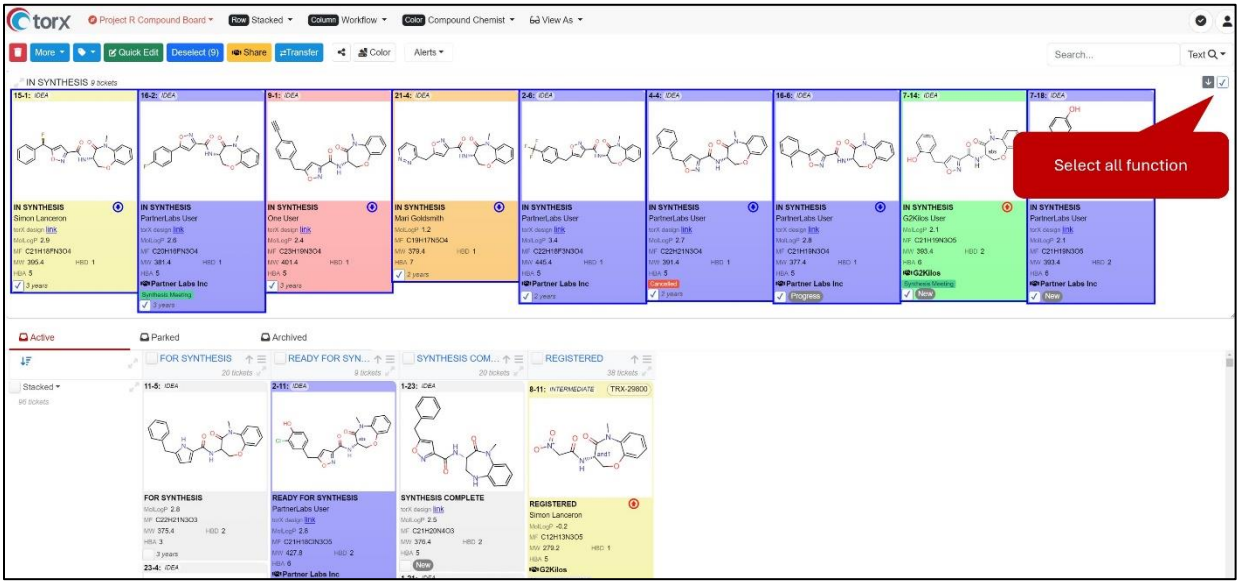
Torx Make and Test updates

Enhancements

Pinned tickets can be bulk selected

The pinning function on a tracking board enables you to draw attention to all the tickets in a particular column by positioning them as a row above the tracking board. This area can be resized and scrolled independently of the main board, and tickets can be dragged and dropped as normal between the pinned row and the rest of the tracking board. This function is particularly useful in scenarios such as presenting work status during team meetings.

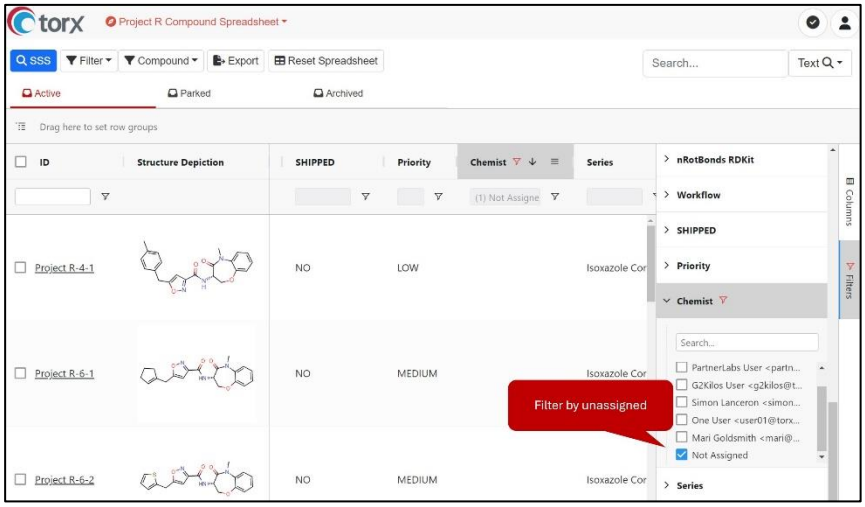
In this version we have added the function to select all the tickets in the pinned section, so that actions can be performed in bulk (such as a quick edit).



Spreadsheet view enhancements

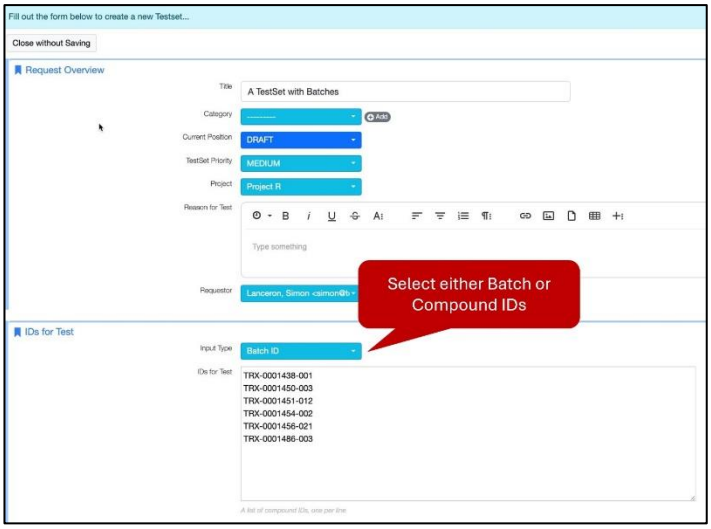
The spreadsheet view in Torx Make and Test gives you ultimate flexibility to visualize your synthesis or testing workload. The spreadsheet can be pivoted and filtered by an extensive list of ticket metadata fields, providing insights into team capacity, progress against high priority work items, and the presence of workflow bottlenecks.

In this release, we have enhanced the spreadsheet view to enable filtering by empty (blank) cells and improved the editing behavior so that selected filters are maintained after performing edits.



Torx Test Project and Orchestrator enhancements

Torx Test enables assignment of assays for creation of test requests at project, DesignSet and compound level. In the latest version, we have made the following improvements:



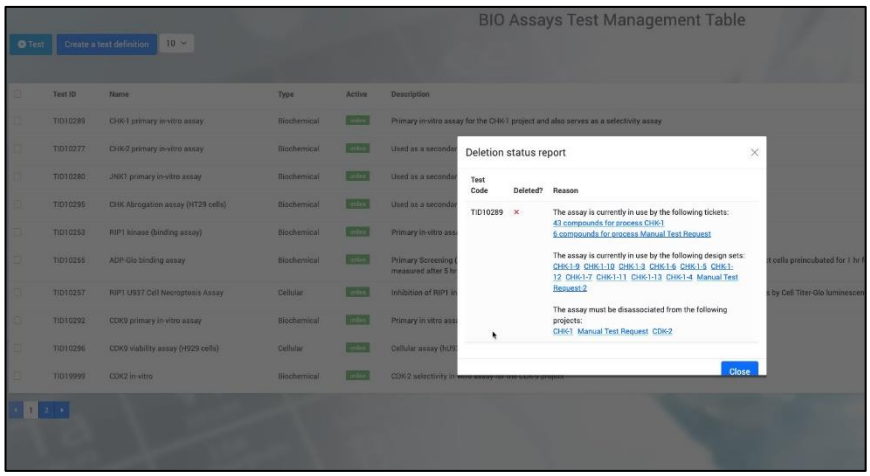
Manual test workflows accommodate batch IDs

The manual test workflow allows you to create tests for a list of items, via a simple text interface. In this latest version, you can now choose from a dropdown menu to select whether you want to create tests for a list of compound IDs or batch IDs.

Improvements to Test Management Table

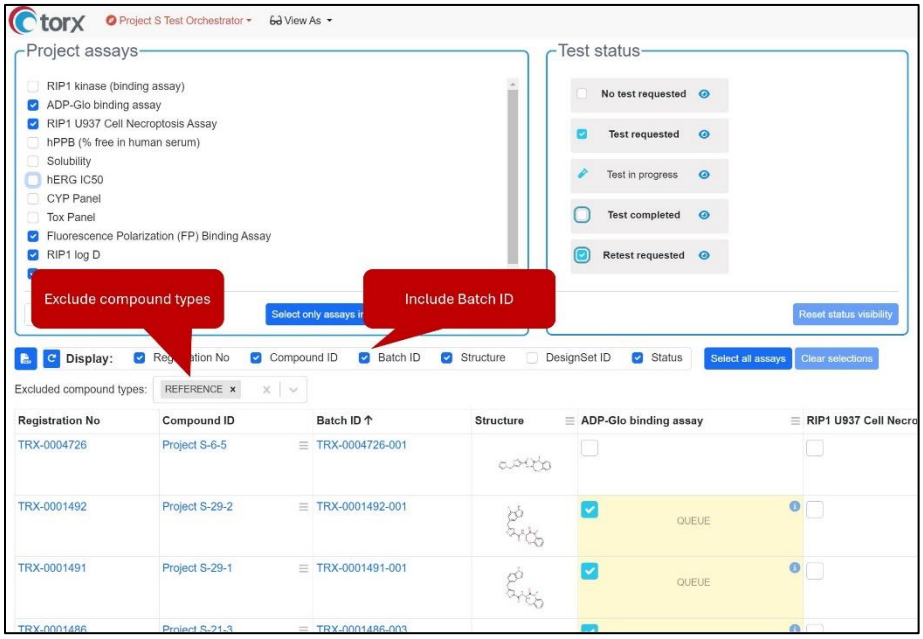
When deleting an assay via the Test Management Table, it is important to understand where that assay is currently in use, especially if it has been assigned as a project default, or where test requests may even be in flight.

Where this is the case, the Test Management Table will now flag an error during the assay deletion process, indicating which test tickets, DesignSets and projects are impacted by the deletion, and provide direct links to the relevant pages in Torx.



Test Orchestrator filtering and heatmap enhancements

Using the Test Orchestrator, you can view an integrated display of chemical structure and assay information and easily search for associated compounds and test requests.



In the latest version it is now possible to include the Batch ID in the heatmap view and filter out certain compound types (e.g. REFERENCE).

Bug fixes, performance, and security

- Addressed issue with spreadsheet where reset button needed to be clicked twice when filters applied and issue with column filter dropdowns.
- We have addressed a vertical scrolling issue on the calendar view where page position in the week view defaults to current time, even after editing or adding a new event.
- We have addressed an issue with the ‘my tickets’ filtering behavior on the calendar view.