



## Torx<sup>®</sup> Quarterly Update

Q4 2023

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## Overview

In the latest version of Torx we have implemented new features and enhancements strongly driven by feedback from our users.

Comparing molecules from across the DMTA cycle is a core capability of Torx which we have made even easier by introducing features such as standardization of 2D molecule orientation, and the ability to select molecules from a connected data source (e.g. a CDMS or data warehouse) to benchmark predicted properties and 3D poses of new design ideas. Facilitating planning and forecasting is always at the forefront of our minds, and this latest version brings enhancements which make it easier to view upcoming synthesis work in calendar format and improve the view of submitted test requests via the Test Orchestrator feature.

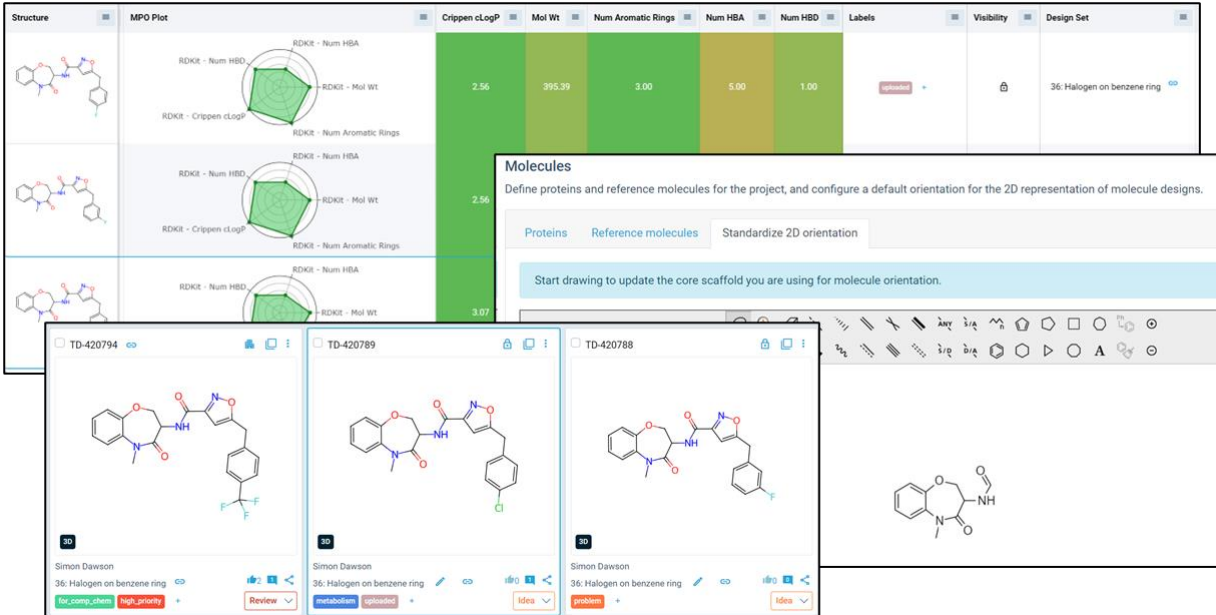
Finally, we have introduced several features across the platform which reduce user effort in routine tasks, such as configuring project settings, defining custom calculations, sending molecules to connected services, and performing bulk ticket updates.

## Torx Design and Analyze updates

### Enhancements

#### Standardize orientation of 2D structures

Torx Design features a user-configurable interface where plugins can be combined to compare 2D and 3D molecule features on a single page. For example, the Data Table plugin is an interactive spreadsheet that provides the main interface to all molecules in a project, whereas the "My Designs" and "Review" plugins are card-based views allowing the user to respectively focus on molecules they have created, or those which are under review by the project team.

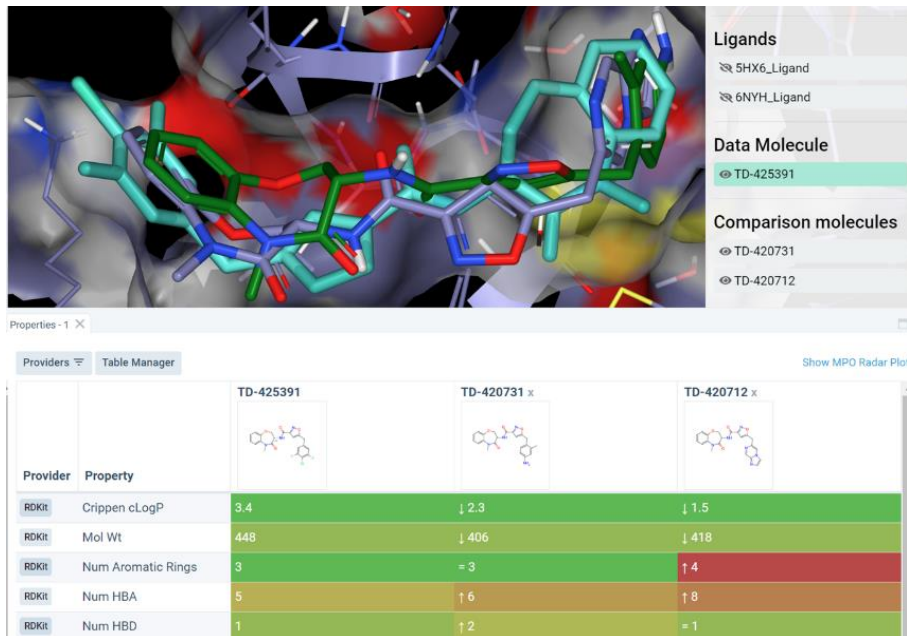


The screenshot displays the Torx Design interface. At the top, there is a navigation bar with tabs for Structure, MPO Plot, Crippen cLogP, Mol Wt, Num Aromatic Rings, Num HBA, Num HBD, Labels, Visibility, and Design Set. Below this is a data table with columns for these metrics. The table contains three rows of data, with the first two rows having a Mol Wt of 395.39 and the third row having a Mol Wt of 3.07. To the right of the table is a 'Molecules' control panel with tabs for Proteins, Reference molecules, and Standardize 2D orientation. The Standardize 2D orientation tab is active, showing a 'Start drawing to update the core scaffold you are using for molecule orientation.' button. Below the table and control panel are three molecule cards, each showing a chemical structure and a 'Review' button. The cards are labeled TD-420794, TD-420789, and TD-420788. The TD-420789 card shows a molecule with a chlorine atom, and the TD-420788 card shows a molecule with a fluorine atom. The bottom right of the screenshot shows a larger molecule structure with a carbonyl group.

In the latest version, you can now set a template to standardize how molecule 2D structures are orientated within a project. Use the interface in the Control Panel to define and save your core scaffold, molecules will then be represented in the same orientation across the various table and card views. In this way, designs can easily be compared regardless of how they have been originally drawn.

## Selecting Data Molecules

Torx uses the concept of Data Sources to gather information from external resources such as SDF and CSV files or connections to your CDMS or data warehouse. Multiple Data Sources can be merged, enabling the creation of Data Sets that combine 2D and 3D data potentially stored across multiple locations. In the latest version, molecules from these external sources ('Data Molecules') can now be selected in the Data Table by clicking on the relevant row.



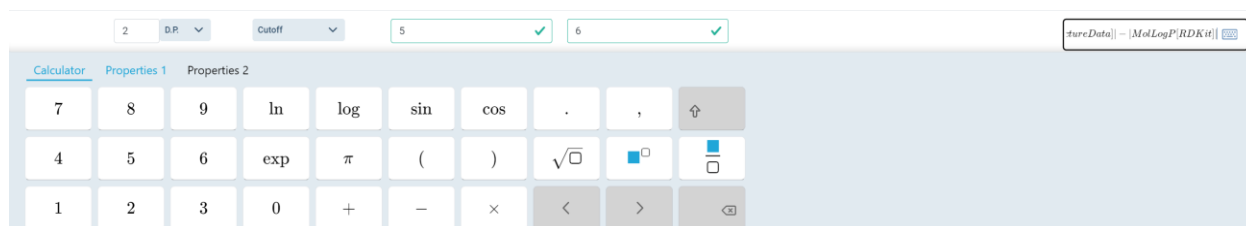
The screenshot displays a 3D molecular model of a ligand bound to a protein. On the right, a sidebar lists 'Ligands' (5HX6\_Ligand, 6NYH\_Ligand), 'Data Molecule' (TD-425391), and 'Comparison molecules' (TD-420731, TD-420712). Below the model is a 'Table Manager' window with a table comparing properties for TD-425391, TD-420731, and TD-420712.

Provider	Property	TD-425391	TD-420731 x	TD-420712 x
RDKit	Crippen cLogP	3.4	↓ 2.3	↓ 1.5
RDKit	Mol Wt	448	↓ 406	↓ 418
RDKit	Num Aromatic Rings	3	= 3	↑ 4
RDKit	Num HBA	5	↑ 6	↑ 8
RDKit	Num HBD	1	↑ 2	= 1

Where a 3D pose is associated with that molecule, it will be shown in the Viewer plugin. This enables you to make better comparisons with Data Molecules using the “Compare” function as their poses can be overlaid with those of your designs, and they can be set as the left-most column in the Properties table (to which the other added molecules are compared).

## Easily create custom calculations

The Torx Data Table enables molecules to be sorted, grouped, and filtered by any metadata field associated with them. Numbers can also be colored according to a fitness function where values are either acceptable or unacceptable, enabling you to rapidly triage your designs.

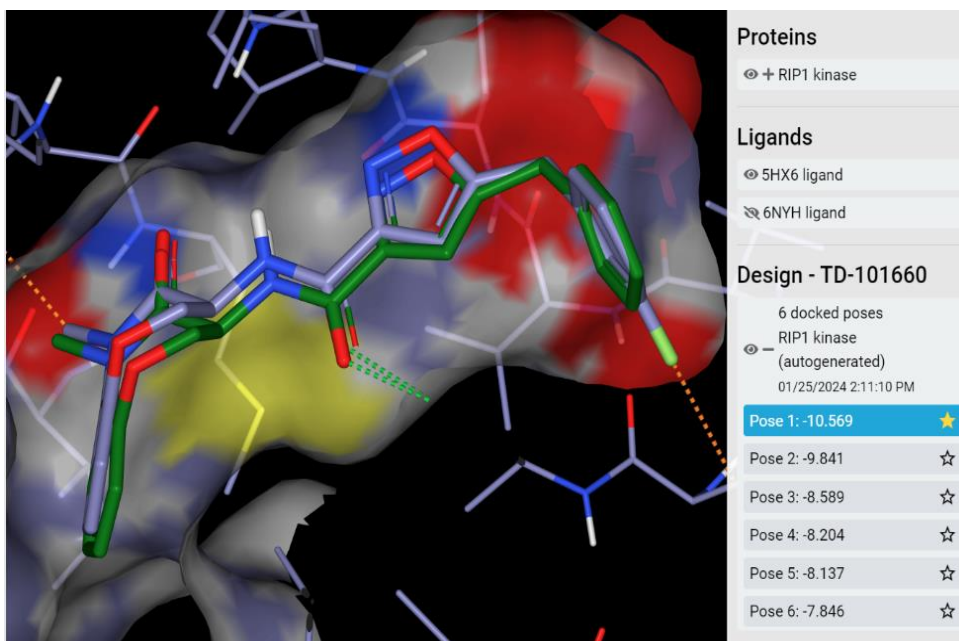


The screenshot shows the 'Calculator' interface with a numeric keypad and various mathematical functions. At the top, there are input fields for 'D.P.' (set to 2) and 'Cutoff' (set to 5 and 6). A search bar contains the formula: `torx[Data] - [MolLogP, RDKit]`.

Calculated columns can also be created from any value, including other calculated columns. The latest version of Design-Analyze features an all-new equation editor for calculated columns, enabling a greater range of functions to be applied via an intuitive user interface.

## Clearer context on docking and alignment experiments

The interactive 3D design of molecules has always been central to Torx. In this latest release, the 3D Viewer plugin has been enhanced to show the ID of the current selected design, the timestamp of the last docking or alignment experiment, and the preset which was used.



## Properties table row ordering

Torx enables results from external property calculation or prediction providers to be presented with molecules in the Data Table and Properties plugins. Project-wide configuration of properties display and coloration according to a fitness function are also supported. In the latest version, we have extended this to include row ordering for the Properties plugin. Rows can be selected and moved up and down the list in the Control Panel through drag and drop, or by using the arrow icons.

**Properties**  
Settings for the properties plugin

Providers: 0 out of 16 selected | Search properties... | Header Structures:

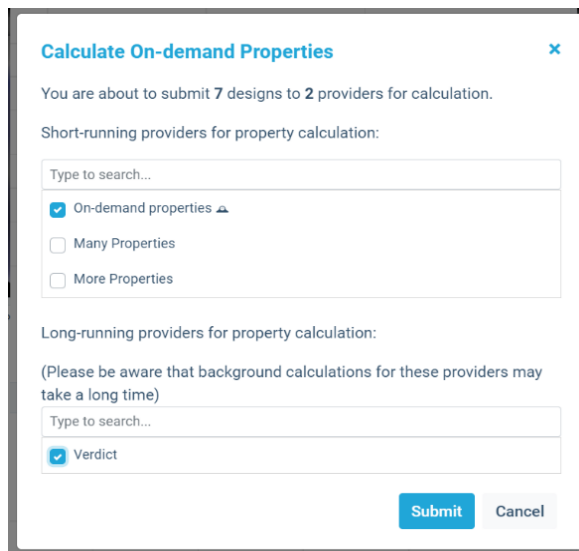
	Provider	Property	Show
⋮	<input type="checkbox"/> RDKit	Crippen cLogP	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Fraction CSP 3	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Heavy Atom Count	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Mol LogP	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Mol Wt	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Num Aromatic Rings	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Num Atom Stereo Centers	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Num Atoms	<input checked="" type="checkbox"/>
⋮	<input type="checkbox"/> RDKit	Num HBA	<input checked="" type="checkbox"/>

A red arrow points to the 'Num Aromatic Rings' row, indicating the row ordering feature.

This means that where team members may need to align their view of the Properties table to an agreed project standard (perhaps in advance of a group meeting) they can do so in a single click.

## Send molecule selections to 'on-demand' providers

Torx was created from the ground up to easily interface to external data and models and hence features a wide range of integration points including predicted physico-chemical properties calculators. We use the concept of 'Property Providers' to seamlessly connect you to these external services, enabling you to view live how changes to a molecule structure affects its predicted properties. In this release, where you have 'On-demand' properties providers integrated with Torx, you can now send multiple molecules to those providers in a single operation. Simply check the molecules in the Data Table that you wish to send, click the 're-calculate properties' icon in the toolbar and then choose from your list of providers in the modal display.



**Calculate On-demand Properties** ✕

You are about to submit 7 designs to 2 providers for calculation.

Short-running providers for property calculation:

Type to search...

- On-demand properties ▲
- Many Properties
- More Properties

Long-running providers for property calculation:

(Please be aware that background calculations for these providers may take a long time)

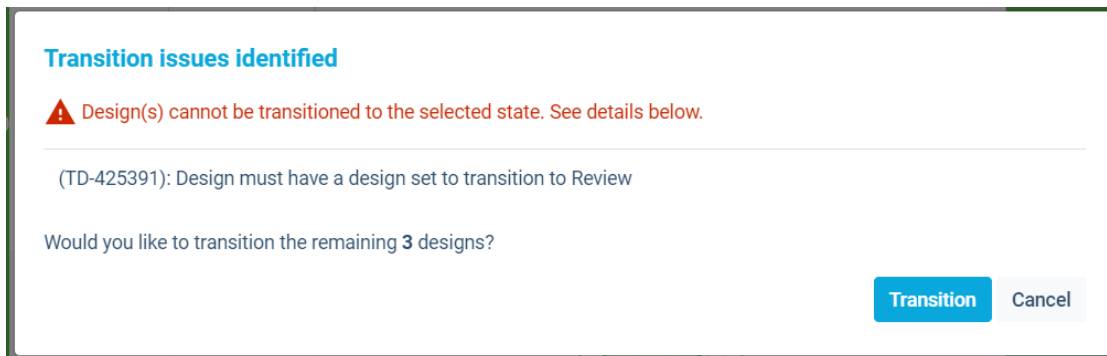
Type to search...

- Verdict

**Submit** **Cancel**

## Workflow transition improvements

Underlying the design process in Torx is a workflow that moves molecules from the initial idea stage through a review system and on to synthesis tracking, registration, and testing. With the latest release, instead of having to completely cancel a bulk workflow state transition of molecules due to issues with a subset of your selection, Torx tells you which molecules are problematic and gives you the option to transition the remainder.



**Transition issues identified**

⚠ Design(s) cannot be transitioned to the selected state. See details below.

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(TD-425391): Design must have a design set to transition to Review

Would you like to transition the remaining 3 designs?

**Transition** **Cancel**

## Bug fixes, performance, and security

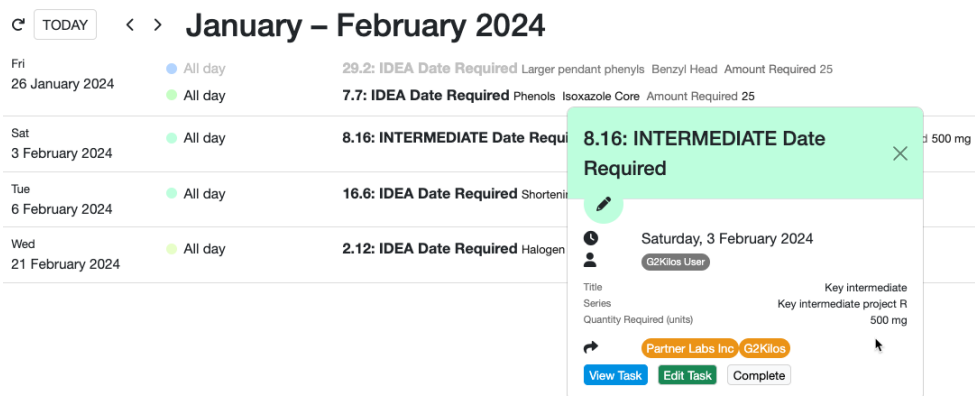
- We have implemented a bug fix where the right edge of the Data Table was hidden by the vertical scrollbar.
- We have implemented a bug fix where grouping by structure for Dataset molecules was not working as expected.
- Various minor security patches and performance enhancements have also been implemented. V2 of our API key format has been introduced and is now used for all newly generated API keys. Valid keys in the previous format remain accepted by the API.

## Torx Make and Test updates

### Enhancements

#### Calendar improvements

The calendar view in Torx Make enables you to easily plan and review deadlines for molecules, intermediates and entire DesignSets, and to understand where work might be falling behind. In the latest version we have introduced a new condensed “Schedule View” making it significantly easier to understand the ordering of time-sensitive tasks.



Calendar view showing tasks for January and February 2024. A task titled "8.16: INTERMEDIATE Date Required" is highlighted in green. The task details show it is for Saturday, 3 February 2024, assigned to G2Kilos User, with a title "Key intermediate", series "Key intermediate project R", and quantity "500 mg". The task is associated with Partner Labs Inc. and G2Kilos. Action buttons for "View Task", "Edit Task", and "Complete" are visible.

We have also improved the view of DesignSet and compound tickets containing date information (e.g. “Date Required”) so that this critical information is easily discoverable.



## 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 better ordering of character and date columns and added the option to pad Torx ID fields when exporting spreadsheet data to file.

## Bulk ticket update enhancements

The bulk ticket update feature enables you to rapidly make changes to multiple compounds via a file based (CSV or SDF) upload. This brings efficiency benefits particularly when dealing with large numbers of compound status updates, where making changes to individual tickets manually would be unwieldy and time consuming. In this latest release we have made enhancements to the handling of errors in the file upload, ensuring issues such as incorrect file formatting can be managed and resolved effectively.

## Torx Test Project and Orchestrator enhancements

Torx Test enables assignment of assays for creation of test requests at project, DesignSet and compound level. 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, the capabilities of Torx Test can now be enabled on an individual project basis, while Test projects can leverage project aliases. This better ensures users have access to only the features and information they need for their role in each project.

As requested in user feedback, we have now added a visual indicator to the Test Orchestrator interface to show where a comment has been left by a test scientist, making communication with test requestors more seamless. DesignSet/TestSet nomenclature in the Orchestrator view is also determined dynamically, avoiding confusion. Finally, the Orchestrator CSV export feature has now been expanded to include physical properties and SMILES.

## Bug fixes, performance, and security

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- We have implemented a bug fix to address where a compound with no tests assigned cannot progress beyond a registered status.
- Associated Test request tickets are now removed when a TestSet or DesignSet is deleted.
- We have addressed styling issues with large cross icons in Torx Test Orchestrator filters when using Safari.