



Contents

Torx Design and Analyze updates.....	1
Enhancements.....	1
Triage designs in the data table with multiparameter optimization.....	1
Categorize designs using labels.....	1
Choose to download either 2D or 3D structures to SDF.....	2
Data Table enhancements.....	2
Protein uploads.....	3
Bug fixes, performance, and security.....	3
Torx Make and Test updates.....	4
Enhancements.....	4
Quick filters.....	4
Ticket selection and export enhancements.....	5
Compound tickets: enlarge image.....	6
Spreadsheet global search.....	6
Filtering by ticket ID.....	7
Project Admins can alter dropdown defaults.....	7
Enhancements to the main dashboard.....	8
Document Drive supports uploads containing multiple files.....	8
Ticket column / row selection.....	8
Torx Test Orchestrator.....	9
Further enhancements, bug fixes, performance and security.....	9

Torx Design and Analyze updates

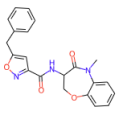
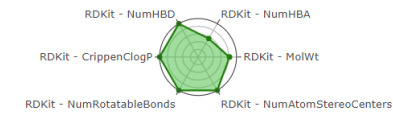
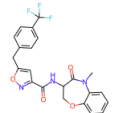
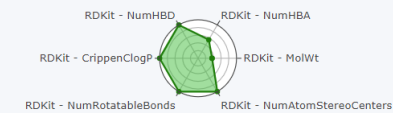
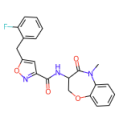
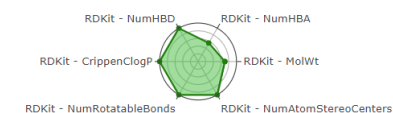
Enhancements

Triage designs in the Data Table with multiparameter optimization

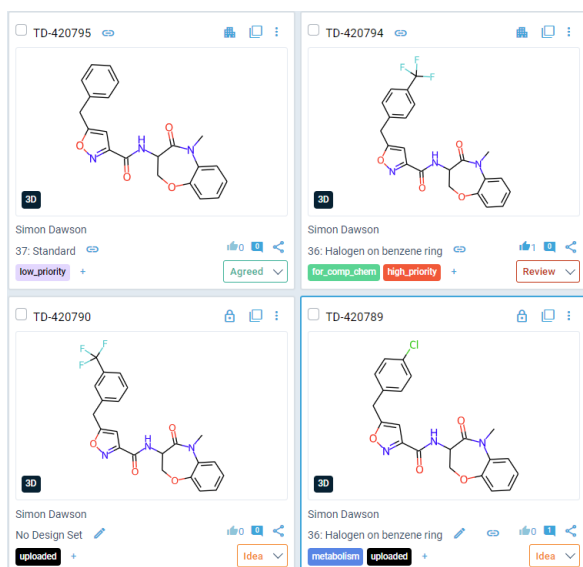
Torx Design now includes the MPO plot and score in the Data Table.

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.

Structure	Molecule Name	Workflow	MPO Plot	MPO Score	CrippenC
	TD-420795	Agreed		0.90	2.42
	TD-420794	Review		0.82	3.44
	TD-420793	Idea		0.88	2.56

Categorize designs using labels

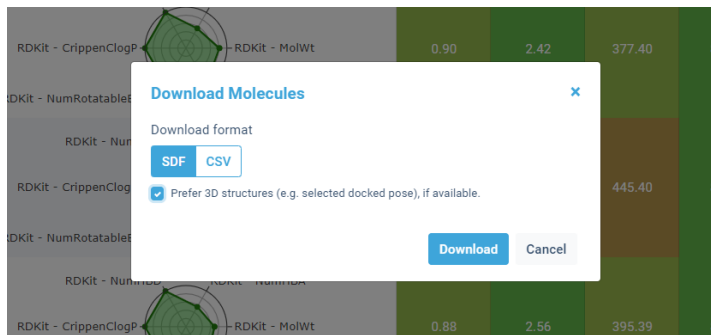


The screenshots show design cards for TD-420795, TD-420794, TD-420790, and TD-420789. Each card displays a chemical structure, a 3D view, and a label. The labels are: 'low_priority' (green), 'high_priority' (red), 'metabolism' (blue), and 'uploader' (orange). The cards also show the user 'Simon Dawson' and the design set name.

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

Show/Hide	Name	Precision	Color Function	Bad1	Good1
<input checked="" type="checkbox"/>	MPO Score <small>MPO</small>	2 D.P.	Cutoff	0.4	1
<input checked="" type="checkbox"/>	CrippenClogP <small>RDKit</small>	2 D.P.	Cutoff	5	3.5
<input checked="" type="checkbox"/>	MolWt <small>RDKit</small>	2 D.P.	Cutoff	500	350

Inherited from properties configuration in the properties plugin

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.

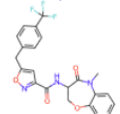
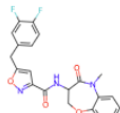
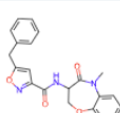
Grouped by "Workflow State"	Structure	Molecule Name	Workflow	MPO Score
Agreed (2)				0.90
		TD-420792	Agreed	0.86
Idea (94)				

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.

<input type="checkbox"/>	Structure	Molecule Name	Workflow
<input checked="" type="checkbox"/>		TD-420794	Review
<input checked="" type="checkbox"/>		TD-420792	Agreed
<input type="checkbox"/>		TD-420795	Agreed

Protein uploads

Ligand detected within protein. Please upload a protein structure that does not include a ligand.

< Projects
Project R
Active

Details Roles Members Plugins Molecules Docking and Alignment presets Properties Settings Data Sources

Molecules
The proteins and reference molecules for the project.

Proteins Reference molecules

Add new protein
Fill in the form below to add a new protein to the project.
You must ensure that the protein structure has been prepared with structural water only, hydrogens present and orientated. The protein must be empty (no ligand).
Please note that once added, the files for proteins cannot be changed.

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

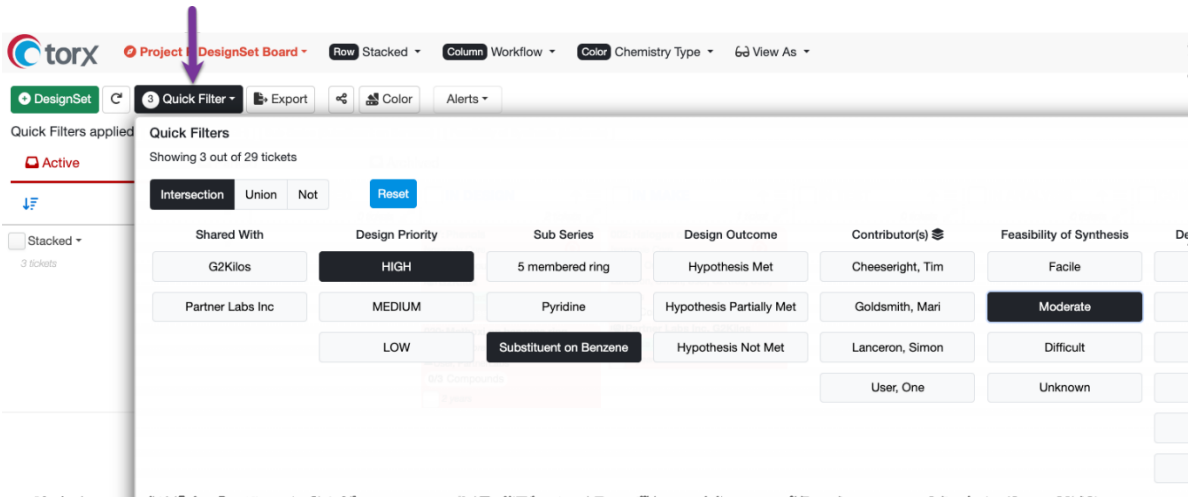
- We have fixed an issue where, after copying a molecule in the Data Table or My Designs plugins, the copied molecule is not selected.
- Various minor security patches and performance enhancements have also been implemented.

Torx Make and Test updates

Enhancements

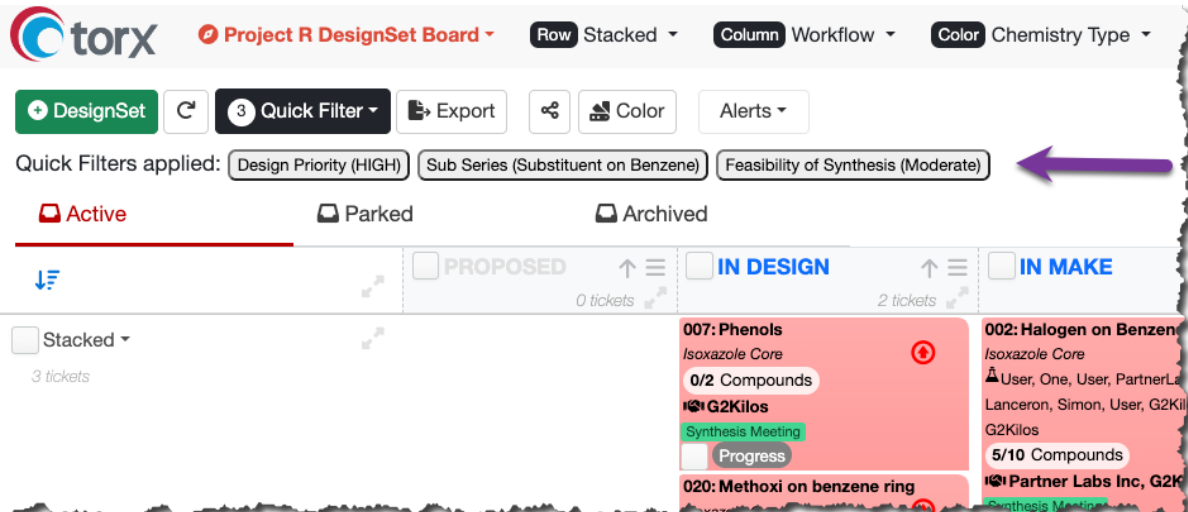
Quick Filters

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.



The screenshot shows the Torx DesignSet Board interface. At the top, there are navigation options: 'Project R DesignSet Board', 'Row Stacked', 'Column Workflow', 'Color Chemistry Type', and 'View As'. Below this, there are buttons for 'DesignSet', 'Quick Filter', 'Export', 'Color', and 'Alerts'. The 'Quick Filter' dialog is open, showing 'Showing 3 out of 29 tickets'. The dialog has three tabs: 'Intersection' (selected), 'Union', and 'Not'. There is a 'Reset' button. The dialog lists several filters: 'Shared With' (G2Kilos, Partner Labs Inc), 'Design Priority' (HIGH, MEDIUM, LOW), 'Sub Series' (5 membered ring, Pyridine, Substituent on Benzene), 'Design Outcome' (Hypothesis Met, Hypothesis Partially Met, Hypothesis Not Met), 'Contributor(s)' (Cheeseright, Tim; Goldsmith, Mari; Lanceron, Simon; User, One), and 'Feasibility of Synthesis' (Facile, Moderate, Difficult, Unknown).

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.

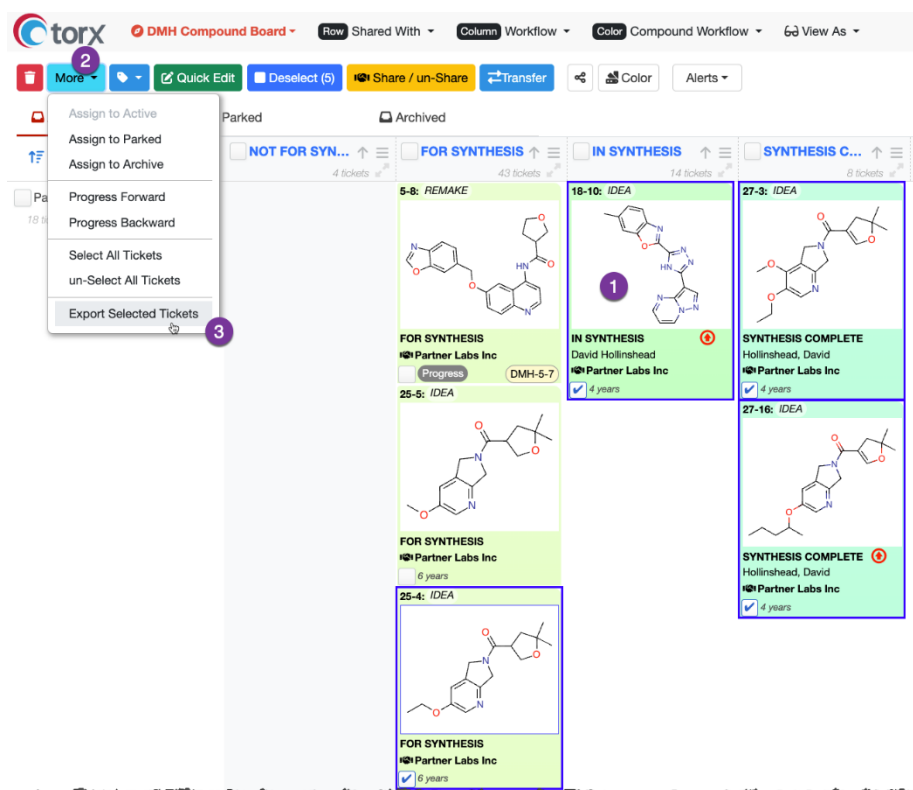


The screenshot shows the Torx DesignSet Board interface with filters applied. The top navigation bar is the same as in the previous screenshot. Below the navigation bar, there are buttons for 'DesignSet', 'Quick Filter', 'Export', 'Color', and 'Alerts'. The 'Quick Filters applied:' section shows three filters: 'Design Priority (HIGH)', 'Sub Series (Substituent on Benzene)', and 'Feasibility of Synthesis (Moderate)'. A purple arrow points to these filter buttons. Below the filters, there are tabs for 'Active', 'Parked', and 'Archived'. The 'Active' tab is selected. The tracking board shows three columns: 'PROPOSED' (0 tickets), 'IN DESIGN' (2 tickets), and 'IN MAKE'. The 'IN DESIGN' column shows two tickets: '007: Phenols Isoxazole Core' and '020: Methoxy on benzene ring'. The 'IN MAKE' column shows one ticket: '002: Halogen on Benzene Isoxazole Core'. The tickets are color-coded: red for 'IN DESIGN' and pink for 'IN MAKE'. The '007: Phenols' ticket has a red circle with a white plus sign. The '020: Methoxy on benzene ring' ticket has a red circle with a white minus sign. The '002: Halogen on Benzene' ticket has a red circle with a white plus sign.

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



The screenshot shows the Torx DMH Compound Board interface. At the top, there are navigation tabs for 'Parked' and 'Archived'. Below these are columns for 'NOT FOR SYN...', 'FOR SYNTHESIS', 'IN SYNTHESIS', and 'SYNTHESIS C...'. A 'More' dropdown menu is open, showing options like 'Assign to Active', 'Assign to Parked', 'Assign to Archive', 'Progress Forward', 'Progress Backward', 'Select All Tickets', 'un-Select All Tickets', and 'Export Selected Tickets'. The 'Export Selected Tickets' option is highlighted with a red circle and the number 3. A red circle with the number 2 is also present near the 'More' button.

This takes you to the standard export page where you can choose to export as CSV, SDF, or SMILES as appropriate.

DMH Downloads

Select the tickets you wish to export and stipulate the required date range.

6 tickets are in your selection

Which tickets do you wish to export?

- Main Tracking Board Tickets
 Compound Tickets

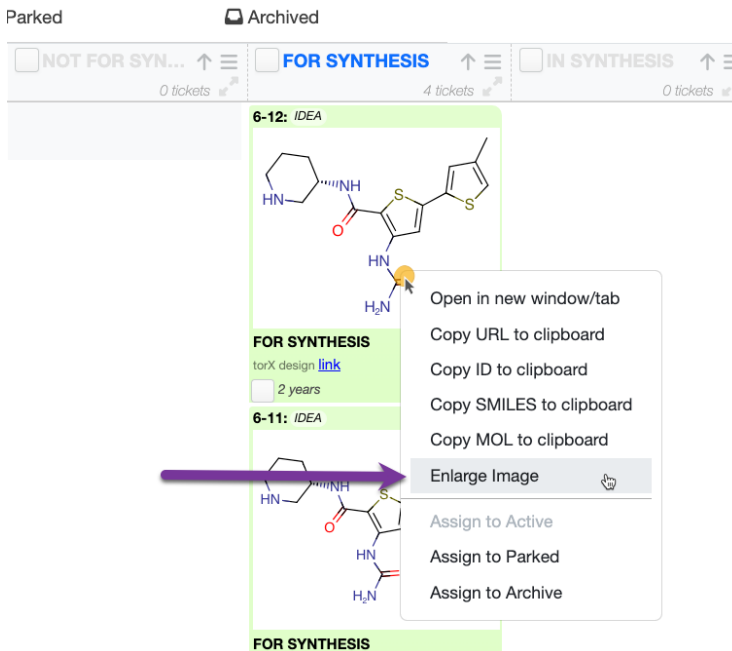
File type to export?

- CSV
 SDFfile
 SMILES

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.



Parked Archived

NOT FOR SYN... 0 tickets FOR SYNTHESIS 4 tickets IN SYNTHESIS 0 tickets

6-12: IDEA

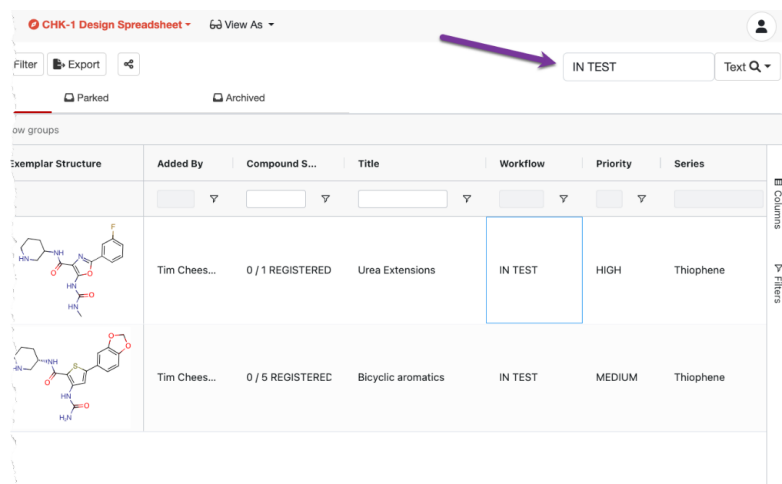
FOR SYNTHESIS
torX design [link](#)
2 years

6-11: IDEA

FOR SYNTHESIS

- Open in new window/tab
- Copy URL to clipboard
- Copy ID to clipboard
- Copy SMILES to clipboard
- Copy MOL to clipboard
- Enlarge Image
- Assign to Active
- Assign to Parked
- Assign to Archive

Spreadsheet Global Search

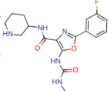
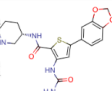


CHK-1 Design Spreadsheet View As

Filter Export Filter

Parked Archived

low groups

Exemplar Structure	Added By	Compound S...	Title	Workflow	Priority	Series
	Tim Chees...	0 / 1 REGISTERED	Urea Extensions	IN TEST	HIGH	Thiophene
	Tim Chees...	0 / 5 REGISTERED	Bicyclic aromatics	IN TEST	MEDIUM	Thiophene

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.

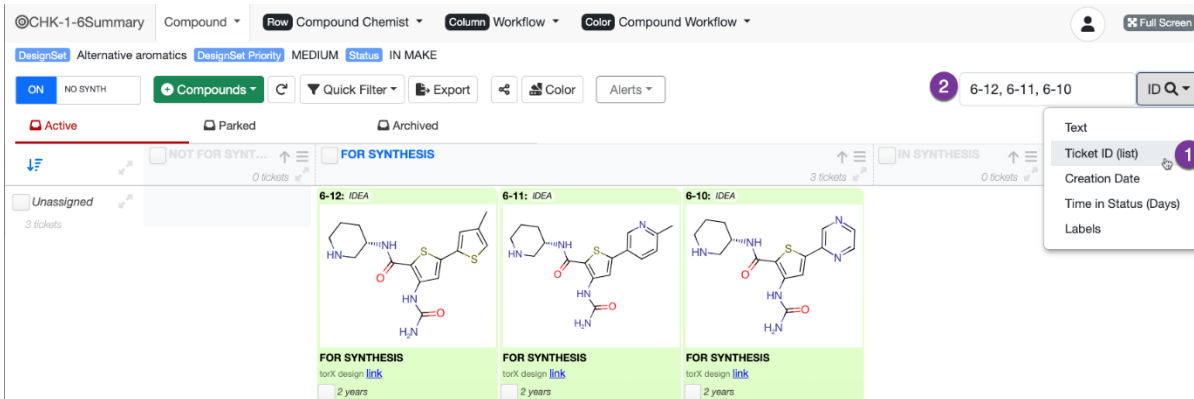
On the spreadsheet there is also now a Reset Spreadsheet button that appears if you have changed the spreadsheet default set-up, i.e., changing column order, grouping by, hiding columns. Clicking the button reverts the spreadsheet back to its original view.



Filter Export Reset Spreadsheet

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).

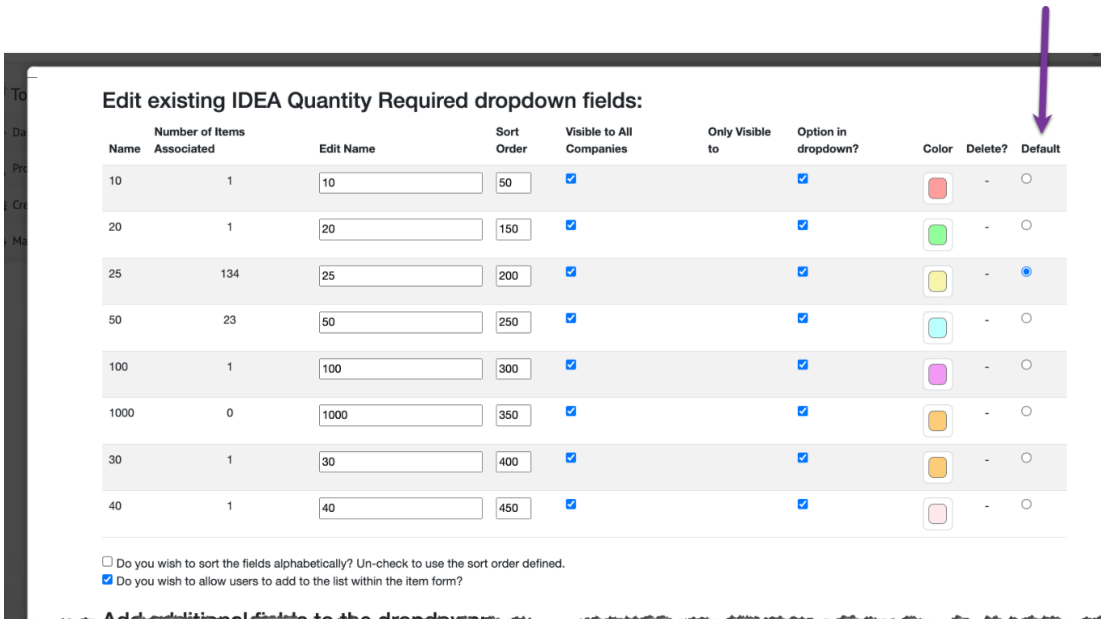


The screenshot shows the Torx tracking board interface. At the top, there are navigation tabs for 'DesignSet', 'Alternative aromatics', 'DesignSet Priority', 'MEDIUM', and 'Status IN MAKE'. Below this, there are filters for 'ON NO SYNTH', 'Compounds', 'Quick Filter', 'Export', 'Color', and 'Alerts'. A search bar contains the text '6-12, 6-11, 6-10'. A dropdown menu is open, showing options: 'Text', 'Ticket ID (list)' (highlighted with a red circle and '1'), 'Creation Date', 'Time in Status (Days)', and 'Labels'. The main board area shows three columns, each with a chemical structure and the text 'FOR SYNTHESIS' and '2 years'.

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).



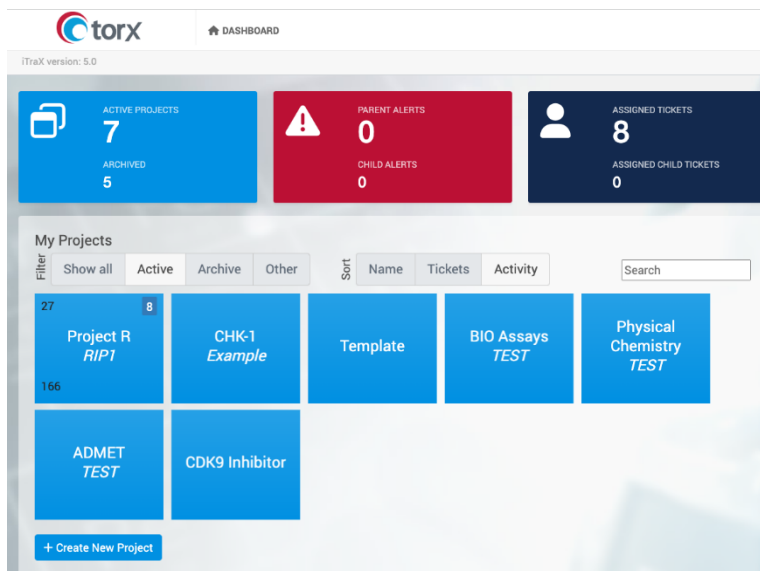
The screenshot shows the 'Edit existing IDEA Quantity Required dropdown fields' admin page. It features a table with the following columns: Name, Number of Items Associated, Edit Name, Sort Order, Visible to All Companies, Only Visible to, Option in dropdown?, Color, Delete?, and Default. A purple arrow points to the 'Default' column.

Name	Number of Items Associated	Edit Name	Sort Order	Visible to All Companies	Only Visible to	Option in dropdown?	Color	Delete?	Default
10	1	10	50	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
20	1	20	150	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
25	134	25	200	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input checked="" type="radio"/>
50	23	50	250	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
100	1	100	300	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
1000	0	1000	350	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
30	1	30	400	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>
40	1	40	450	<input checked="" type="checkbox"/>		<input checked="" type="checkbox"/>		-	<input type="radio"/>

Do you wish to sort the fields alphabetically? Un-check to use the sort order defined.
 Do you wish to allow users to add to the list within the item form?

Enhancements to the main dashboard

The main Torx Make dashboard now has an updated color scheme and UI, and improved performance.



The dashboard shows the following statistics:

- ACTIVE PROJECTS: 7
- ARCHIVED: 5
- PARENT ALERTS: 0
- CHILD ALERTS: 0
- ASSIGNED TICKETS: 8
- ASSIGNED CHILD TICKETS: 0

My Projects

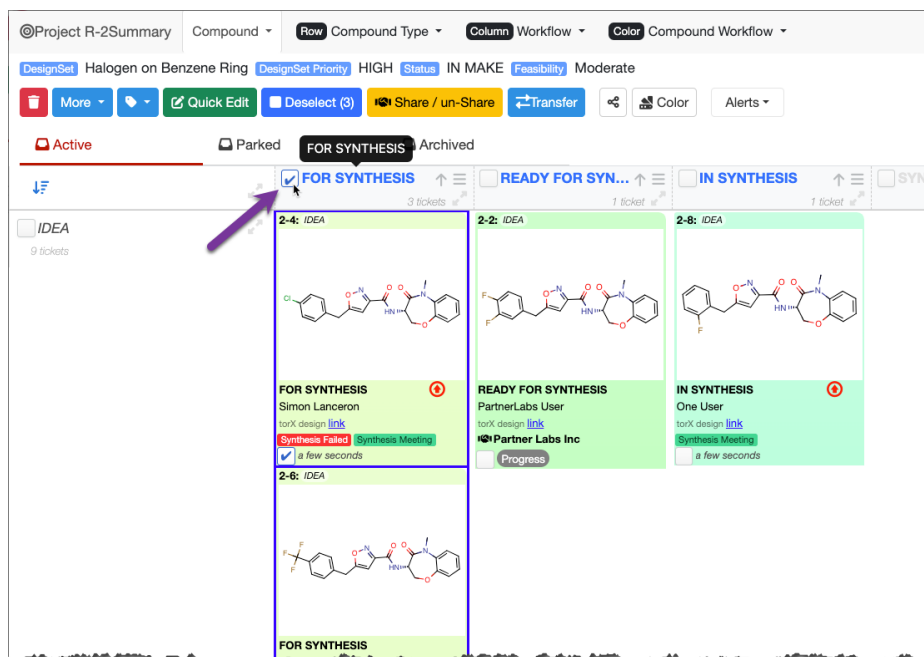
Filter	Show all	Active	Archive	Other	Sort	Name	Tickets	Activity
27	8	Project R <i>RIP1</i>	CHK-1 <i>Example</i>	Template	BIO Assays <i>TEST</i>	Physical Chemistry <i>TEST</i>		
166		ADMET <i>TEST</i>	CDK9 Inhibitor					

+ Create New Project

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



The tracking board displays a grid of tickets with the following headers:

- FOR SYNTHESIS (2 tickets)
- READY FOR SYN... (1 ticket)
- IN SYNTHESIS (1 ticket)

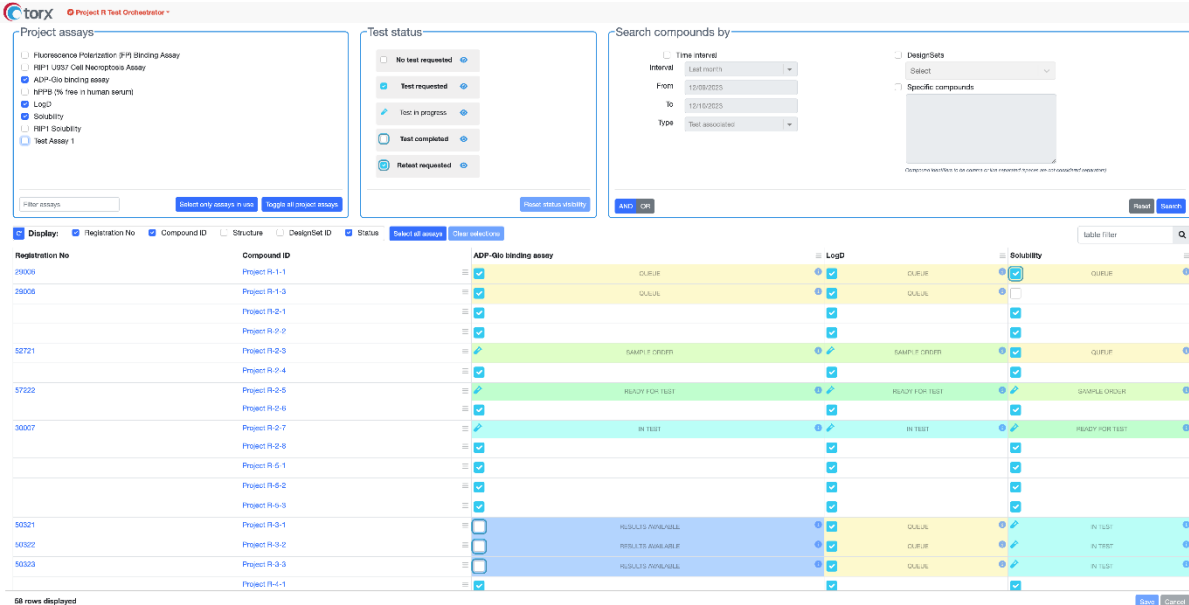
Individual ticket details include:

- 2-4: IDEA** (FOR SYNTHESIS): Simon Lanceron, torX design [link](#), **Synthesis Failed**, [Synthesis Meeting](#), a few seconds.
- 2-2: IDEA** (READY FOR SYNTHESIS): PartnerLabs User, torX design [link](#), [Partner Labs Inc](#), (Progress).
- 2-8: IDEA** (IN SYNTHESIS): One User, torX design [link](#), [Synthesis Meeting](#), a few seconds.

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.



The screenshot displays the Torx Test Orchestrator interface. It includes a sidebar for 'Project assays' with filters for Fluorescence Polarization (FPI) Binding Assay, RPH1 U937 Cell Neutrophils Assay, ADP-Glo Binding Assay, HPLS 26-Hes in human serum, LogD, Solubility, RPH1 Solubility, and Test Assay 1. The 'Test status' section shows buttons for 'No test requested', 'Test requested', 'Test in progress', 'Test completed', and 'Retest requested'. The 'Search compounds by' section has filters for 'Time interval' (Last month), 'From' (12/09/2023), 'To' (12/15/2023), 'Type' (Test associated), 'DesignSets', and 'Specific compounds'. The main table displays test requests with columns for Registration No, Compound ID, Assay Name, Status, LogD, and Solubility. The table shows various test requests with their respective statuses and associated compounds.

Registration No	Compound ID	ADP-Glo binding assay	LogD	Solubility
28009	Project R-1-1	QUELIE	QUELIE	QUELIE
28006	Project R-1-3	QUELIE	QUELIE	QUELIE
	Project R-2-1			
	Project R-2-2			
52721	Project R-2-3	SAMPLE CREDIT	SAMPLE CREDIT	QUELIE
	Project R-2-4			
57222	Project R-2-5	READY FOR TEST	READY FOR TEST	SAMPLE CREDIT
	Project R-2-6			
30007	Project R-2-7	IN TEST	IN TEST	READY FOR TEST
	Project R-2-8			
	Project R-5-1			
	Project R-5-2			
	Project R-5-3			
50321	Project R-3-1	RESULTS AVAILABLE	QUELIE	IN TEST
50322	Project R-3-2	RESULTS AVAILABLE	QUELIE	IN TEST
50323	Project R-3-3	RESULTS AVAILABLE	QUELIE	IN TEST
	Project R-4-1			

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.