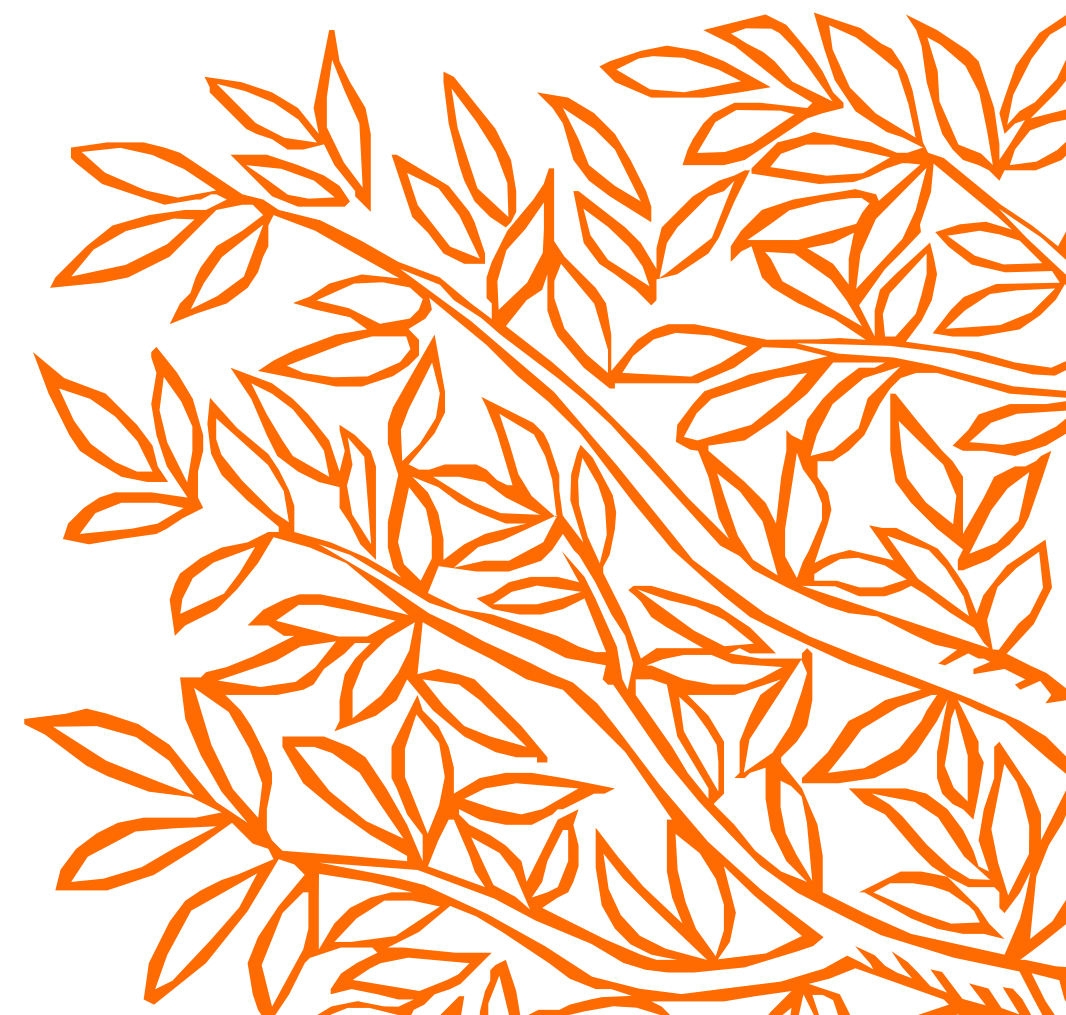




Reaxys®

Reaxys Predictive Retrosynthesis powered by Pending.AI

Quick Reference Guide



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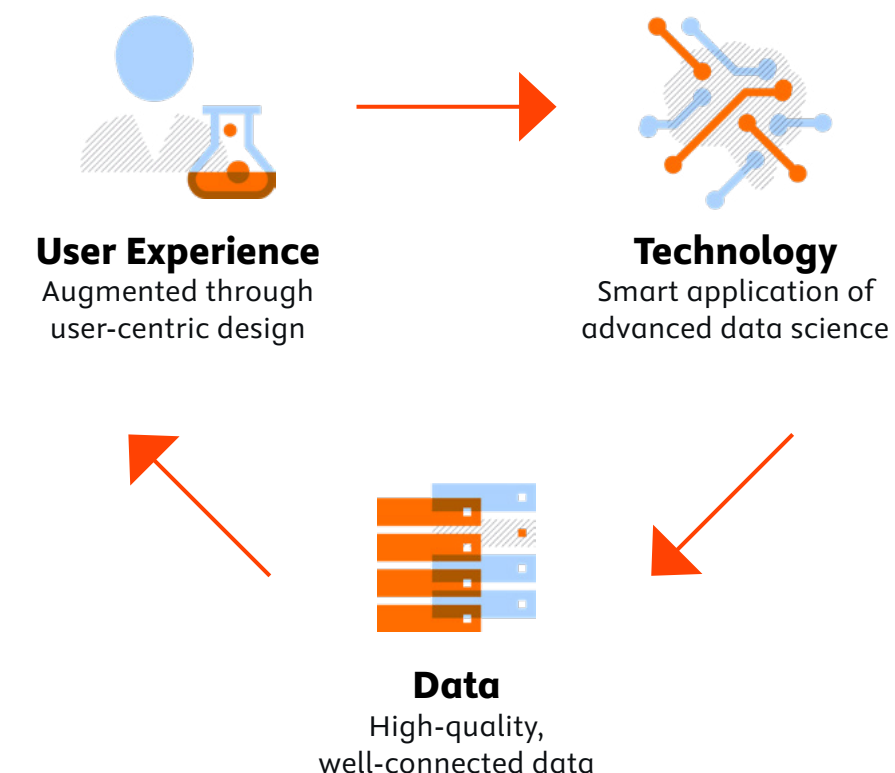
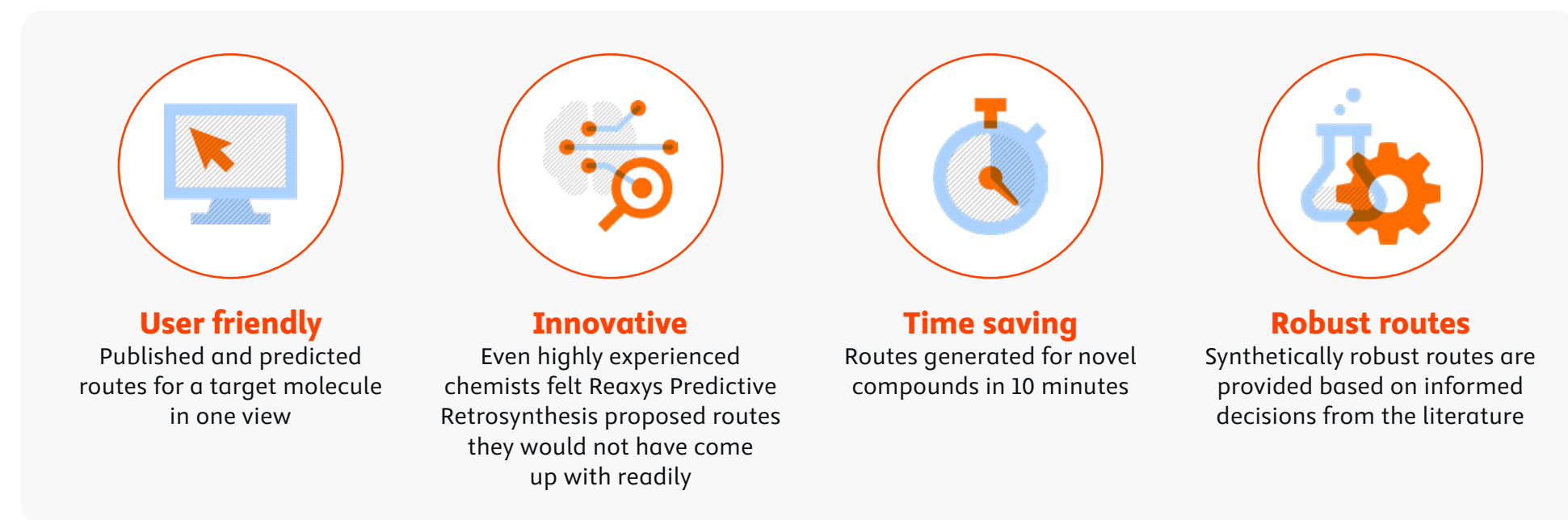
1. Introduction

What is Reaxys Predictive Retrosynthesis powered by Pending.AI?

The Reaxys Predictive Retrosynthesis powered by Pending.AI module is designed to drive idea generation, time savings and cost control in synthetic chemistry projects. It provides fast predictions of synthesis routes to known and unknown small organic molecules. The module combines high-quality reaction data from Reaxys with state-of-the-art AI & ML technologies from our partner Pending.AI, in an easy-to-use interface.

The Reaxys Predictive Retrosynthesis powered by Pending.AI module includes access to unique Reaxys content, including supporting literature references, experimental procedures, commercial availability of starting materials and much more.

What are the key benefits when using Reaxys Predictive Retrosynthesis?



2. How-to guide

In this section you will find important tips and tricks to help you start using Reaxys Predictive Retrosynthesis.

2.1. Getting started

To use the predictive retrosynthesis Pending.AI module, you will need to login at [Reaxys.com](https://www.reaxys.com) and click on Retrosynthesis.

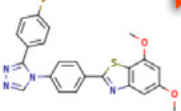
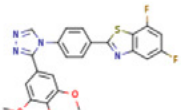
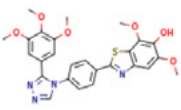
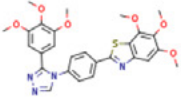
The screenshot displays the Reaxys web application interface. At the top, the navigation bar includes the Reaxys logo, a search bar, and tabs for 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted with a red arrow), 'History', and 'Alerts'. A user profile for 'Martina Stella' is visible on the right. Below the navigation bar, a header section states 'Search substances, reactions, documents and bioactivity data' with a link to 'Import'. The main search area features a 'Search Reaxys' input field containing the text 'Documents, e.g. Tetrahedron, 2014, 70, 2343' and a 'Find >' button. Below the search field is an 'AND' section with a 'Draw' button. At the bottom, a 'Content Overview' section shows statistics: 287M Substances, 68M Reactions, 117M Documents, 45M Patents, and 48M Bioactivities. The footer contains the Elsevier logo, remote access links, a cookie notice, and a feedback button.

To start a new project, follow the orange arrows to move to the drawing page.

Reaxys® Quick search Query builder Results Retrosynthesis History Alerts Martina Stella

My Synthesis Projects 0 selected Delete

Draw

No.	Date	Project name		No. of routes
2412682	14 Nov 2024	Project #2412682	<div>Draw new structure</div>  <div>Edit</div>	Predicted 16 Published 0 View
2412677	14 Nov 2024	Project #2412677	 <div>Edit</div>	Predicted 12 Published 0 View
2412625	14 Nov 2024	Project #2412625	 <div>Edit</div>	Predicted 12 Published 0 View
2412619	14 Nov 2024	Project #2412619	 <div>Edit</div>	Predicted 12 Published 2 Feedback

Once on the drawing page, there are several options to customize your plan.

The screenshot displays the Reaxys Retrosynthesis interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (active), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. The main workspace is the 'Structure editor selected: MarvinJS' (with ChemDrawJS as an option). A toolbar at the top of the editor contains various drawing tools. The central canvas shows the 'Marvin JS by Chemaxon' logo. On the right, the 'Parameters' panel is open, showing settings for 'Predicted' routes, 'Length and depth of routes' (Full routes: 20, Last step only), 'Diversity of routes' (Allow, identical reaction steps per project: 3, identical building blocks per project: 3), 'Processing time' (Standard, Extended), and 'Select Building Block Libraries' (Standard Lab Chemicals (STD), Commercial Substances in 10 days (RCS10D), Commercial Substances >10 days (RCS>10D), Commercial Substances <\$10/g (RCS\$10), Natural Products (NATP), Reaxys Starting Materials Occur 3 (RSM3), Reaxys Starting Materials Occur 4 (RSM4), Reaxys Starting Materials Occur gte 5 (RSM5)). At the bottom right, it says 'Powered by Reaxys AI' and has a 'Feedback' button. At the bottom left of the editor, there are buttons for 'Clear', 'Cancel', and 'Synthesize'.

1. Draw your molecule of interest using either MarvinJS or ChemdrawJS
2. Use the *Insert structure from name* feature to add a molecule using a SMILES, InChI or CAS number
3. Alter the parameters to tailor to your synthesis needs (see next image)
4. Once happy, click *Synthesize* to begin the project

Parameters

☒ Predicted ⓘ

Length and depth of routes ⓘ

☒ Full routes: 20 ▼

☐ Last step only

Diversity of routes ⓘ

Allow

3 ▼ identical reaction steps per project

3 ▼ identical building blocks per project

Processing time ⓘ

☒ Standard ☐ Extended

Select Building Block Libraries ⓘ

☐ Standard Lab Chemicals (STD)

☒ Commercial Substances in 10 days (RCS10D)

☒ Commercial Substances >10 days (RCS>10D)


☐ Commercial Substances <\$10/g (RCS\$10)

☒ Natural Products (NATP)

☐ Reaxys Starting Materials Occur 3 (RSM3)

☐ Reaxys Starting Materials Occur 4 (RSM4)

☒ Reaxys Starting Materials Occur gte 5 (RSM5)

Powered by  PendingAI

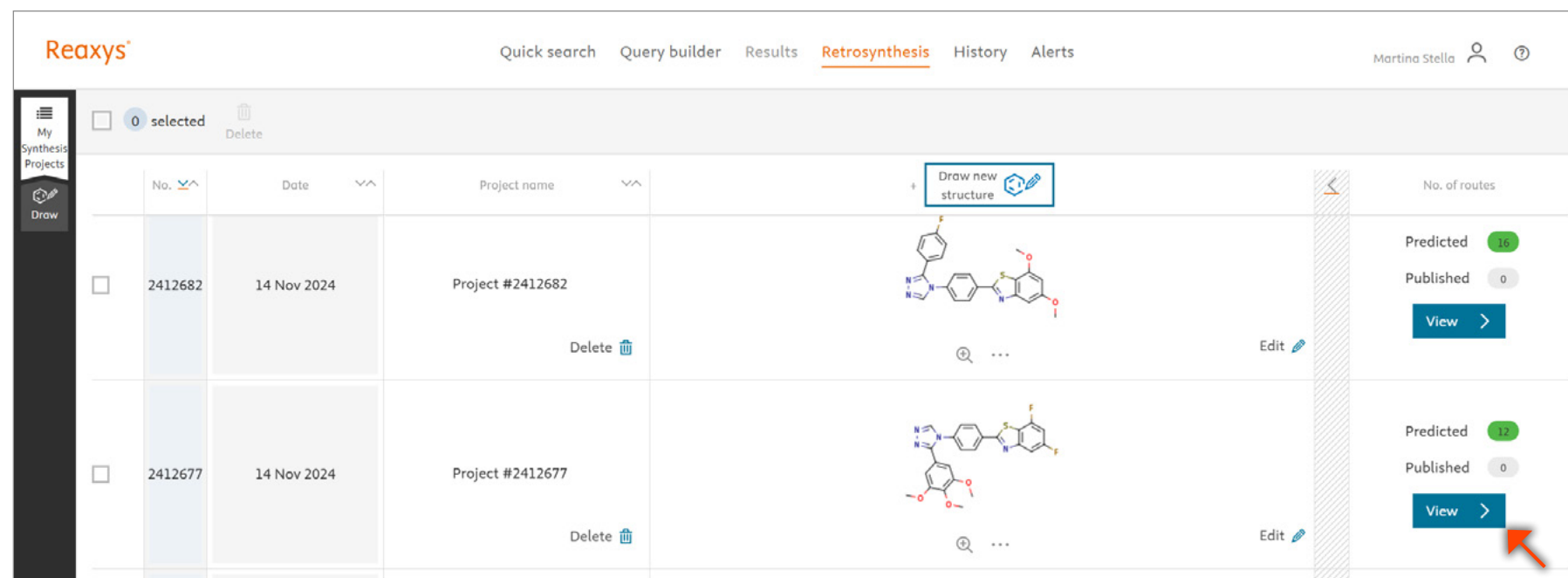
Feedback

Selecting parameters

- Use the last step only feature if your original project provided no routes
- Alter the diversity of synthesis plans as you see fit
- Select extended processing time in case no results occur
- Toggle building block libraries to ensure the routes lead to starting materials you can access or prefer

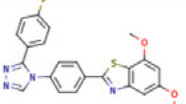
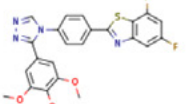
2.2. View the results

Once you've clicked *Synthesize*, you will return to the project page and any published routes of your molecule of interest can be reviewed while you wait for the predicted routes. Once the project is complete, click *View* to evaluate the results.



Reaxys® Quick search Query builder Results **Retrosynthesis** History Alerts Martina Stella

0 selected Delete

No.	Date	Project name	Chemical structure	No. of routes
2412682	14 Nov 2024	Project #2412682		Predicted 16 Published 0 View >
2412677	14 Nov 2024	Project #2412677		Predicted 12 Published 0 View >

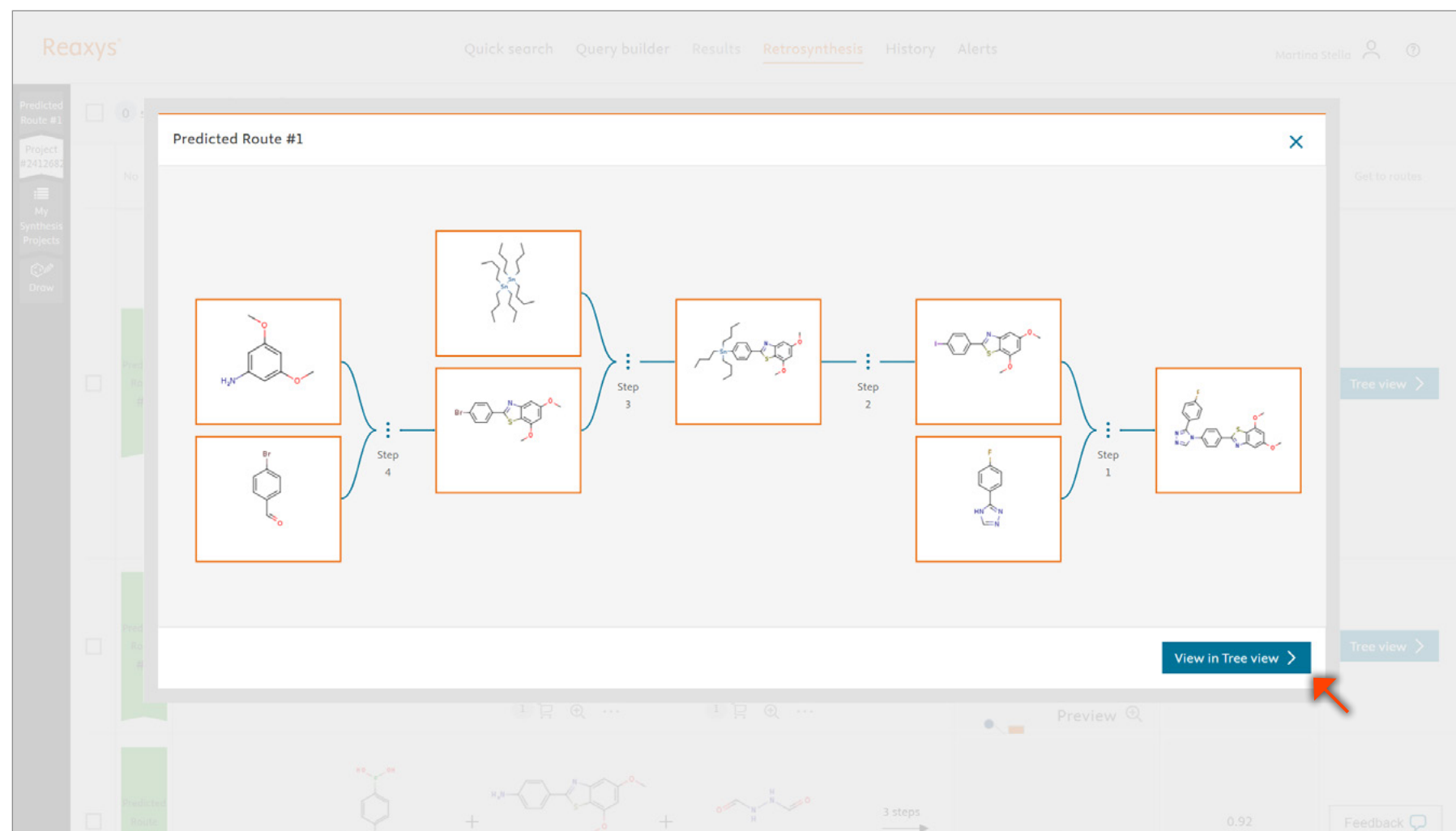
On the review screen it is easy to quickly analyze both published and predicted routes in one view.

The screenshot displays the Reaxys Retrosynthesis review interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (active), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. The left sidebar shows 'Project #2412682', 'My Synthesis Projects', and a 'Draw' button. The main area shows three 'Predicted Route' entries, each with a green banner label. Each route is presented in a row with columns for building blocks, steps, topology, score, and a 'Get to routes' button.

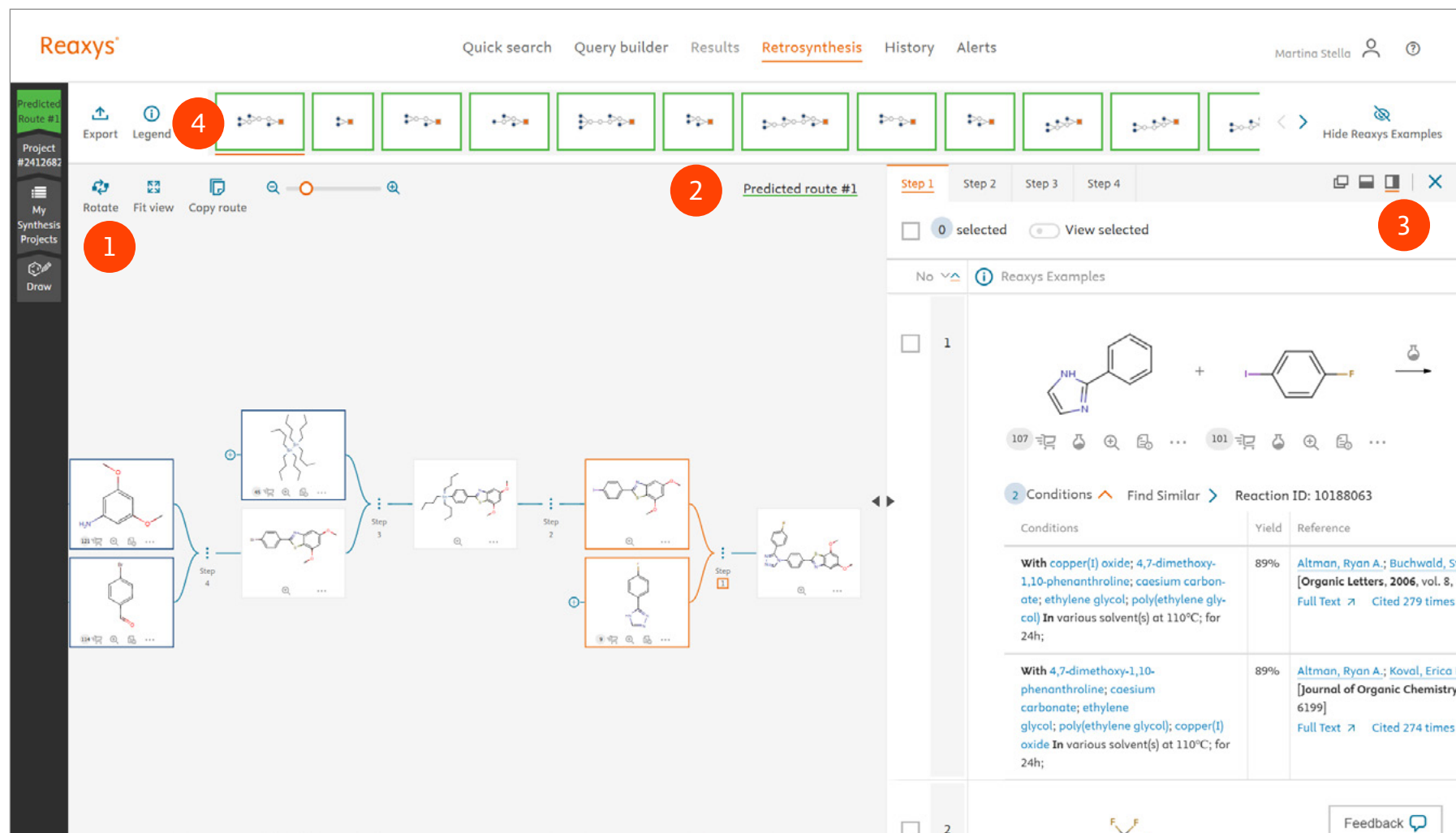
	Building blocks to target	No. of steps	Route topology	Score	Get to routes
Predicted Route #1	9 + 45 + 121 + 114	4 steps	Preview	0.95	Tree view >
Predicted Route #2	1 + 1	1 step	Preview	0.92	Tree view >
Predicted Route #3	128 + 2 + 80	3 steps	Preview	0.92	Tree view > Feedback

1. Easily view the number of steps
2. Review the route topology to see how branched the routes are
3. The routes are ranked by the algorithm so you can analyze the best routes first
4. Click the preview of a given route to see a full view of the route

From the route preview you can see all the steps in one view. Clicking *View in Tree view* allows you to view more details of your preferred route.



2.3. Analyzing the routes



1. Use the rotate and zoom functions to make it easier to view what you need in one screen
2. The route topology previews allow you to easily switch between routes for quick comparisons
3. Alter how you view the literature that informed the routes to fit your preferences; see the screenshot below for the alternative view
4. Copy entire synthesis plans to the clipboard for use in external editor or applications, such as Revvity ChemDraw

Alternative view

Reaxys®

Quick searchQuery builderResultsRetrosynthesisHistoryAlerts

Martina Stella

Predicted Route #1

Project #2412682

My Synthesis Projects

Draw

ExportLegend

RotateFit viewCopy route

Step 1Step 2Step 3Step 4

0 selectedView selected

NoReaxys Examples

1

107101

2 ConditionsFind SimilarReaction ID: 10188063

Predicted route #1

Feedback

2.4. Selecting a route to begin the synthesis

Once you have selected your view style, you can review the literature that informed the results.

The screenshot displays the Reaxys Retrosynthesis interface. On the left, a vertical sidebar shows the 'Predicted Route #1' and a 'My Synthesis Projects' section. The main area is divided into two panels. The left panel shows a retrosynthetic tree for 'Predicted route #1', with steps 1, 2, 3, and 4. The right panel shows a list of 'Reaxys Examples' for the selected reaction. The first example (Reaction ID: 25781103) is highlighted with a red circle '1' and a green background. The second example is highlighted with a red circle '2' and a green background. The interface includes a top navigation bar with 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. A user profile 'Martina Stella' is visible in the top right corner. The bottom right corner has a 'Feedback' button.

No.	Reaxys Examples	Score
2	<p>1 Conditions Find Similar > Reaction ID: 25781103</p> <p>Conditions: With peracetic acid; sodium hydroxide; [¹²⁵I] sodium iodide; sodium iodide In water; acetic acid</p> <p>Yield: 94%</p> <p>Reference: Current Patent Assignee: GE HEALTHCARE - WO2006/32911, 2006, A2 Location in patent: Page/Page column 50; 51 Full Text Details Abstract</p>	1
3	<p>Conditions: With peracetic acid; sodium hydroxide; [¹²⁵I] sodium iodide; sodium iodide In water; acetic acid</p> <p>Yield: 94%</p> <p>Reference: Current Patent Assignee: GE HEALTHCARE - WO2006/32911, 2006, A2 Location in patent: Page/Page column 50; 51 Full Text Details Abstract</p>	1

1. View the conditions and experimental procedures that informed the route
2. The similarity score prioritizes published reactions which are more similar to the predicted reaction for ease of reviewing

The predictive retrosynthesis module always ends in purchasable starting materials to begin the synthesis. Click on Commercial Substances to select the supplier based on stock availability, price, pack size etc. You can see these details when you hover your cursor over the shopping cart icon.

When you are satisfied with the route, click on *Export* on the top left corner to export the data and share it with your colleagues or to include it in your electronic lab notebook.

Export the routes in a variety of formats with the structures and experimental procedures included.

The screenshot displays the Reaxys Retrosynthesis module interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (active), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. The left sidebar shows 'Project #2412682', 'My Synthesis Projects', and 'Draw'. The main workspace shows 'Predicted route #1' with a sequence of chemical structures connected by arrows, labeled 'Step 3' and 'Step 2'. A 'Substance Availability' pop-up is visible for a starting material, showing 'Commercial Suppliers' and 'Accelrys' ACD'. A detailed view of a starting material (a brominated benzene derivative) is shown on the right, with a tooltip displaying 'Shipping time: Up to 5 days', 'Best price: 1 USD/g', and 'Largest available package size: Up to 10 kg'. The 'Export reactions' dialog box is open, showing options to 'Choose a format' (Microsoft Word), 'Export' (All available data or Selected examples only), and 'Additional options' (Include structures, Include experimental procedure, Include a description in the document). A disclaimer is also present: 'Disclaimer: please refer to our Terms and Conditions before downloading data.'



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