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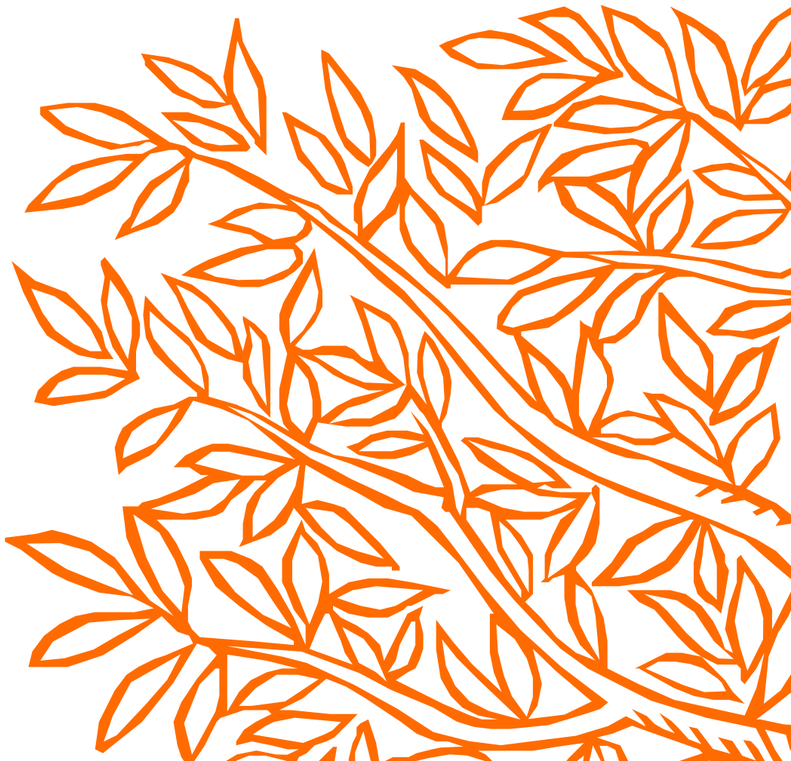
Reaxys®

Reaxys Predictive Retrosynthesis powered by Pending.AI

Quick Reference Guide



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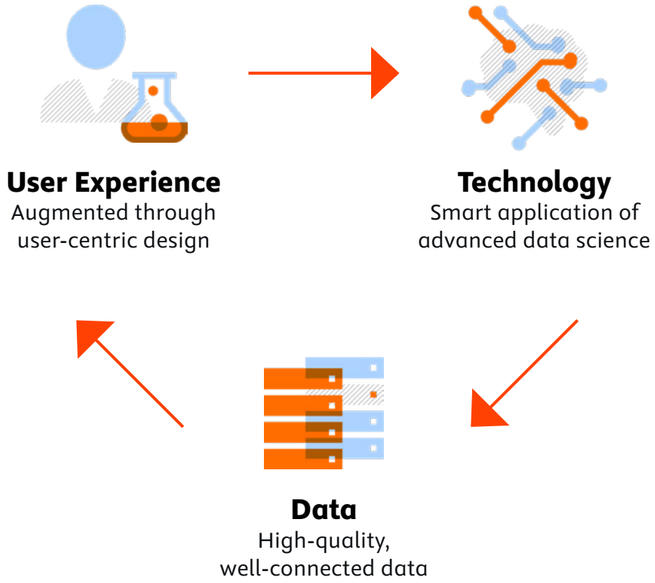
1. Introduction

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?

User friendly
Published and predicted routes for a target molecule in one view

Innovative
Even highly experienced chemists felt Reaxys Predictive Retrosynthesis proposed routes they would not have come up with readily

Time saving
Routes generated for novel compounds in 10 minutes

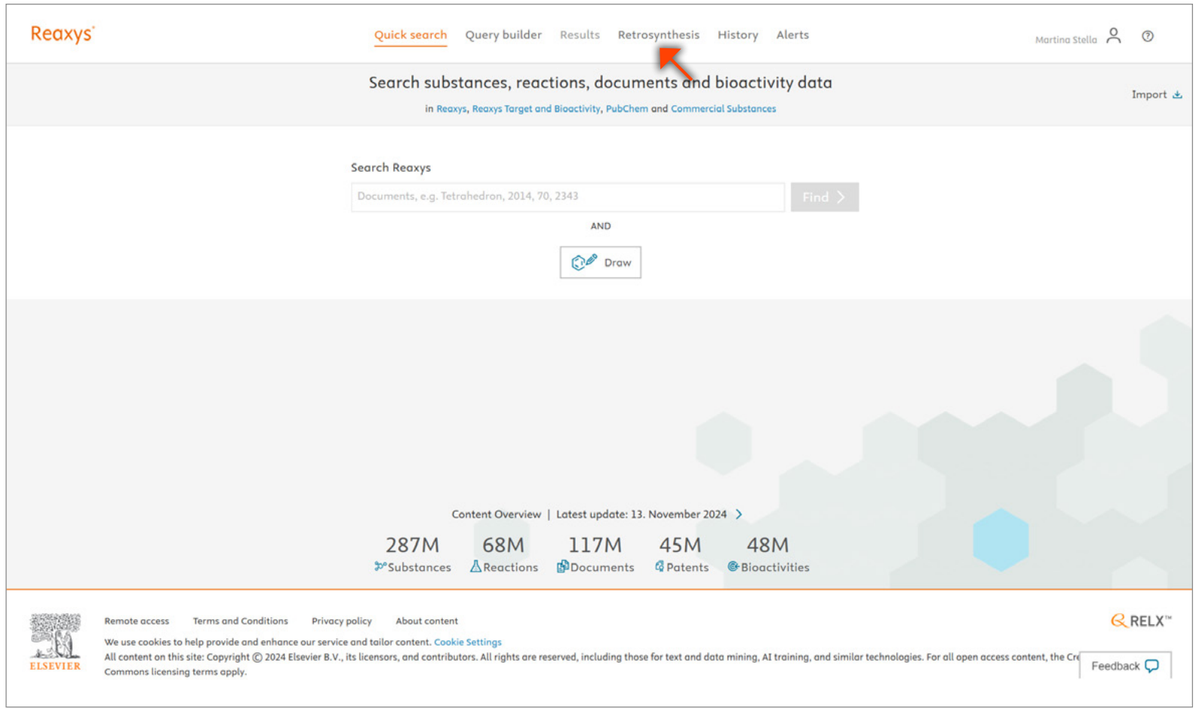
Robust routes
Synthetically robust routes are provided based on informed decisions from the literature

2. How-to guide

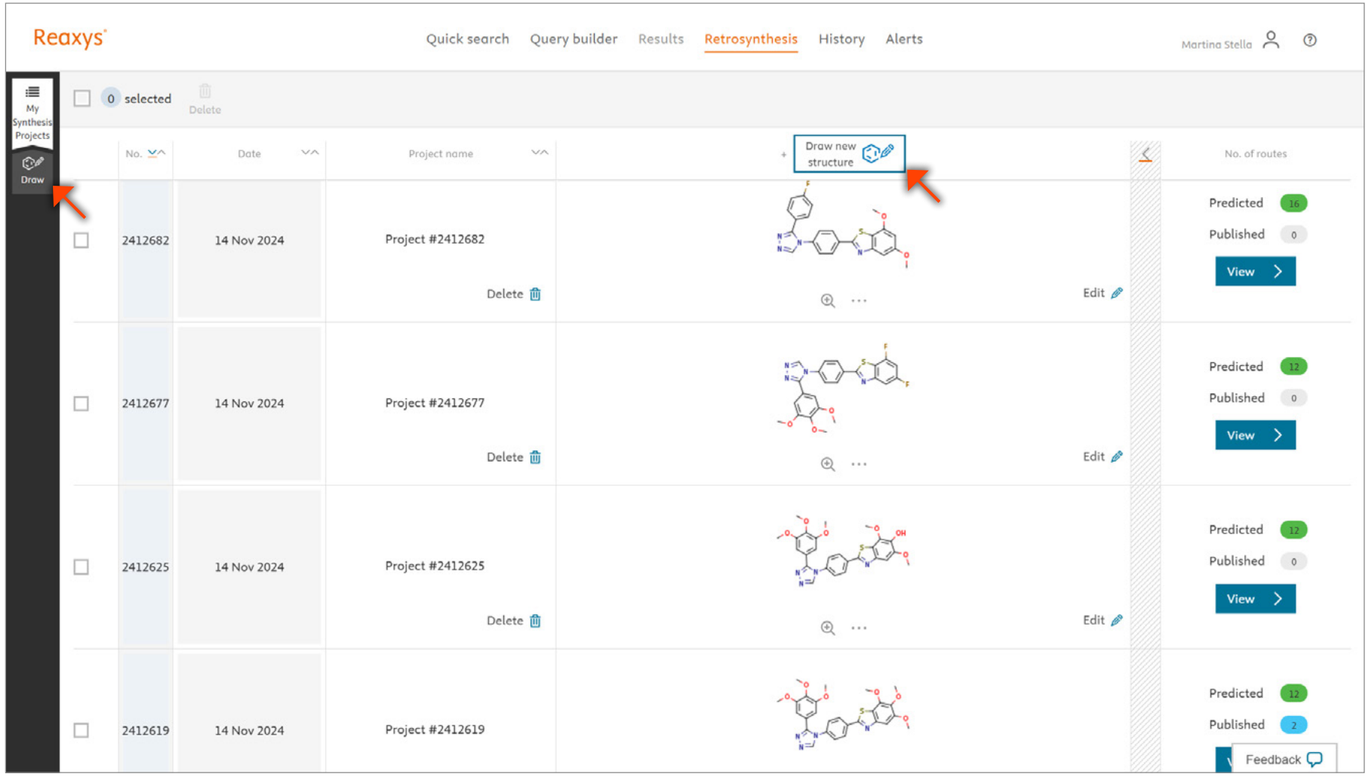
In this section you will find important tips and tricks to help you start using Reaxys Predictive Retrosynthesis.

2.1. Getting started

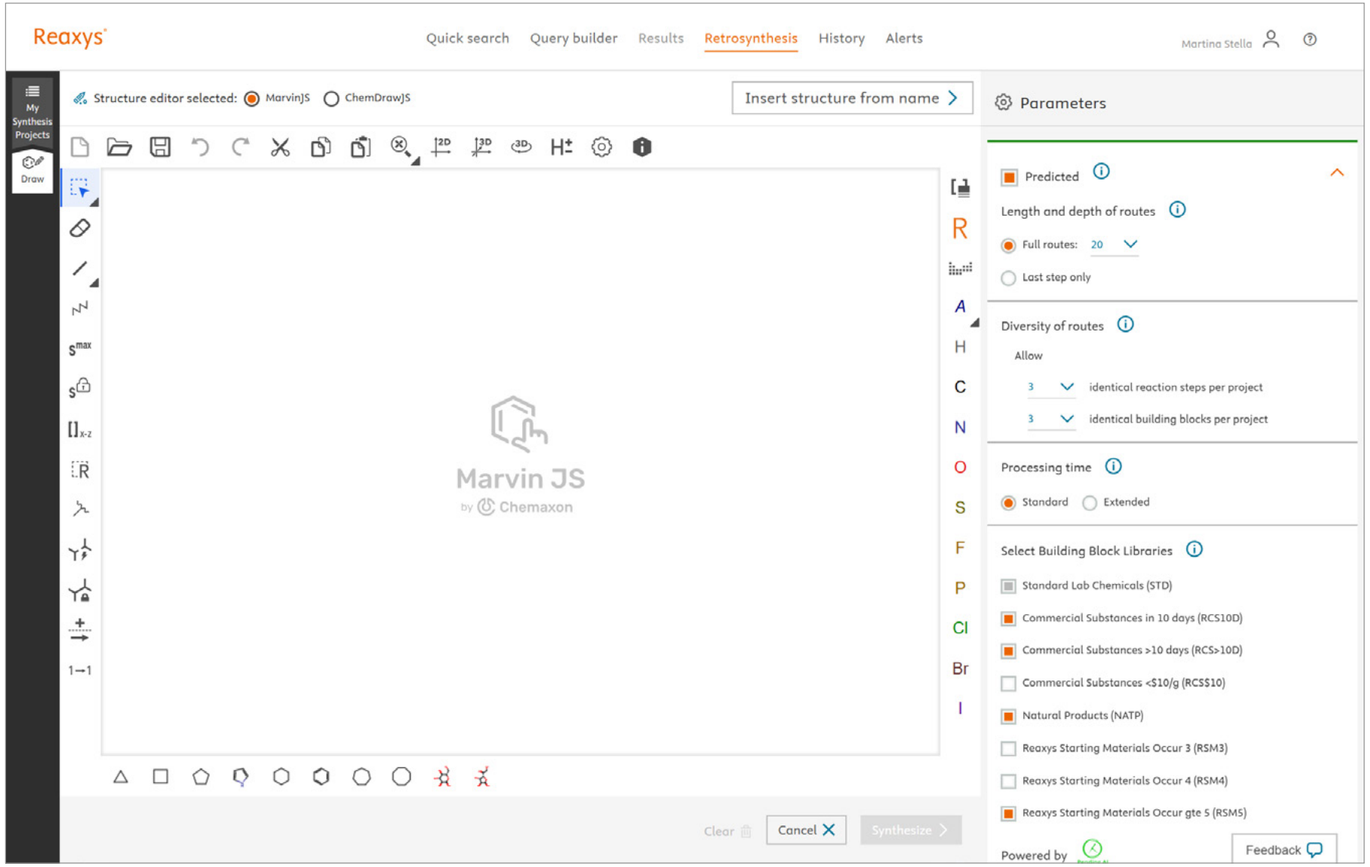
To use the predictive retrosynthesis Pending.AI module, you will need to login at Reaxys.com and click on Retrosynthesis.



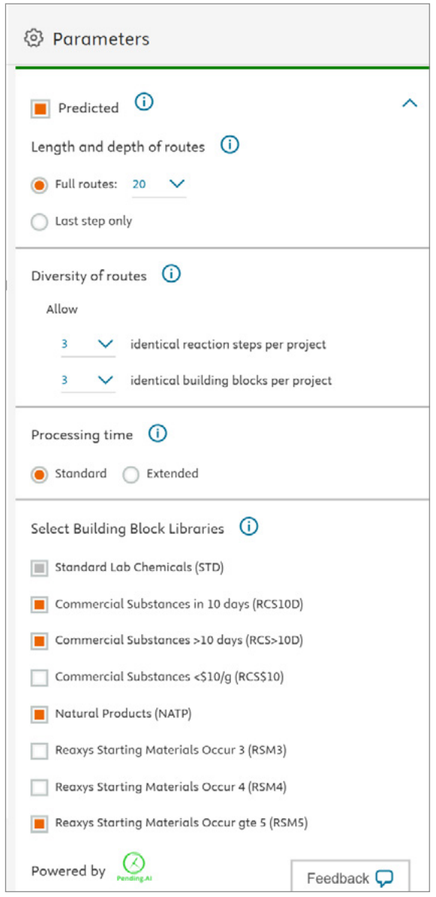
To start a new project, follow the orange arrows to move to the drawing page.



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



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

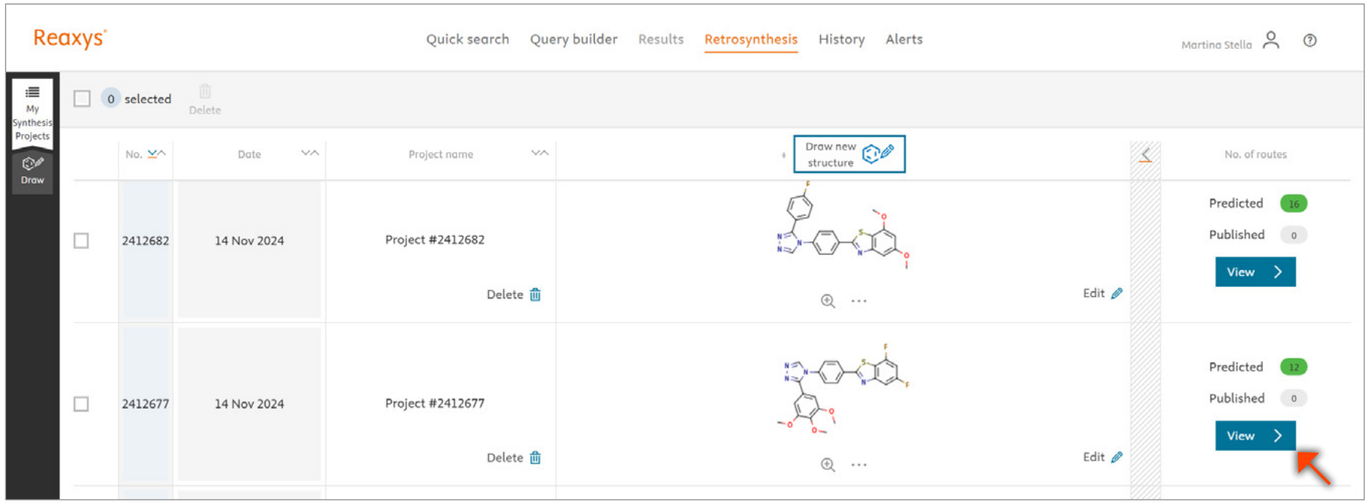


Selecting parameters

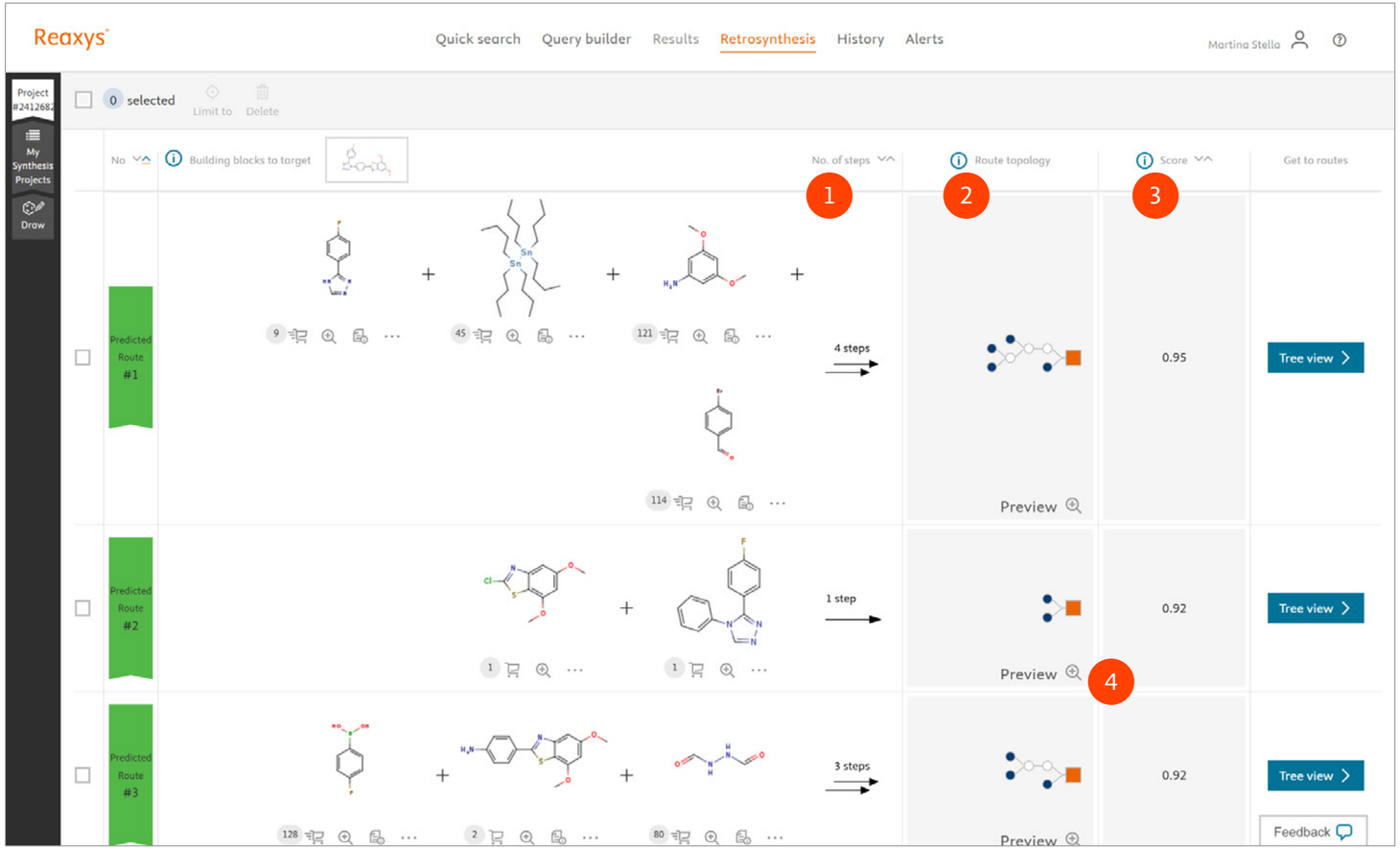
- Use the last step only feature if your original project provided no routes
- Alter the diversity of synthesis plans as you see fit
- Select extended processing time in case no results occur
- Toggle building block libraries to ensure the routes lead to starting materials you can access or prefer

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.

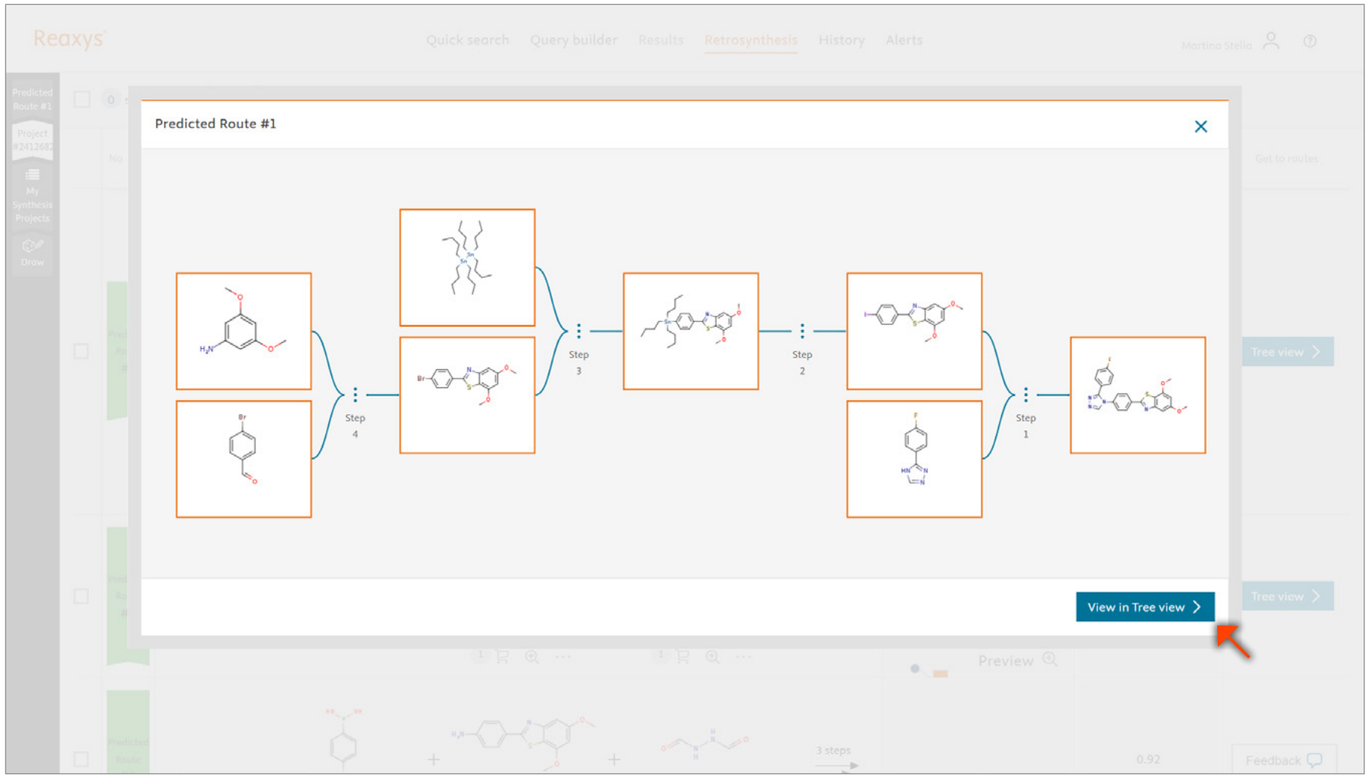


On the review screen it is easy to quickly analyze both published and predicted routes in one view.

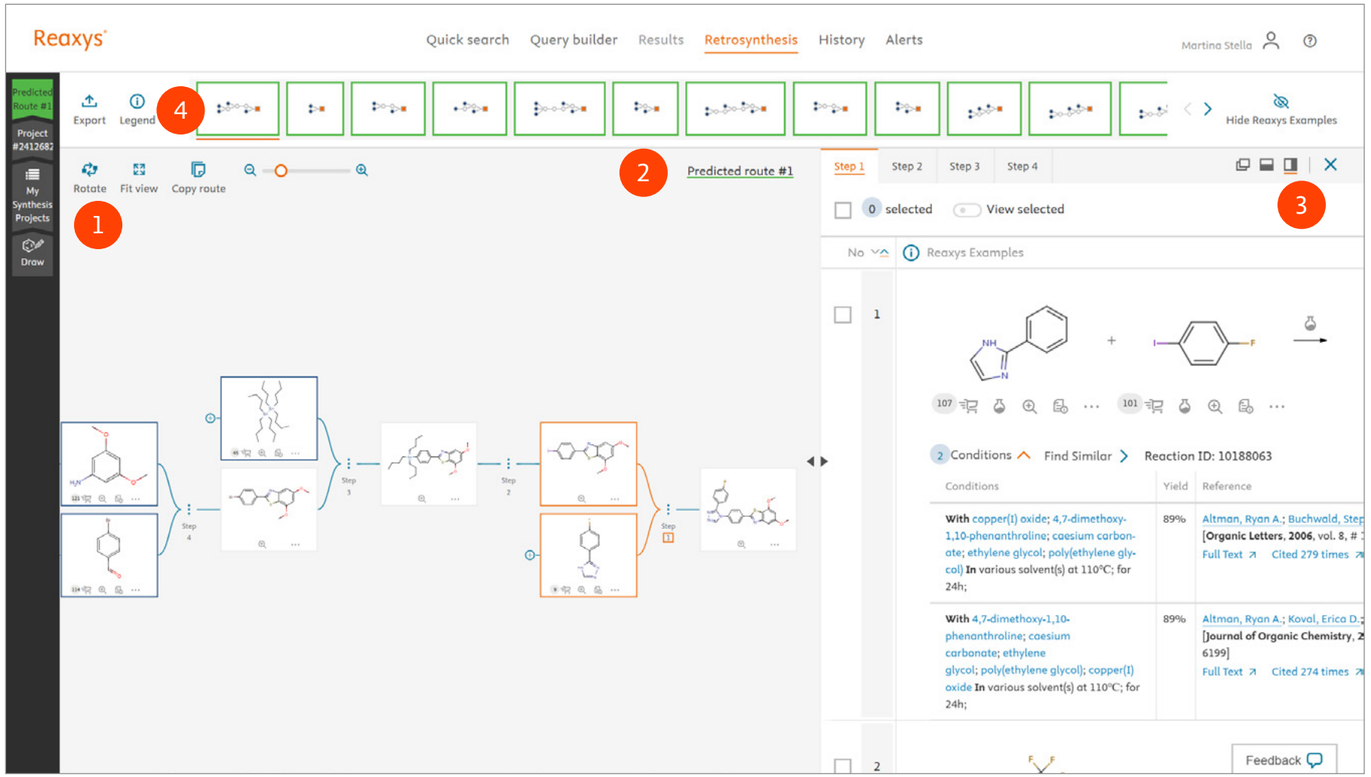


1. Easily view the number of steps
2. Review the route topology to see how branched the routes are
3. The routes are ranked by the algorithm so you can analyze the best routes first
4. Click the preview of a given route to see a full view of the route

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.

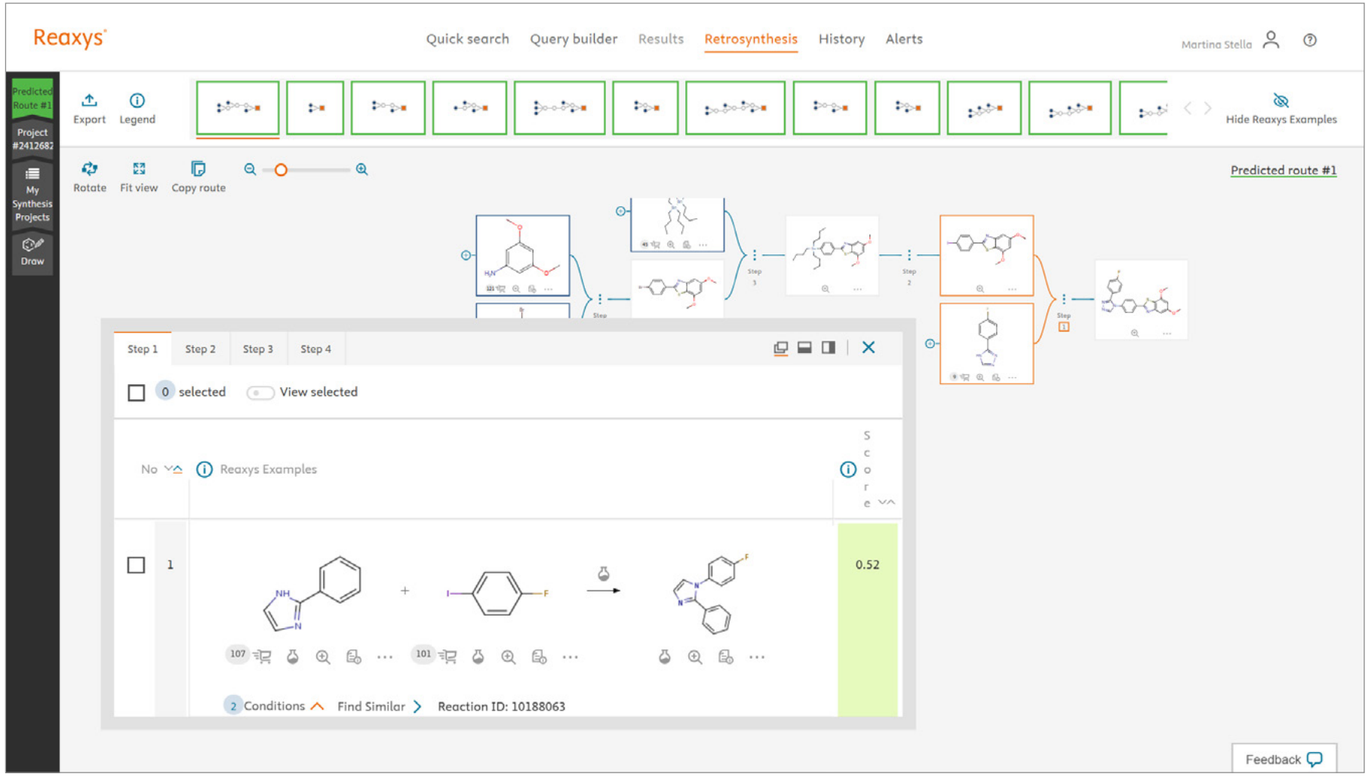


2.3. Analyzing the routes



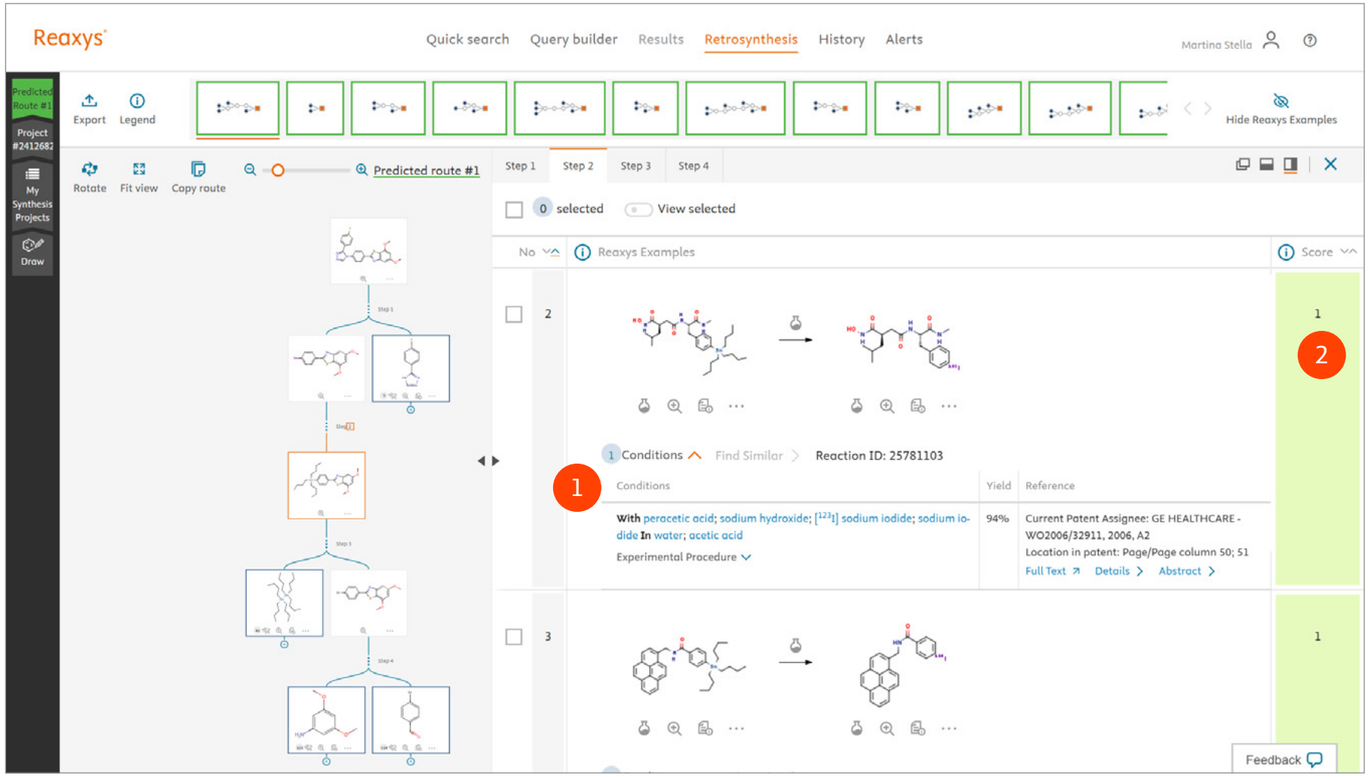
1. Use the rotate and zoom functions to make it easier to view what you need in one screen
2. The route topology previews allow you to easily switch between routes for quick comparisons
3. Alter how you view the literature that informed the routes to fit your preferences; see the screenshot below for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

Alternative view



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.

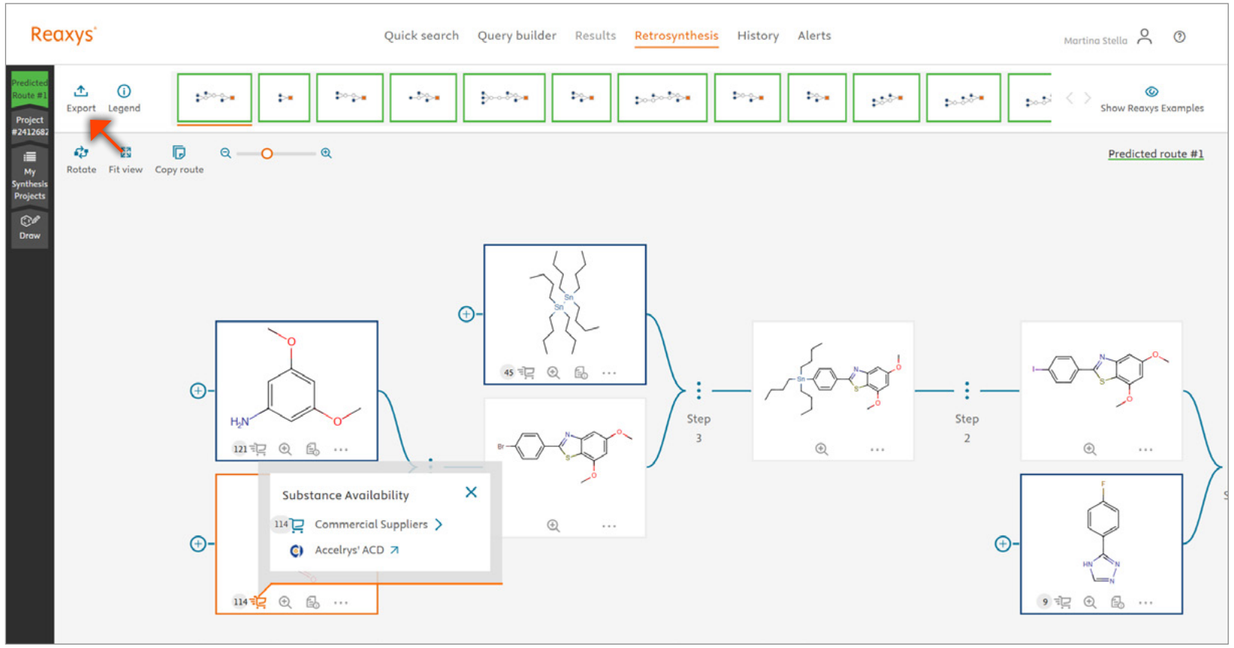


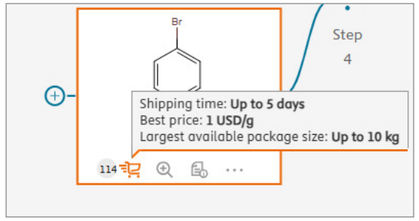
1. View the conditions and experimental procedures that informed the route
2. The similarity score prioritizes published reactions which are more similar to the predicted reaction for ease of reviewing

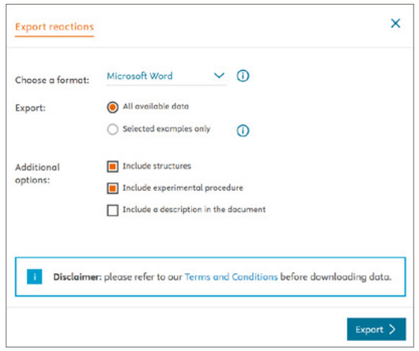
The predictive retrosynthesis module always ends in purchasable starting materials to begin the synthesis. Click on Commercial Substances to select the supplier based on stock availability, price, pack size etc. You can see these details when you hover your cursor over the shopping cart icon.

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.







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