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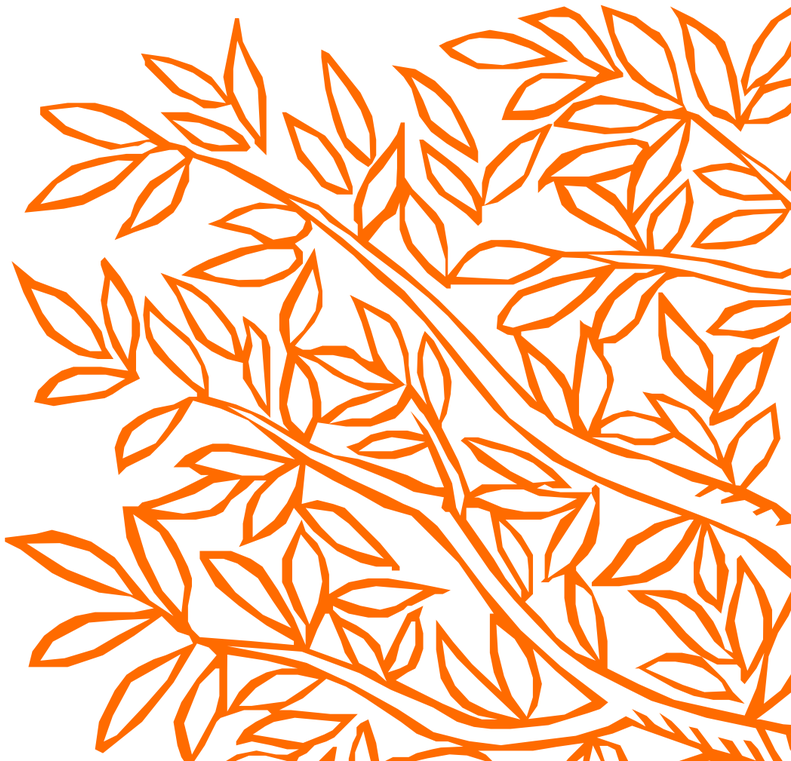
Reaxys®

Reaxys Predictive Retrosynthesis powered by Iktos

Quick Reference Guide



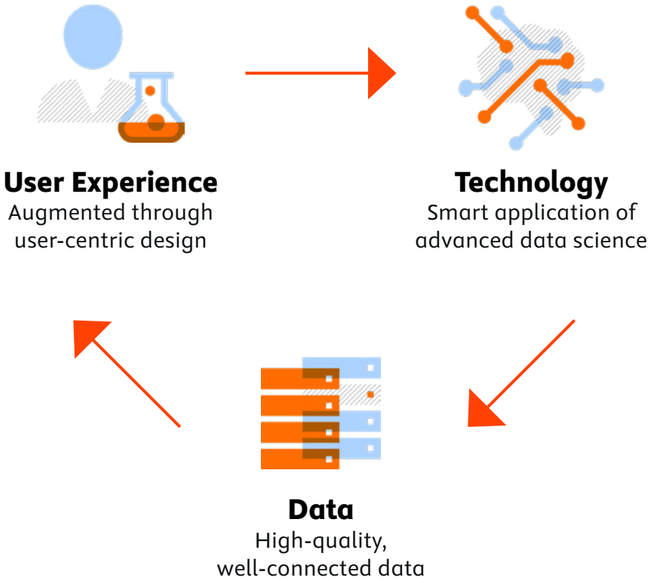
Contents

1. Introduction

What is Reaxys Predictive Retrosynthesis powered by Iktos?

The Reaxys Predictive Retrosynthesis powered by Iktos 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 Iktos, in an easy-to-use interface.

Unique to the Reaxys Predictive Retrosynthesis module, routes include access to 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

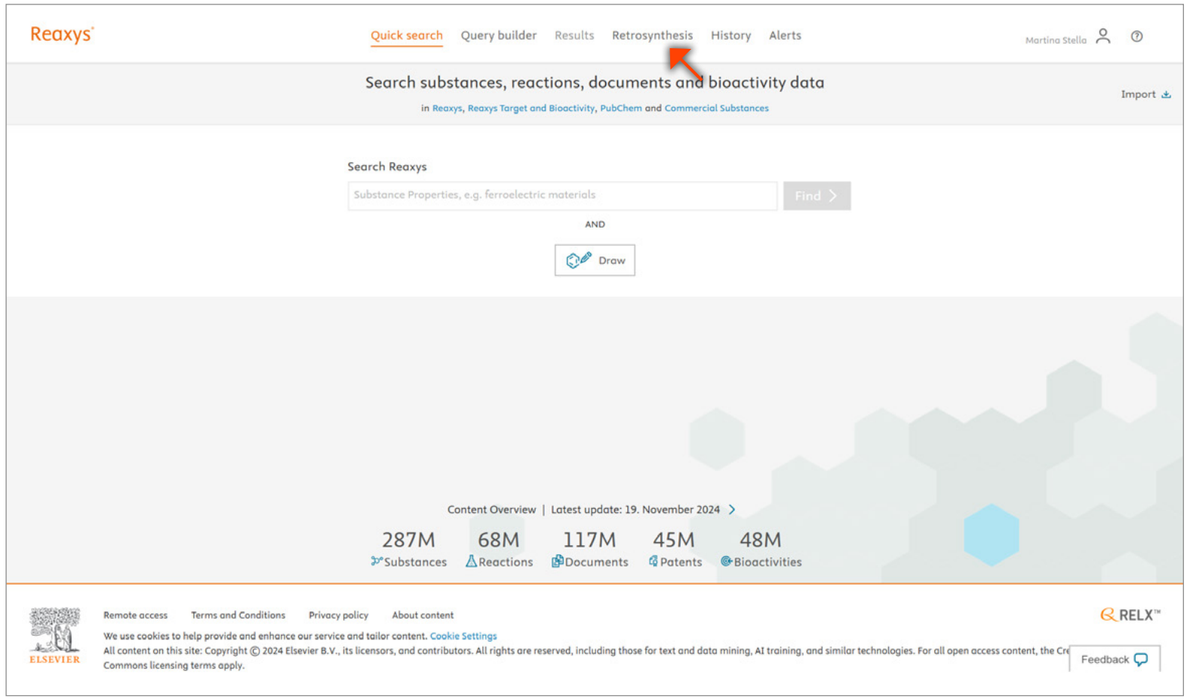
Robust routes
Synthetically robust routes are provided based on informed decisions from the literature

2. How-to guide

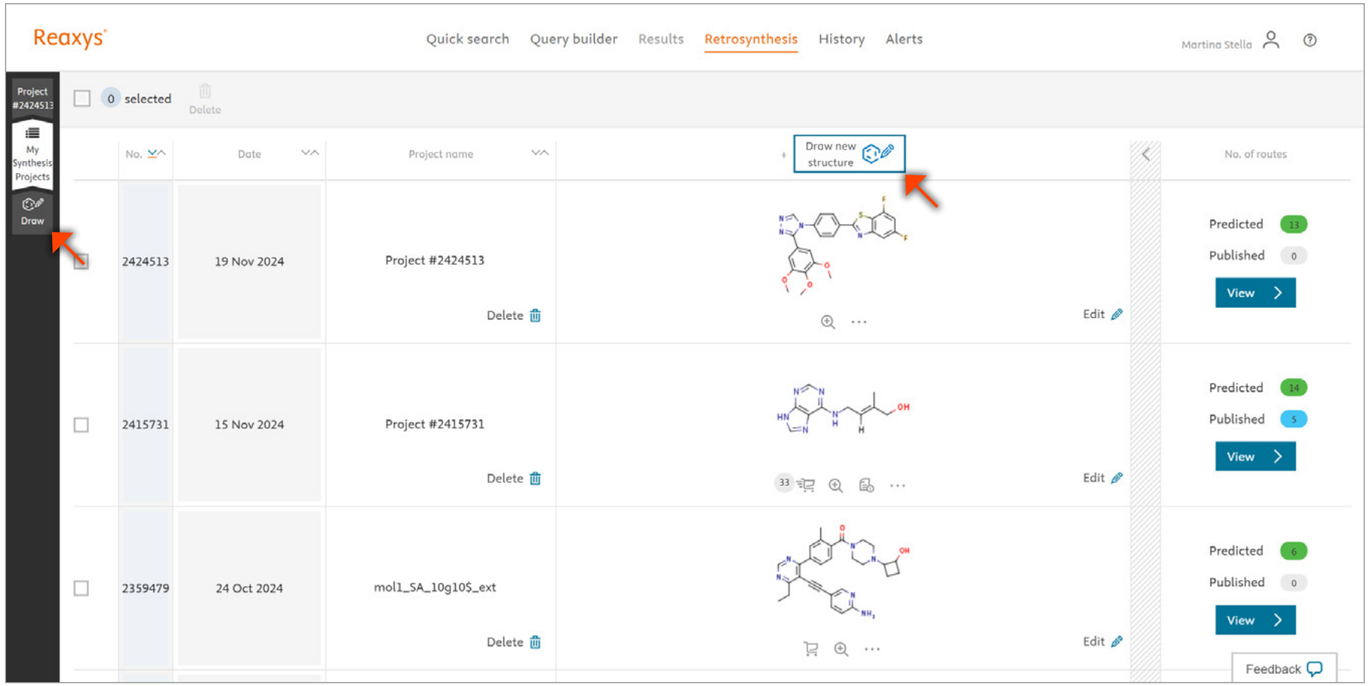
In this section you will find important tips and tricks to help you get started using Reaxys Predictive Retrosynthesis powered by Iktos.

2.1. Getting started

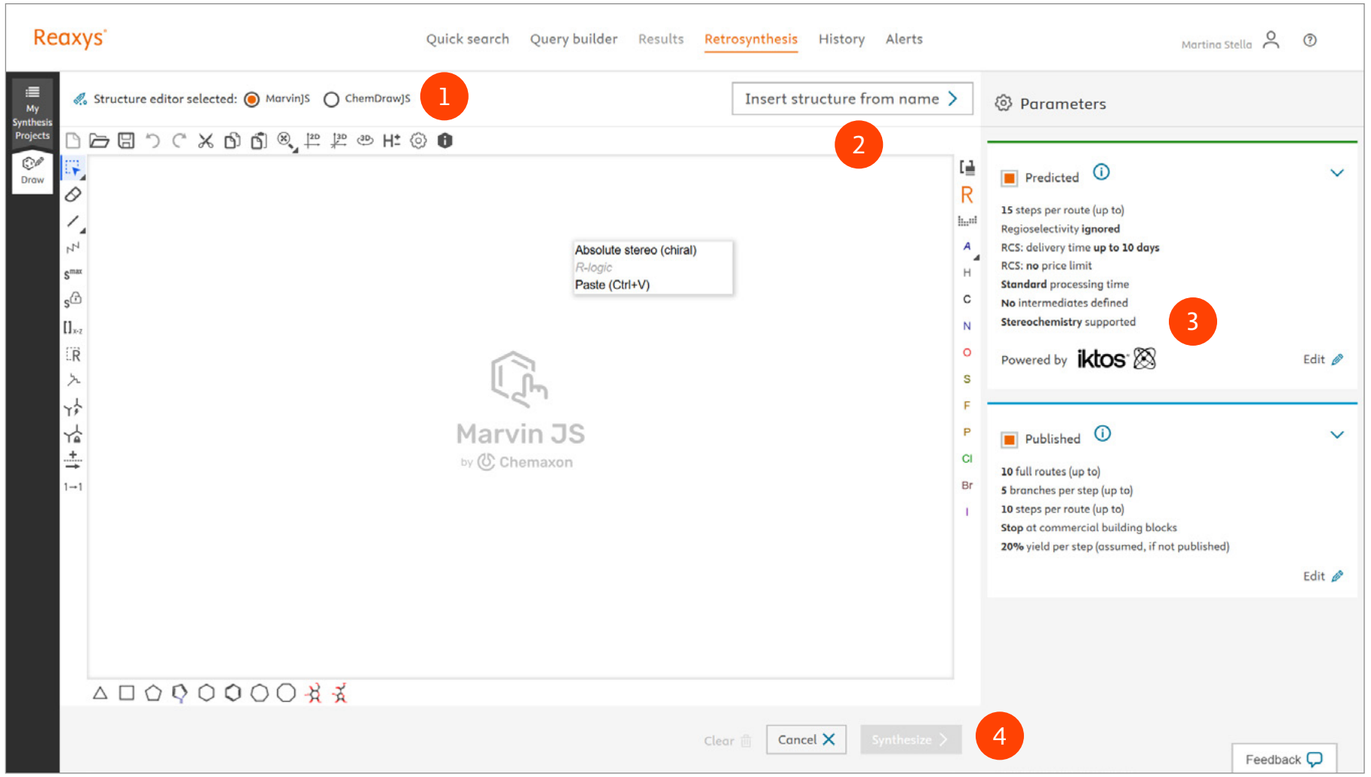
To use the predictive retrosynthesis module Iktos, you will need to login at Reaxys.com and click on *Retrosynthesis*.



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

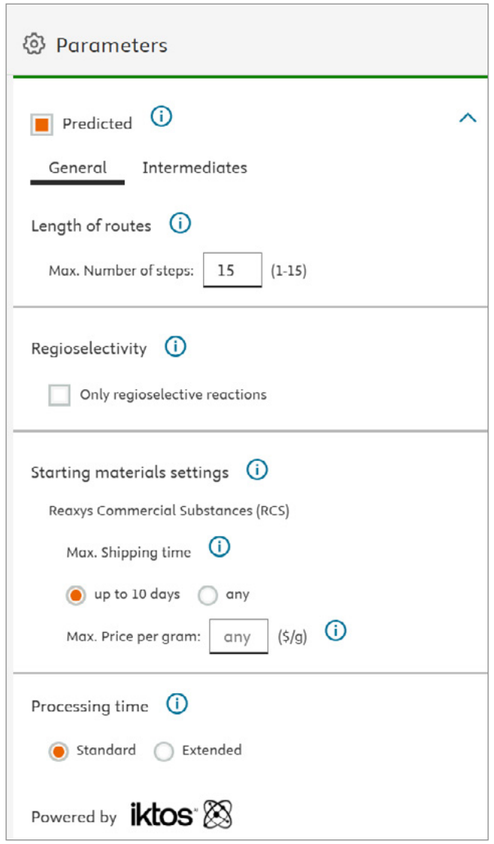


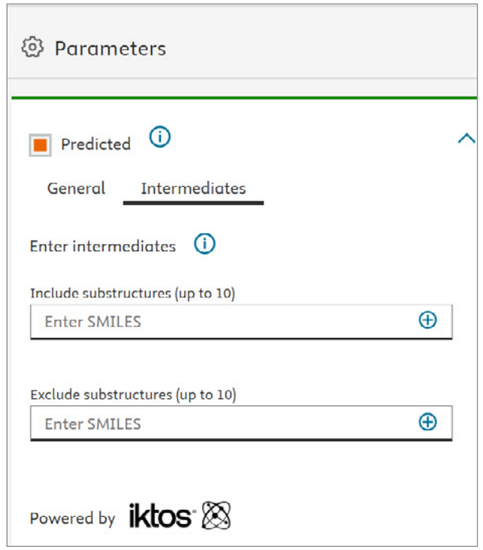
Once on the drawing page, there are several options to customize your plan.



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 it to your synthesis needs (see next image)
4. Once you are happy, click *Synthesize* to begin the project

iktos AI



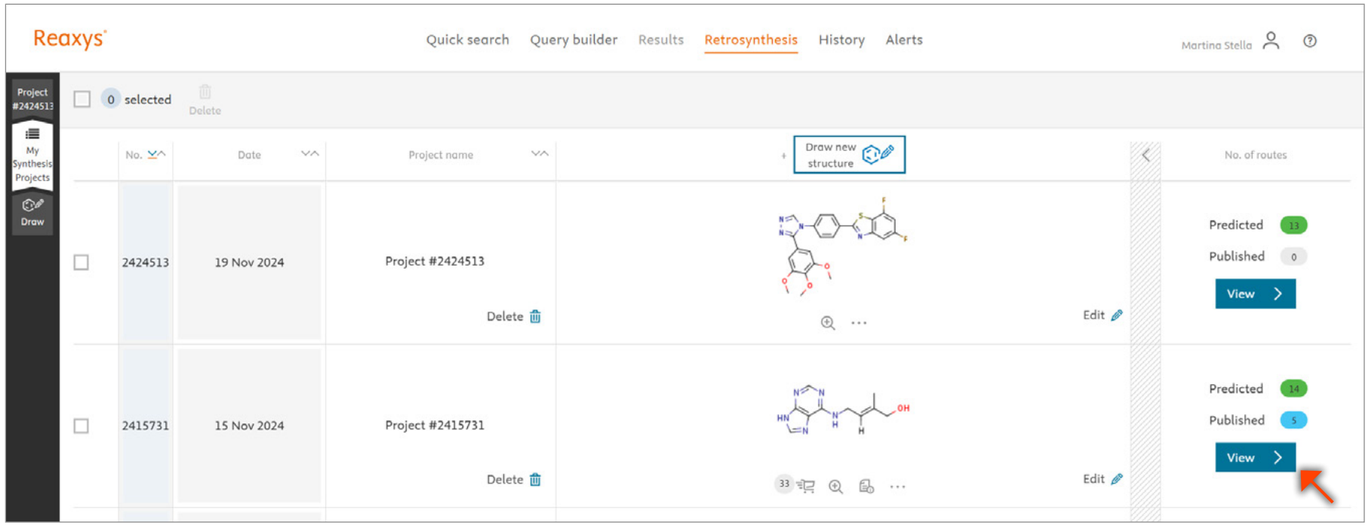


Selecting parameters

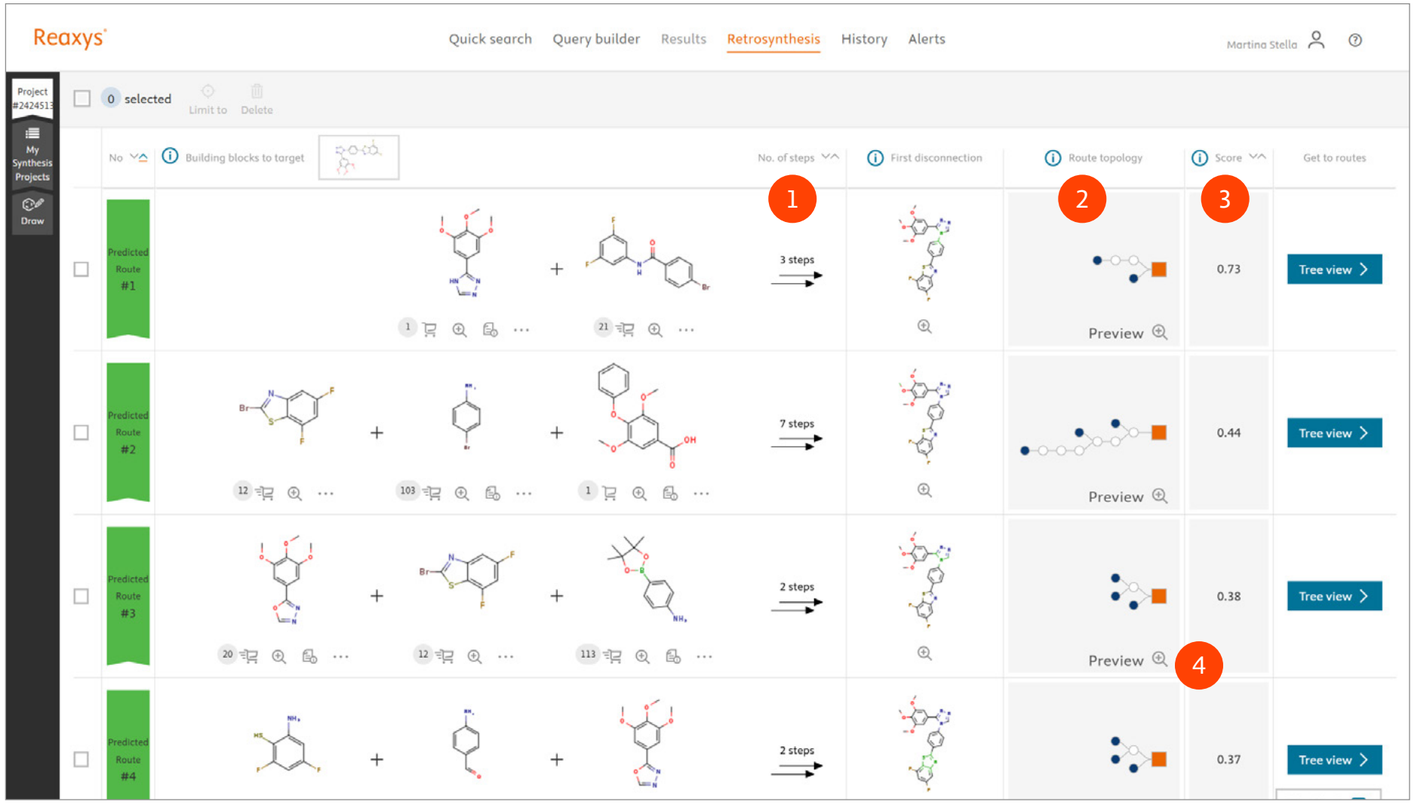
- Adjust length of routes
- Add/remove regioselectivity filter
- Adjust building blocks settings form Reaxys Commercial Substances
  - Select any delivery time to increase the pool size of building blocks or define max price per grom to limit the set
- Add/remove intermediate substructures
  - Utilize Smiles to define intermediates for the reactions
- Extend processing time to increase the number and diversity in the routes

2.2. View the results

Once you've clicked *Synthesize*, you will return to the project page. Since creation of published retrosynthesis routes is fast, published routes for 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.

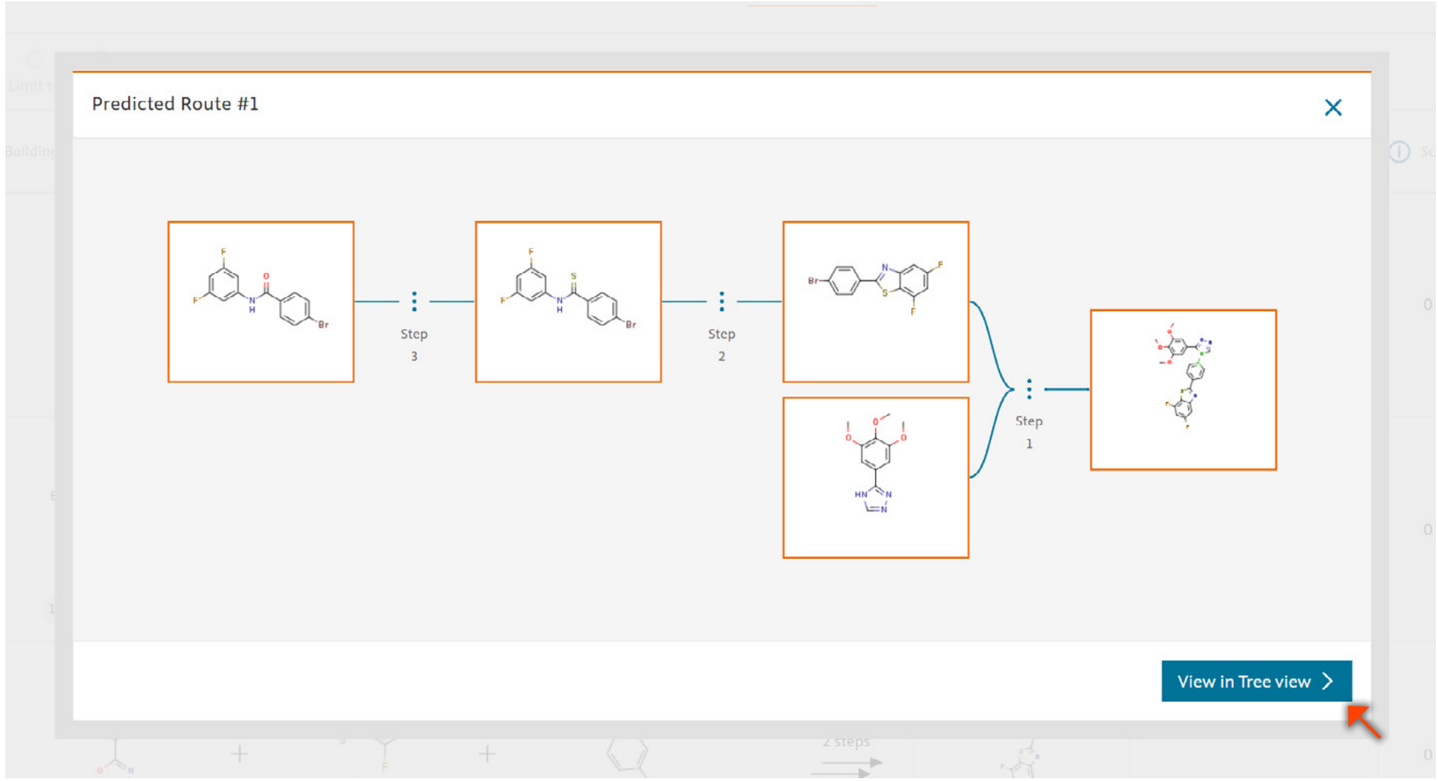


On the Routes Overview screen, it is easy to quickly analyze both published and predicted routes in one view

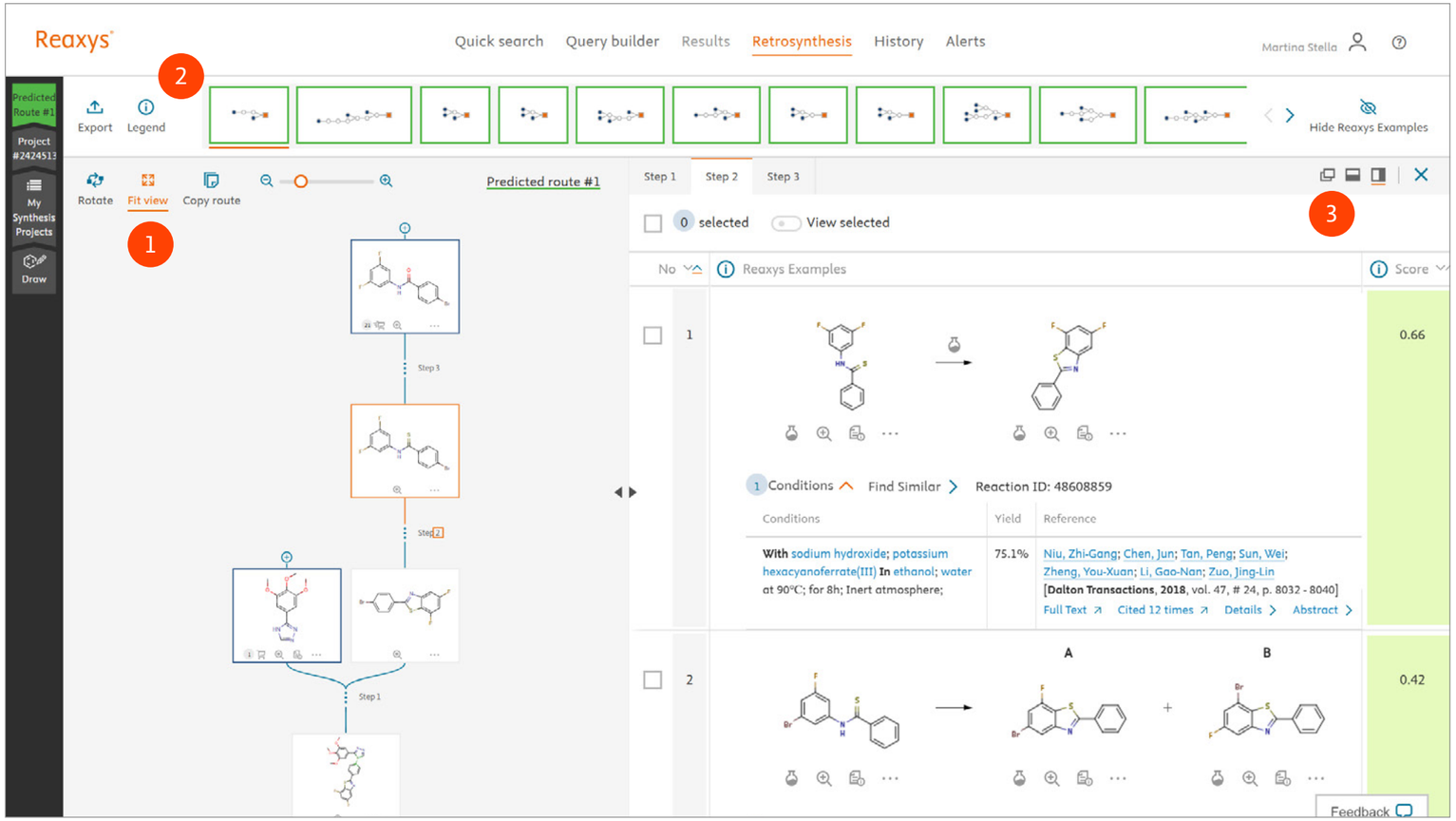


1. Clearly view the number of steps
2. Review the route topology to see how branched the routes are
3. The predicted routes are ranked by a synthetic accessibility score so you can analyze the best routes first
4. Click the preview of a given route to see a full view of the route, or click the nodes to see the structures involved in 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.

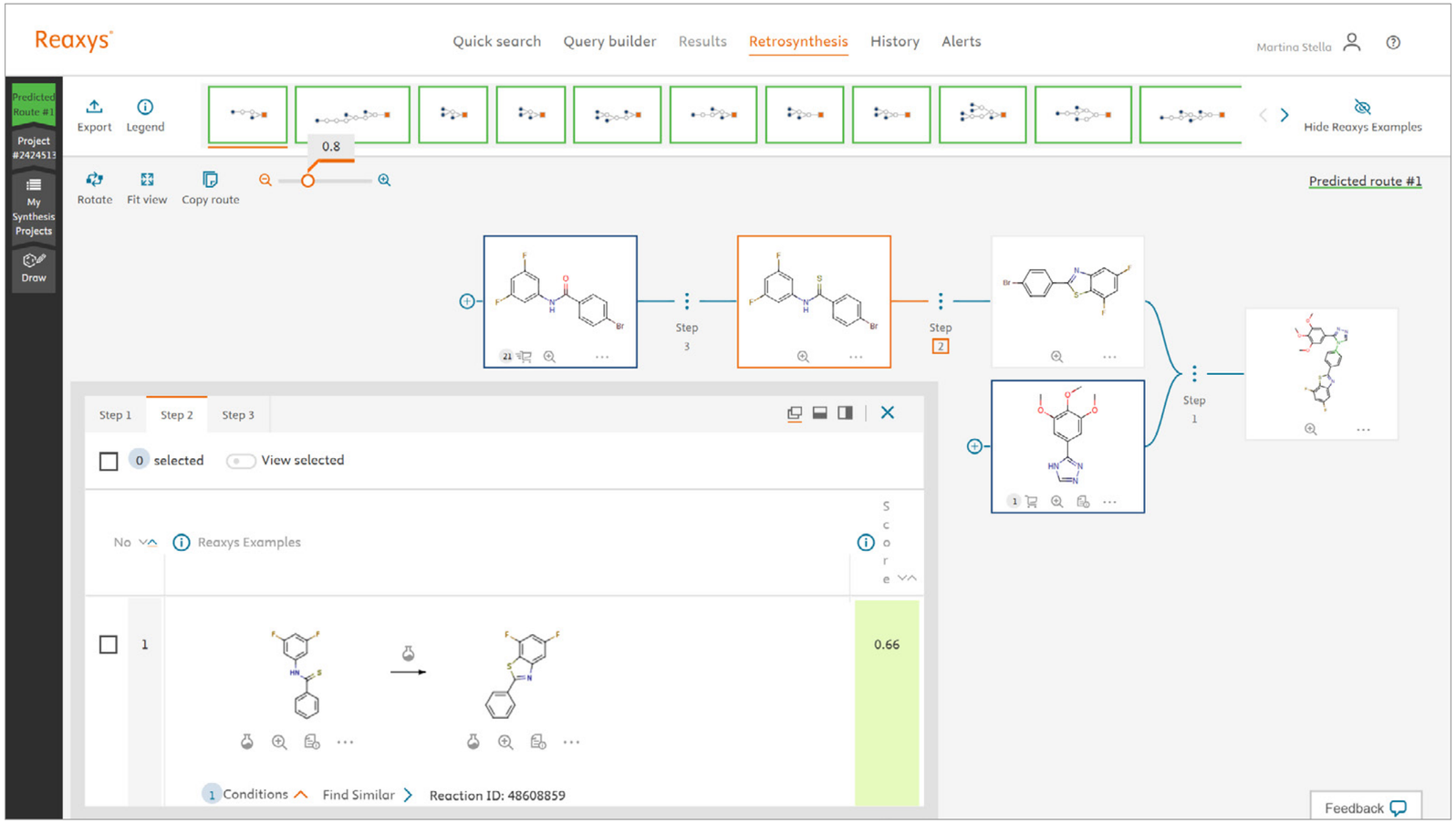


2.3. Analyzing the routes

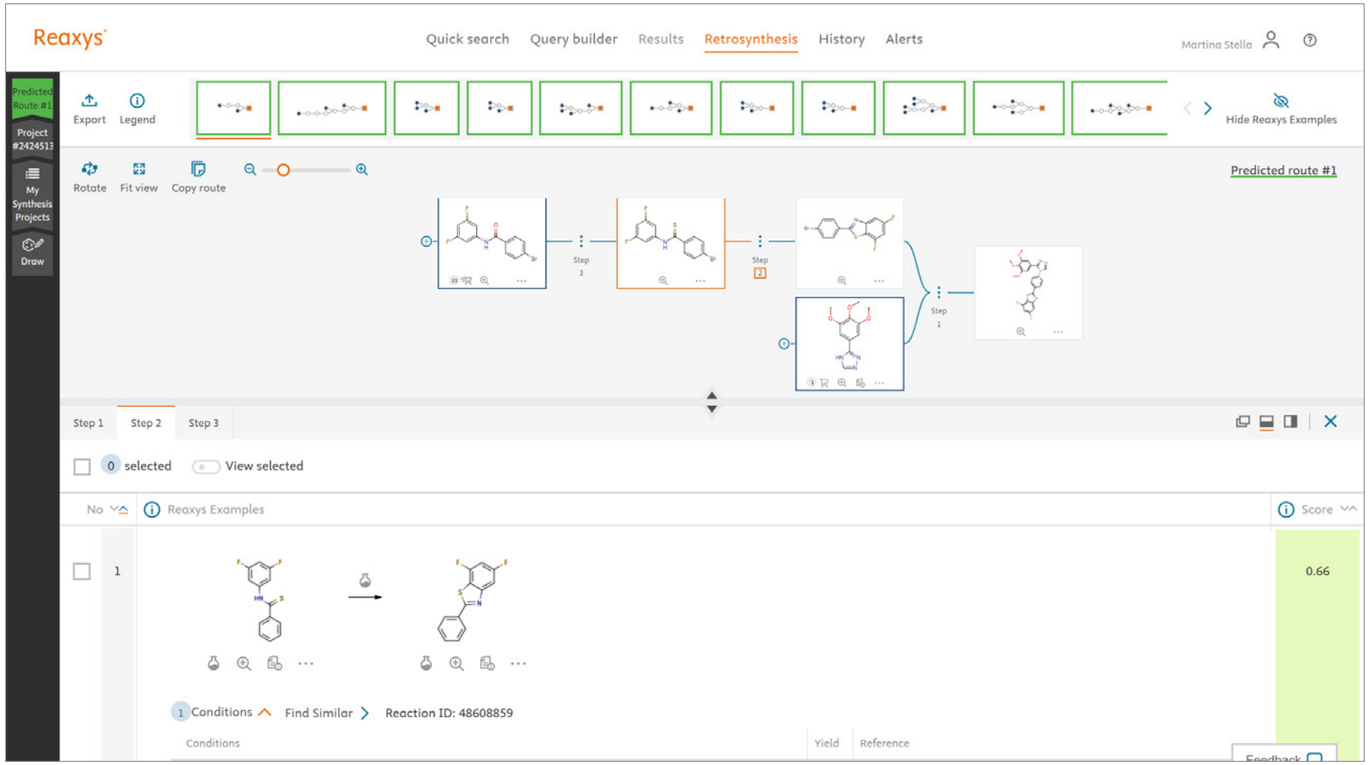


1. Use the rotate and zoom functions to make it easier to view what you need in one screen
2. The route topology previews allow you to easily switch between routes for quick comparisons
3. Alter how you view the literature that informed the routes to fit your preferences and see the screenshots below for the alternative views

Alternative view A

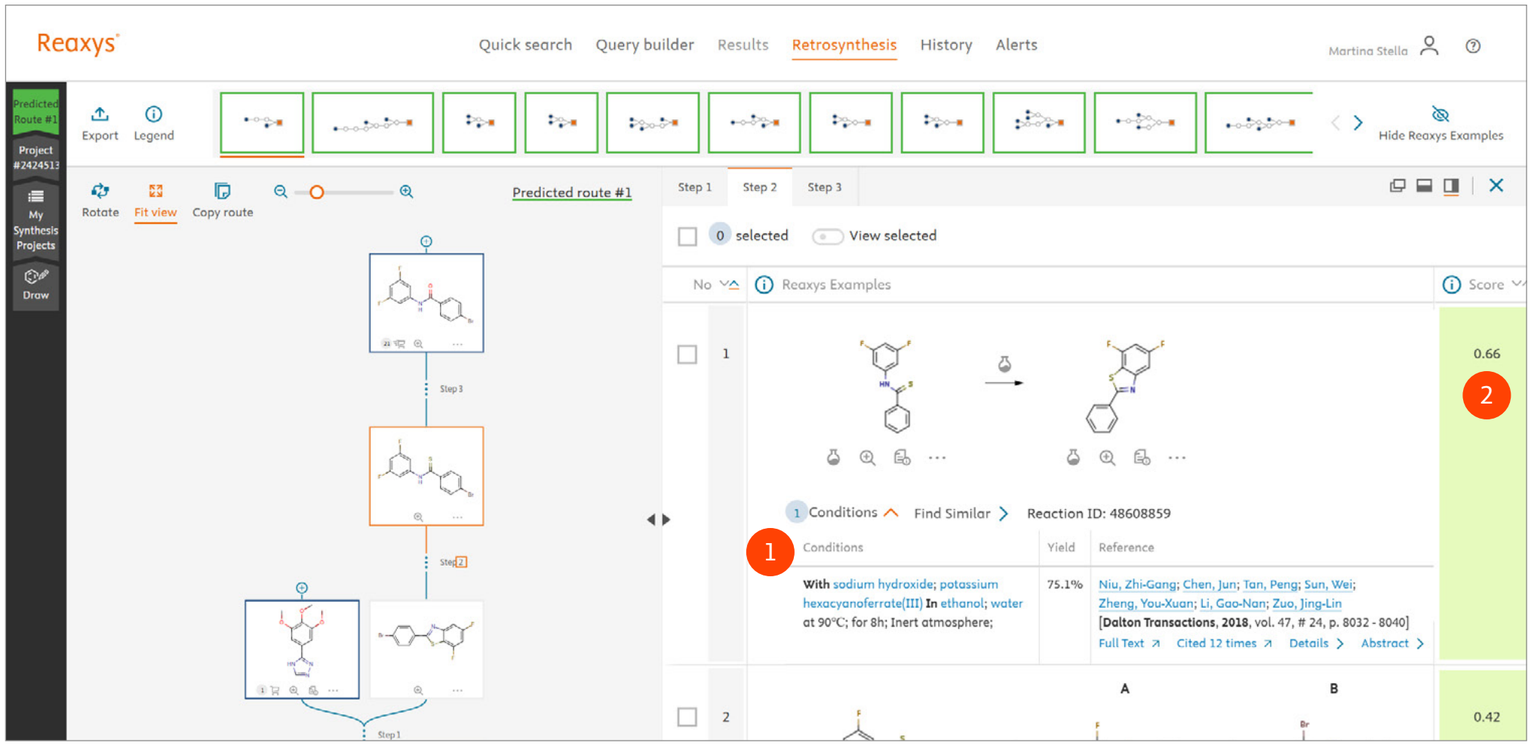


Alternative view B



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.

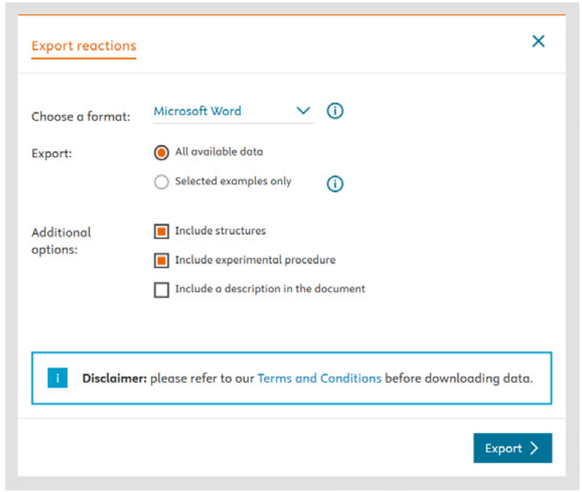


1. View the conditions and experimental procedures that informed the route
2. The similarity score prioritizes published reactions which are more similar to the predicted reaction for ease of reviewing

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.

You may also use the button *Copy route* to copy the entire route into the clipboard for pasting it into your preferred editor.



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