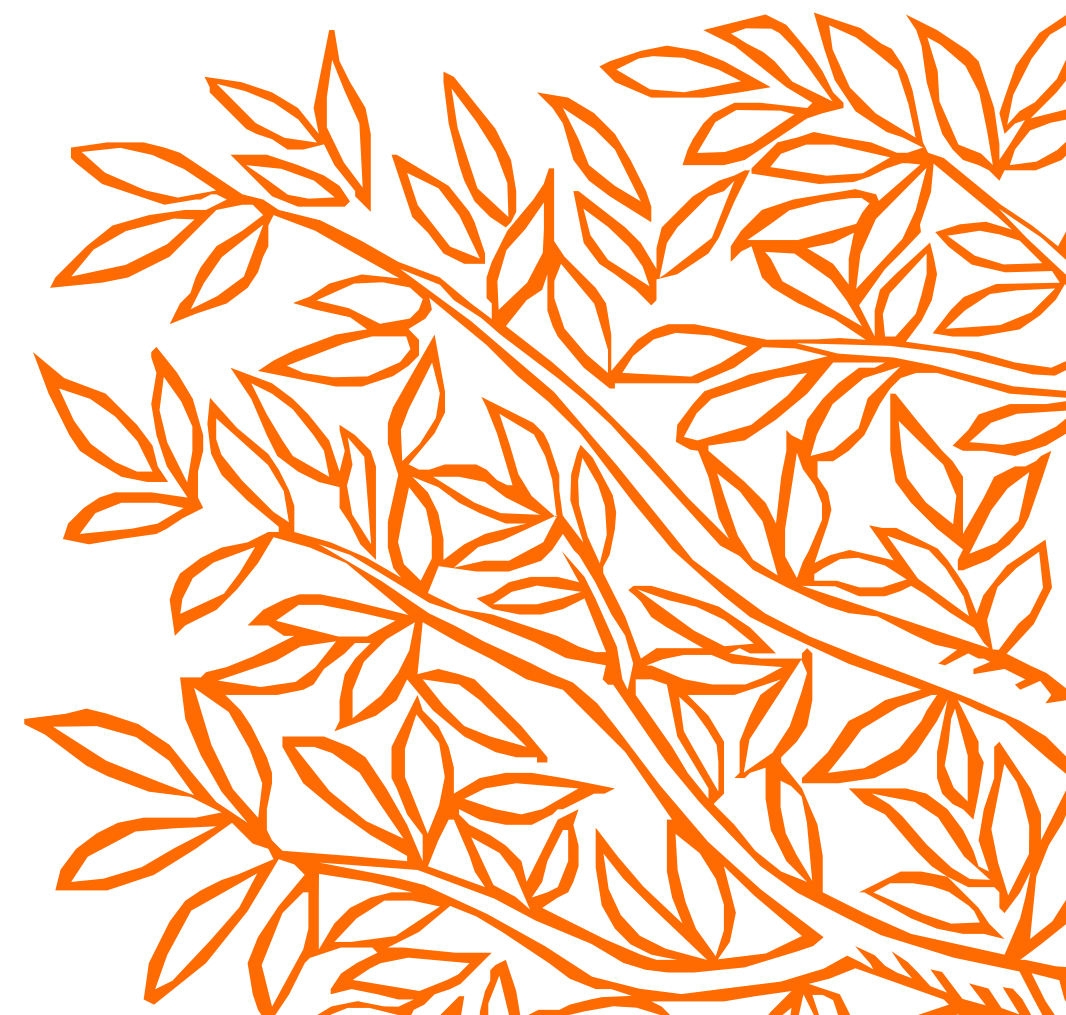




Reaxys®

Reaxys Predictive Retrosynthesis powered by Iktos

Quick Reference Guide



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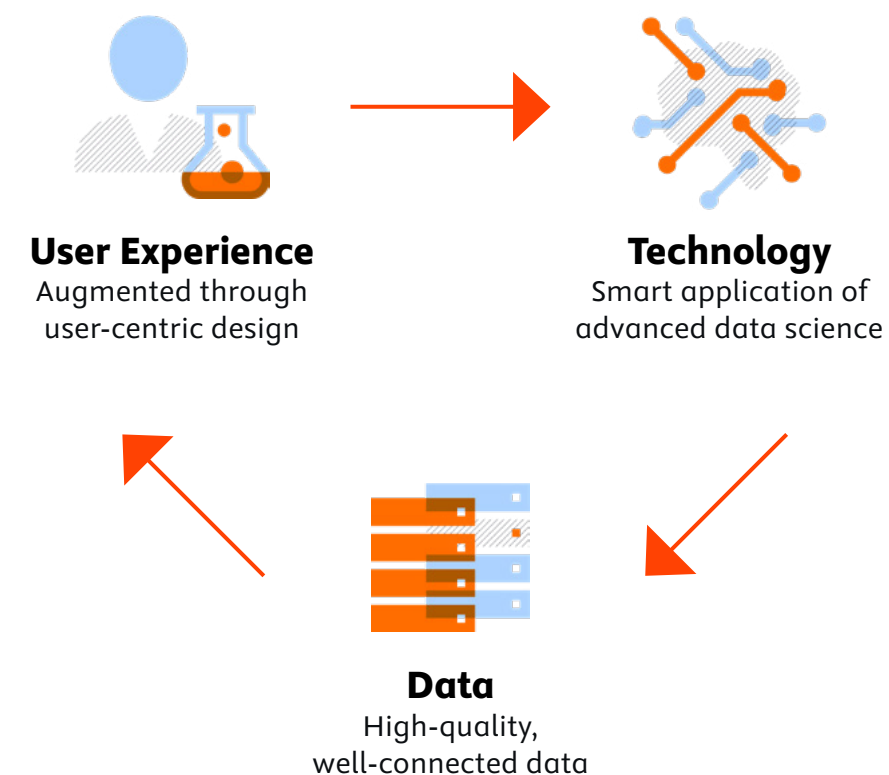
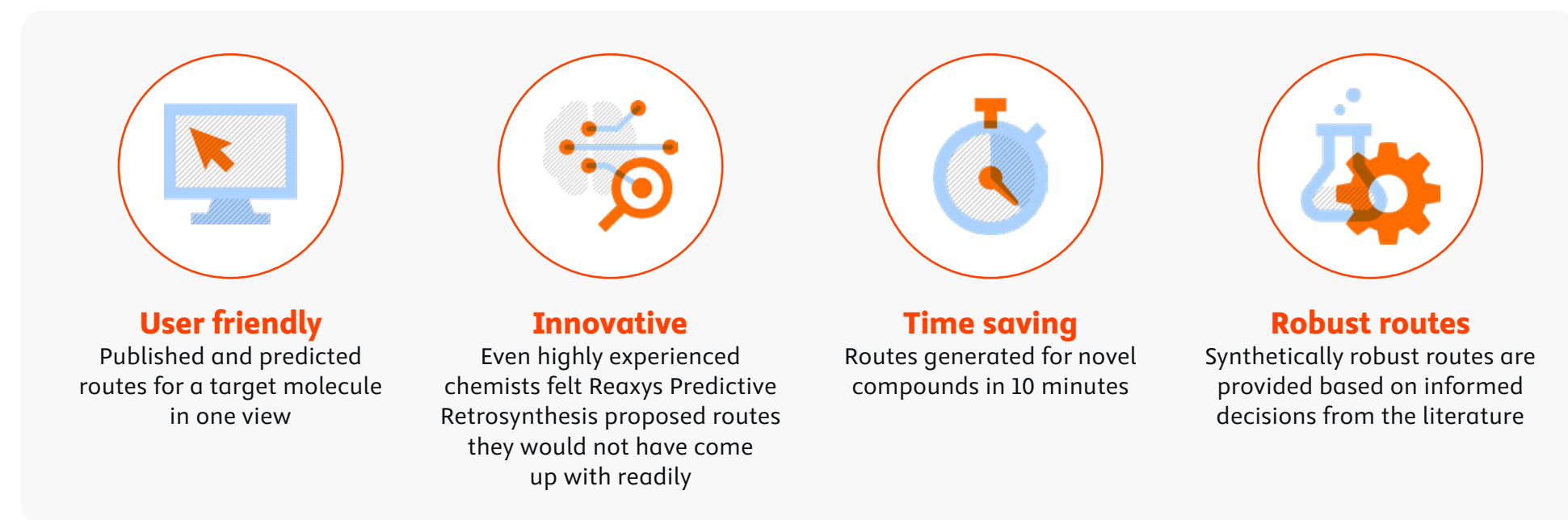
1. Introduction

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?



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](https://reaxys.com) and click on *Retrosynthesis*.

The screenshot displays the Reaxys website interface. At the top, the Reaxys logo is on the left, and navigation links (Quick search, Query builder, Results, Retrosynthesis, History, Alerts) are in the center. A red arrow points to the 'Retrosynthesis' link. On the right, the user 'Martina Stella' is logged in. Below the navigation bar is a search bar with the placeholder text 'Search substances, reactions, documents and bioactivity data'. Below the search bar is a 'Search Reaxys' section with a text input field containing 'Substance Properties, e.g. ferroelectric materials' and a 'Find >' button. Below the input field is an 'AND' button and a 'Draw' button. At the bottom, there is a 'Content Overview' section with a 'Latest update: 19. November 2024' link. Below this are five statistics: 287M Substances, 68M Reactions, 117M Documents, 45M Patents, and 48M Bioactivities. The footer contains the Elsevier logo, links for Remote access, Terms and Conditions, Privacy policy, and About content, a cookie notice, and a Feedback button.

Reaxys®

Quick search Query builder Results Retrosynthesis History Alerts

Martina Stella

Search substances, reactions, documents and bioactivity data

in Reaxys, Reaxys Target and Bioactivity, PubChem and Commercial Substances

Import

Search Reaxys

Substance Properties, e.g. ferroelectric materials Find >

AND

Draw

Content Overview | Latest update: 19. November 2024 >

287M 68M 117M 45M 48M

Substances Reactions Documents Patents Bioactivities

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RELX™

Feedback

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

Project #2424513 0 selected Delete

My Synthesis Projects Draw

No.	Date	Project name	Chemical structure	No. of routes
2424513	19 Nov 2024	Project #2424513 Delete	<div>Draw new structure</div> Edit	Predicted 13 Published 0 View
2415731	15 Nov 2024	Project #2415731 Delete	Edit	Predicted 14 Published 5 View
2359479	24 Oct 2024	mol1_SA_10g10\$_ext Delete	Edit	Predicted 6 Published 0 View Feedback

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

The screenshot shows the Reaxys Retrosynthesis interface. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. The interface is divided into three main sections:

- Left Panel (Callout 1):** Contains 'My Synthesis Projects' and a 'Draw' button. Below this is a vertical toolbar with various chemical drawing tools.
- Central Canvas (Callout 2):** The main workspace for drawing molecules. It features a 'Structure editor selected' dropdown with 'MarvinJS' and 'ChemDrawJS' options. A text box above the canvas says 'Insert structure from name >'. The canvas itself displays the 'Marvin JS by Chemaxon' logo and a context menu with options like 'Absolute stereo (chiral)', 'R-logic', and 'Paste (Ctrl+V)'.
- Right Panel (Callout 3):** Contains 'Parameters' for the retrosynthesis. It has two sections: 'Predicted' and 'Published'. The 'Predicted' section lists parameters like '15 steps per route (up to)', 'Regioselectivity ignored', 'RCS: delivery time up to 10 days', 'RCS: no price limit', 'Standard processing time', 'No intermediates defined', and 'Stereochemistry supported'. The 'Published' section lists '10 full routes (up to)', '5 branches per step (up to)', '10 steps per route (up to)', 'Stop at commercial building blocks', and '20% yield per step (assumed, if not published)'. Both sections have an 'Edit' button.

At the bottom of the interface, there are buttons for 'Clear', 'Cancel', 'Synthesize', and 'Feedback'.

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



Parameters

☒ Predicted ⓘ

General

Intermediates

Length of routes ⓘ

Max. Number of steps: (1-15)

Regioselectivity ⓘ

☐ Only regioselective reactions

Starting materials settings ⓘ

Reaxys Commercial Substances (RCS)

Max. Shipping time ⓘ

☒ up to 10 days
 ☐ any

Max. Price per gram: (\$/g) ⓘ

Processing time ⓘ

☒ Standard
 ☐ Extended

Powered by **iktos**

Parameters

☒ Predicted ⓘ

General

Intermediates

Enter intermediates ⓘ

Include substructures (up to 10)

ⓘ

Exclude substructures (up to 10)

ⓘ

Powered by **iktos**

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 gram 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.

The screenshot displays the Reaxys interface for the Retrosynthesis section. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. On the left, a sidebar shows 'Project #2424513', 'My Synthesis Projects', and a 'Draw' button. The main area features a table of projects:

No.	Date	Project name	Chemical Structure	No. of routes
2424513	19 Nov 2024	Project #2424513		Predicted: 13 Published: 0 View >
2415731	15 Nov 2024	Project #2415731		Predicted: 14 Published: 5 View >

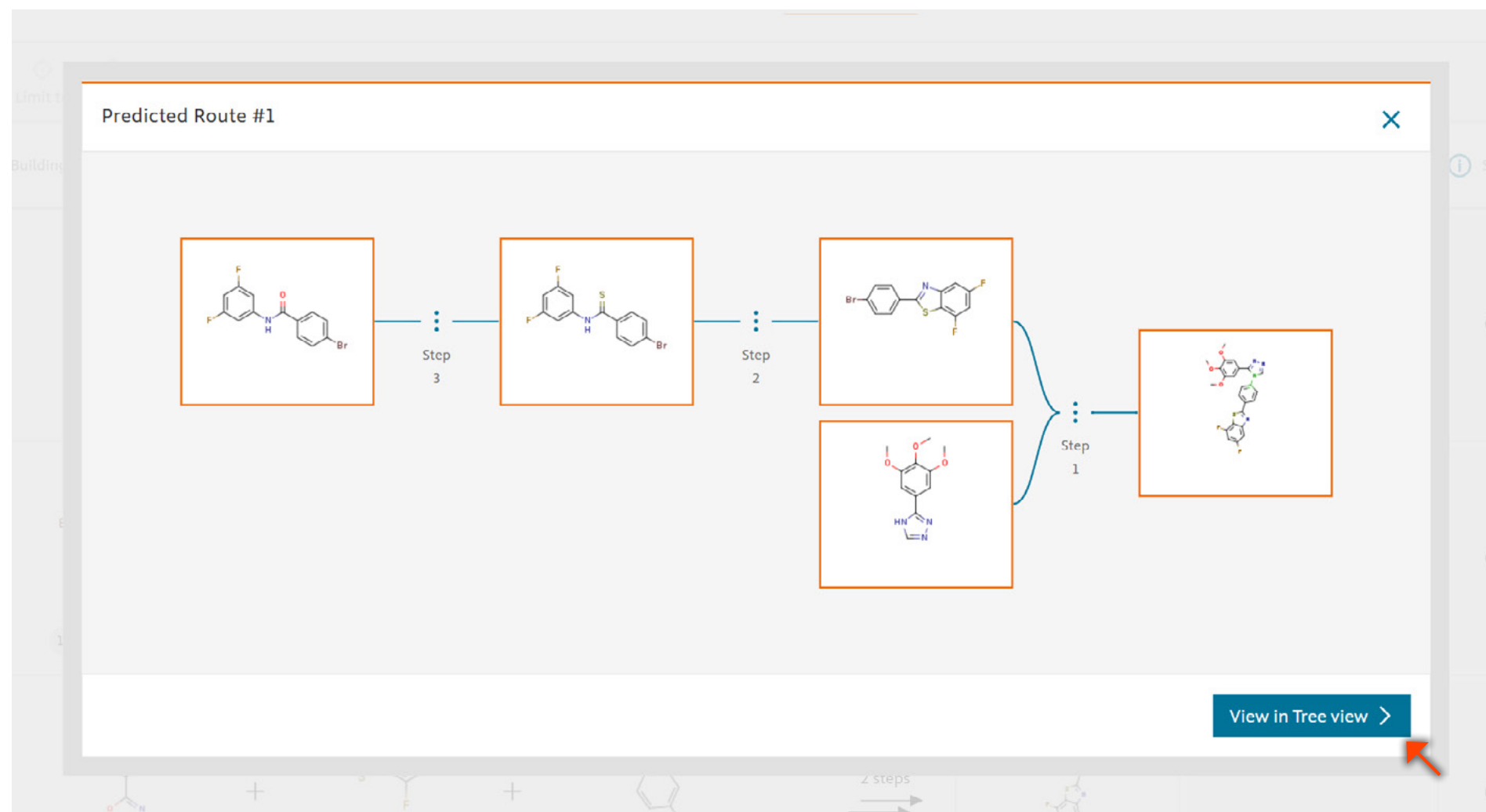
A red arrow points to the 'View >' button for Project #2415731.

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

	No. of steps	First disconnection	Route topology	Score	Get to routes
Predicted Route #1	3 steps			0.73	Tree view >
Predicted Route #2	7 steps			0.44	Tree view >
Predicted Route #3	2 steps			0.38	Tree view >
Predicted Route #4	2 steps			0.37	Tree 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

The screenshot displays the Reaxys Retrosynthesis interface. On the left, a vertical sidebar contains navigation options: 'Project #2424513', 'My Synthesis Projects', and 'Draw'. The main workspace is divided into several sections. At the top, a horizontal toolbar includes 'Export', 'Legend', and a series of icons for manipulating the route. Below this, a 'Predicted route #1' is shown, consisting of three steps (Step 1, Step 2, Step 3) connected by arrows. The first step is highlighted with a red box and a red circle labeled '1'. The second step is highlighted with a red box and a red circle labeled '2'. The third step is highlighted with a red box and a red circle labeled '3'. To the right of the route, a table lists reaction examples. The first example (Reaction ID: 48608859) shows a reaction with a score of 0.66. The second example shows a reaction with a score of 0.42. The table includes columns for 'Conditions', 'Yield', and 'Reference'. The 'Conditions' column for the first reaction reads: 'With sodium hydroxide; potassium hexacyanoferrate(III) In ethanol; water at 90°C; for 8h; Inert atmosphere;'. The 'Yield' column for the first reaction reads: '75.1%'. The 'Reference' column for the first reaction reads: 'Niu, Zhi-Gang; Chen, Jun; Tan, Peng; Sun, Wei; Zheng, You-Xuan; Li, Gao-Nan; Zuo, Jing-Lin [Dalton Transactions, 2018, vol. 47, # 24, p. 8032 - 8040]'. The 'Reference' column for the second reaction reads: 'A B'. The 'Score' column for the first reaction reads: '0.66'. The 'Score' column for the second reaction reads: '0.42'. A 'Feedback' button is located at the bottom right of the table.

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

Reaxys

Quick search Query builder Results **Retrosynthesis** History Alerts

Martina Stella

Predicted Route #1

Export Legend

Rotate Fit view Copy route

My Synthesis Projects Draw

0.8

Predicted route #1

Step 1 Step 2 Step 3

0 selected View selected

No	Reaxys Examples	Score
1		0.66

Conditions Find Similar Reaction ID: 48608859

Feedback

Alternative view B

Reaxys®

[Quick search](#)
[Query builder](#)
[Results](#)
[Retrosynthesis](#)
[History](#)
[Alerts](#)

Martina Stella

Predicted Route #1

Project #2424513

My Synthesis Projects

Draw

Export

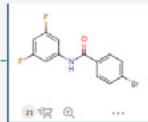
Legend

Rotate

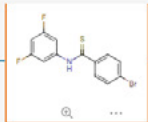
Fit view

Copy route


Step 3

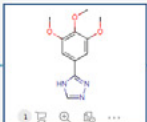


Step 2

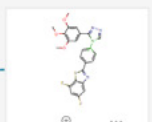


Step 1





Step 1



Step 1

Step 2

Step 3


0 selected

View selected

No

Reaxys Examples

1



1

Conditions

Find Similar

Reaction ID: 48608859

Yield

Reference

Score

0.66

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 contains navigation options: 'Predicted Route #1', 'Project #2424513', 'My Synthesis Projects', and 'Draw'. The main workspace shows a 'Predicted route #1' with three steps. Step 1 is highlighted, showing a reaction between a substituted benzene derivative and a thiazole derivative. To the right, a table lists 'Reaxys Examples' of similar reactions. The first example (ID: 48608859) has a score of 0.66 and is highlighted with a red circle '2'. The second example has a score of 0.42. A red circle '1' highlights the 'Conditions' column header in the table.

No	Reaxys Examples	Score						
1	<p>1 Conditions Find Similar > Reaction ID: 48608859</p> <table border="1"> <thead> <tr> <th>Conditions</th> <th>Yield</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>With sodium hydroxide; potassium hexacyanoferrate(III) In ethanol; water at 90°C; for 8h; Inert atmosphere;</td> <td>75.1%</td> <td>Niu, Zhi-Gang; Chen, Jun; Tan, Peng; Sun, Wei; Zheng, You-Xuan; Li, Gao-Nan; Zuo, Jing-Lin [Dalton Transactions, 2018, vol. 47, # 24, p. 8032 - 8040] Full Text Cited 12 times Details Abstract ></td> </tr> </tbody> </table>	Conditions	Yield	Reference	With sodium hydroxide; potassium hexacyanoferrate(III) In ethanol; water at 90°C; for 8h; Inert atmosphere;	75.1%	Niu, Zhi-Gang; Chen, Jun; Tan, Peng; Sun, Wei; Zheng, You-Xuan; Li, Gao-Nan; Zuo, Jing-Lin [Dalton Transactions, 2018, vol. 47, # 24, p. 8032 - 8040] Full Text Cited 12 times Details Abstract >	0.66
Conditions	Yield	Reference						
With sodium hydroxide; potassium hexacyanoferrate(III) In ethanol; water at 90°C; for 8h; Inert atmosphere;	75.1%	Niu, Zhi-Gang; Chen, Jun; Tan, Peng; Sun, Wei; Zheng, You-Xuan; Li, Gao-Nan; Zuo, Jing-Lin [Dalton Transactions, 2018, vol. 47, # 24, p. 8032 - 8040] Full Text Cited 12 times Details Abstract >						
2	<p>A B</p>	0.42						

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.

Export reactions [X]

Choose a format: **Microsoft Word** [v] [i]

Export: ☒ All available data ☐ Selected examples only [i]

Additional options: ☒ Include structures ☒ Include experimental procedure ☐ Include a description in the document

[i] **Disclaimer:** please refer to our [Terms and Conditions](#) before downloading data.

Export >



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