



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?



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



User Experience

Augmented through user-centric design



Technology

Smart application of advanced data science



Data

High-quality, well-connected data



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.

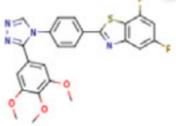
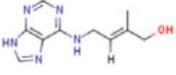
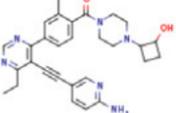
2.1. Getting started

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

The screenshot displays the Reaxys website interface. At the top left is the Reaxys logo. The navigation menu includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. A red arrow points to the 'Retrosynthesis' menu item. The user profile 'Martina Stella' is visible in the top right. Below the navigation is a search bar with the text 'Search substances, reactions, documents and bioactivity data' and an 'Import' button. The main search area contains a search input field with the text 'Substance Properties, e.g. ferroelectric materials' and a 'Find >' button. Below the search input is an 'AND' button and a 'Draw' button with a chemical structure icon. At the bottom of the page, there is a 'Content Overview' section with the latest update date '19. November 2024'. Below this are five data points: '287M Substances', '68M Reactions', '117M Documents', '45M Patents', and '48M Bioactivities'. The footer includes the Elsevier logo, 'Remote access', 'Terms and Conditions', 'Privacy policy', 'About content', 'RELX™' logo, and a 'Feedback' button.

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

The screenshot displays the Reaxys Retrosynthesis interface. At the top, there is a navigation bar with 'Quick search', 'Query builder', 'Results', 'Retrosynthesis' (highlighted), 'History', and 'Alerts'. The user 'Martina Stella' is logged in. On the left, a sidebar contains 'My Synthesis Projects' and a 'Draw' button, both highlighted with orange arrows. The main area shows a table of projects with columns for 'No.', 'Date', 'Project name', 'Chemical structure', and 'No. of routes'. The first row is selected and highlighted in blue. A 'Draw new structure' button is overlaid on the first row's structure column, also highlighted with an orange arrow. The table contains three rows of project data, each with a chemical structure, a 'Delete' button, and an 'Edit' button. The right side of the interface shows statistics for the selected project: 'Predicted' (13) and 'Published' (0) routes, with a 'View' button. A 'Feedback' button is located at the bottom right.

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 >
2359479	24 Oct 2024	mol1_SA_10g10S_ext		Predicted: 6 Published: 0 View >

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

The screenshot shows the Reaxys Retrosynthesis interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis (selected), History, and Alerts. The user's name, Martina Stella, is visible in the top right. On the left, there is a sidebar with 'My Synthesis Projects' and a 'Draw' button. The main workspace is labeled 'Structure editor selected: MarvinJS ChemDrawJS' with a red circle '1' next to the MarvinJS radio button. Below this is a toolbar with various drawing tools. The central canvas displays the 'Marvin JS by Chemaxon' logo and a context menu with options: 'Absolute stereo (chiral)', 'R-logic', and 'Paste (Ctrl+V)'. A red circle '2' is placed over the 'Insert structure from name >' input field. On the right, the 'Parameters' panel is open, showing two sections: 'Predicted' and 'Published'. The 'Predicted' section includes 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'. A red circle '3' is placed over the 'Stereochemistry supported' parameter. The 'Published' section includes '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)'. At the bottom of the interface, there are buttons for 'Clear', 'Cancel', 'Synthesize', and 'Feedback'. A red circle '4' is placed over the 'Synthesize' button.

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

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Parameters

Predicted ⓘ

General Intermediates

Enter intermediates ⓘ

Include substructures (up to 10)

ⓘ

Exclude substructures (up to 10)

ⓘ

Powered by **iktos**

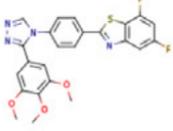
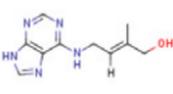
Selecting parameters

- 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 Retrosynthesis interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Retrosynthesis (active), History, and Alerts. The user's name, Martina Stella, is visible in the top right. Below the navigation, there is a header for the project list: Project #2424513, 0 selected, and a Delete button. The main table lists two projects:

No.	Date	Project name	Chemical structure	No. of routes
2424513	19 Nov 2024	Project #2424513		Predicted: 33 Published: 0 View >
2415731	15 Nov 2024	Project #2415731		Predicted: 14 Published: 5 View >

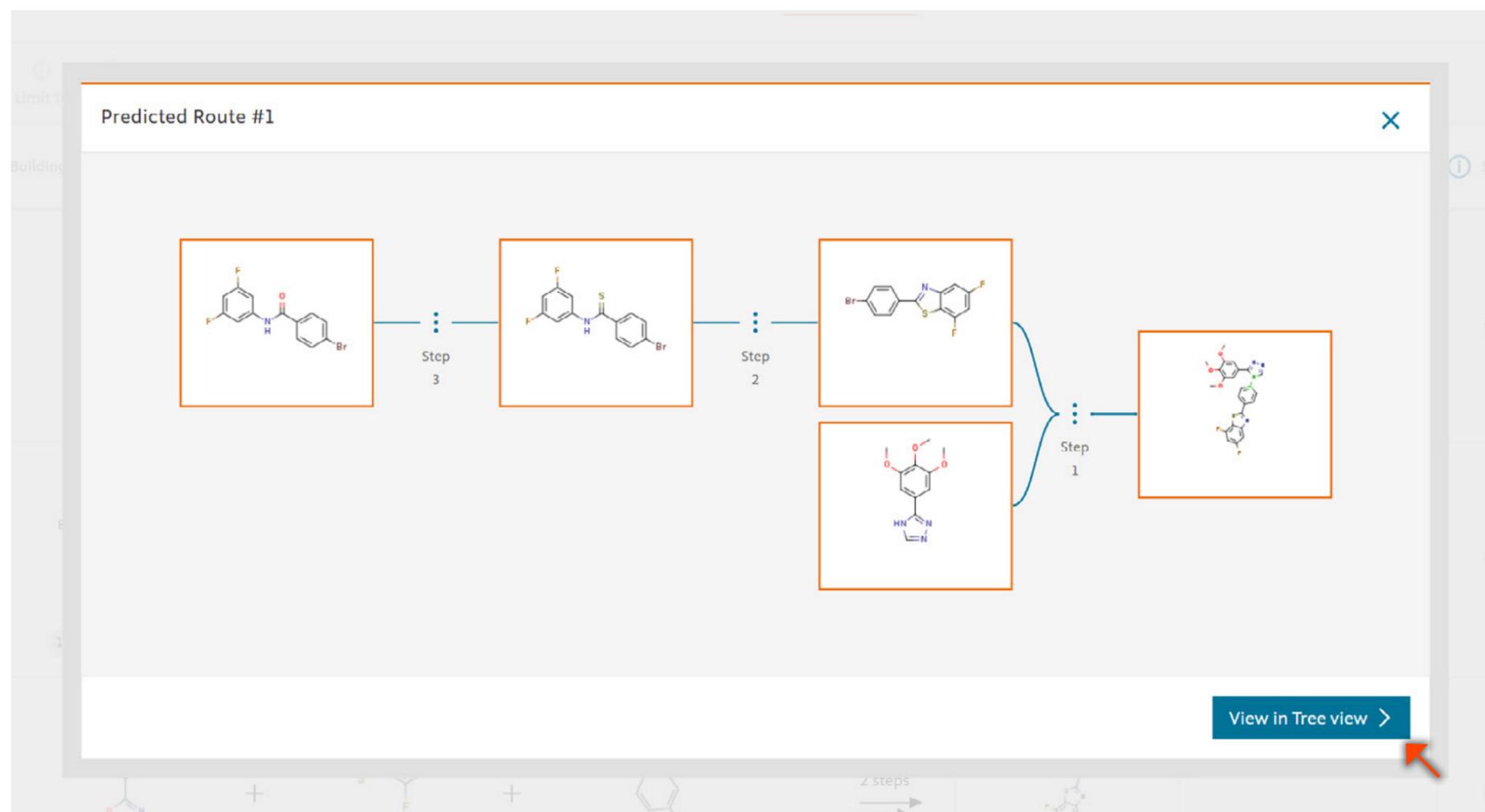
The interface also includes a sidebar on the left with 'My Synthesis Projects' and 'Draw' options, and a 'Draw new structure' button above the table. A red arrow points to the 'View >' button for the second project.

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

	Building blocks to target	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 like 'Export', 'Legend', 'Rotate', 'Fit view', and 'Copy route'. The main workspace shows a 'Predicted route #1' with three steps. A red circle '1' highlights the 'Fit view' button. A red circle '2' highlights a row of route topology preview thumbnails. A red circle '3' highlights the 'View selected' button in the reaction list.

The reaction list on the right shows two examples:

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
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2		0.42						

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

Export Legend 0.8 Hide Reaxys Examples

Rotate Fit view Copy route **Predicted route #1**

Step 1 Step 2 Step 3

0 selected View selected

No Reaxys Examples

Score	Reaction	Score
1		0.66

1 Conditions Find Similar Reaction ID: 48608859

Feedback

Alternative view B

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

Project #2424513 Predicted Route #1

Export Legend

Rotate Fit view Copy route

Hide Reaxys Examples

Predicted route #1

Step 1 Step 2 Step 3

0 selected View selected

No Reaxys Examples

	Score
<p>1</p> <p>1 Conditions Find Similar Reaction ID: 48608859</p> <p>Conditions Yield Reference</p>	0.66

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 'Predicted Route #1' and 'Project #2424513'. The main workspace is divided into three steps: Step 1, Step 2, and Step 3. A table on the right lists similar reactions with their conditions, yields, and references. The first reaction (ID: 48608859) is highlighted with a red circle '2' next to its score of 0.66. A red circle '1' is placed over the 'Conditions' column of the first row.

No.	Reaxys Examples	Score
1	<p>1 Conditions Find Similar Reaction ID: 48608859</p> <p>Conditions: With sodium hydroxide; potassium hexacyanoferrate(III) in ethanol; water at 90°C; for 8h; Inert atmosphere;</p> <p>Yield: 75.1%</p> <p>Reference: 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</p>	0.66
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 [i]
 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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