

# Optimize synthesis planning

Reaxys Predictive Retrosynthesis, *powered by Iktos*, combines AI with high-quality reaction data to deliver more efficient synthesis routes quickly.

Monte Carlo tree search and forward synthesis prediction combine to generate diverse and robust retrosynthetic routes, considering chemo-, regio- and stereo-selectivity.

## Tailor searches to project needs

- Dynamic price control on starting materials
- Shipping time filter
- Include and/or exclude intermediates
- Break or protect bonds



**16.3M**

chemical reactions



**453K**

retrosynthetic rules



**<10**

minutes  
to get results



**150M**

commercially  
available materials



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# Explore the intuitive interface of Reaxys Predictive Retrosynthesis

The screenshot displays the Reaxys Predictive Retrosynthesis interface. On the left, a vertical sidebar contains navigation options like 'Project 271745', 'My synthesis projects', and 'Browse'. The main workspace shows a 'Predicted route #15' with three steps. Step 1 is highlighted with a red box and a '2' callout. Step 2 is highlighted with a red box and a '5' callout. Step 3 is highlighted with a red box and a '1' callout. A top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Retrosynthesis', 'History', and 'Alerts'. A toolbar at the top left has 'Export' (6) and 'Legend' (4) buttons. On the right, a detailed view of a reaction is shown, including 'Reaxys Examples', 'Conditions', 'Yield', and 'Reference' (1). The 'Reference' section contains the text: 'Current Patent Assignee: BRISTOL MYERS SQUIBB - US2016/115126, 2016, A1 Location in patent: Paragraph 0302-0303 Full Text Details Abstract'. Below this, the 'Intermediate 2C: 4-Bromo-5-fluoro-2,3-dimethyl-1H-indole-7-carboxylic acid' is detailed with its experimental procedure and mass spectrum data. A 'Feedback' button is located at the bottom right of the interface.

## Scientifically robust predictions

- 1 Link to literature that informed the routes
- 2 End in purchasable starting materials
- 3 Access experimental procedures to execute plans

## Intuitive experience

- 4 Published, predicted and custom routes in one view
- 5 Tailor results by editing synthesis routes
- 6 Export easily to collaborate on route design

## Customizable

- Integrate reaction data
- Select preferred vendors
- Integrate starting materials

## More routes, faster with API

Reaxys Predictive Retrosynthesis offers an API to process more molecules, faster.

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