

Reaxys®

# Predictive Retrosynthesis

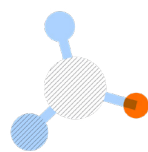
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Synthetic planning AI technology able to rapidly generate diverse and robust retrosynthetic routes while considering **chemo-, regio- and stereo-selectivity**.



## Ideate quickly

Get results in **less than 10 minutes**, including literature references and experimental procedures.



## Control selectivity

**Chemo-selectivity:** Protection/deprotection strategies taken into account by design.

**Regio-selectivity filter:** avoid routes which contain reaction steps with uncertain regioselectivity.

**Stereo-selectivity:** supported by chiral pool approach.



ELSEVIER

No.	Building blocks to target	No. of steps	First disconnection	Route topology	Score	Get to routes
1		1 step			0.63	<a href="#">See view</a>
2		2 steps			0.62	<a href="#">See view</a>
3		3 steps			0.61	<a href="#">See view</a>
4		4 steps			0.61	<a href="#">See view</a>

Enter intermediates ⓘ

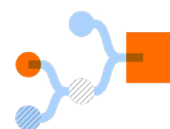
Include substructures (up to 10)

Enter SMILES

Exclude substructures (up to 10)

Enter SMILES

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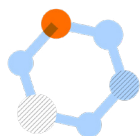
## Tailor searches to project needs

Use **dynamic price control** on starting materials and shipping time filter.

Set **route length**, define **bonds to break** and **intermediates** to be included and/or excluded.

The superior **technology developed by Iktos** is trained on the largest reaction dataset available for modelling applications. Access it via **Reaxys' user-friendly interface** or API.

## What is the technology used?



A **template-based neural network** approach predicts reaction steps for a target molecule and ranks them based on feasibility, novelty and diversity.



A **forward reaction algorithm** estimates the validity of the disconnections, excluding invalid reactions based on literature precedents.



**Protection and deprotection strategies** enable **chemo-selectivity**.

A **neural network** predicts the most probable regioisomer. Users can filter out routes that might have **regio-selectivity** issues.



**Monte Carlo Tree Search (MCTS)** algorithm quickly propagates retrosynthesis routes back to commercially available compounds. **Stereocenters** are taken from chiral building blocks applying chiral pool approach.



A **proprietary scoring function** is used to reward the MCTS algorithm to search novel and diverse routes, and to rank the final selected routes.

16.8 million

unique chemical  
reactions

100 million

commercially  
available materials

425,000

retrosynthetic rules

<10 minutes

to get results



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