Reaxys®

Predictive Retrosynthesis

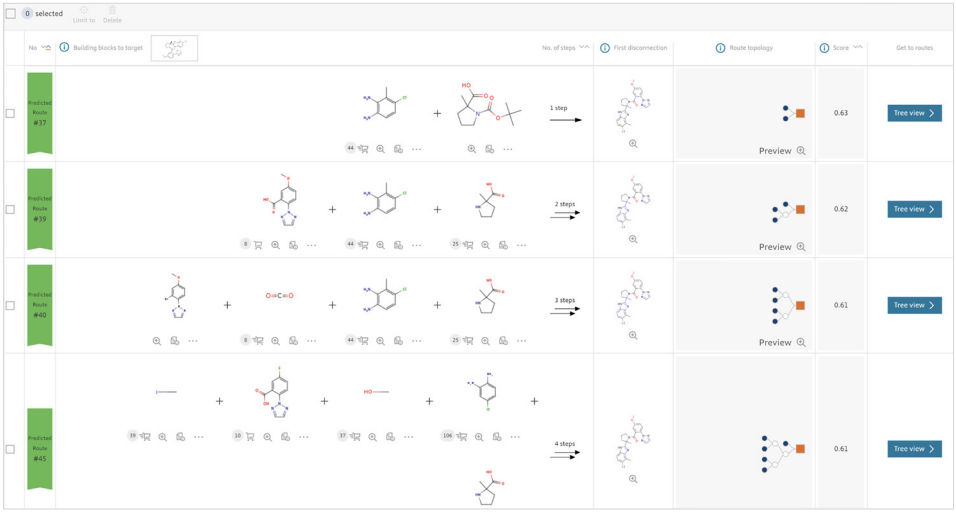
Powered by

iktos AI

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.

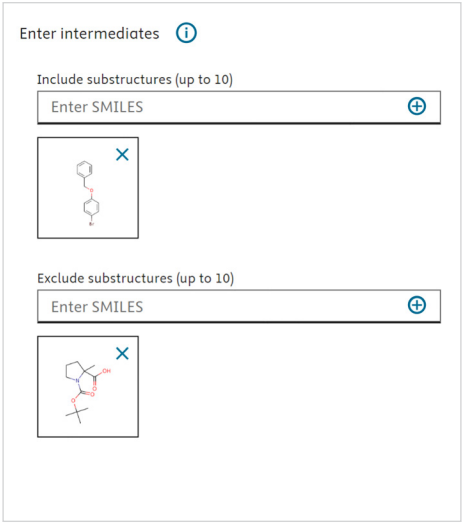


Control selectivity

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.



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.

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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	100 million	425,000	<10 minutes
unique chemical reactions	commercially available materials	retrosynthetic rules	to get results

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