



Superior technology

- 3 neural networks
- Monte Carlo tree search
- Results in 10 minutes



Unmatched data set

- >15M single step reactions
- >100M virtual negative reactions
- >400k auto-extracted rules



Customizable

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

The screenshot displays the Reaxys Predictive Retrosynthesis interface. On the left, a reaction tree shows the synthesis of a target molecule through three steps (Step 1, Step 2, Step 3), with confidence scores of 0.99. Numbered callouts 1 through 6 highlight specific features: 1 points to a reaction step in the tree, 2 points to a starting material, 3 points to a reaction condition, 4 points to a search filter, 5 points to a reaction step, and 6 points to a navigation menu. On the right, a detailed view of a reaction step is shown, including the reaction scheme, conditions, and a reference to a scientific paper.



Scientifically robust predictions

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



Intuitive experience

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

