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Reaxys®

Reaxys in practice

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Reaxys Content development

1817: First edition of Gmelin Handbook

1881: First edition of Beilstein Handbook

1989: Beilstein and Gmelin database go online

1992: CrossFire launched

2009: Reaxys launched

2013/2014: Complete overhaul of Reaxys and content expansion including RMC

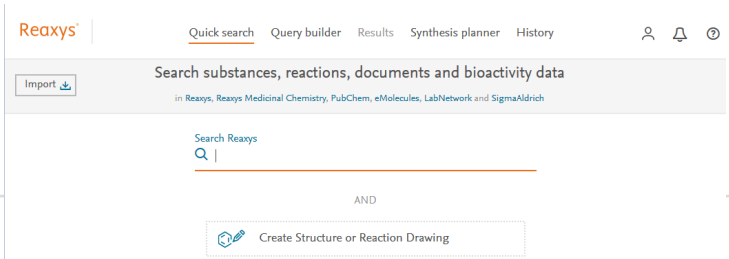
2016: New Reaxys launched

2017: New Reaxys Medicinal Chemistry (RMC) module

2020: Reaxys Commercial Substances

2021: Patent Expansion to 100+ PO's

2021: Predictive Retrosynthesis (AI based Synthesis prediction}



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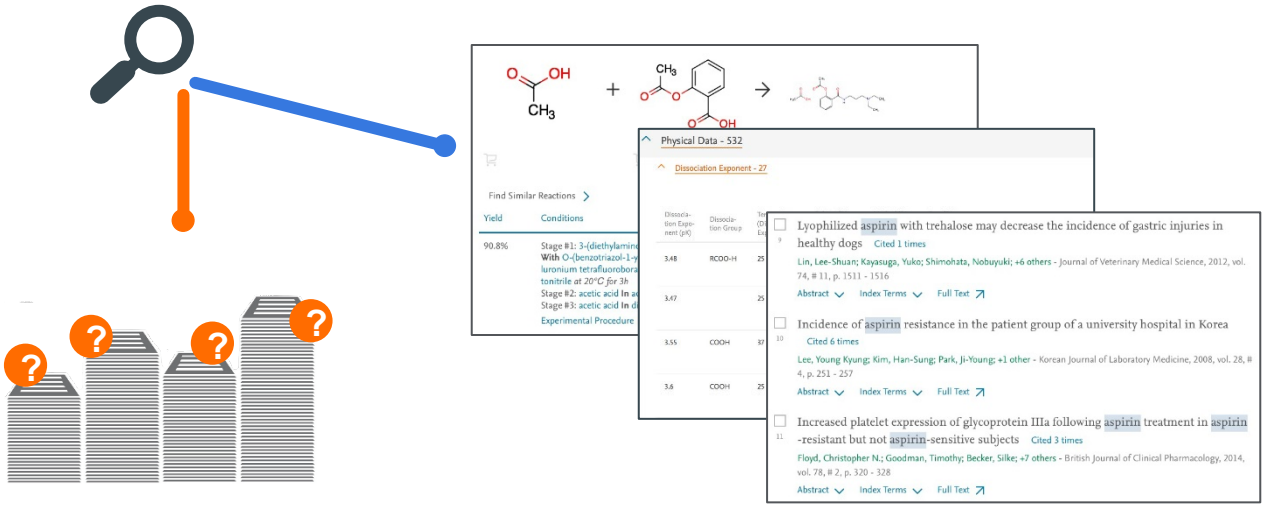
The core of our philosophy: Reaxys aims to deliver immediate access to information



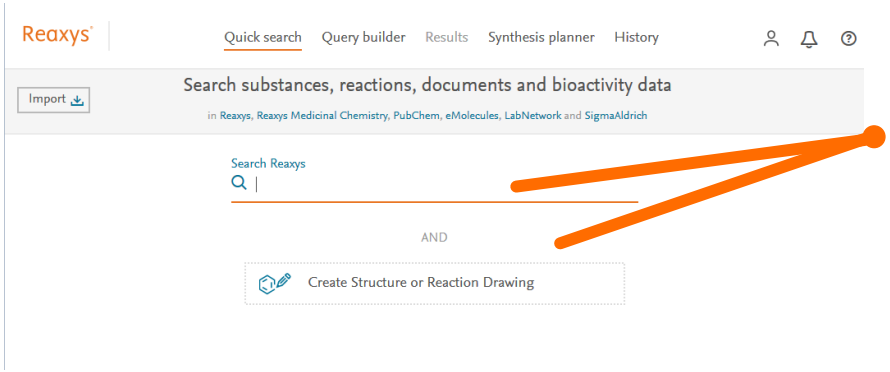
Instead of **delivering lists of references** that may be relevant to a query…

… Reaxys strives to **deliver relevant answers on the spot:**

- References ranked by relevance
- Reactions with experimental details
- Substances with extensive properties

Focus on **using** information, not searching for information

Using a clean and streamlined user interface



The vast majority of scientists perform text or structure searches and prefer the intuitive, simple and familiar.

So, Reaxys places powerful text and structure searches front and center on a single, easy-to-use interface.

Everyone can leverage the full capabilities of Reaxys, from first-year students to expert users

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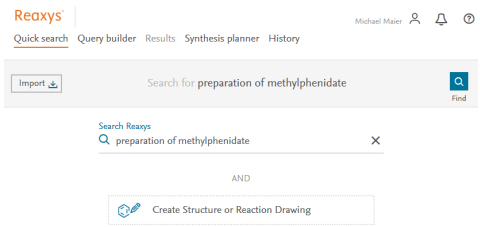
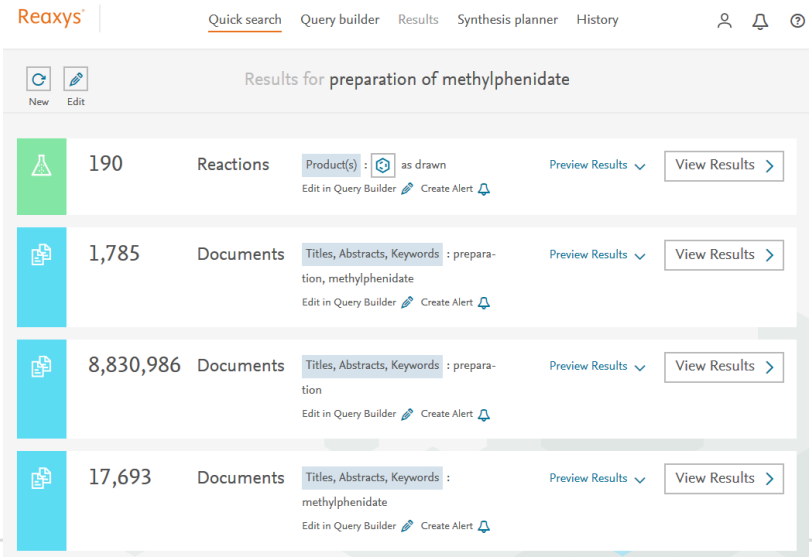
Retrieving relevant answers and anticipating needs – providing options



1 Reaxys interprets either natural language, or truncation and operators

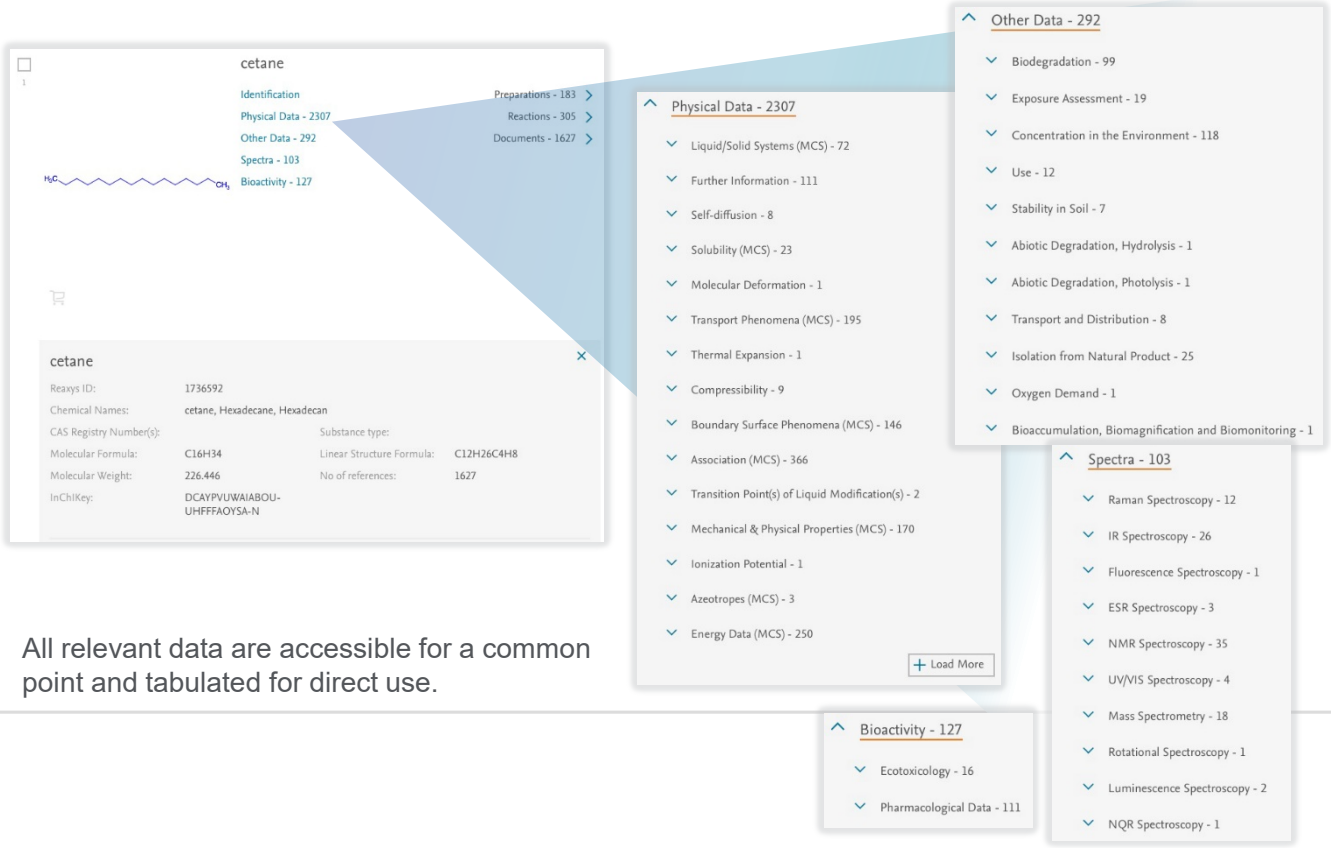
2 Reaxys recognizes search intention (reactions)

3 Reaxyx delivers a ranked list of alternative results suggestions



Get intended answers directly, plus relevant results you may not have considered

Presenting standardized, normalized and collated data in one record for quick and easy access



All relevant data are accessible for a common point and tabulated for direct use.

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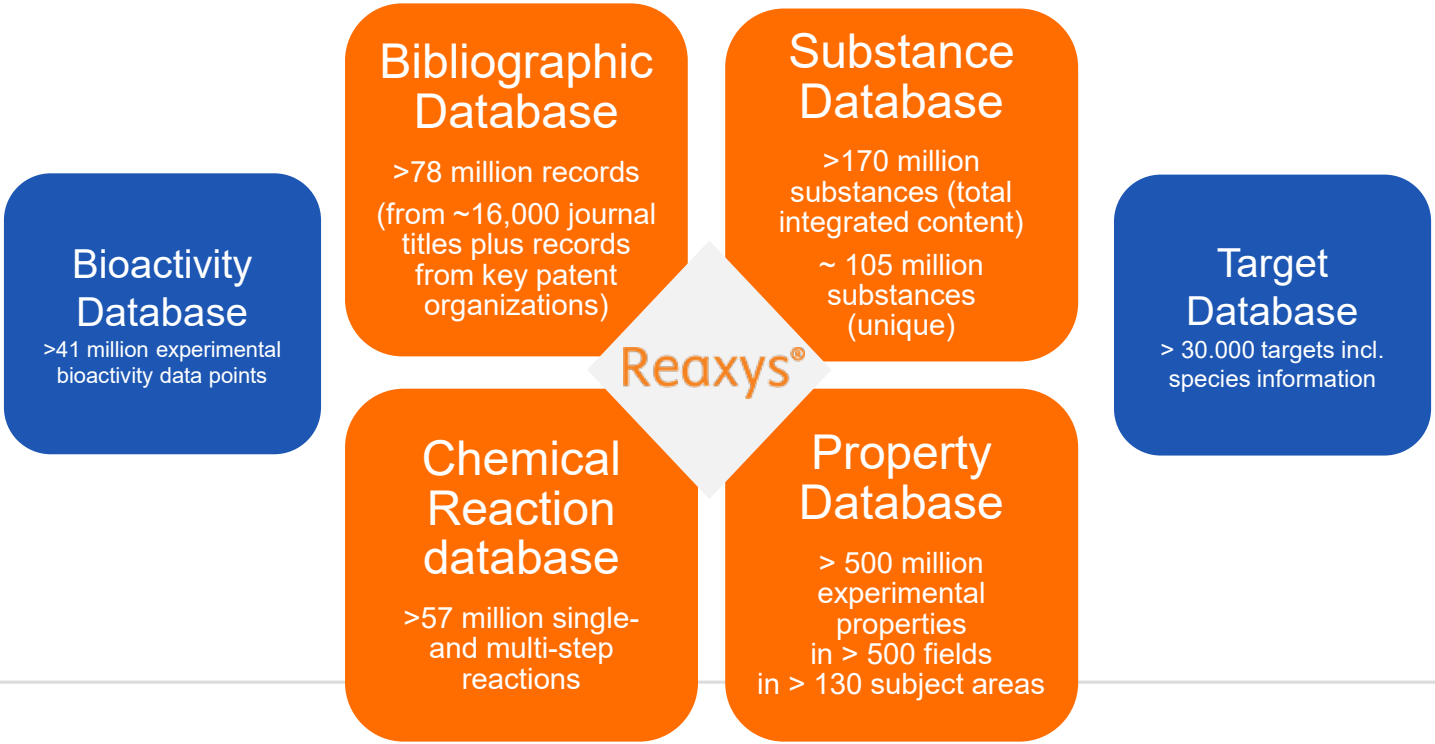
Our Chemistry solution - Reaxys and Reaxys Medicinal Chemistry - comprises 6 core databases



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NEW Reaxys Retrosynthesis

Easy access to optimal synthesis routes

New Reaxys Retrosynthesis

We have completely redesigned the Synthesis Planner feature in Reaxys.
All the information you need to select the best route to make compound, **in one view**

Access experimental procedures with literature references.

Purchase building blocks. Easily check the availability of starting materials.

Collaborate – Manage your projects and export data for easy collaboration.

Integrate – Option to integrate our awarding winning predictive retrosynthesis module

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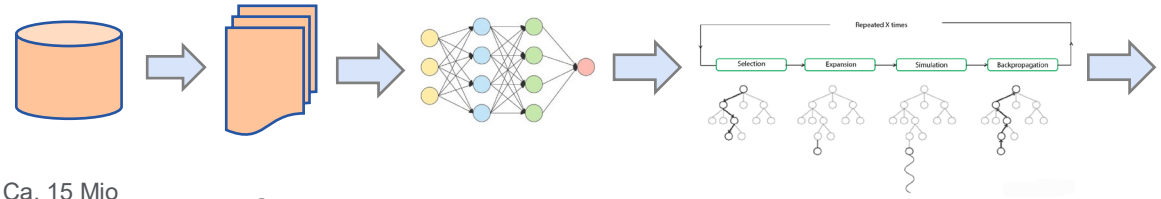
How it was created: Reaxys Retrosynthesis in a nutshell

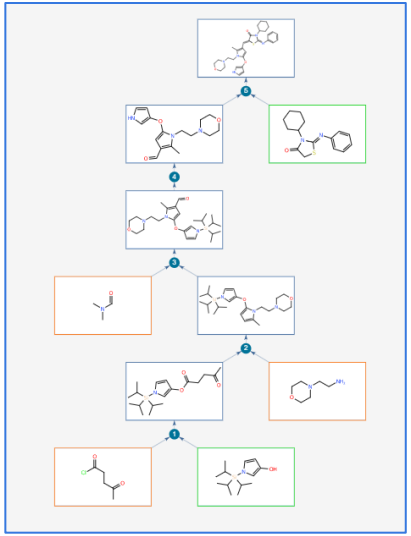
- Combining Reaxys reaction knowledge base and 3N-MCTS technology to create outstanding retrosynthesis application



Ca. 15 Mio single-step reactions of small organic molecules

Ca. 400.000 reaction rules

3 neural networks and Monte-Carlo-Tree-Search



Segler, M., Preuss, M. & Waller, M. Planning chemical syntheses with deep neural networks and symbolic AI. Nature 555, 604–610 (2018). https://doi.org/10.1038/nature25978

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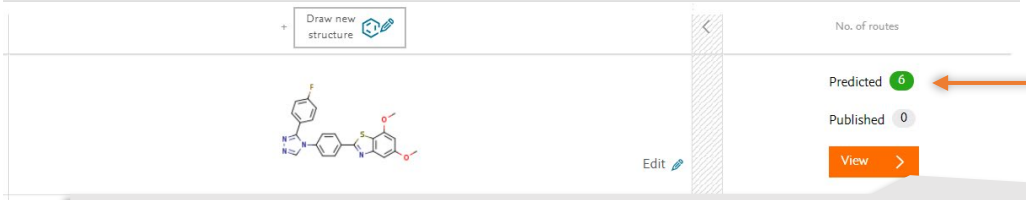
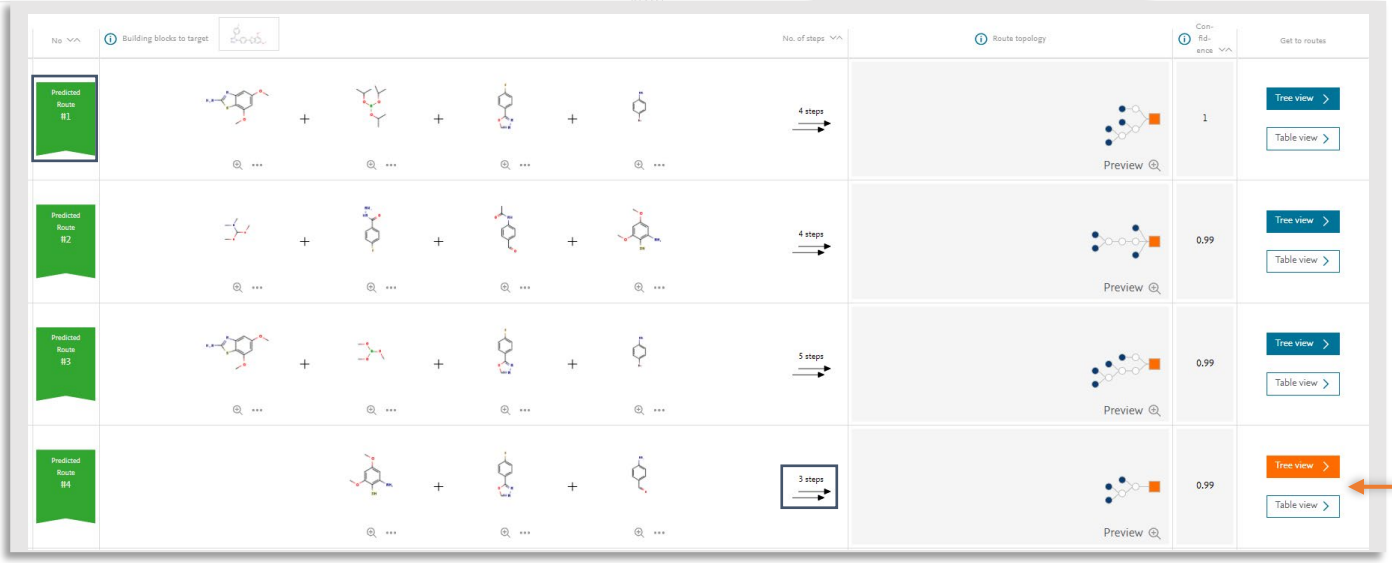
Result of Predictive Retrosynthesis



The Predictive retrosynthesis module provides **6 routes to a novel compound in just 10 minutes**



A route to the molecule of interest can be executed in just 3 steps from commercially available building blocks

Choose between the tree view and the table view to further evaluate the results

Reaxys® Advisors

Do you want to become Reaxys Advisor?

- Are you **chemistry enthusiast** and (can become) **passionate Reaxys user?**
- As **Reaxys Advisor** you will **help** scientist to find the shortest path from chemistry question to relevant answer
- As **Reaxys Advisors** you will **enjoy rewards**, **get into spotlight**, and open doors to accelerate your careers!

More information at *https://www.elsevier.com/reaxysadvisors*

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What Reaxys Advisors have to say?

“Applying for Reaxys Advisor program was one of the best decisions I made. I feel that the program will help me improve my communication and public speaking abilities, while also giving me the chance to receive awesome rewards.”

Roxana

“I am really happy that I can learn how to use Reaxys and that with this opportunity I can help my friends too and share my experience with colleagues and fellow researchers. On top of that, there are some amazing rewards which can help a newcomer to build his/her scientific carrier!”

Yvette

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Thank you

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