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Reaxys®

Reaxys in practice

Piotr Golkiewicz

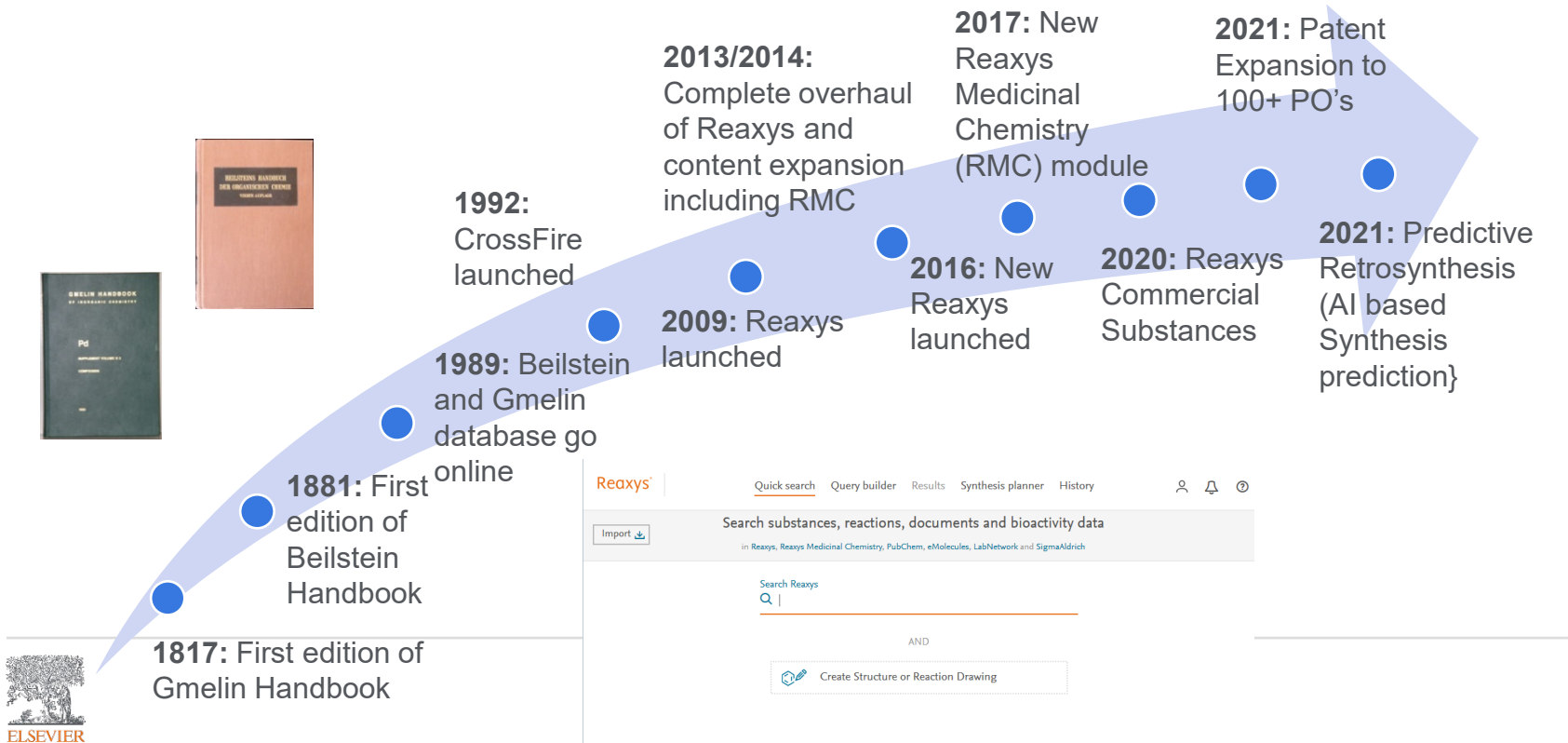
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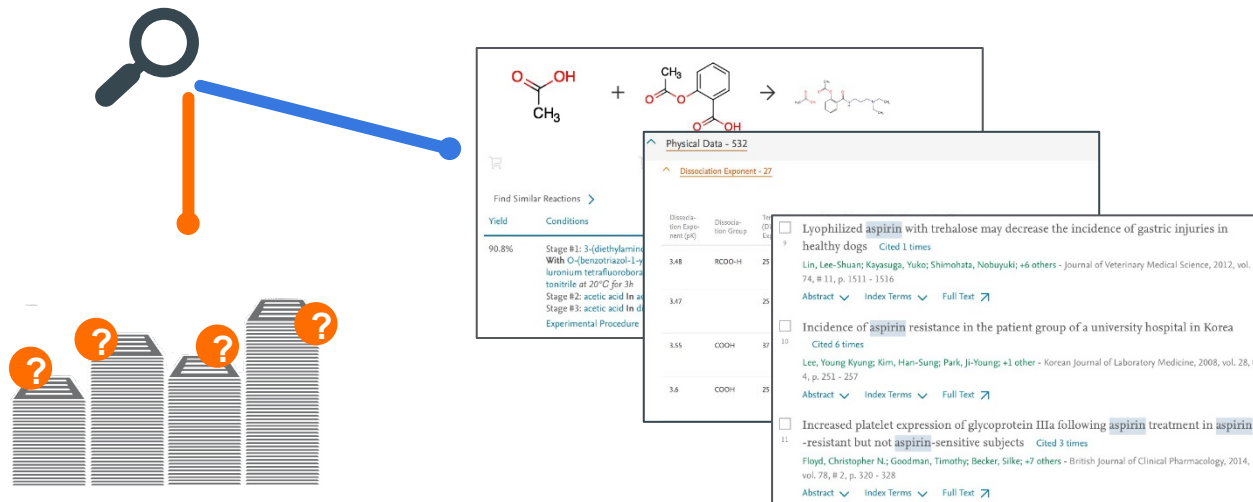
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Reaxys Content development



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



Find Similar Reactions >

| Yield | Conditions |
|-------|---|
| 90.8% | Stage #1: 3-(diethylamino) With O-(benzotriazol-1-yl)uronium tetrafluoroborate in acetonitrile at 20°C for 3h |
| | Stage #2: acetic acid In ac |
| | Stage #3: acetic acid In d |
| | Experimental Procedure |

Physical Data - 532

Dissociation Exponent - 27

Find Similar Reactions >

Yield

Conditions

90.8%

Stage #1: 3-(diethylamino) With O-(benzotriazol-1-yl)uronium tetrafluoroborate in acetonitrile at 20°C for 3h

Stage #2: acetic acid In ac

Stage #3: acetic acid In d

Experimental Procedure

3.48

RCOOH

25

3.47

25

3.55

COOH

19

3.8

COOH

25

Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs Cited 1 times

Lin, Lee-Shuan; Kayasuga, Yuko; Shimohata, Nobuyuki; +6 others - Journal of Veterinary Medical Science, 2012, vol. 74, # 11, p. 1511 - 1516

Abstract Index Terms Full Text

Incidence of aspirin resistance in the patient group of a university hospital in Korea Cited 6 times

Lee, Young Kyung; Kim, Han-Sung; Park, Ji-Young; +1 other - Korean Journal of Laboratory Medicine, 2008, vol. 28, # 4, p. 251 - 257

Abstract Index Terms Full Text

Increased platelet expression of glycoprotein IIIa following aspirin treatment in aspirin-resistant but not aspirin-sensitive subjects Cited 3 times

Floyd, Christopher M.; Goodman, Timothy; Becker, Silke; +7 others - British Journal of Clinical Pharmacology, 2014, vol. 78, # 2, p. 320 - 328

Abstract Index Terms Full Text

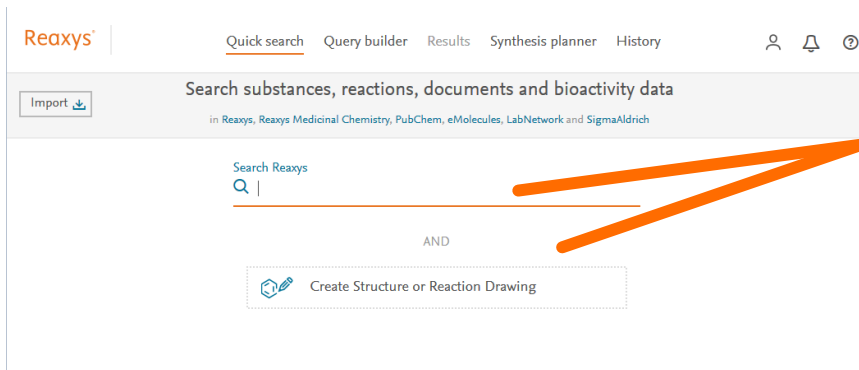
Instead of **delivering lists of references** that may be relevant to a query...

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

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

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.

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 Reaxys delivers a ranked list of alternative results suggestions

The image shows a two-part screenshot of the Reaxys web application. The top part shows the search input field with the text 'preparation of methylphenidate'. The bottom part shows the search results page, which is titled 'Results for preparation of methylphenidate'. The results are ranked and categorized as follows:

| Category | Count | Search Criteria | Actions |
|-----------|-----------|--|--|
| Reactions | 190 | Product(s) : as drawn | Preview Results, View Results, Edit in Query Builder, Create Alert |
| Documents | 1,785 | Titles, Abstracts, Keywords : preparation, methylphenidate | Preview Results, View Results, Edit in Query Builder, Create Alert |
| Documents | 8,830,986 | Titles, Abstracts, Keywords : preparation | Preview Results, View Results, Edit in Query Builder, Create Alert |
| Documents | 17,693 | Titles, Abstracts, Keywords : methylphenidate | Preview Results, View Results, Edit in Query Builder, Create Alert |

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

The image displays a user interface for a chemical data record. The main window shows the chemical name 'cetane' and its structure. Below this, a table lists key identifiers: Reaxys ID (1736592), Chemical Names (cetane, Hexadecane, Hexadecan), CAS Registry Number(s) (C16H34), Molecular Formula (C16H34), Molecular Weight (226.446), InChIKey (DCAYPVUWAIBOU-UHFFFAOYSA-N), Substance type, Linear Structure Formula (C12H26C4H8), and No of references (1627). To the right, three panels are expanded from a central point, showing categorized data:

- Physical Data - 2307**
 - Liquid/Solid Systems (MCS) - 72
 - Further Information - 111
 - Self-diffusion - 8
 - Solubility (MCS) - 23
 - Molecular Deformation - 1
 - Transport Phenomena (MCS) - 195
 - Thermal Expansion - 1
 - Compressibility - 9
 - Boundary Surface Phenomena (MCS) - 146
 - Association (MCS) - 366
 - Transition Point(s) of Liquid Modification(s) - 2
 - Mechanical & Physical Properties (MCS) - 170
 - Ionization Potential - 1
 - Azeotropes (MCS) - 3
 - Energy Data (MCS) - 250
- Other Data - 292**
 - Biodegradation - 99
 - Exposure Assessment - 19
 - Concentration in the Environment - 118
 - Use - 12
 - Stability in Soil - 7
 - Abiotic Degradation, Hydrolysis - 1
 - Abiotic Degradation, Photolysis - 1
 - Transport and Distribution - 8
 - Isolation from Natural Product - 25
 - Oxygen Demand - 1
 - Bioaccumulation, Biomagnification and Biomonitoring - 1
- Spectra - 103**
 - Raman Spectroscopy - 12
 - IR Spectroscopy - 26
 - Fluorescence Spectroscopy - 1
 - ESR Spectroscopy - 3
 - NMR Spectroscopy - 35
 - UV/VIS Spectroscopy - 4
 - Mass Spectrometry - 18
 - Rotational Spectroscopy - 1
 - Luminescence Spectroscopy - 2
 - NQR Spectroscopy - 1

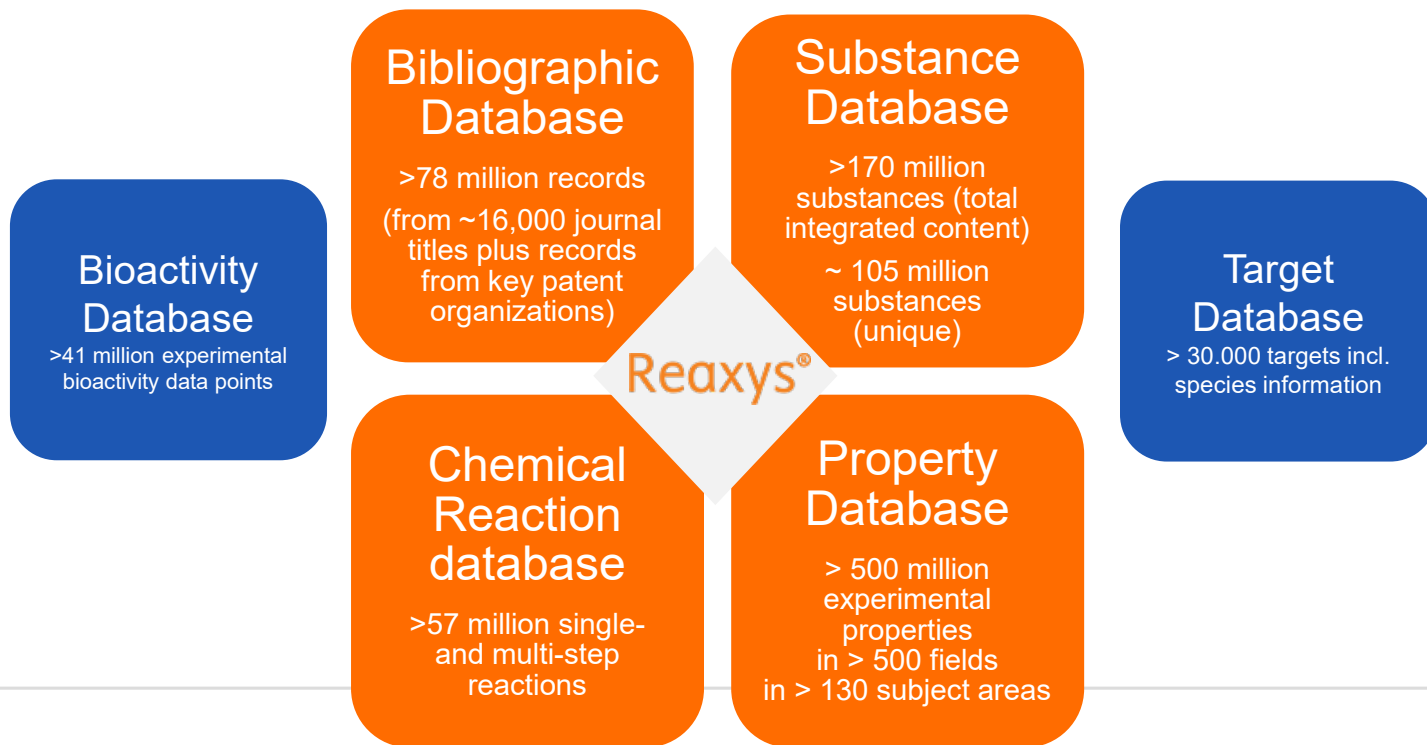
Additional panels shown include:

- Bioactivity - 127**
 - Ecotoxicology - 16
 - Pharmacological Data - 111

A '+ Load More' button is visible at the bottom of the Physical Data panel.

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

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





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.



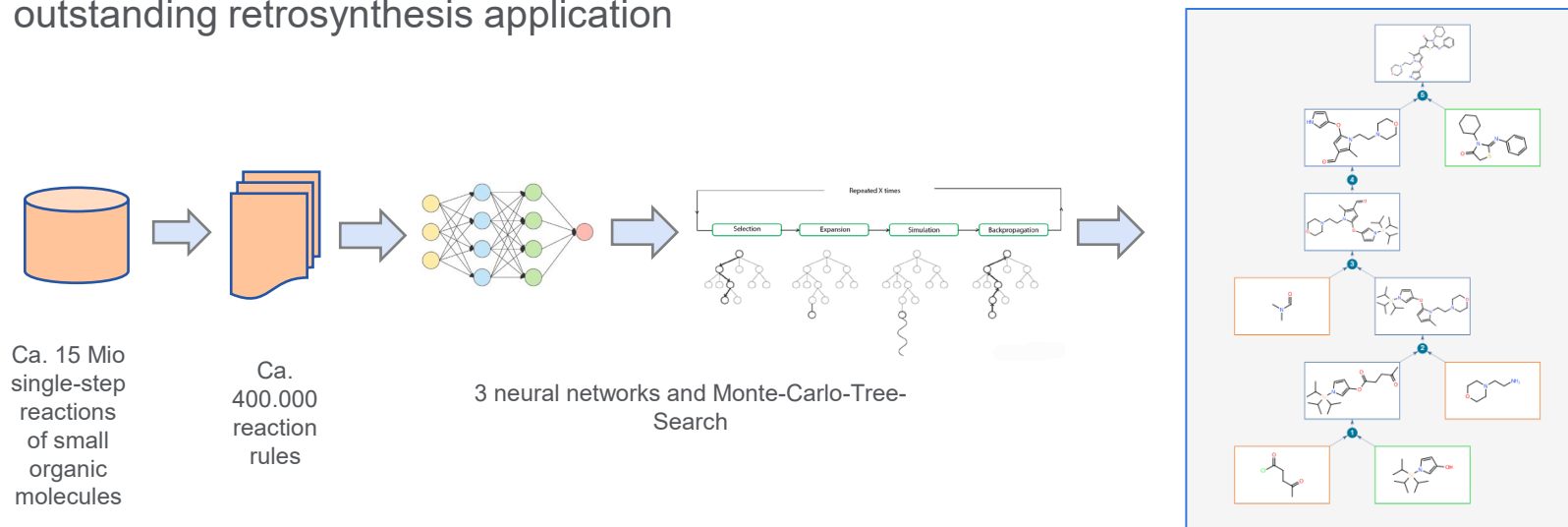
Collaborate – Manage your projects and export data for easy collaboration.



Integrate – Option to integrate our awarding winning predictive retrosynthesis module

How it was created: Reaxys Retrosynthesis in a nutshell

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



Result of Predictive Retrosynthesis



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

No.

Building blocks to target

No. of steps

Route topology

Confidence

Get to routes

| Predicted Route | Building blocks | No. of steps | Route topology | Confidence | Get to routes |
|--------------------|-----------------|--------------|----------------|------------|---|
| Predicted Route #1 | | 4 steps | | 1 | Tree view Table view |
| Predicted Route #2 | | 4 steps | | 0.99 | Tree view Table view |
| Predicted Route #3 | | 5 steps | | 0.99 | Tree view Table view |
| Predicted Route #4 | | 3 steps | | 0.99 | Tree view Table view |

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>



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





Thank you

Reaxys®

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