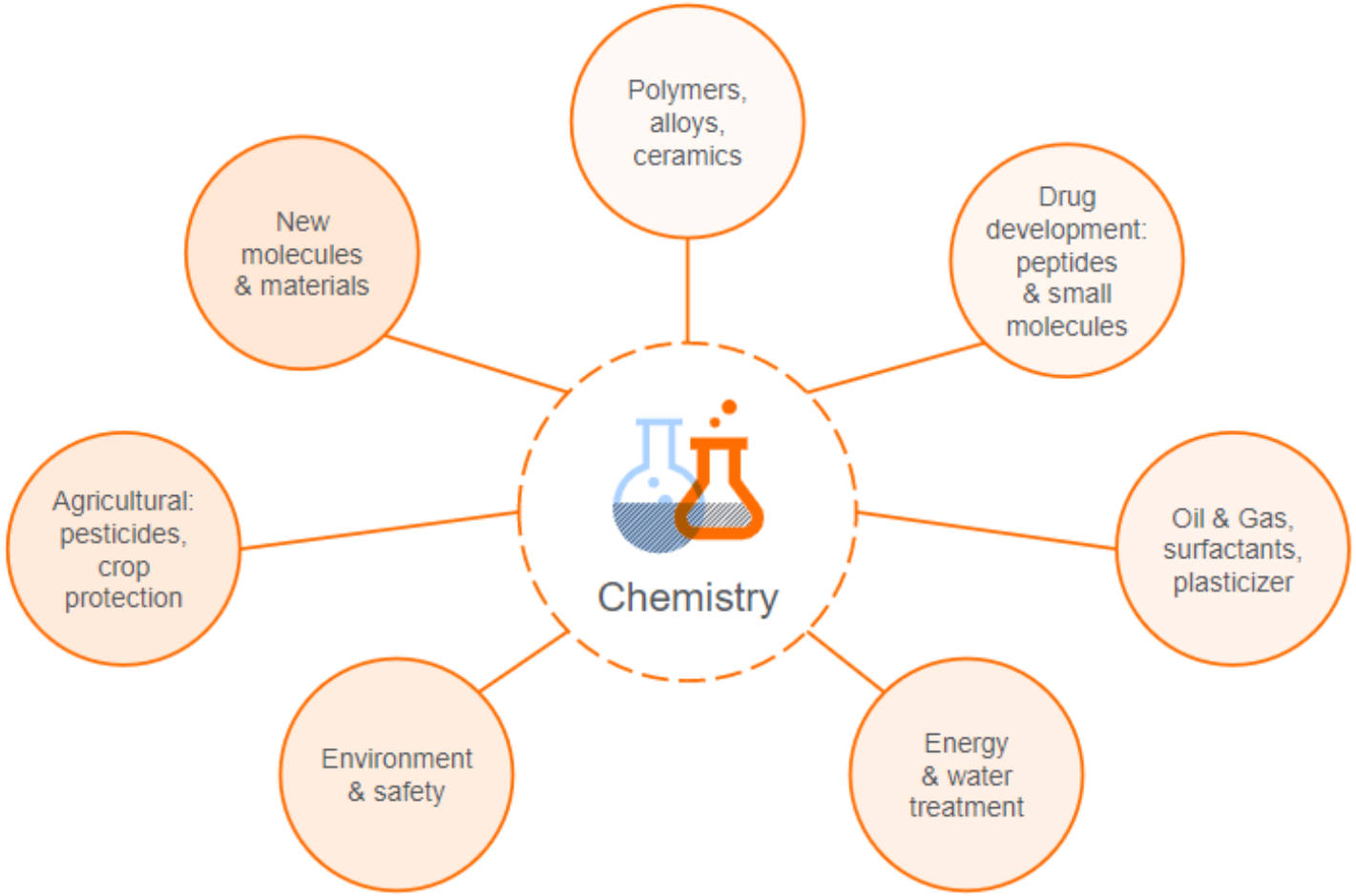
Reaxys®

Introduction to Reaxys Academic Edition

06 March 2025

Dr. Giulia Moncelsi – Chemistry Solution Engineer

Chemistry is at the heart of solving research problems as a central science



Navigating a growing sea of chemical information

>55% of chemists spend more than 5 hours each week on data and literature retrieval

Reaxys' journey: evolving to navigate the sea of information

1881: First edition of Beilstein Handbook of Organic Chemistry

1817: First edition of Gmelin Handbook of organometallic and inorganic compounds

1989: Beilstein and Gmelin database go online

1992: CrossFire launched

2009: Reaxys launched

2013/2014: Complete revamp of **Reaxys** and content expansion

2016: New **Reaxys** UI launched

2017: Reaxys Bioactivity & Targets module

2020: Reaxys Commercial Substances

2021: Patent Expansion to 46 M patents

2021: Predictive Retrosynthesis (AI-based synthesis prediction)

2024: IKTOS AI Retrosynthesis

Reaxys supports:

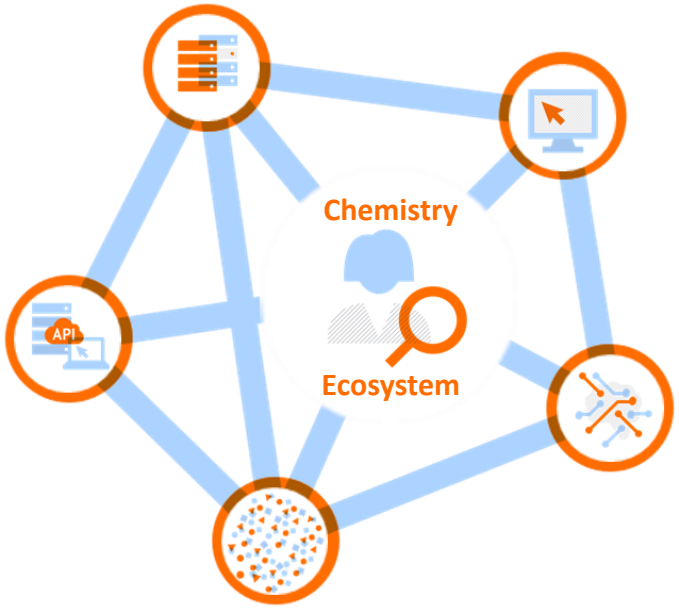
Research

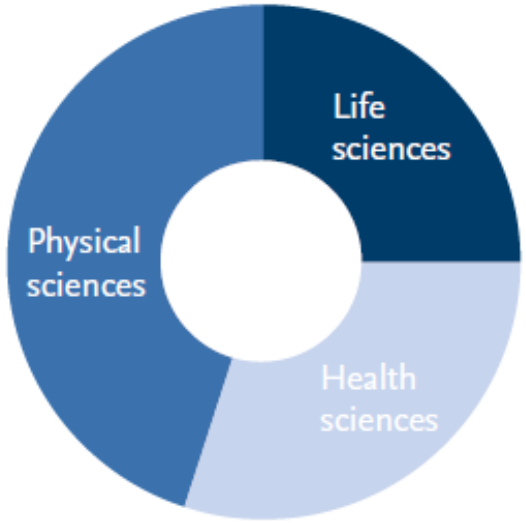
Teaching & Learning

Reaxys Academic Edition

Reaxys Then & Now: https://pharma.elsevier.com/chemistry/reaxys-then-now/

Reaxys impacts fields beyond the Chemistry ecosystem





Physical sciences, including:
- Chemistry
- Chemical engineering
- Material sciences

Life sciences, including:
- Biochemistry
- Pharmacology
- Toxicology
- Biological sciences

Health sciences, including:
- Medicine

...is relevant to a large spectrum of other disciplines

Material sciences
Environmental sciences
Geological Sciences
Archeology
Paleontology
Nanotechnology

Agricultural sciences
Food sciences
Hydrology
Limnology
Toxicology
Surface science
Clinical sciences

Molecular Biology
Cellular Biology
Pharmacology
Biochemistry
Biomedicine
Biotechnology

And many more...

Uses across disciplines

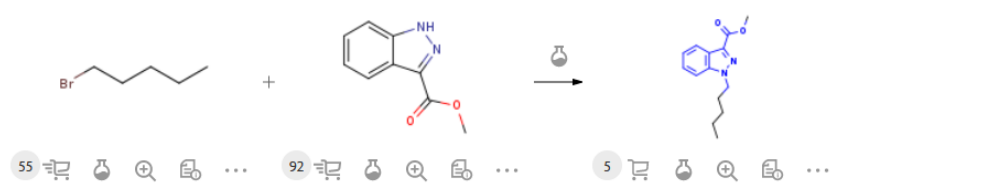
Reaxys serves the needs of a varying profile of chemist

I am a chemist where I mainly search using **structures**

I am a chemist where I search using **structures** and **text**

I am a chemist where I search using **text** because structure searches are difficult or not possible

Type of search	
	• **Structure** search (Reaxys strength): substances, reaction, properties that have been extracted by structure • Text search done to retrieve reaction/ structure/ property related information
	• **Text** search: use of keywords and Boolean for document discovery & retrieval • Text search supports interdisciplinary fields where chemistry is combined with other subjects, e.g. **polymers, chemical engineering, material science**, etc and structure search is too complex or not an option



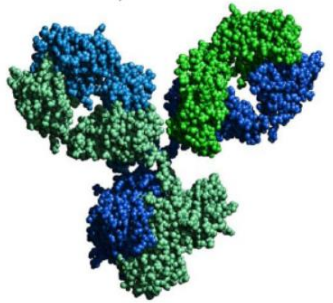
2 Hits | 8 Conditions | Find Similar | Reaction ID: 41428311

Conditions	Yield
Stage #1: methyl 1H-indazole-3-carboxylate **With** sodium hydride **In** tetrahydrofuran at 0°C; for 1h; **Stage #2:** 1-Bromopentane **In** tetrahydrofuran at 50°C; for 24h; regioselective reaction; Experimental Procedure	89%
With potassium *tert*-butylate **In** tetrahydrofuran at 0 - 20°C; for 48h; regioselective reaction;	84%

Large molecule researcher: search information using text search

Large Molecule Drug
Human Growth Hormone
~3,000 atoms

Large Biologic
Herceptin
~25,000 atoms



Chemical Engineer: physical processes for wastewater treatment

Material scientist: advances in hair fibre reinforcement techniques of concrete

Our information security standards are certified

Reaxys has obtained the ISO 27001 Information Security System Management certification

Your confidentiality is our key priority

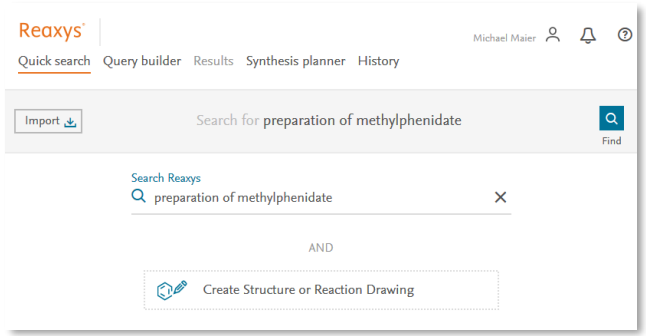
You can trust Reaxys to confidently perform searches on proprietary research to strengthen your IP portfolio.

- ✓ Reaxys maintains certified high standards for security practices
- ✓ Reaxys continuously improves its information security practices

ELSEVIER Reaxys®

Reaxys in action

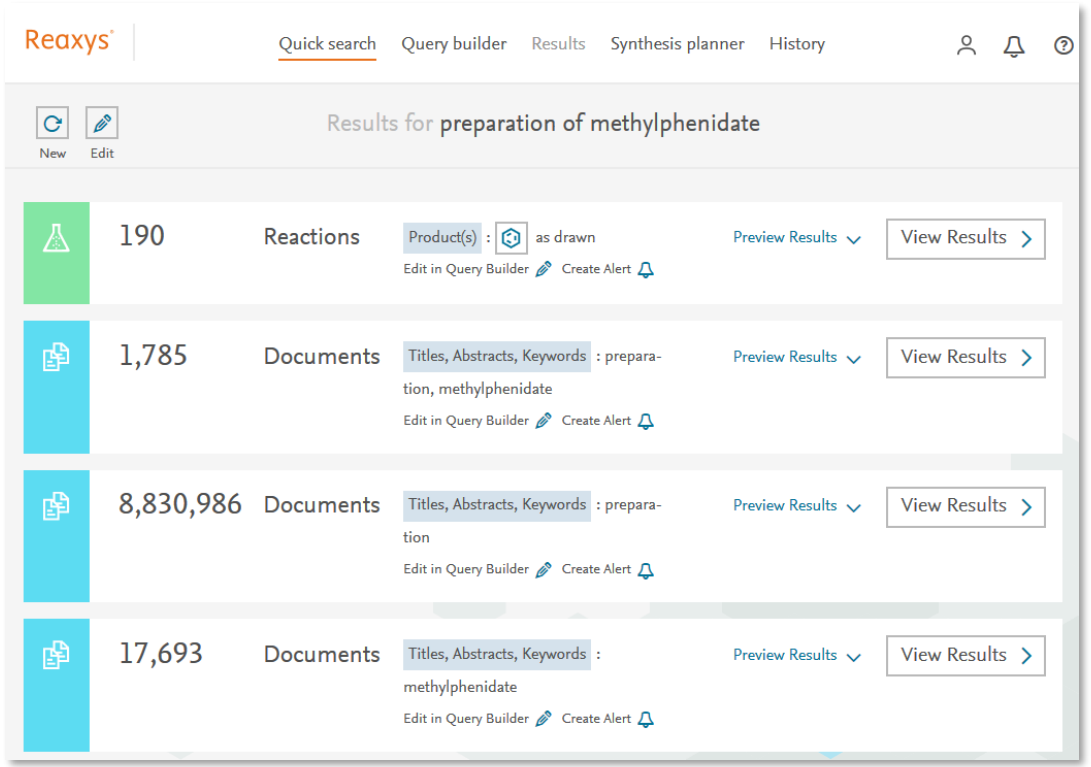
Reaxys produces results set adjusted to your needs



1 Reaxys interprets keyword(s) as well as special characters: truncations, wildcards and operators

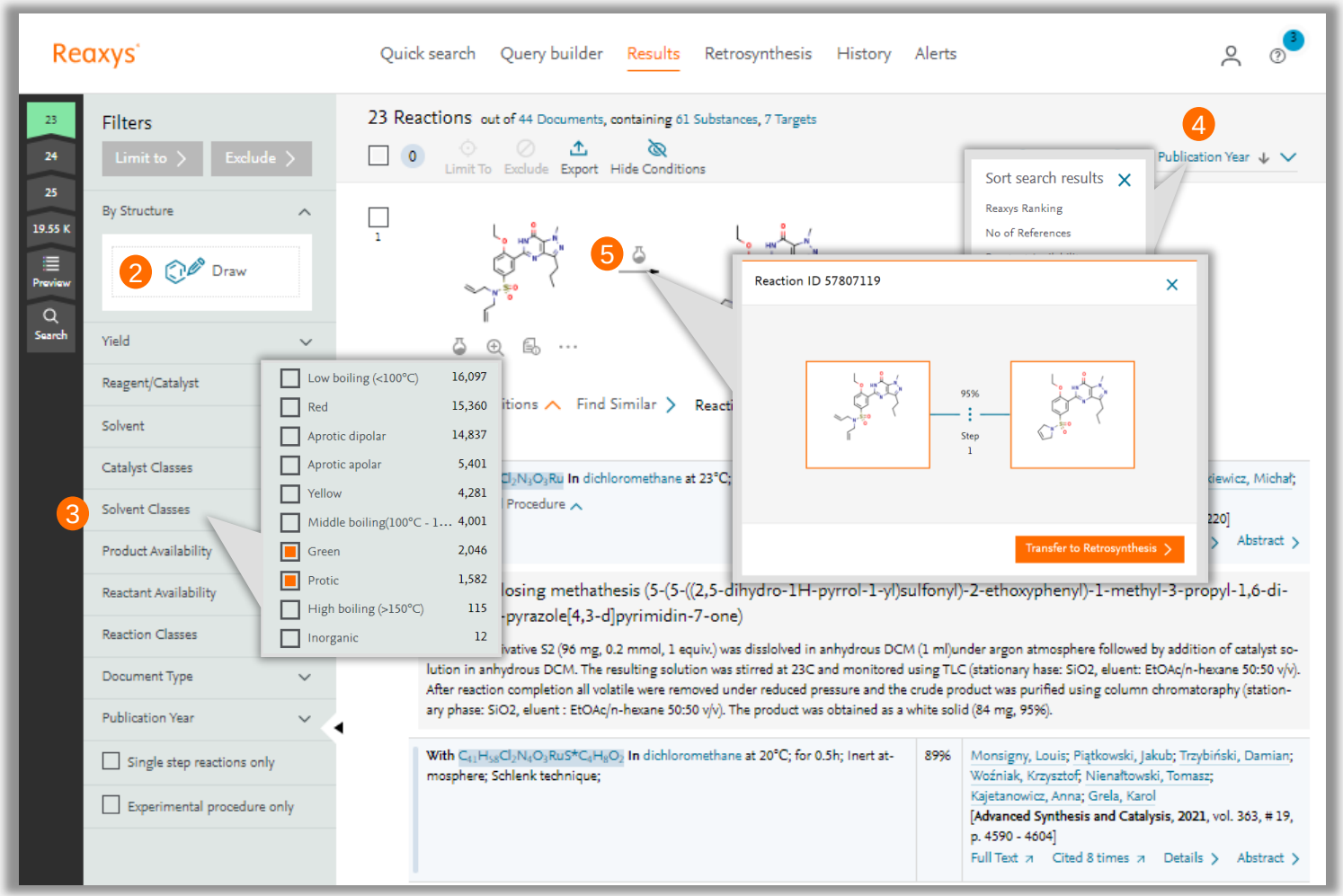
2 Reaxys recognises your search intention

3 Reaxys produces a list of results with options: intended answers plus relevant results you may not have considered



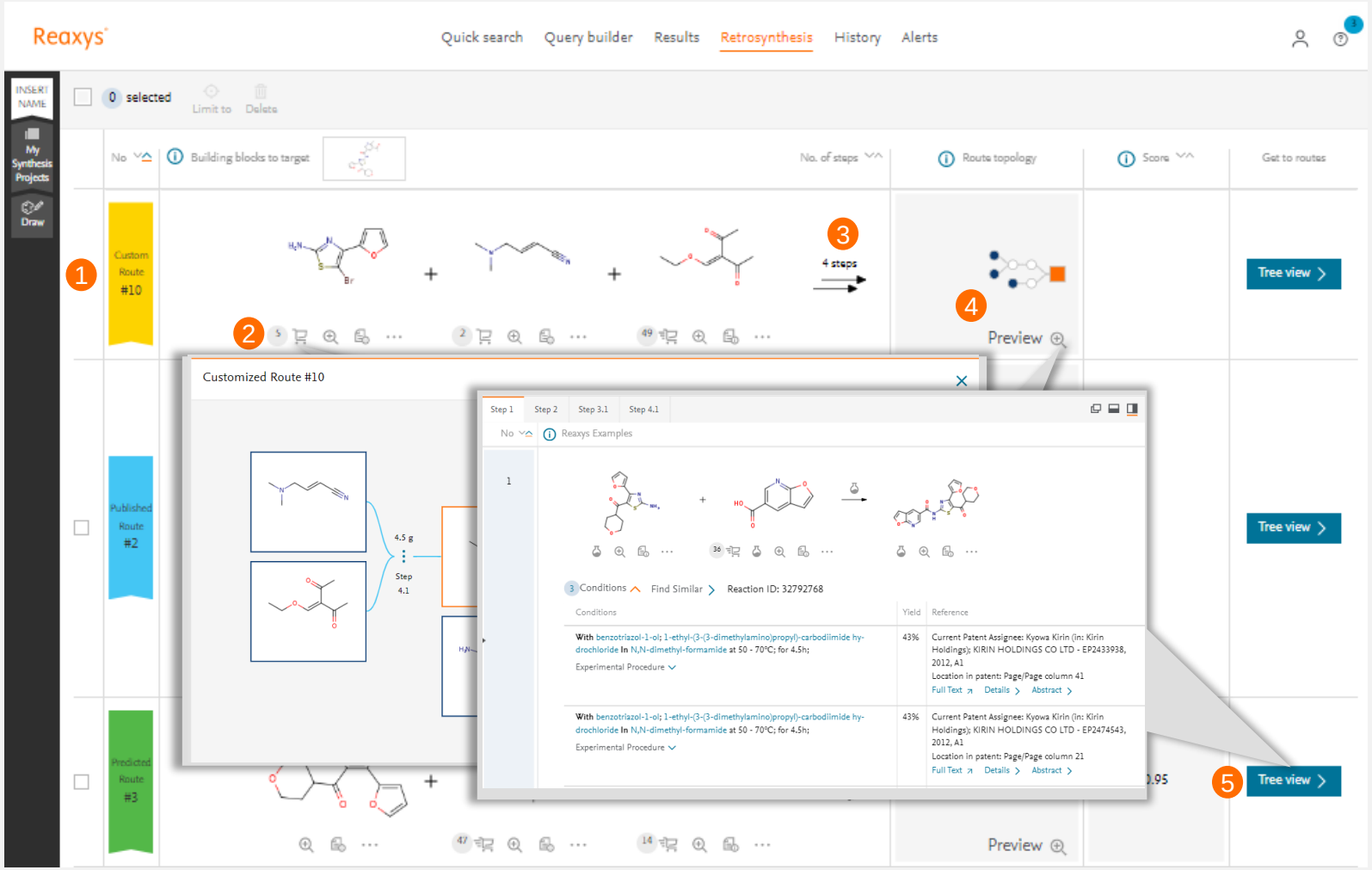
Focus on **using** information, not searching for information

Discover new experimental procedures and verify results



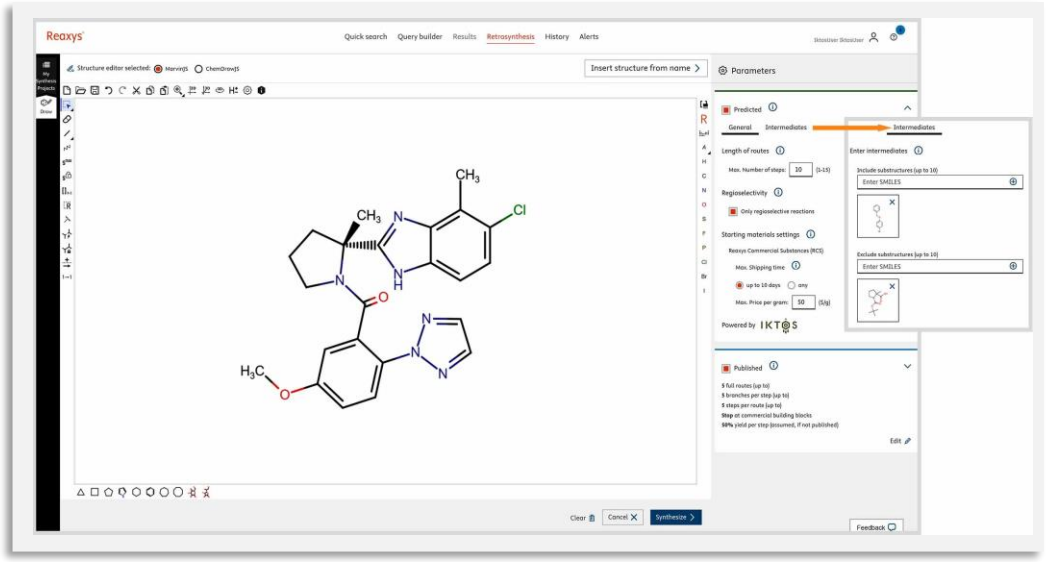
1. Review excerpted experimental information including purification techniques
2. Filter by substructure to ensure the most relevant results
3. Narrow by multiple filter options including green principles, yield and catalyst classes
4. Sort the content by citations, relevance or publication year
5. Utilize the retrosynthesis feature to discover new chemistry

Quickly identify synthesis routes and assess costs

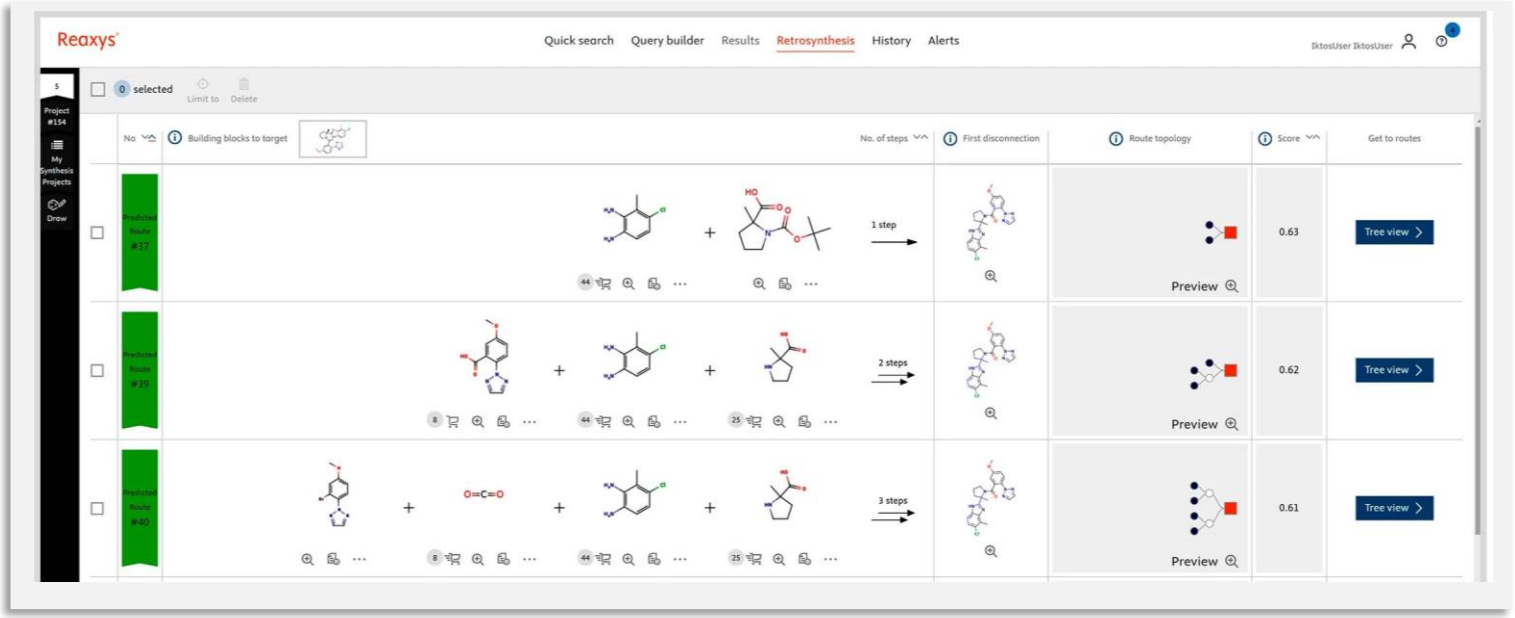


1. View published, predicted & customized routes in one view
2. Assess the commercially availability of starting materials needed for synthesis
3. View of the number of steps in synthesis plan to enable faster prioritization of shorter routes
4. Preview the route diversity with ease using the route topology
5. Discover real examples of the predicted steps in the only chemistry database that provides published examples linked to the routes in a single view

Results of Predictive Retrosynthesis

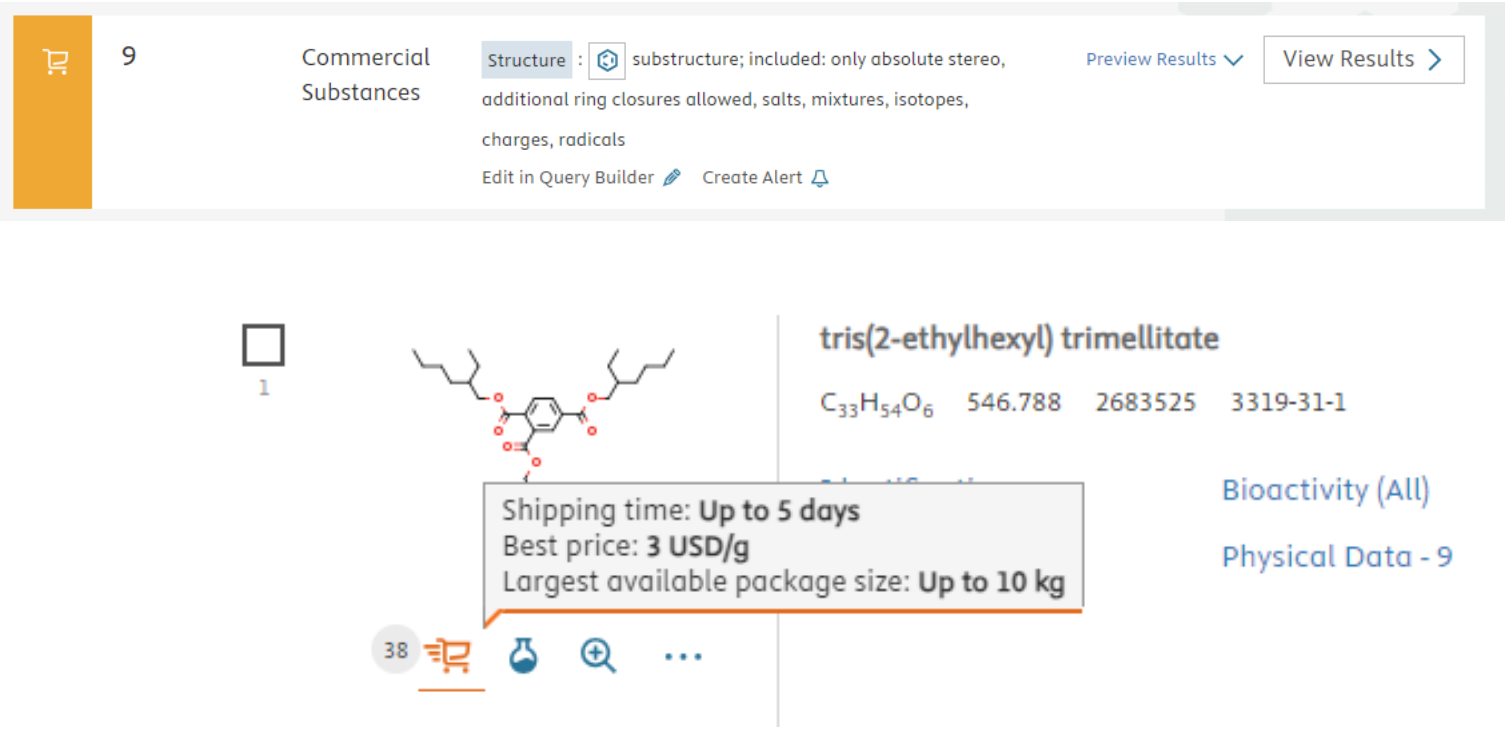


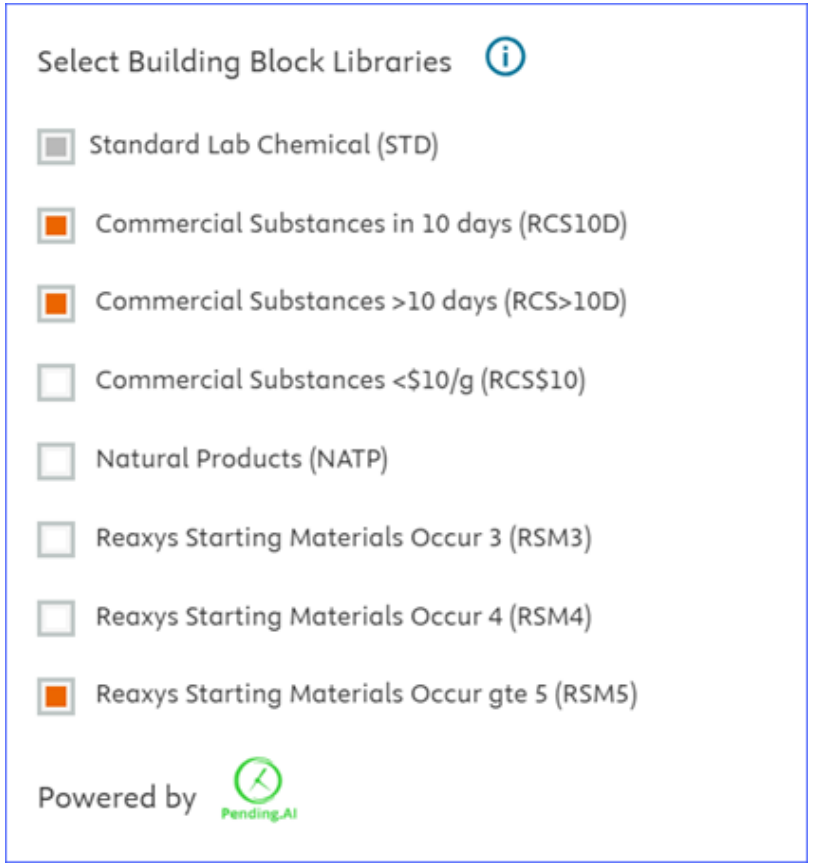
The Predictive retrosynthesis modules powered by Pending.AI or IKTOS can be switched on within the Retrosynthesis planner and provide routes to a novel compound in under 30 minutes



Routes to the molecule of interest are executed in just few steps from commercially available building blocks

Commercial substances and suppliers' information

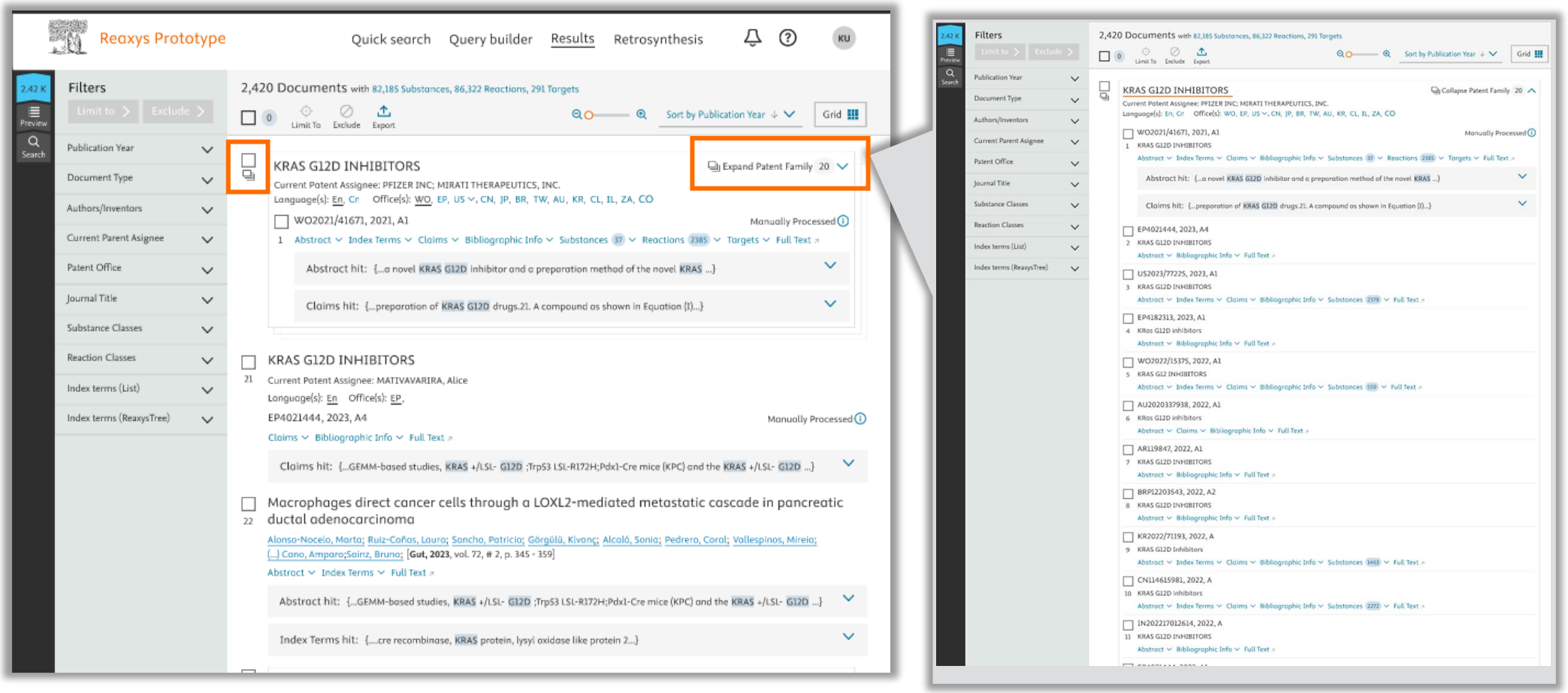




- Reaxys now includes > 500 commercial suppliers and growing, within a dedicated searching environment
- Both PendingAI and IKTOS use Reaxys commercial substances (RCS) as building block library (100M compounds)
- Features available: Preferred supplier, product level selection for export,…

Press release example: Merck adds Chemical Products to Reaxys' Chemistry Database
Commercial suppliers can apply for their products to be included in Reaxys via the supplier portal

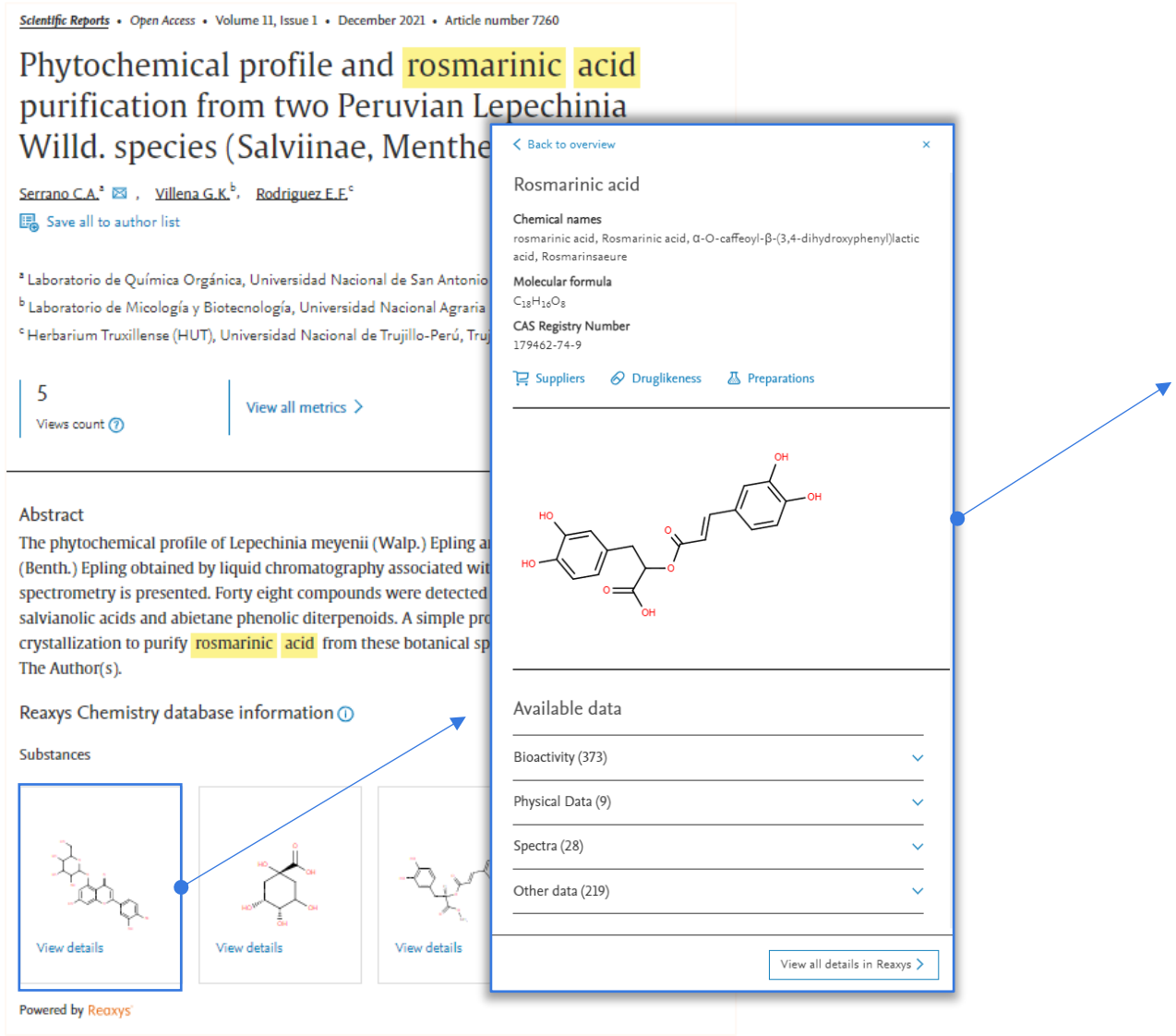
Patent discoverability and family member grouping for faster reviewing and better analysis of results



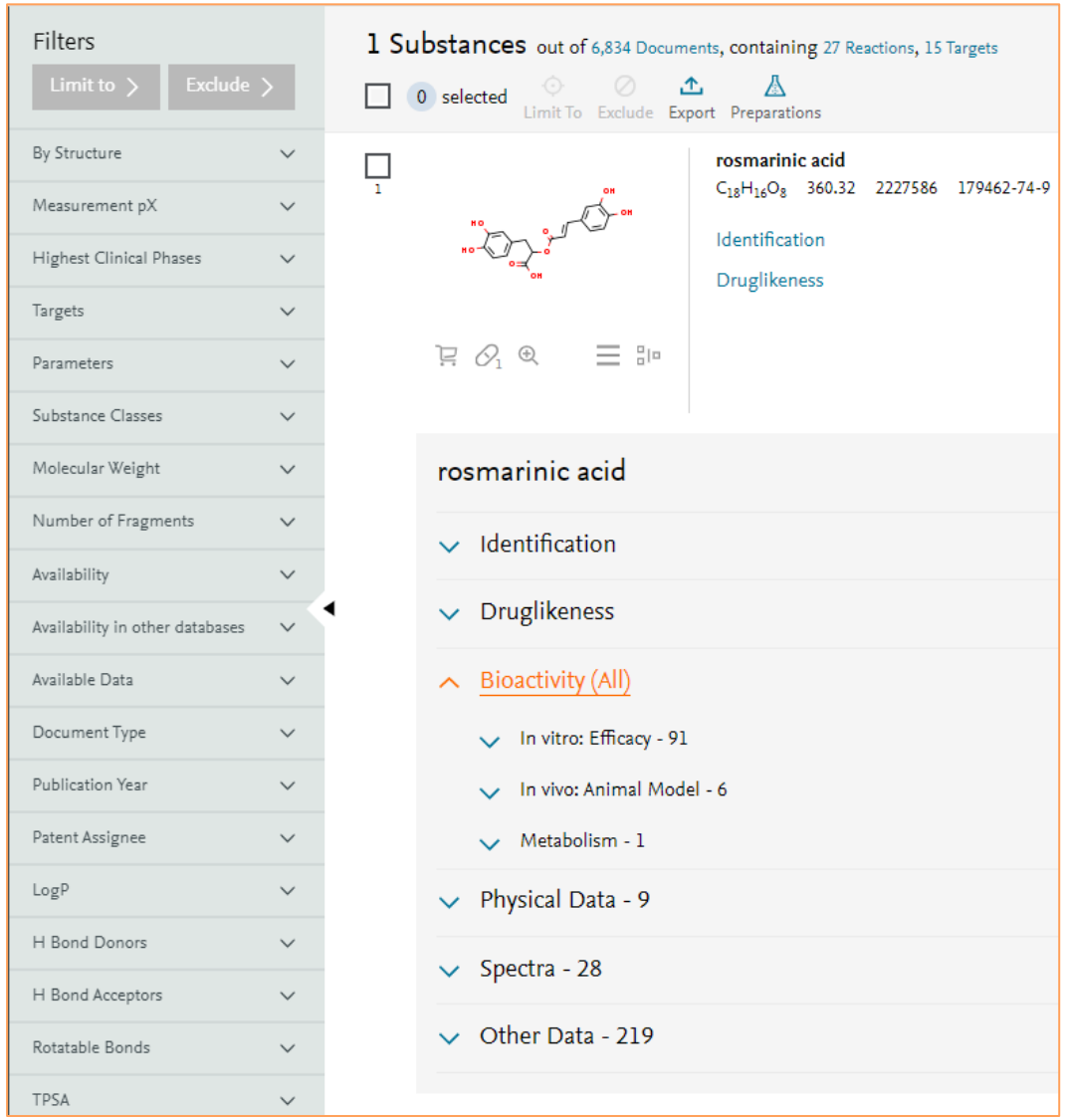
For a comprehensive study and comparison on patent content and searches of known chemistry databases:
https://www.tprinternational.com/patcid-ibm-patent-chemical-structure-database-part-2/

Reaxys linking with Scopus and ScienceDirect

Scopus



Reaxys



Answer questions for hit-to-lead and lead optimization

- ✓ **What** substances interact with my target?
- ✓ **What** type of interactions occur between my substance and my target?
- ✓ **What** interactions do other substances with similar structures have?
- ✓ **What** is the comparative affinity of different substances for my targets?

Medicinal chemists

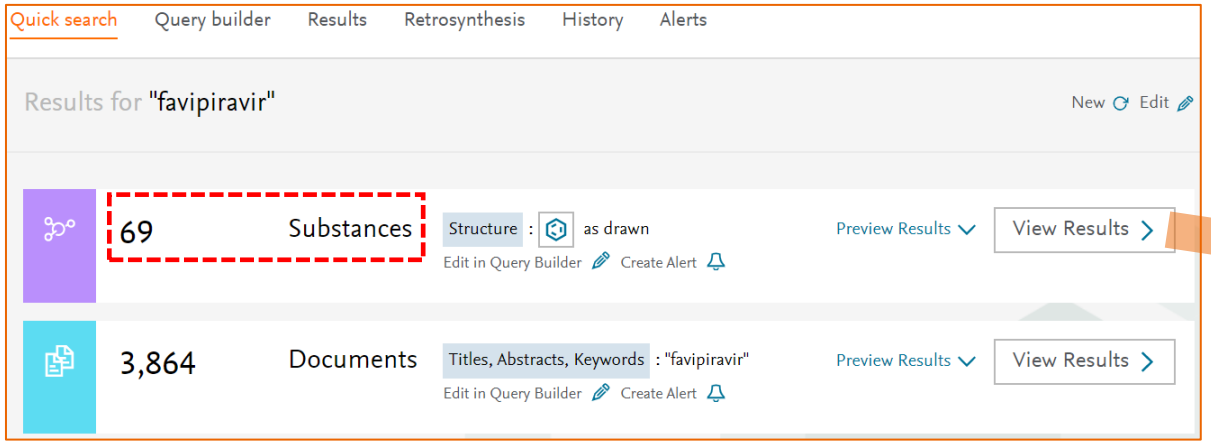
Computational chemists

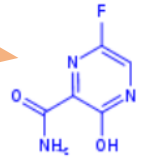
Toxicologists, pharmacologists and others

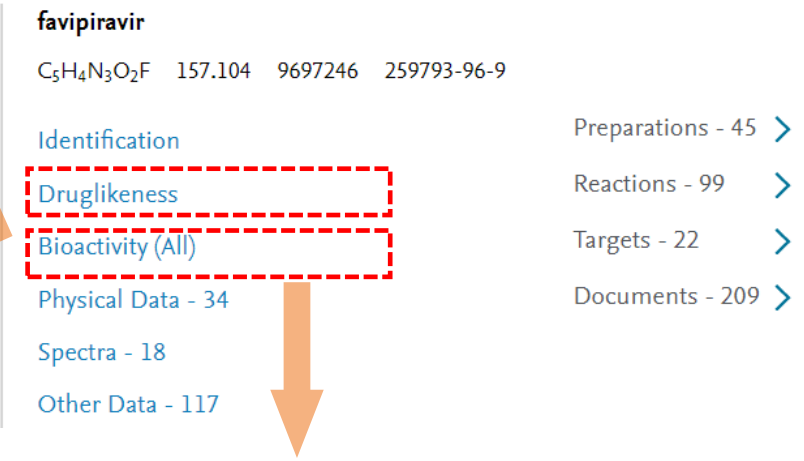
Bioactivity of a substance and pharmacy targets

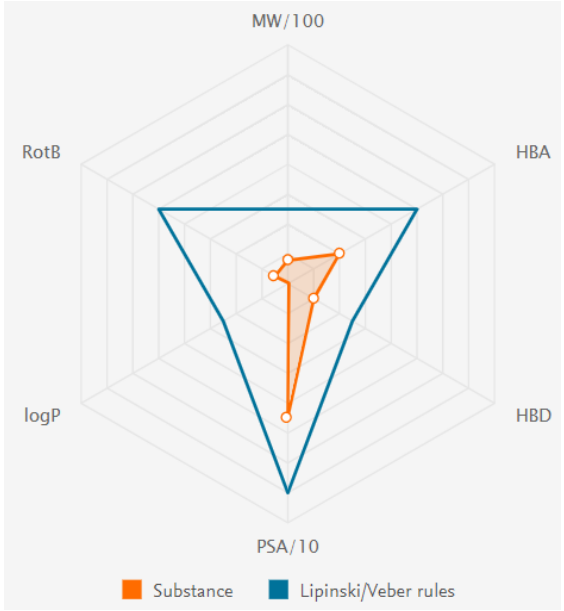
1 Search of bioactivity properties from substance

Favipiravir is an antiviral medication used to treat influenza. It is also being studied to treat several other viral infections, including SARS-CoV-2.

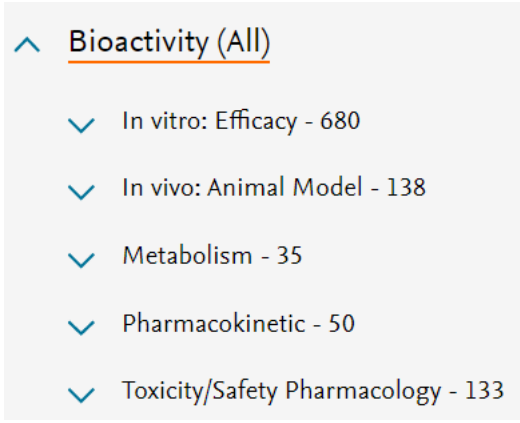








Using Lipinski's and Veber's rules of thumb to evaluate druglikeness.



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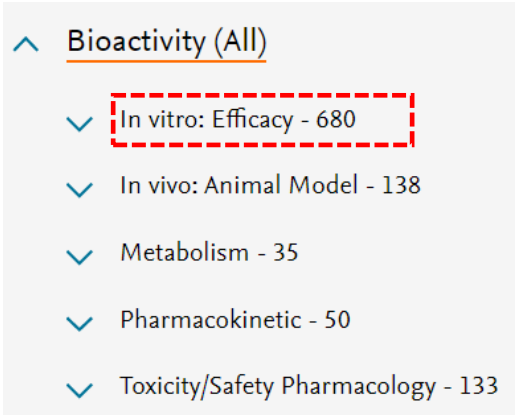
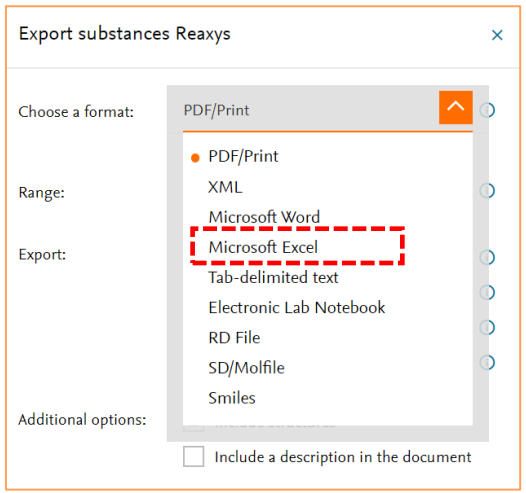
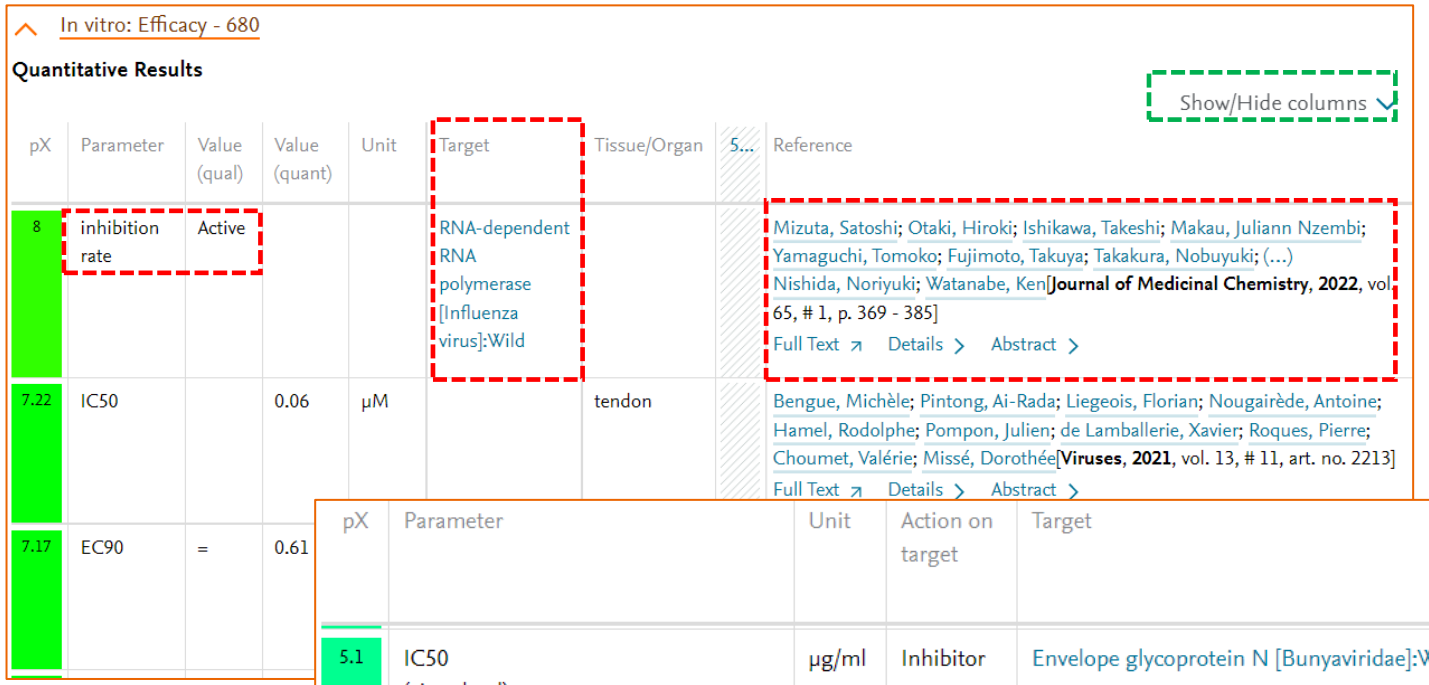
Bioactivity of a substance and pharmacy targets

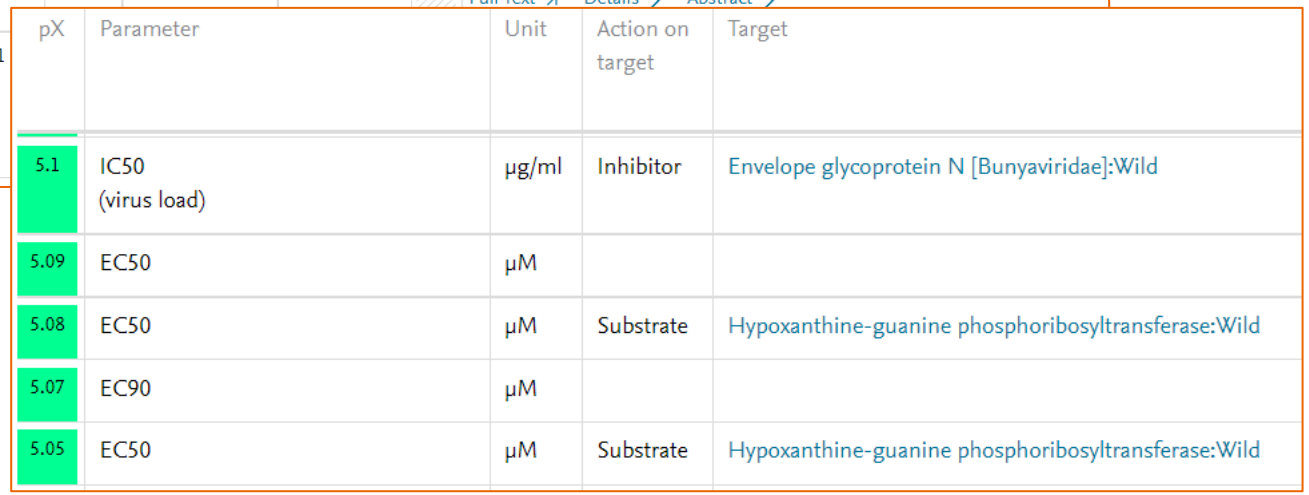
2 *In Vitro*

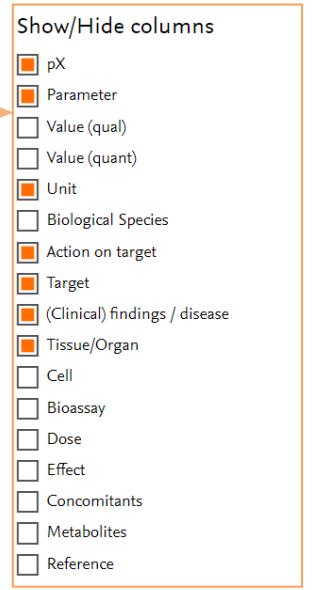
In vitro is a process performed or taking place in a test tube, culture dish, or elsewhere outside a living organism.











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Bioactivity of a substance and pharmacy targets

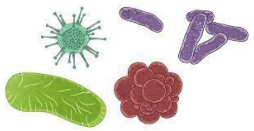
3 *In Vivo*

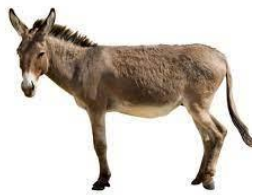
- Bioactivity (All)
  - In vitro: Efficacy - 680
  - In vivo: Animal Model - 138
  - Metabolism - 35
  - Pharmacokinetic - 50
  - Toxicity/Safety Pharmacology - 133

In vitro is a process performed or taking place in a living organism.

pX	Parameter	Value (qual)	Biological Species	(Clinical) findings / disease	Animal Model	Route of administration	5...	Reference
1	body weight change	Not active	Hartley guinea pig		experimental viral infection	oral administration		Anantpadma, Manu; Comer, Jason E.; Davey, Robert A.; Dyall, Julie; Ekins, Sean; Freiberg, Alexander N.; Holbrook, Michael R.; (...) Massey, Christopher; Zhou, Huanying[**Antiviral Research**, **2020**, vol. 181] Full Text ↗ Cited 4 times ↗ Details > Abstract >
1	percentage change (viral RNA and infectious + more	Not active	C57BL 6 mouse	immunocompetent		oral administration		Bengue, Michèle; Pintong, Ai-Rada; Liegeois, Florian; Nougairède, Antoine; Hamel, Rodolphe; Pompon, Julien; de Lamballerie, Xavier; Roques, Pierre; Choumet, Valérie; Missé, Dorothée[**Viruses**, **2021**, vol. 13, # 11, art. no. 2213] Full Text ↗ Details > Abstract >

Various biological species: more than 65.000





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Bioactivity of a substance and pharmacy targets

4 Metabolism and Pharmacokinetic

- Bioactivity (All)
  - In vitro: Efficacy - 680
  - In vivo: Animal Model - 138
  - Metabolism - 35
  - Pharmacokinetic - 50
  - Toxicity/Safety Pharmacology - 133

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Tissue/Organ	Cell fraction	Dose
3.22	Km (Michaelis constant)		602	µM	human	liver	Cytosol (pooled)	5 - 2000 µM
3.21	Km (Michaelis constant)		616	µM	Macaca fascicularis	liver	Cytosol (pooled)	5 - 2000 µM

Parameter	Value (quant)	Unit	Biological Species	(Clinical) findings / disease	Route of administration	Dose	Dosing regimen	1...	Reference
Rac (Ctrough) (based on drug concentration at 12 h + more	6	no unit	Syrian hamster		intraperitoneal administration	18.75 mg/day	Repeated		Driouich, Jean-Sélim; Cochin, Maxime; Lingas, Guillaume; Moureau, Grégory; Touret, Franck; Petit, Paul-Rémi; Piorkowski, Géraldine; (...) Solas, Caroline; Nougairède, Antoine[**Nature Communications**, **2021**, vol. 12, # 1] Full Text ↗ Cited 35 times ↗ Details › Abstract ›
Cmax	178.7	µg/ml	BALB/cA mouse	Healthy	oral administration	100 mg/kg	Single		Moshikur, Rahman Md; Ali, Md. Korban; Wakabayashi, Rie; Moniruzzaman, Muhammad; Goto, Masahiro[**Molecular Pharmaceutics**, **2021**, vol. 18, # 8, p. 3108 - 3115] Full Text ↗ Cited 3 times ↗ Details › Abstract ›
tmax	0.75	h	BALB/cA mouse	Healthy	oral administration	100 mg/kg	Single		Moshikur, Rahman Md; Ali, Md. Korban; Wakabayashi, Rie; Moniruzzaman, Muhammad; Goto, Masahiro[**Molecular Pharmaceutics**, **2021**, vol. 18, # 8, p. 3108 - 3115]

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Bioactivity of a substance and pharmacy targets

5 Toxicity / Safety Pharmacology

- Bioactivity (All)
  - In vitro: Efficacy - 680
  - In vivo: Animal Model - 138
  - Metabolism - 35
  - Pharmacokinetic - 50
  - Toxicity/Safety Pharmacology - 133

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Cell	Dose	2...	Effect
	body weight loss (Normalized)	Active			Syrian hamster		75 mg/kg		toxic substance
	CC50 (cytotoxic concentration)		2633	µM		Vero C1008 cell line			cytotoxic agent
	cell viability percentage		101.38	%		Vero C1008 cell line	0.41 µM		cytotoxic agent

Reaxys

What's been delivered to Reaxys between 2022 and 2024

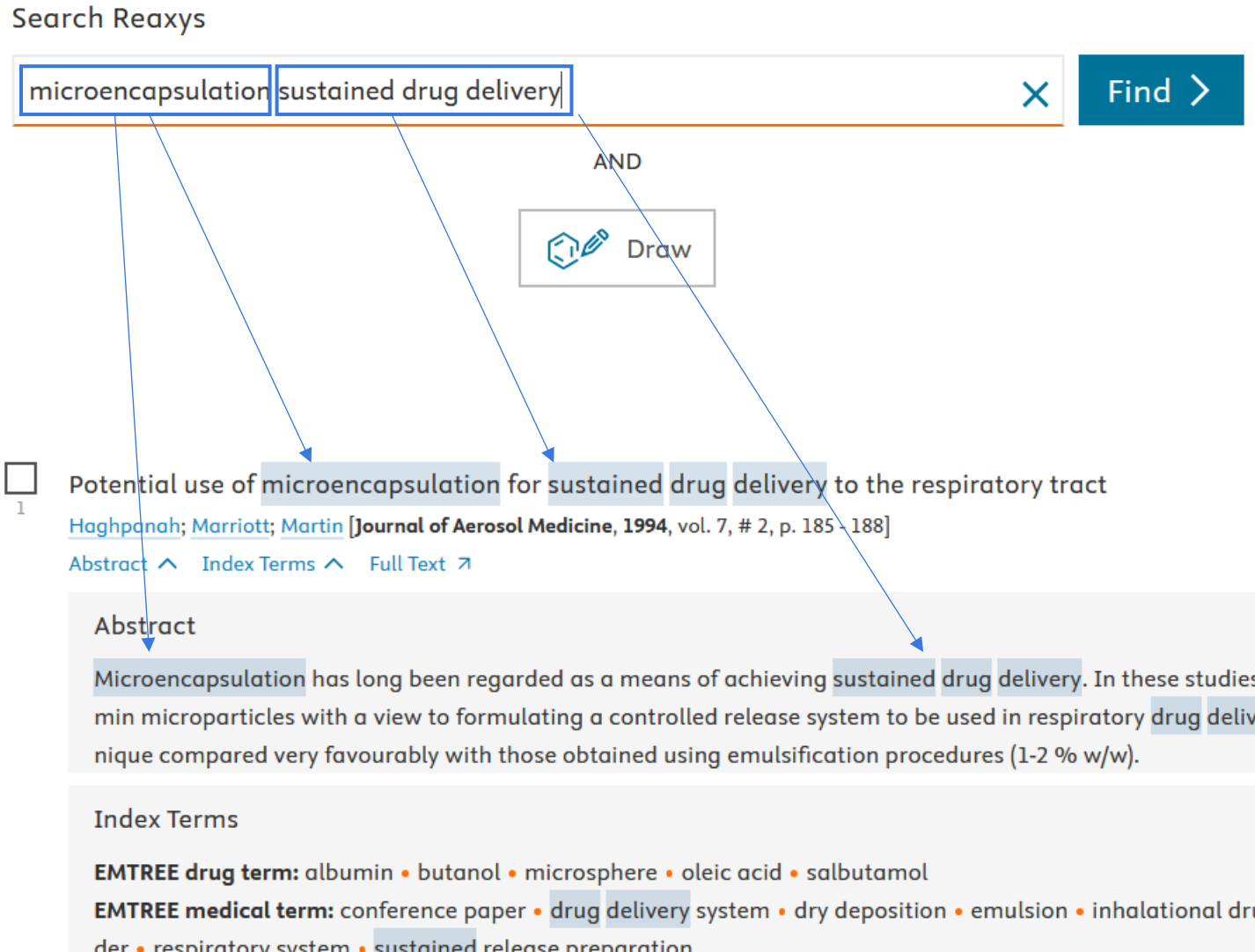
Content Expansion	• Expansion of patents from 12 patent offices to 105 patent offices • From 16,000 journals to 18,000 journals • Expansion of Asian language patent for target & bioactivity data • CAS numbers expansion • Reaxys Commercial Substances expansion to >500 suppliers
Search & User Experience	• Email alerting service • Target & Bioactivity visualization & export improvements • Document discoverability enhancements via new relevancy ranking and addition of keywords • *Best in class* **author name** search for better discoverability of information • **Patent family member grouping** for faster reviewing and better analysis • Substance discoverability enhancements via tab-based design
Data and Predictive Technologies	• Predictive retrosynthesis from Iktos and PendingAI • Predictive retrosynthesis API from Iktos and PendingAI • Machine learning optimised Reaxys reactions dataset

Reaxys innovations coming in future

- Continuous content expansion & refinement to maintain comprehensiveness
- Enhancing user experience for a more intuitive experience and quicker information retrieval
- Technological advancements to improve the quality and diversity of our offerings
- Predictive retrosynthesis enhancements to continue reducing time & effort in synthesis planning

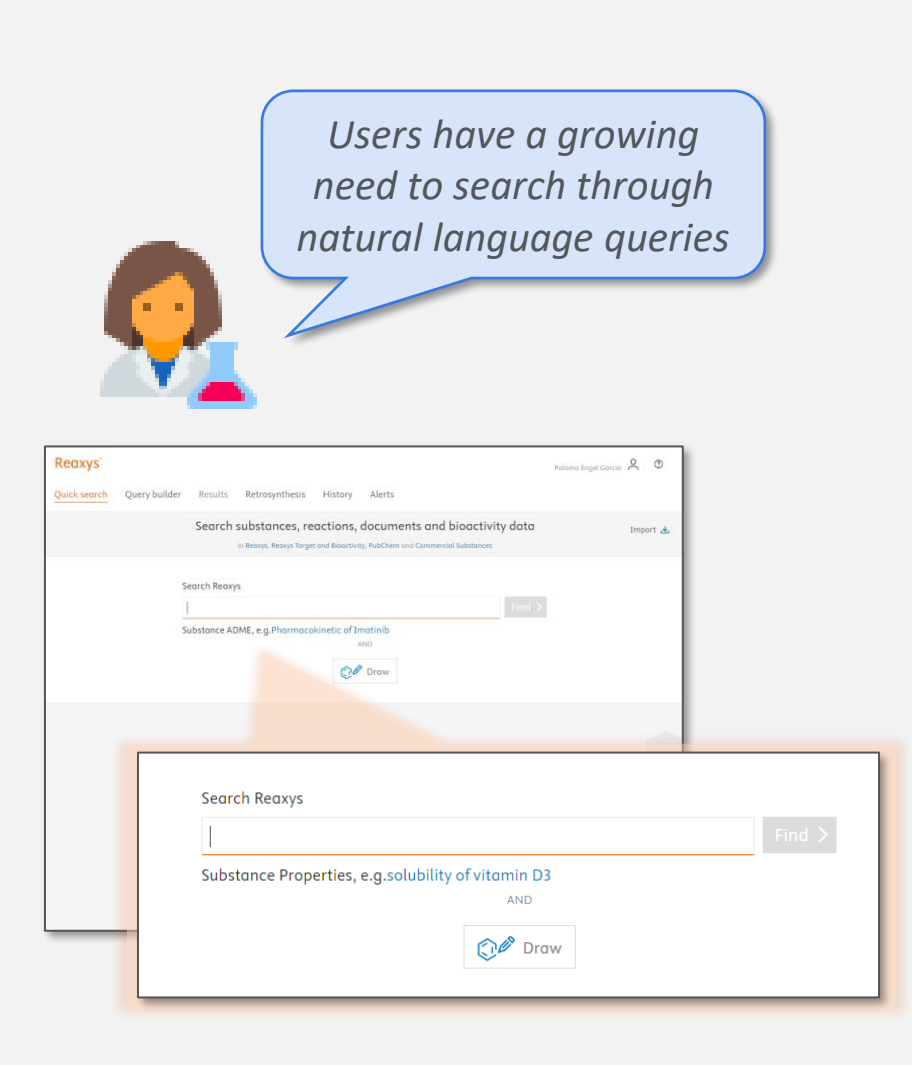
Enhancing text search for document discovery

Text search today: Ontology supported Lexical search



- Relies query term matching in title, abstract and keywords
- Not designed for natural language querying
- Does not consider context of a query
- Inflexible to spelling mistakes
- Requires user intervention if results are not as expected→ Query Builder

Improving natural language based searching requires multiple initiatives



Initiatives to improve natural language-based searching

Lexical

- Enhancements in keyword search, with new document relevancy ranking for improved document discoverability through **lexical** search
- Improved author name search for better discoverability of information

Semantic

- **Experimentation** with **vector** driven semantic **search** for the improved discoverability of unstructured text information

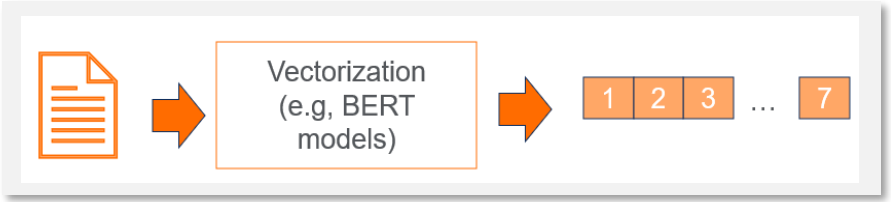
LLM

- **Research** into LLM-driven database search agent to support complex searches over Reaxys structured data fields

What is vector search

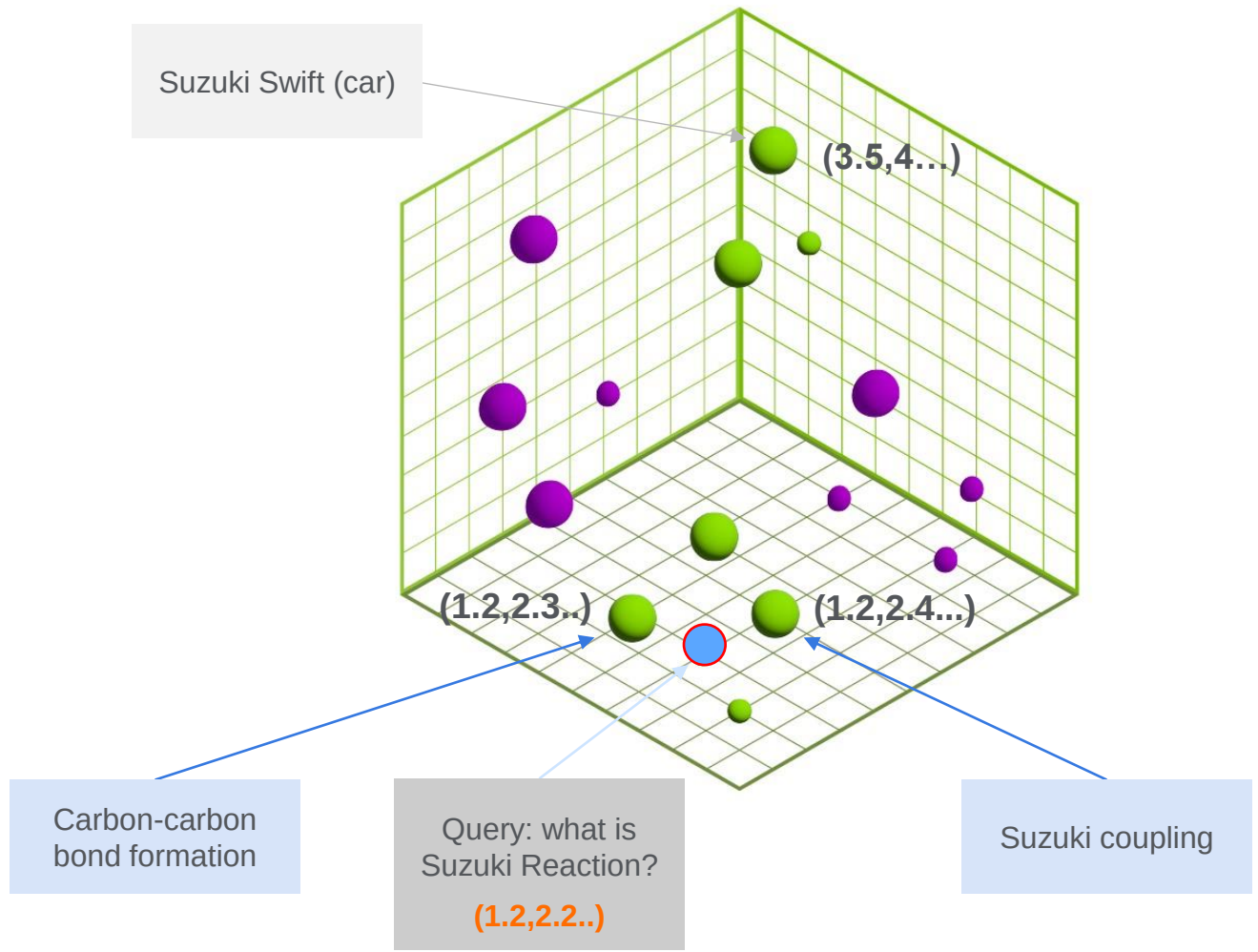
Vectors and the vectorisation of Reaxys data to enable smarter search

Content in Reaxys documents is transformed into vectors, represented as numerical values and stored in a vector database



User query is also converted into vectors and represented as numerical values

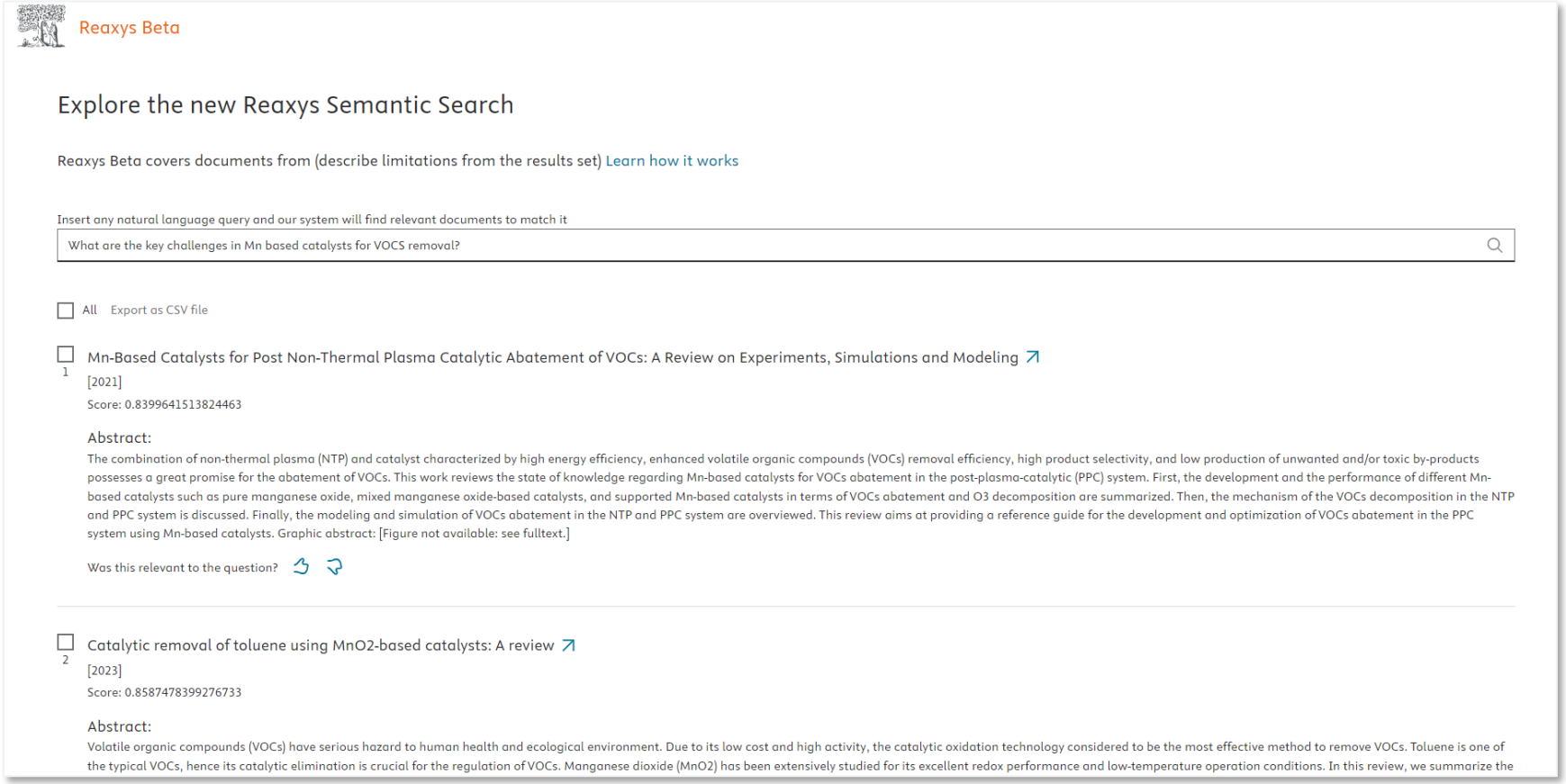
Similarity search between query vectors and content vectors, stored in the data base, returns the results which are semantically closest neighbours to the query vector



Source: https://opendatascience.com/a-gentle-introduction-to-vector-search/

Currently the model is trained to answer chemistry related questions on ***Title & abstracts (2021-2023*** **content)**

Reaxys Vector Search: First-in-class vector search for chemistry to enhance discoverability of documents through natural language querying



- ✓ Retrieve comprehensive results for natural language query type
- ✓ Initial evaluation shows positive results
- ✓ Beta version for customer evaluation is almost ready

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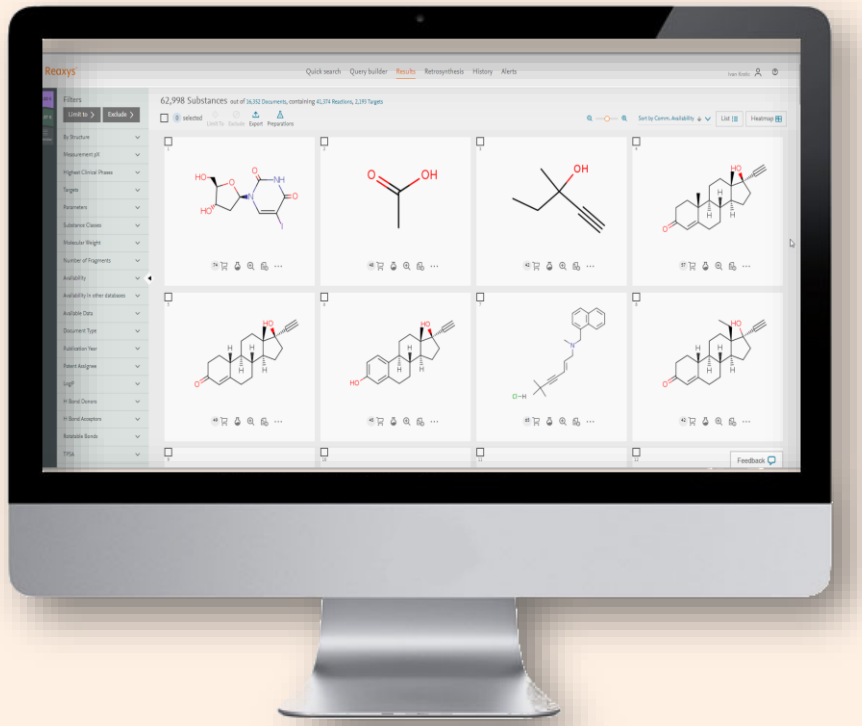

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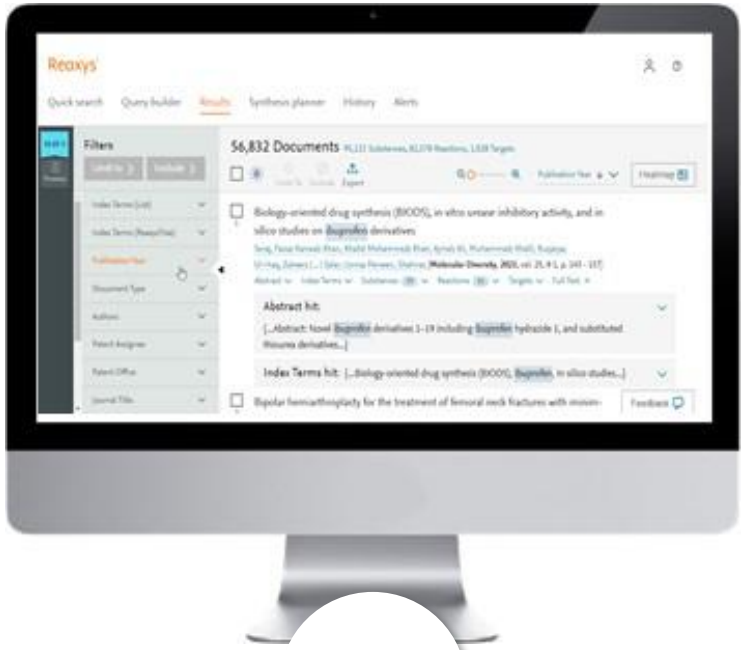

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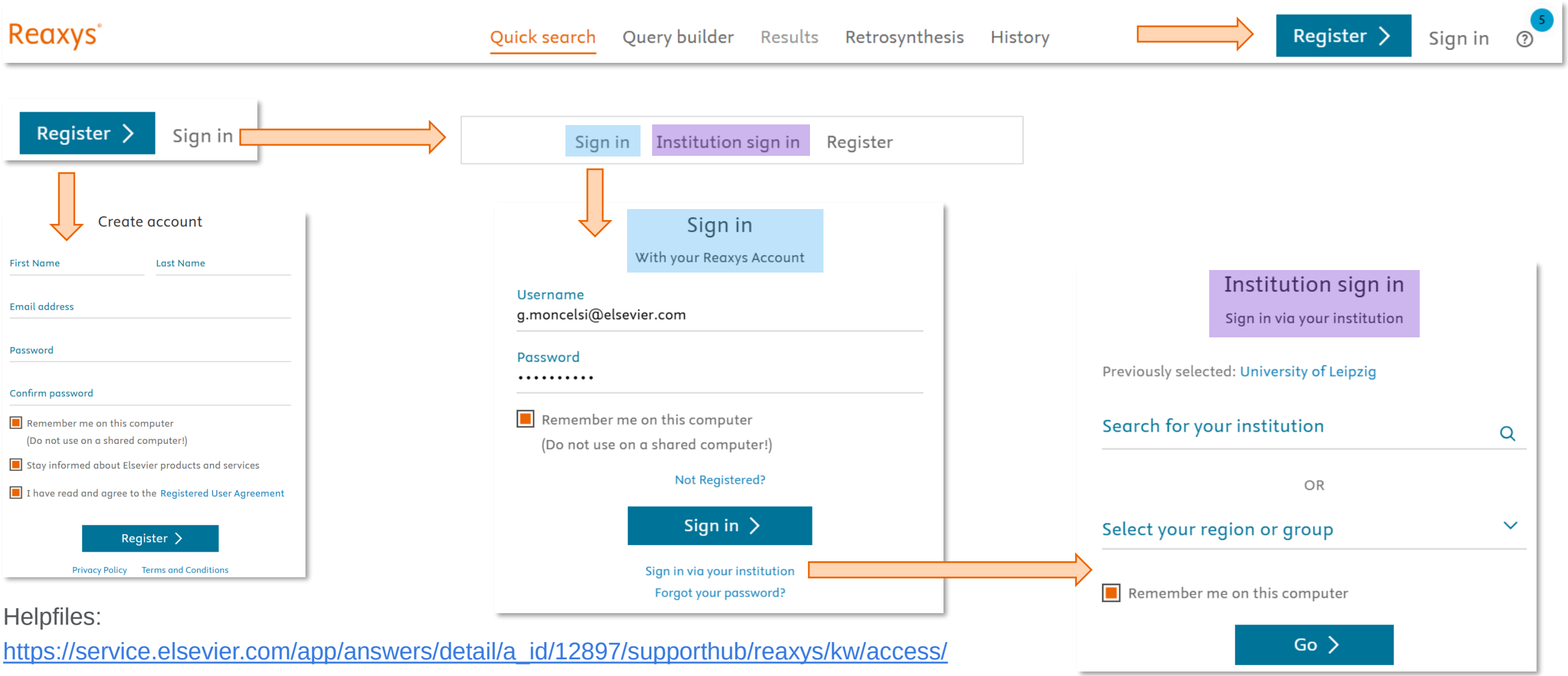

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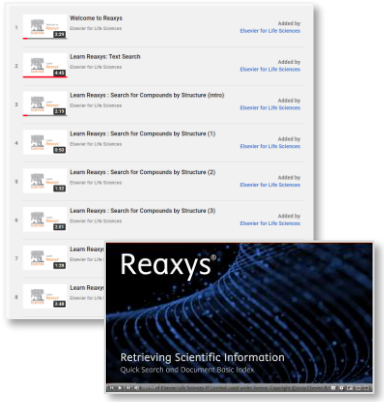

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Please reach out with any questions to:

- Dr. Giulia Moncelsi, g.moncelsi@elsevier.com