

Reaxys®

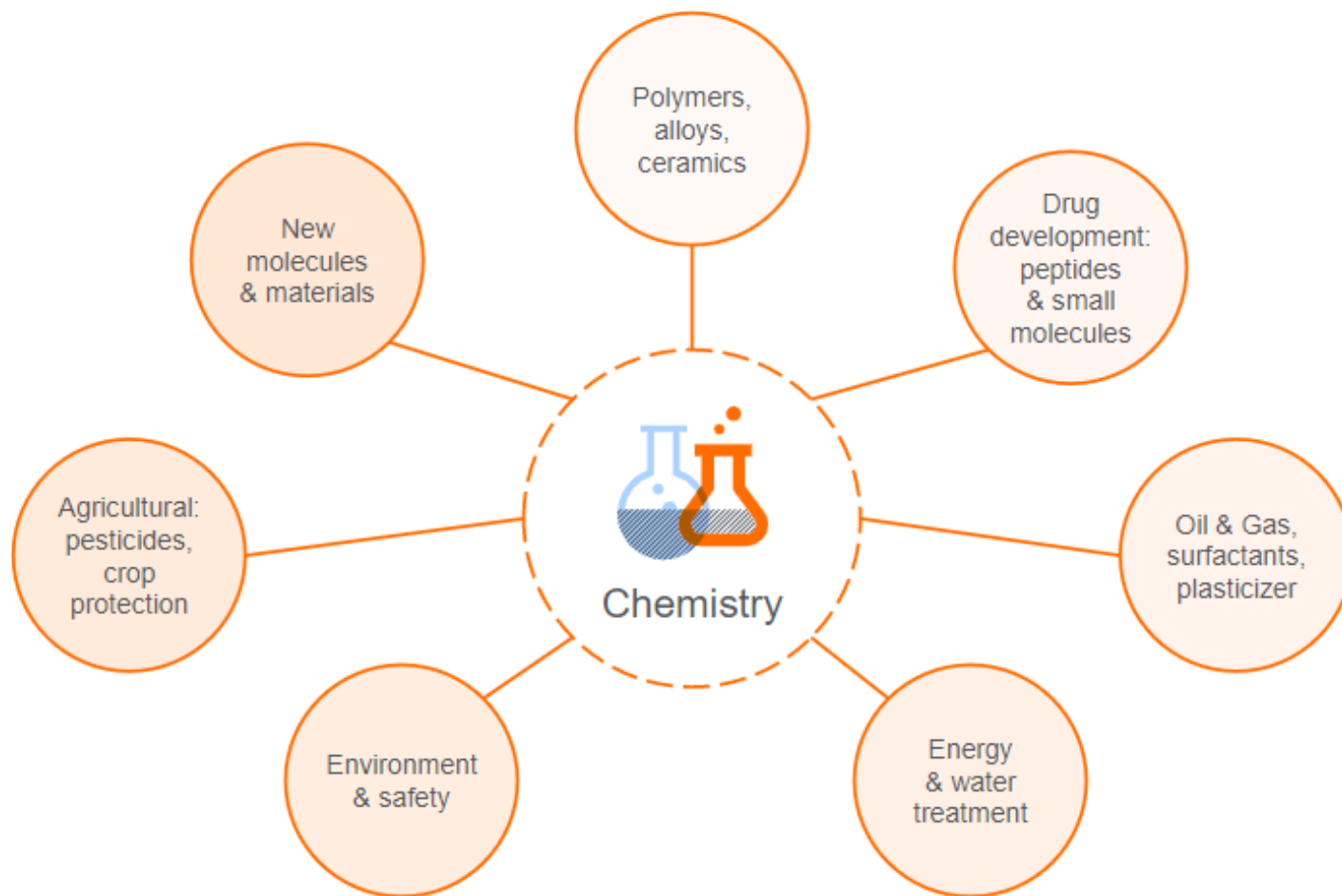
Introduction to Reaxys Academic Edition

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

1992: CrossFire launched

1989: Beilstein and Gmelin database go online

2013/2014: Complete revamp of Reaxys and content expansion

2009: Reaxys launched

2017: Reaxys Bioactivity & Targets module

2016: New Reaxys UI launched

2021: Patent Expansion to 46 M patents

2020: Reaxys Commercial Substances

2024: IKTOS AI Retrosynthesis

2021: Predictive Retrosynthesis (AI-based synthesis prediction)

Reaxys supports:



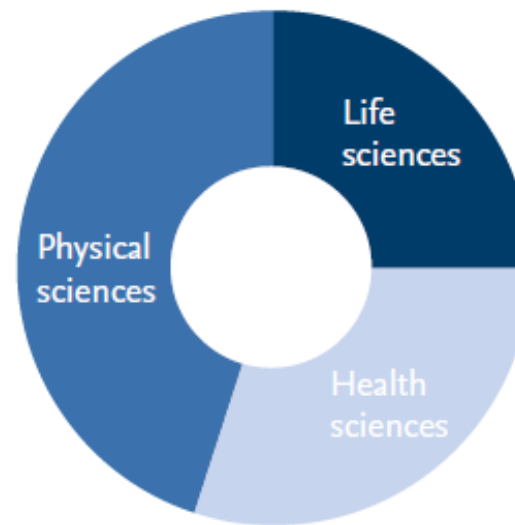
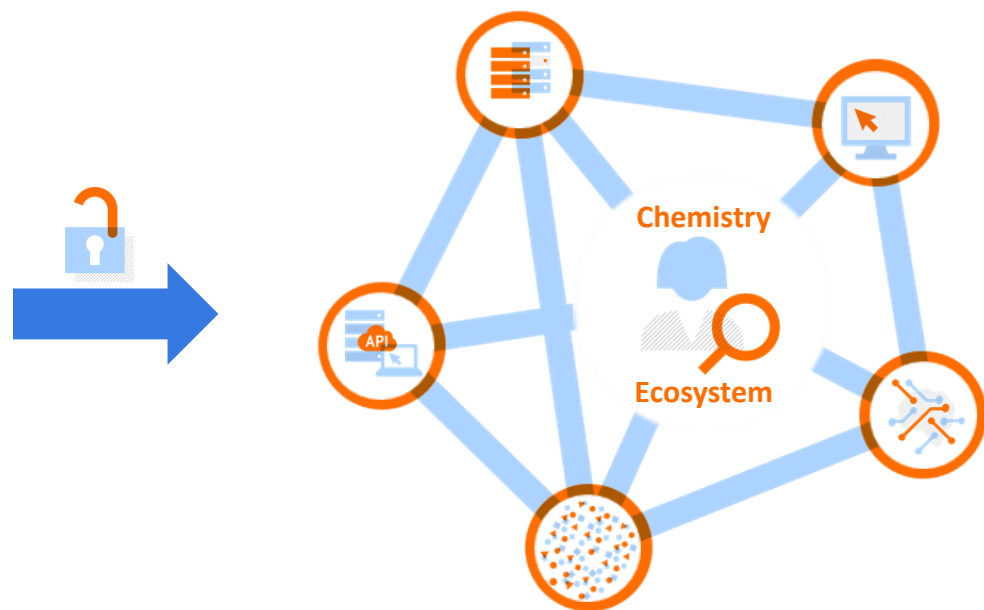
Research



Teaching & Learning

Reaxys Academic Edition

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**



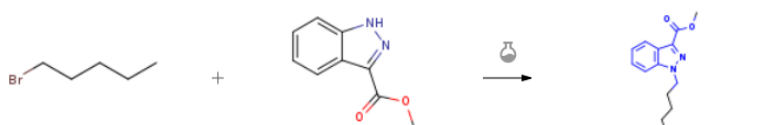
I am a chemist where I search using **text** because structure searches are difficult or not possible

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

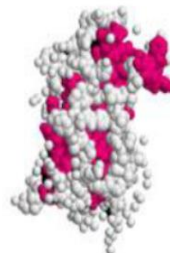


2 Hits 8 Conditions Find Similar Reaction ID: 41428311

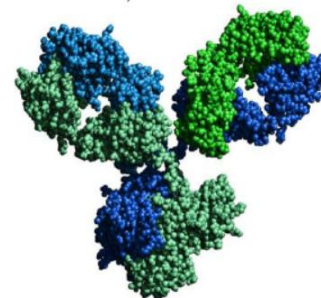
Conditions	Yield
Stage #1: methyl 1H-indazole-3-carboxylate With sodium hydride In tetrahydrofuran at 0°C; for 1h; Stage #2: 1-Bromopentane In tetrahydrofuran at 50°C; for 24h; regioselective reaction;	89%
Experimental Procedure	
With potassium tert-butyrate In tetrahydrofuran at 0 - 20°C; for 48h; regioselective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



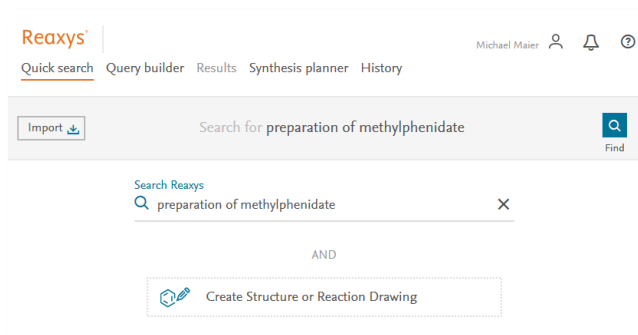


Reaxys®

Reaxys in action



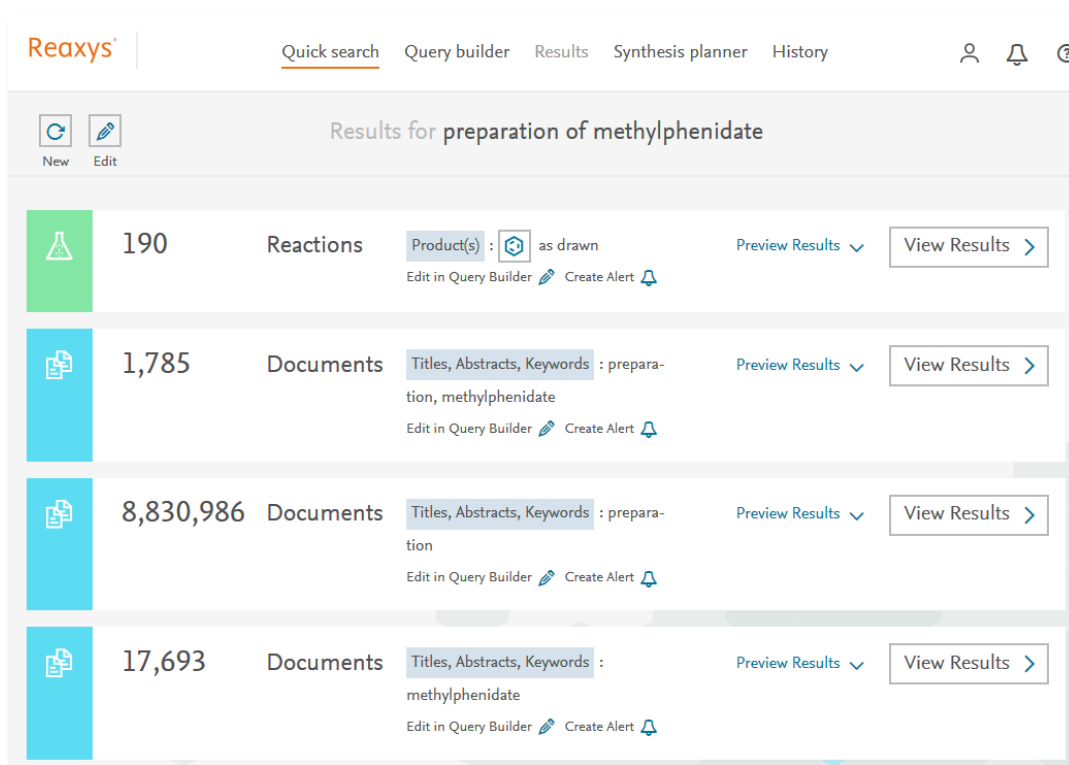
Reaxys produces results set adjusted to your needs



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



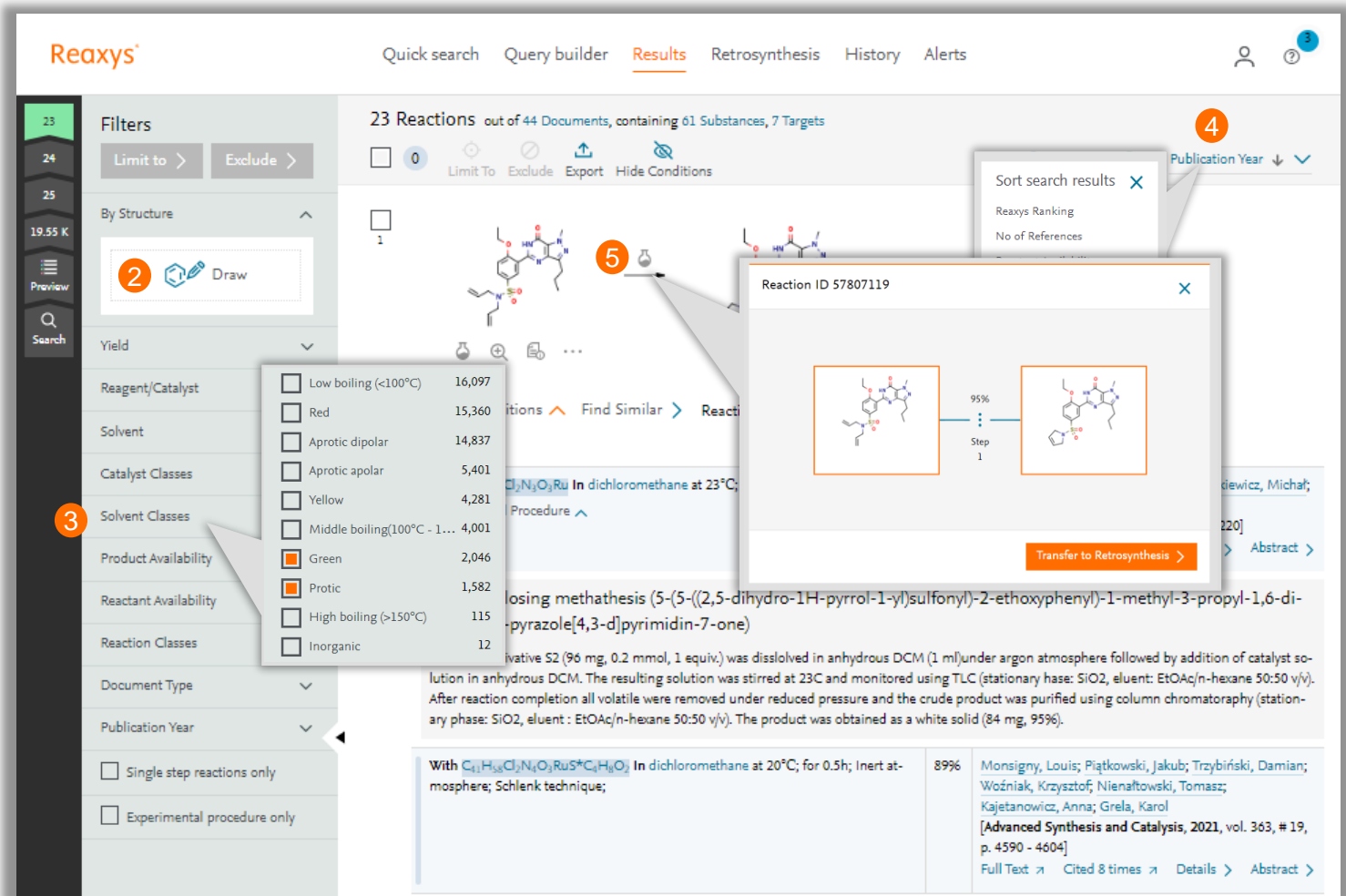
Reaxys
Quick search Query builder Results Synthesis planner History

Results for preparation of methylphenidate

190	Reactions	Product(s) : as drawn	Preview Results	View Results
1,785	Documents	Titles, Abstracts, Keywords : preparation, methylphenidate	Preview Results	View Results
8,830,986	Documents	Titles, Abstracts, Keywords : preparation	Preview Results	View Results
17,693	Documents	Titles, Abstracts, Keywords : methylphenidate	Preview Results	View Results

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

Discover new experimental procedures and verify results



Reaxys

Quick search Query builder **Results** Retrosynthesis History Alerts

23 Reactions out of 44 Documents, containing 61 Substances, 7 Targets

Limit To Exclude Export Hide Conditions

Sort search results
Reaxys Ranking
No of References

Reaction ID 57807119

95%
Step 1

Transfer to Retrosynthesis

Using methathesis (5-(5-((2,5-dihydro-1H-pyrrol-1-yl)sulfonyl)-2-ethoxyphenyl)-1-methyl-3-propyl-1,6-dihydropyrazolo[4,3-d]pyrimidin-7-one)

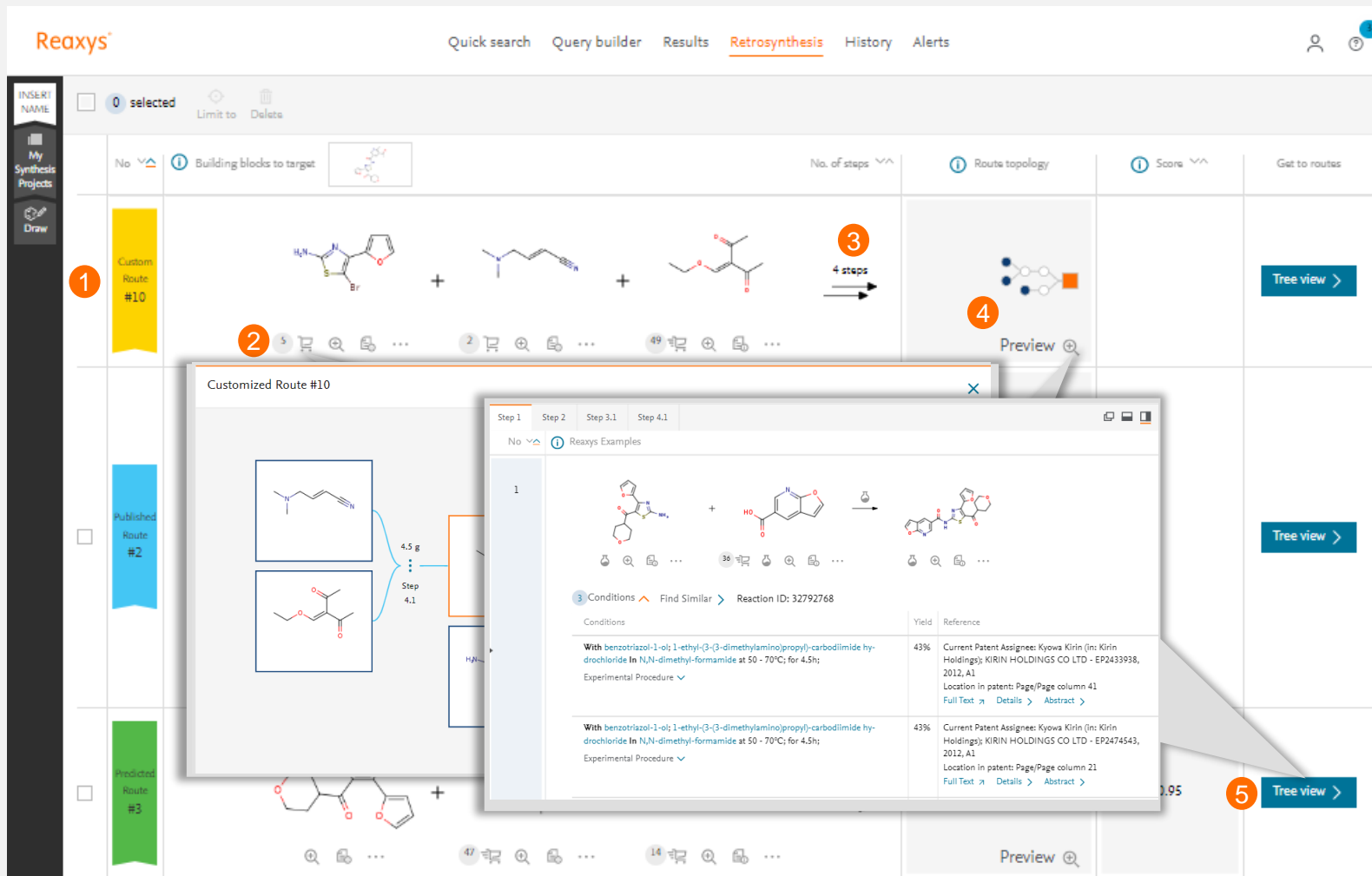
With $C_{11}H_{18}Cl_2N_4O_2RuS^+C_8H_8O_2$ In dichloromethane at 20°C, for 0.5h; Inert atmosphere; Schlenk technique;

89%

Monsigny, Louis; Piątkowski, Jakub; Trzybiński, Damian; Woźniak, Krzysztof; Nienafłowski, Tomasz; Kajetanowicz, Anna; Greła, Karol
[Advanced Synthesis and Catalysis, 2021, vol. 363, # 19, p. 4590 - 4604]
Full Text Cited 8 times Details Abstract

- 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

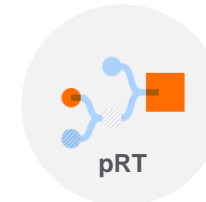
Quickly identify synthesis routes and assess costs



The screenshot displays the Reaxys Retrosynthesis interface. At the top, there are navigation options: Quick search, Query builder, Results, Retrosynthesis (selected), History, and Alerts. The main area shows a search for a target molecule (a benzimidazole derivative) with building blocks to target. Three routes are listed: Custom Route #10 (yellow), Published Route #2 (blue), and Predicted Route #3 (green). The Custom Route #10 is expanded, showing a 4-step synthesis plan. A 'Preview' window is open, showing a reaction step (Step 1) with conditions and references. The conditions are: With benzotriazol-1-yl; 1-ethyl-3-(3-dimethylamino)propyl)-carbodiimide hydrochloride in N,N-dimethyl-formamide at 50 - 70°C; for 4.5h; Experimental Procedure. The yield is 43%. The reference is: Current Patent Assignee: Kyowa Kirin (In: Kirin Holdings); KIRIN HOLDINGS CO LTD - EP2433938, 2012, A1. Location in patent: Page/Page column 41. Full Text > Details > Abstract >

- 1 View published, predicted & customized routes in one view
- 2 Assess the commercial 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 screenshot shows the Reaxys Retrosynthesis interface. On the left, a target molecule is displayed in a structure editor. On the right, the 'Parameters' panel is open, showing options for 'Predicted' and 'Intermediates'. The 'Predicted' section includes 'Length of routes' (set to 10), 'Regioselectivity', and 'Starting materials settings'. The 'Intermediates' section includes 'Enter intermediates' and 'Include substructures (up to 10)'. The interface is powered by IKTOS.

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



The screenshot shows the 'Results' tab of the Reaxys Retrosynthesis interface. It displays a table of predicted routes for a target molecule. The table has columns for 'Building blocks to target', 'No. of steps', 'First disconnection', 'Route topology', 'Score', and 'Get to routes'. Three routes are shown:

Route	Building blocks to target	No. of steps	Score
Predicted Route #37	[Chemical structures]	1 step	0.63
Predicted Route #38	[Chemical structures]	2 steps	0.62
Predicted Route #40	[Chemical structures]	3 steps	0.61

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



Commercial substances and suppliers' information



9 Commercial Substances

Structure : substructure; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals

Edit in Query Builder Create Alert

Preview Results View Results

1

tris(2-ethylhexyl) trimellitate

$C_{33}H_{54}O_6$ 546.788 2683525 3319-31-1

Shipping time: **Up to 5 days**
Best price: **3 USD/g**
Largest available package size: **Up to 10 kg**

Bioactivity (All)
Physical Data - 9

38

- 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,...

Select Building Block Libraries

- Standard Lab Chemical (STD)
- Commercial Substances in 10 days (RCS10D)
- Commercial Substances >10 days (RCS>10D)
- Commercial Substances <\$10/g (RCS\$10)
- Natural Products (NATP)
- Reaxys Starting Materials Occur 3 (RSM3)
- Reaxys Starting Materials Occur 4 (RSM4)
- Reaxys Starting Materials Occur gte 5 (RSM5)

Powered by PendingAI

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



Reaxys Prototype

Quick search Query builder Results Retrosynthesis

2,420 Documents with 82,185 Substances, 86,322 Reactions, 291 Targets

Limit to Exclude

Publication Year Document Type Authors/Inventors Current Parent Assignee Patent Office Journal Title Substance Classes Reaction Classes Index terms (List) Index terms (ReaxysTree)

KRAS G12D INHIBITORS
Current Patent Assignee: PFIZER INC; MIRATI THERAPEUTICS, INC.
Language(s): En, Cr Office(s): WO, EP, US, CN, JP, BR, TW, AU, KR, CL, IL, ZA, CO

WO2021/41671, 2021, A1
1 Abstract Index Terms Claims Bibliographic Info Substances 37 Reactions 2385 Targets Full Text

Abstract hit: {...a novel KRAS G12D inhibitor and a preparation method of the novel KRAS ...}

Claims hit: {...preparation of KRAS G12D drugs.21. A compound as shown in Equation (1)...}

Expand Patent Family 20

KRAS G12D INHIBITORS
21 Current Patent Assignee: MATIVAVARIRA, Alice
Language(s): En Office(s): EP
EP4021444, 2023, A4
Claims Bibliographic Info Full Text

Claims hit: {...GEMM-based studies, KRAS +/-LSI- G12D ;Trp53 LSI-R172H;Pdx1-Cre mice (KPC) and the KRAS +/-LSI- G12D ...}

Macrophages direct cancer cells through a LOXL2-mediated metastatic cascade in pancreatic ductal adenocarcinoma
Alonso-Nocelo, Marta; Ruiz-Cañás, Laura; Sancho, Patricia; Górgüla, Kivanc; Alcalá, Sonia; Pedrero, Coral; Vallespino, Mireia; (...) Cano, Amparo; Sainz, Bruno; [Gut, 2023, vol. 72, # 2, p. 345 - 359]
Abstract Index Terms Full Text

Abstract hit: {...GEMM-based studies, KRAS +/-LSI- G12D ;Trp53 LSI-R172H;Pdx1-Cre mice (KPC) and the KRAS +/-LSI- G12D ...}

Index Terms hit: {...cre recombinase, KRAS protein, lysyl oxidase like protein 2...}

2,420 Documents with 82,185 Substances, 86,322 Reactions, 291 Targets

Limit to Exclude

Publication Year Document Type Authors/Inventors Current Parent Assignee Patent Office Journal Title Substance Classes Reaction Classes Index terms (List) Index terms (ReaxysTree)

KRAS G12D INHIBITORS
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Language(s): En, Cr Office(s): WO, EP, US, CN, JP, BR, TW, AU, KR, CL, IL, ZA, CO

WO2021/41671, 2021, A1
1 KRAS G12D INHIBITORS
Abstract Index Terms Claims Bibliographic Info Substances 37 Reactions 2385 Targets Full Text

Abstract hit: {...a novel KRAS G12D inhibitor and a preparation method of the novel KRAS ...}

Claims hit: {...preparation of KRAS G12D drugs.21. A compound as shown in Equation (1)...}

EP4021444, 2023, A4
2 KRAS G12D INHIBITORS
Abstract Bibliographic Info Full Text

US2023/77225, 2023, A1
3 KRAS G12D INHIBITORS
Abstract Index Terms Claims Bibliographic Info Substances 378 Full Text

EP4182313, 2023, A1
4 KRAS G12D inhibitors
Abstract Bibliographic Info Full Text

WO2022/15375, 2022, A1
5 KRAS G12D INHIBITORS
Abstract Index Terms Claims Bibliographic Info Substances 359 Full Text

AU2020337938, 2022, A1
6 KRAS G12D inhibitors
Abstract Claims Bibliographic Info Full Text

AR119847, 2022, A1
7 KRAS G12D INHIBITORS
Abstract Bibliographic Info Full Text

BRPI2203543, 2022, A2
8 KRAS G12D INHIBITORS
Abstract Bibliographic Info Full Text

KR2022/71193, 2022, A
9 KRAS G12D Inhibitors
Abstract Index Terms Claims Bibliographic Info Substances 1463 Full Text

CN114615981, 2022, A
10 KRAS G12D inhibitors
Abstract Index Terms Claims Bibliographic Info Substances 2272 Full Text

IN202217012614, 2022, A
11 KRAS G12D INHIBITORS
Abstract Bibliographic Info Full Text

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

Scientific Reports • Open Access • Volume 11, Issue 1 • December 2021 • Article number 7260

Phytochemical profile and rosmarinic acid purification from two Peruvian *Lepechinia* Willd. species (Salviinae, Mentheae)

Serrano C.A.^a, Villena G.K.^b, Rodriguez E.E.^c

Save all to author list

^aLaboratorio de Química Orgánica, Universidad Nacional de San Antonio

^bLaboratorio de Micología y Biotecnología, Universidad Nacional Agraria

^cHerbarium Truxillense (HUT), Universidad Nacional de Trujillo-Perú, Trujillo

5

Views count

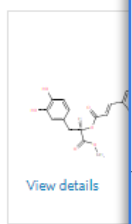
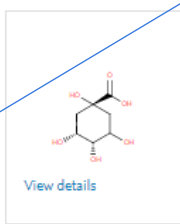
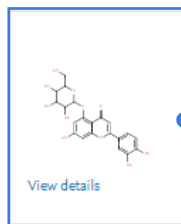
View all metrics

Abstract

The phytochemical profile of *Lepechinia meyenii* (Walp.) Epling et Benth. Epling obtained by liquid chromatography associated with spectrometry is presented. Forty eight compounds were detected salvanolic acids and abietane phenolic diterpenoids. A simple crystallization to purify rosmarinic acid from these botanical species. The Author(s).

Reaxys Chemistry database information

Substances



View all details in Reaxys

Powered by Reaxys

Back to overview

Rosmarinic acid

Chemical names
rosmarinic acid, Rosmarinic acid, α-O-caffeoyl-β-(3,4-dihydroxyphenyl)lactic acid, Rosmarinsaeure

Molecular formula
C₁₈H₁₆O₈

CAS Registry Number
179462-74-9

Suppliers Druglikeness Preparations

Available data

- Bioactivity (373)
- Physical Data (9)
- Spectra (28)
- Other data (219)

View all details in Reaxys

Reaxys

Filters

Limit to > Exclude >

- By Structure
- Measurement pX
- Highest Clinical Phases
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Availability in other databases
- Available Data
- Document Type
- Publication Year
- Patent Assignee
- LogP
- H Bond Donors
- H Bond Acceptors
- Rotatable Bonds
- TPSA

1 Substances

out of 6,834 Documents, containing 27 Reactions, 15 Targets

0 selected

Limit To Exclude Export Preparations

rosmarinic acid
C₁₈H₁₆O₈ 360.32 2227586 179462-74-9

Identification
Druglikeness

rosmarinic acid

- Identification
- Druglikeness
- Bioactivity (All)
 - In vitro: Efficacy - 91
 - In vivo: Animal Model - 6
 - Metabolism - 1
- Physical Data - 9
- Spectra - 28
- Other Data - 219



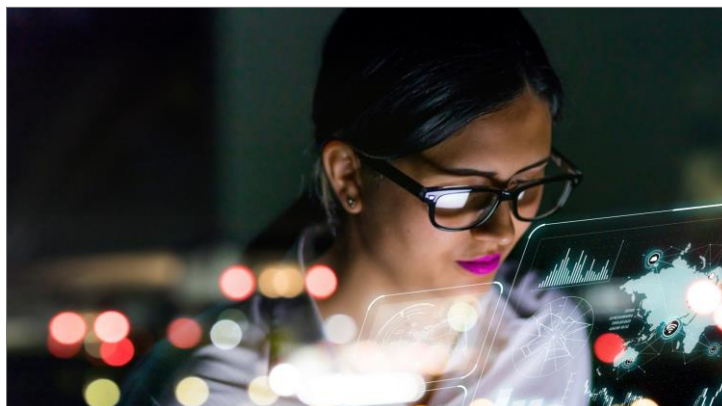
Answer questions for hit-to-lead and lead optimization



- ✓ **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

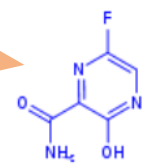
Favipiravir is an antiviral medication used to treat influenza. It is also being studied to treat several other viral infections, including SARS-CoV-2.

Quick search Query builder Results Retrosynthesis History Alerts

Results for "favipiravir" New Edit

69 Substances Structure : as drawn Preview Results View Results >

3,864 Documents Titles, Abstracts, Keywords : "favipiravir" Preview Results View Results >



favipiravir
C₅H₄N₃O₂F 157.104 9697246 259793-96-9

Identification Preparations - 45 >

Druglikeness Reactions - 99 >

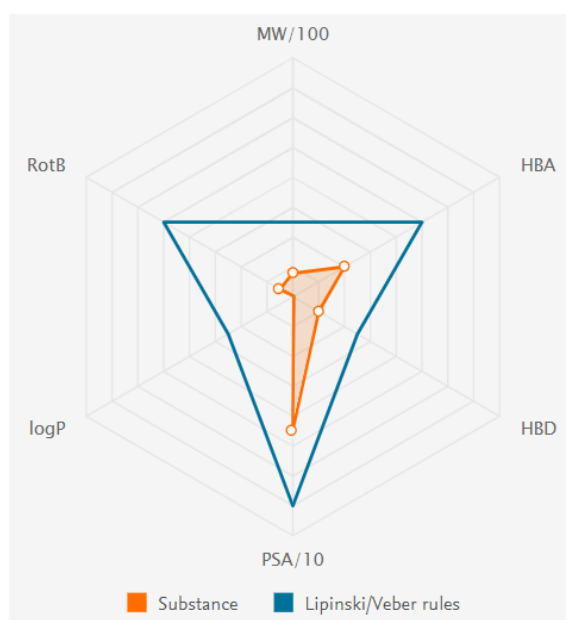
Bioactivity (All) Targets - 22 >

Physical Data - 34 Documents - 209 >

Spectra - 18

Other Data - 117

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



Bioactivity (All)

- ✓ In vitro: Efficacy - 680
- ✓ In vivo: Animal Model - 138
- ✓ Metabolism - 35
- ✓ Pharmacokinetic - 50
- ✓ Toxicity/Safety Pharmacology - 133

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.

^ Bioactivity (All)

- ✓ In vitro: Efficacy - 680
- ✓ In vivo: Animal Model - 138
- ✓ Metabolism - 35
- ✓ Pharmacokinetic - 50
- ✓ Toxicity/Safety Pharmacology - 133

^ In vitro: Efficacy - 680

Quantitative Results

pX	Parameter	Value (qual)	Value (quant)	Unit	Target	Tissue/Organ	5...	Reference
8	inhibition rate	Active			RNA-dependent RNA polymerase [Influenza virus]:Wild			Mizuta, Satoshi; Otaki, Hiroki; Ishikawa, Takeshi; Makau, Juliann Nzembi; Yamaguchi, Tomoko; Fujimoto, Takuya; Takakura, Nobuyuki; (...) Nishida, Noriyuki; Watanabe, Ken [Journal of Medicinal Chemistry, 2022, vol. 65, # 1, p. 369 - 385] Full Text > Details > Abstract >
7.22	IC50		0.06	µM		tendon		Bengue, Michèle; Pintong, Ai-Rada; Liegeois, Florian; Nougairède, Antoine; Hamel, Rodolphe; Pompon, Julien; de Lamballerie, Xavier; Roques, Pierre; Choumet, Valérie; Missé, Dorotheé [Viruses, 2021, vol. 13, # 11, art. no. 2213] Full Text > Details > Abstract >
7.17	EC90	=	0.61					

Show/Hide columns

Show/Hide columns

- pX
- Parameter
- Value (qual)
- Value (quant)
- Unit
- Biological Species
- Action on target
- Target
- (Clinical) findings / disease
- Tissue/Organ
- Cell
- Bioassay
- Dose
- Effect
- Concomitants
- Metabolites
- Reference

Export substances Reaxys

Choose a format: PDF/Print

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Tab-delimited text
- Electronic Lab Notebook
- RD File
- SD/Molfile
- Smiles

Additional options: Include a description in the document

pX	Parameter	Unit	Action on target	Target
5.1	IC50 (virus load)	µg/ml	Inhibitor	Envelope glycoprotein N [Bunyaviridae]:Wild
5.09	EC50	µM		
5.08	EC50	µM	Substrate	Hypoxanthine-guanine phosphoribosyltransferase:Wild
5.07	EC90	µM		
5.05	EC50	µM	Substrate	Hypoxanthine-guanine phosphoribosyltransferase:Wild

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

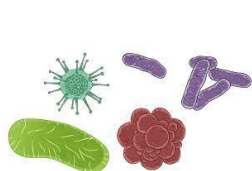


In vitro is a process performed or taking place in a living organism.

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[<i>Antiviral Research</i> , 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[<i>Viruses</i> , 2021, vol. 13, # 11, art. no. 2213] Full Text ↗ Details > Abstract >



Various biological species: more than 65.000



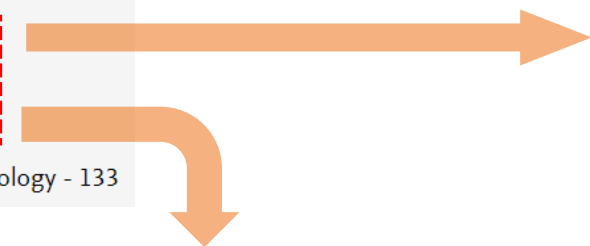
Bioactivity of a substance and pharmacy targets

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 (Ctough) (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]

Bioactivity of a substance and pharmacy targets

5 Toxicity / Safety Pharmacology

^ Bioactivity (All)

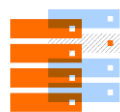
- ✓ In vitro: Efficacy - 680
- ✓ In vivo: Animal Model - 138
- ✓ Metabolism - 35
- ✓ Pharmacokinetic - 50
- ✓ Toxicity/Safety Pharmacology - 133

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



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



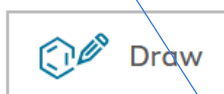
Enhancing text search for document discovery

Text search today: Ontology supported Lexical search

Search Reaxys

microencapsulation sustained drug delivery

AND



1 Potential use of microencapsulation for sustained drug delivery to the respiratory tract

[Haghpanah](#); [Marriott](#); [Martin](#) [[Journal of Aerosol Medicine](#), 1994, vol. 7, # 2, p. 185-188]

[Abstract](#) [Index Terms](#) [Full Text](#)

[Cited 2 times](#)

Abstract

Microencapsulation has long been regarded as a means of achieving sustained drug delivery. In these studies, a spray drying technique was used to produce salbutamol-loaded albumin microparticles with a view to formulating a controlled release system to be used in respiratory drug delivery. Encapsulation efficiencies (40-60 % w/w) obtained using this technique compared very favourably with those obtained using emulsification procedures (1-2 % w/w).

Index Terms

EMTREE drug term: albumin • butanol • microsphere • oleic acid • salbutamol

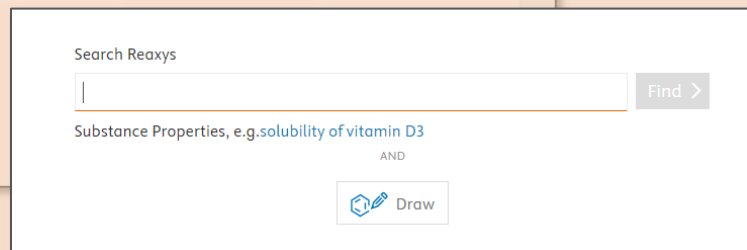
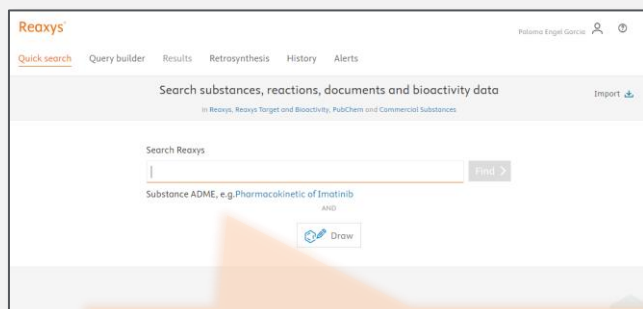
EMTREE medical term: conference paper • drug delivery system • dry deposition • emulsion • inhalational drug administration • microencapsulation • nebulizer • particle size • powder • respiratory system • sustained release preparation

- 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

Users have a growing need to search through natural language queries



Initiatives to improve natural language-based searching

Lexical

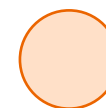


Enhancements in keyword search, with new document relevancy ranking for improved document discoverability through **lexical** search



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



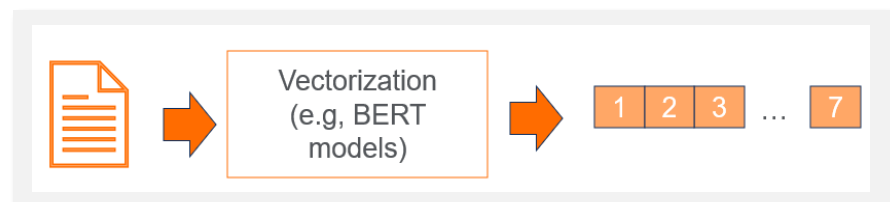
What is vector search



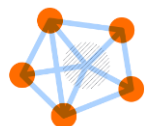
Vectors and the vectorisation of Reaxys data to enable smarter search



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



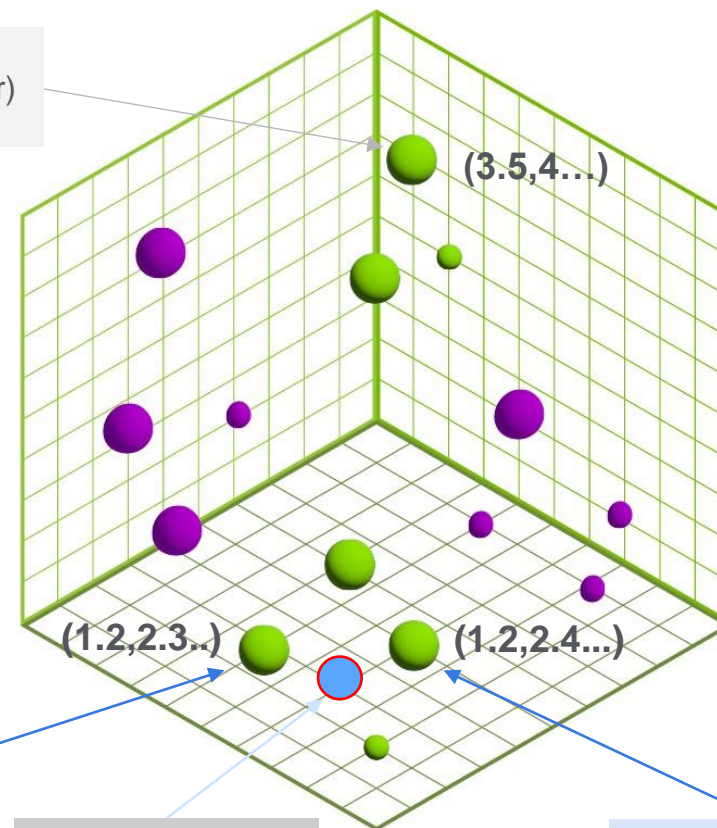
User query is also converted into vectors and represented as numerical values



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

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

Suzuki Swift (car)



Carbon-carbon bond formation


Query: what is Suzuki Reaction?
(1.2, 2.2..)

Suzuki coupling



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



 Reaxys Beta

Explore the new Reaxys Semantic Search

Reaxys Beta covers documents from (describe limitations from the results set) [Learn how it works](#)

Insert any natural language query and our system will find relevant documents to match it

All [Export as CSV file](#)

Mn-Based Catalysts for Post Non-Thermal Plasma Catalytic Abatement of VOCs: A Review on Experiments, Simulations and Modeling [↗](#)
1
[2021]
Score: 0.8399641513824463

Abstract:
The combination of non-thermal plasma (NTP) and catalyst characterized by high energy efficiency, enhanced volatile organic compounds (VOCs) removal efficiency, high product selectivity, and low production of unwanted and/or toxic by-products possesses a great promise for the abatement of VOCs. This work reviews the state of knowledge regarding Mn-based catalysts for VOCs abatement in the post-plasma-catalytic (PPC) system. First, the development and the performance of different Mn-based catalysts such as pure manganese oxide, mixed manganese oxide-based catalysts, and supported Mn-based catalysts in terms of VOCs abatement and O3 decomposition are summarized. Then, the mechanism of the VOCs decomposition in the NTP and PPC system is discussed. Finally, the modeling and simulation of VOCs abatement in the NTP and PPC system are overviewed. This review aims at providing a reference guide for the development and optimization of VOCs abatement in the PPC system using Mn-based catalysts. Graphic abstract: [Figure not available: see fulltext.]

Was this relevant to the question? [↺](#) [↻](#)

Catalytic removal of toluene using MnO2-based catalysts: A review [↗](#)
2
[2023]
Score: 0.8587478399276733

Abstract:
Volatile organic compounds (VOCs) have serious hazard to human health and ecological environment. Due to its low cost and high activity, the catalytic oxidation technology considered to be the most effective method to remove VOCs. Toluene is one of the typical VOCs, hence its catalytic elimination is crucial for the regulation of VOCs. Manganese dioxide (MnO2) has been extensively studied for its excellent redox performance and low-temperature operation conditions. In this review, we summarize the

- ✓ 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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287 M
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48 M
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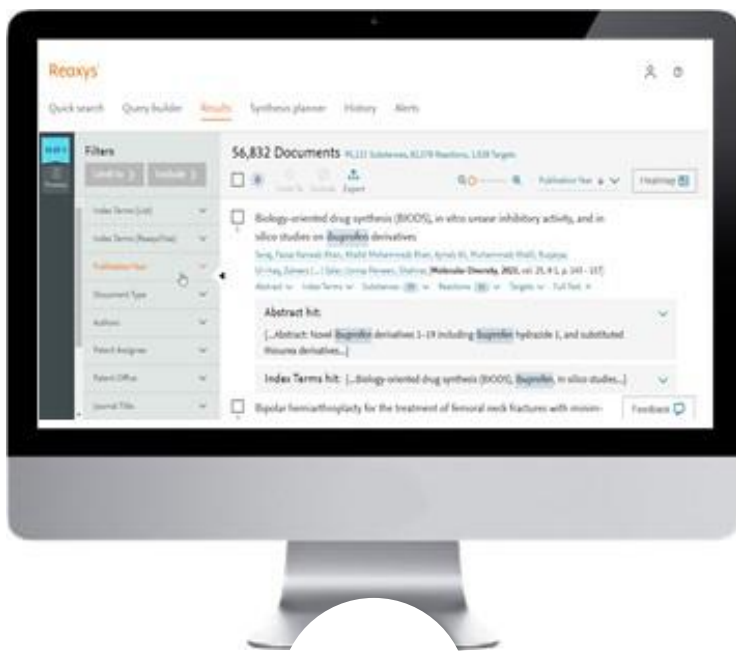
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Core content



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With 48 million bioactivity data points, to achieve rapid hit identification and lead optimization.

Additional content and features included



Predictive Retrosynthesis:

A best-in-class innovation redesigned for synthetic and medicinal chemists, to boost success rates in synthesis route design and prediction.

Additional content and features included



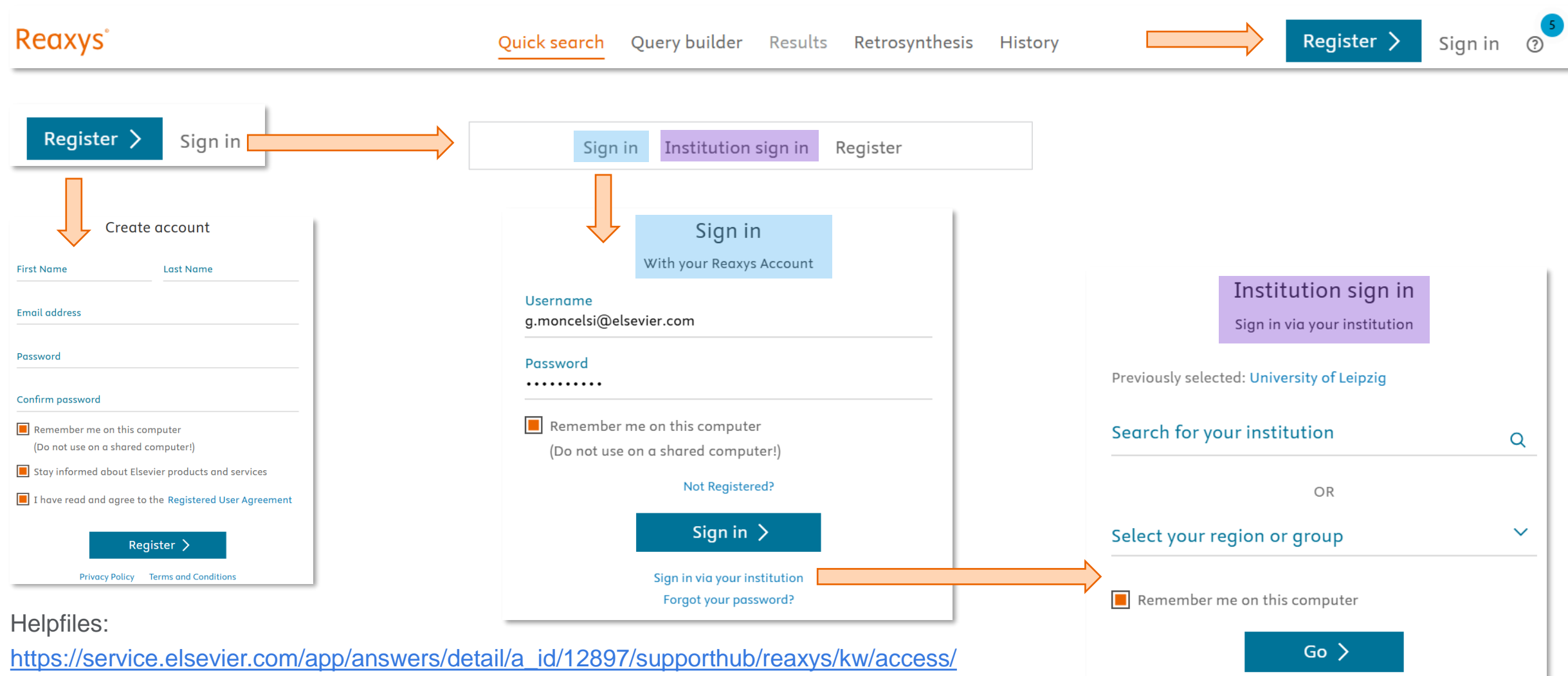
Reaxys®

Learning resources



How to access Reaxys

Reaxys URL: <https://www.reaxys.com>



The image shows the Reaxys website interface with three sequential screens for user access, connected by orange arrows:

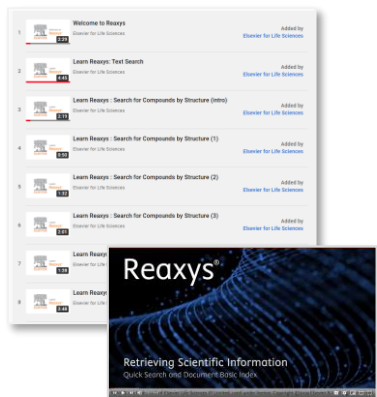
- Navigation Bar:** Features the Reaxys logo, a search bar, and menu items: Quick search, Query builder, Results, Retrosynthesis, History, Register >, and Sign in. A notification badge with the number 5 is next to Sign in.
- Registration Screen:** Titled "Create account", it includes fields for First Name, Last Name, Email address, Password, and Confirm password. It also has checkboxes for "Remember me on this computer", "Stay informed about Elsevier products and services", and "I have read and agree to the Registered User Agreement". A "Register >" button is at the bottom.
- Sign-in Screen:** Titled "Sign in With your Reaxys Account", it includes fields for Username (g.moncelsi@elsevier.com) and Password. It has a "Remember me on this computer" checkbox and a "Sign in >" button. Links for "Not Registered?", "Sign in via your institution", and "Forgot your password?" are also present.
- Institution Sign-in Screen:** Titled "Institution sign in Sign in via your institution", it shows "Previously selected: University of Leipzig", a search bar for institutions, an "OR" separator, a dropdown for "Select your region or group", and a "Remember me on this computer" checkbox. A "Go >" button is at the bottom.

Helpfiles:

https://service.elsevier.com/app/answers/detail/a_id/12897/supporthub/reaxys/kw/access/

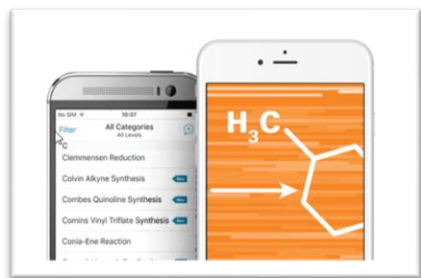
https://service.elsevier.com/app/answers/detail/a_id/28070/supporthub/reaxys/kw/access/

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- **Reaxys Academy** is a self-paced, online chemistry training for librarians, researchers, instructors and students. Designed to support learning and teaching chemistry concepts, and to use digital chemistry tools efficiently. Includes post-course quizzes and certificates of completion.

- **Reaxys Retrosynthesis** is a vital tool when teaching advanced synthesis courses



- **ReactionFlash** app makes learning named reactions easy and fun, by providing access to over 1000 Named Reactions and examples in Reaxys

Link:



Link:



Reaxys 101 Self-paced course



This course is ideal for librarians, educators, researchers and students who are looking to get an introduction to Reaxys or enhance their skills and understanding of Reaxys as a platform for research.

Designed by chemists, Reaxys is a web-based, chemical search engine that allows you to search for chemical reactions, (parts of) chemical structures and substance properties. Approximate time to complete – 30-45 minutes.

Introduction to Reaxys

- [Welcome to Reaxys](#)

Conducting textual searches

- [Literature Search: How to retrieve documents for a topic of interest](#)
- [Search for Reaction by text terms](#)

Searching by structure

- [An introduction to searching for compounds by structure in Reaxys](#)
- [How to create a structure drawing from a substance name in Reaxys](#)
- [How to create a structure](#)

[Take the quiz](#)

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Reaxys can broaden the understanding of chemistry for any level of student: from undergraduate and graduate to post-graduate and beyond.

Chemists need exposure to relevant chemistry databases early in their careers to effectively learn chemistry, gain chemistry digital literacy skills, and be well-prepared for their research projects and labs. Approximate time to complete – 45-60 minutes.

Obtaining reaction data

- [How to obtain UV/Vis and IR spectroscopic data](#)
- [How to obtain characterization data on pH indicators](#)
- [How to obtain pKa data of phenols](#)
- [Vickers hardness of lanthanoids](#)

Working with chemical reactions

- [How to identify named reactions](#)
- [The Diels-Alder cycloaddition reaction](#)
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Thank you

Please reach out with any questions to:

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

