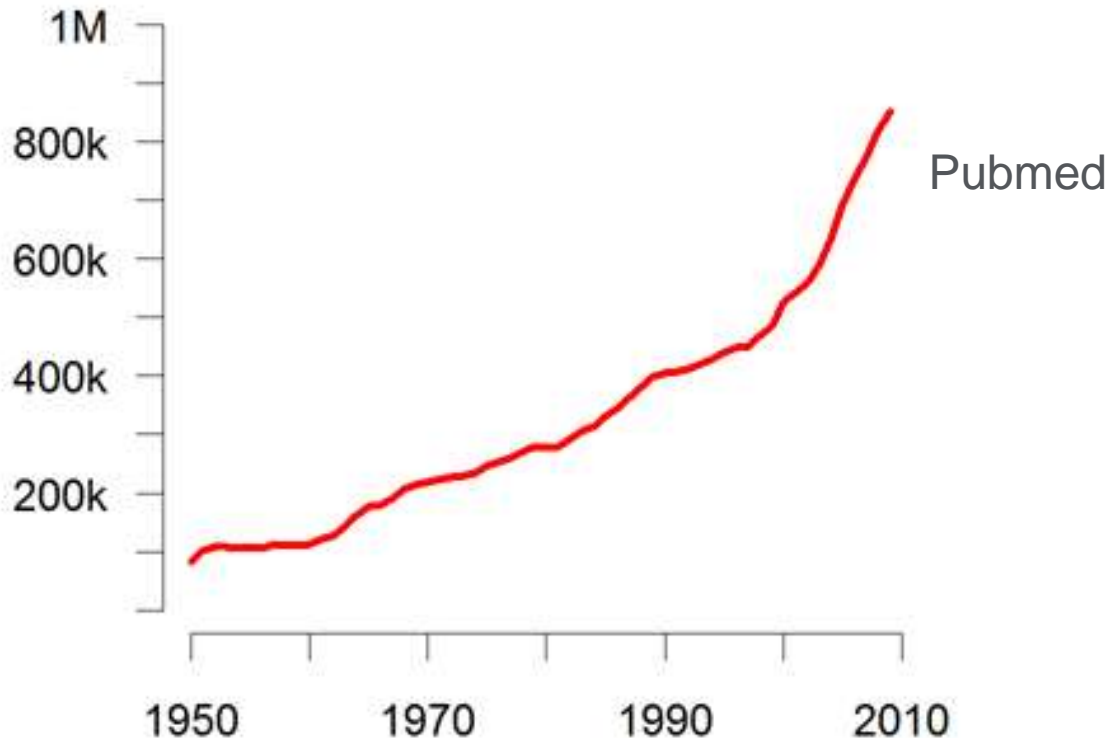


Introduction to Reaxys 2017

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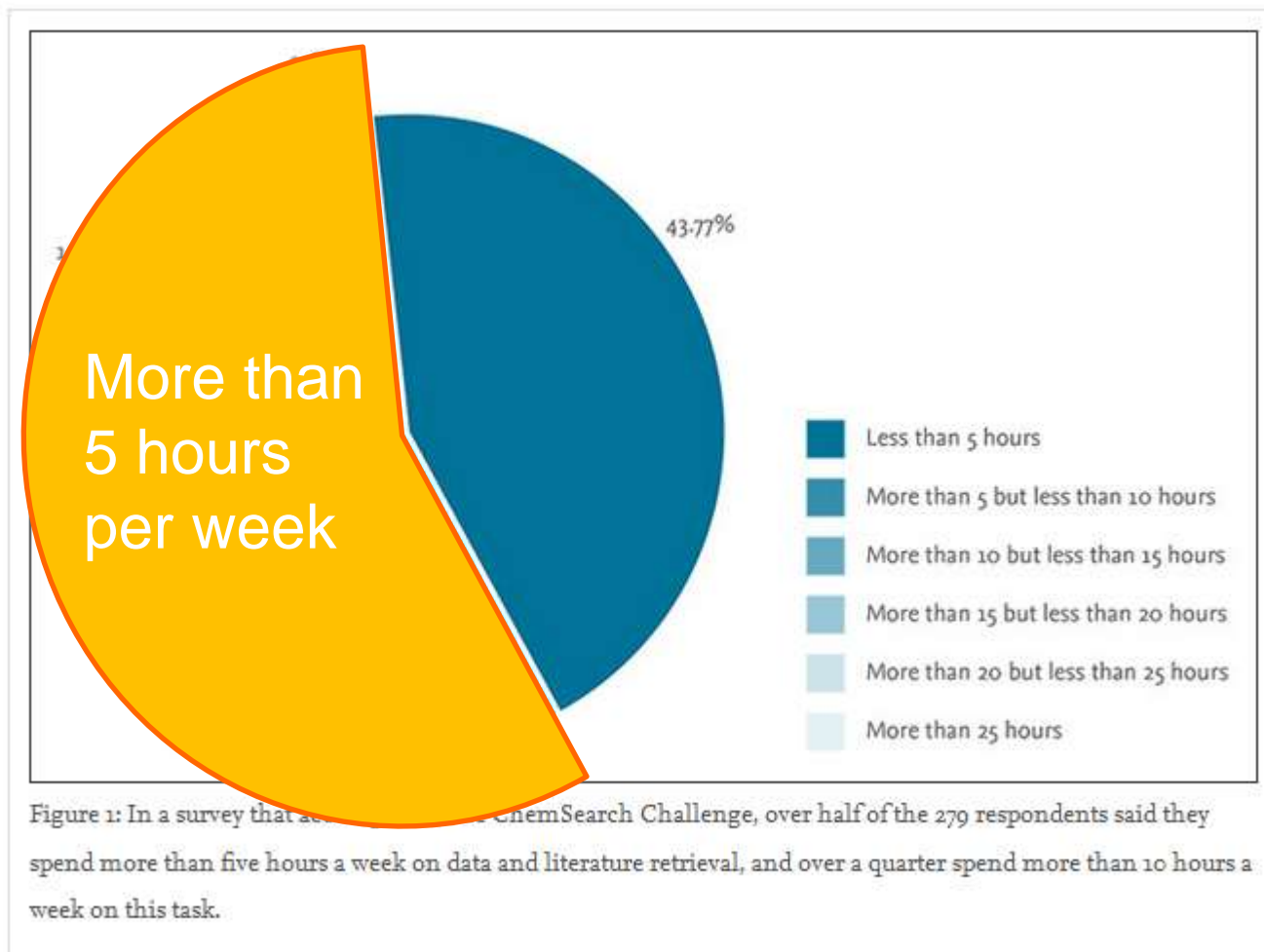
Number of scientific publications grows exponentially



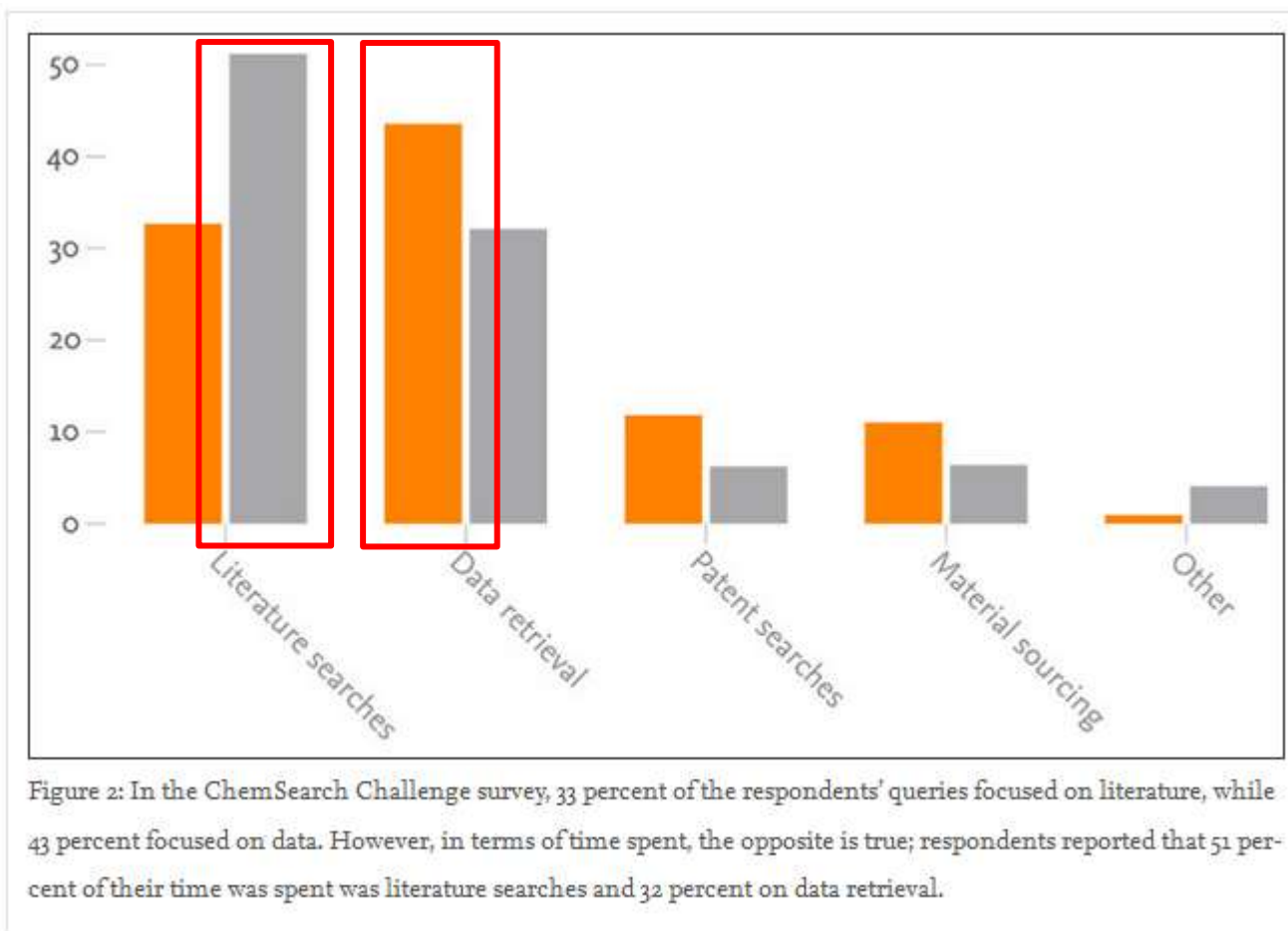
... as grows their dispersion ...



„recent estimates from Google analytics suggest as many as 42% of highly cited papers appear in journals that are not traditionally highly cited”

Time spent on literature searching



What do researchers search for (Life Science) ?



-  — What sort of info they search
-  — Time spent on searching

Serving the life sciences space

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN

Characterize
targets & analyze
disease pathways

 **PATHWAY STUDIO™**

Characterize & discover
molecules
Identify & confirm lead
compounds

 **REAXYS®**
Medicinal Chemistry
 **REAXYS®**

Translate preclinical
data in humans
(Translational)

 **PHARMAPENDIUM™**

Monitor drug adverse
events &
real-world evidence
data in literature

 **EMBASE™**

Biology

Chemistry

Pharmacy

Bio-medicine

Bio-chemistry

Discovery

Pre-clinical

Clinical

Post-launch

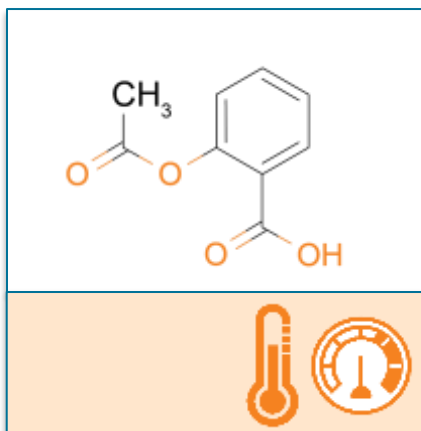
Broader full-text indexing
of biomedical content

ScienceDirect

 **EMBASE™**

Scopus

Reaxys is a powerful allround research solution for facts and literature



>100 M Substance records with **>500 M** excerpted facts on their **properties**: physical, chemical, spectral, ecological, bioactivity



>41 M Reaction records including excerpted data on reaction conditions, solvents, catalyst, yield



>52 M Document records from 16,000 journals and patents describing applications in material sciences, biomedicine, technology, geosciences, engineering, environmental sciences, pharmacology...




Chemistry fundamentals

Uses across disciplines

What does Reaxys2017 look like?

A clean, streamlined user interface fits to how YOU search and grants access to unparalleled content

Reaxys®


Elsevier Reaxys   


Search substances, reactions, documents and bioactivity data in [Reaxys](#), [PubChem](#) and [eMolecules](#)

Quick Search

Query Builder

Saved Searches

 Substance Property, e.g. [ferroelectric materials](#)

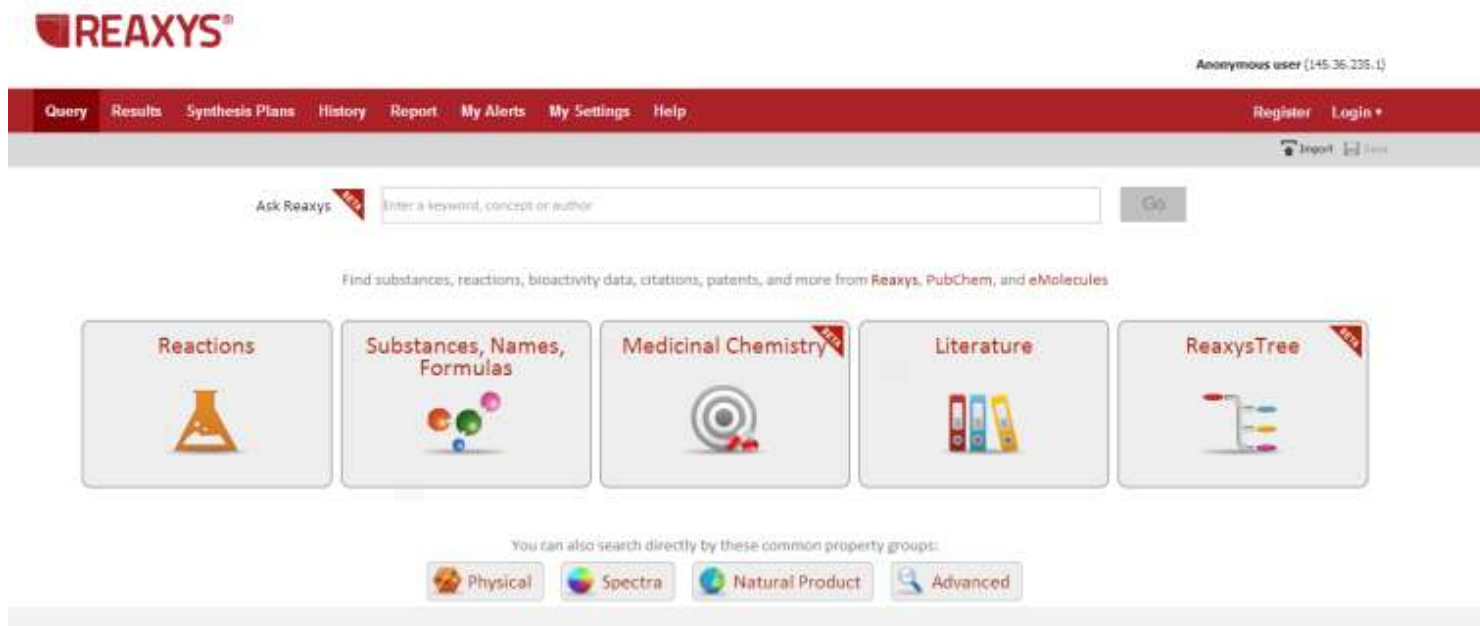
 Create Structure or Reaction Drawing

Search >

Old interface

SEARCH

REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION



A clean, streamlined user interface fits to how YOU search and grants access to unparalleled content

The image shows a screenshot of the Reaxys website interface. At the top left is the 'Reaxys' logo. To its right are links for 'Elsevier Reaxys', a user profile icon, a search icon, and a menu icon. Below the header is a grey banner with the text: 'Search substances, reactions, documents and bioactivity data in Reaxys, PubChem and eMolecules'. Underneath the banner are three tabs: 'Quick Search' (which is underlined), 'Query Builder', and 'Saved Searches'. Below the tabs is a search input field containing the text 'Substance Property, e.g. ferroelectric materials'. Below the input field is a dashed box containing a chemical structure icon and the text 'Create Structure or Reaction Drawing'. To the right of the input field is a blue 'Search >' button. Three orange lines with circular endpoints point to specific features: one points to the 'Quick Search' tab, another points to the 'Query Builder' tab, and a third points to the search input field. Three text annotations are placed around the interface: 'Common search types using natural language and familiar terms' points to the search input field; 'Build your own queries by combining diverse intelligent search fields' points to the 'Query Builder' tab; and 'For Quick Search, simply enter a search phrase and/or draw a structure.' points to the search input field.

Reaxys®

Elsevier Reaxys

Search substances, reactions, documents and bioactivity data in Reaxys, PubChem and eMolecules

Quick Search Query Builder Saved Searches

Substance Property, e.g. ferroelectric materials

Create Structure or Reaction Drawing

Search >

Common search types using natural language and familiar terms

Build your own queries by combining diverse intelligent search fields

For **Quick Search**, simply enter a search phrase and/or draw a structure.

Quick Search recognizes search intention and lists alternative hitsets

Search Reaxys
Q esterification of benzoic acid

Create Structure or Reaction Drawing

Interprets natural language ①

② Recognizes search intention (reactions)

③ Delivers a ranked list of alternative results suggestions

Count	Category	Preview Results	View Results
82	Reactions	Preview Results ▼	View Results >
399	Documents	Preview Results ▼	View Results >
21316	Documents	Preview Results ▼	View Results >
48655	Documents	Preview Results ▼	View Results >

Alternatively, use **Query Builder** to create your own targeted queries without being an expert

The screenshot shows the Reaxys Query Builder interface. At the top, a search bar is labeled with a circled '4' and the text 'Enter search terms and click Search.' Below this is a toolbar with icons for Structure, Formula, Number, IChIndex, Favourites, Save to file, Save form, Reset form, and Delete. The main workspace is divided into two sections. The top section, labeled 'Structure', contains a 'Create Structure / Reaction Drawing' button. The bottom section is a query builder area with a dropdown menu set to 'AND'. It contains two query boxes: 'Melting Point' and 'Boiling Point'. An orange arrow points from the 'AND' dropdown to a circled '3' with the text 'Combine them with operators'. Another orange arrow points from the 'Boiling Point' query box to a circled '2' with the text 'Drag and drop them into a query'. On the right side, a 'Search properties' panel is visible, listing various properties such as Autoignition, Azeotropes (MCS), Boiling Point, Boundary Surface Phenomena (MCS), Bulk Viscosity, Chromatographic Data, Circular Dichroism, Complex Phase Equilibria (MCS), Compressibility, Conformation, Critical Density, Critical Micelle Concentration (MCS), Critical Pressure, Critical Temperature, and Critical Volume. An orange bracket on the right side of this panel is labeled with a circled '1' and the text 'Search Querylets'.

4 Enter search terms and click Search.

1 Search Querylets

3 Combine them with operators

2 Drag and drop them into a query

Each record retrieved offers multiple touch points to discover more within and outside of Reaxys

Display associated index terms

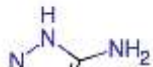
☐ Fused heterocyclic compounds bearing bridgehead nitrogen as potent HIV-1 NNRTIs.
Part 1: Design, synthesis and biological evaluation of novel 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives
Tian, Ye Du, Deping; Rao, Diwanar; +6 others - Bioorganic and Medicinal Chemistry, 2014, vol. 22, # 7, p. 2052 - 2059
Abstract ^ Index Terms ^ Substances ^ Reactions ^ Full Text ^

Cited 1 times

View citing articles in Scopus

Abstract:

In our continuous efforts to identify novel potent HIV-1 NNRTIs, a novel class of 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives were rationally designed, synthesized and evaluated for their anti-HIV activities in MT4 cell. Most of the tested compounds displayed excellent activity against wild-type HIV-1 with IC_{50} values ranging from 5.98 to 0.07 μ M. Among the active compounds, 5a was found to be the most potent.



3(5)-aminopyrazole

Identification -

Spectra - 5

Physical Data - 11

Preparations - 4

Reactions - 232

Documents - 211

See other reactions

Access references

3(5)-aminopyrazole

Reaxys ID:

605752

Chemical Name:

3(5)-aminopyrazole, 7-aminopyrazole

CAS Registry Number(s)

100000000

Molecular Formula:

C₄H₅N₃

Molecular Weight:

81.0808

isChiral

Y

Substance type:

Linear Structure Formula

No. of references:

211

C₄H₅N₃

211

Identification -

Spectra - 5

Physical Data - 11

Other Thermodynamic Data - 1

Boiling Point - 7

Melting Point - 5

View property data

Check availability

Options ^

Options ^

Find Similar Reactions >

Yield	Conditions	Reference
73.2%	With sodium in ethanol, T=80 °C; D=5 h	

Experimental Procedure ^

Access Substance record

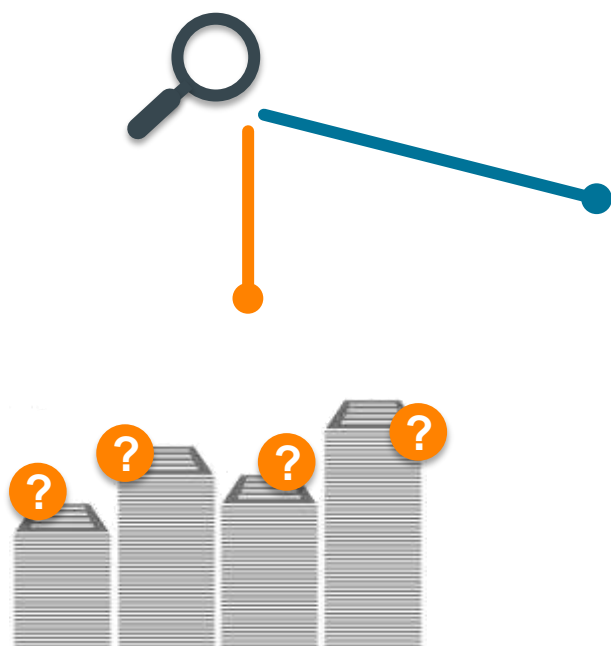
Examine experimental conditions

Experimental Procedure

3-Aminopyrazole (1) (20mmol, 1.0equiv) and diethyl malonate (22mmol, 1.1equiv) were added to a freshly made solution of sodium metal (40mmol, 2equiv) in ethanol (100mL). The mixture was heated to reflux and stirred for 5h. After the reaction, the solution was cooled to room temperature and filtered. The obtained solid was washed with ethanol and dissolved in water (50mL). Then the solution was acidified to pH 1-2 using concentrated HCl in an ice-bath. The precipitate was filtered, washed with water and dried to give light yellow powder (2), yield 73.2%. mp: 152.2 °C (decolor), 174.3 °C (decolor) (lit. 152-153 °C (decolor), 174-175 °C (decolor)).

What is unique about Reaxys2016?

Reaxys2016 aims to deliver immediate access to information



Chemical reaction scheme showing the synthesis of aspirin from acetic acid and salicylic acid.

Find Similar Reactions >

Yield	Conditions
93.8%	Stage #1: 3-(diethylamino) With O-(benzotriazol-1-yl) isomium tetrafluoroborate tosylate at 20°C for 3h Stage #2: acetic acid in Stage #3: acetic acid in d Experimental Procedure

Physical Data - 332

Classification Experiment - 21

Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs. Cited 1 times
Lin, Lee-Shuan; Kayazawa, Yuko; Shimahata, Nobuyuki; et al. 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-Yeong; et al. 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
Flejd, Christopher N.; Goodman, Timothy; Becker, Saba; et al. British Journal of Clinical Pharmacology, 2014, vol. 78, # 2, p. 329 - 329
Abstract Index Terms Full Text

While the philosophy of other solutions is to **deliver 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

How does it do that?

Excerpted data are standardized, normalized and collated into one record for quick and easy access

The image displays a user interface for chemical data, specifically for the compound 'cetane'. The main window shows a list of data categories with their respective counts: Identification, Physical Data - 2307, Other Data - 292, Spectra - 103, Bioactivity - 127, Preparations - 183, Reactions - 305, and Documents - 1627. A blue arrow points from the 'Physical Data - 2307' category to a detailed view of that category. This detailed view lists various physical properties and their counts: 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, and Energy Data (MCS) - 250. A '+ Load More' button is visible at the bottom right of this panel. To the right, another panel shows 'Other Data - 292' with categories like 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, and Bioaccumulation, Biomagnification and Biomonitoring - 1. Below this, a 'Spectra - 103' panel lists categories such as 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, and NQR Spectroscopy - 1. At the bottom, a 'Bioactivity - 127' panel lists Ecotoxicology - 16 and Pharmacological Data - 111. On the left, a detailed view of 'cetane' is shown, including its chemical structure, CAS Registry Number (1736592), Chemical Names (cetane, Hexadecane, Hexadecan), CAS Registry Number(s), Substance type, Molecular Formula (C16H34), Linear Structure Formula (C12H26C4H8), Molecular Weight (226.446), No. of references (1627), and InChIKey (DCAYPVUWAIABOU, LHHFFADYSA-N).

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

Bioactivity - 127

- ✓ Ecotoxicology - 16
- ✓ Pharmacological Data - 111

cetane

Heavy ID: 1736592

Chemical Names: cetane, Hexadecane, Hexadecan

CAS Registry Number(s): Substance type:

Molecular Formula: C16H34 Linear Structure Formula: C12H26C4H8

Molecular Weight: 226.446 No. of references: 1627

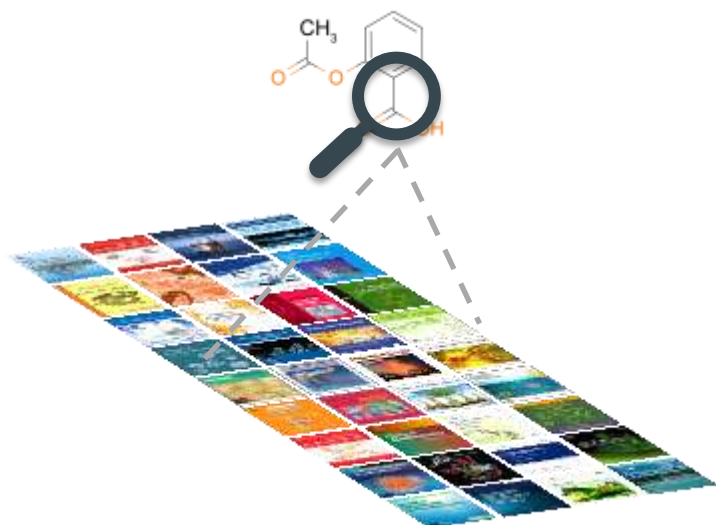
InChIKey: DCAYPVUWAIABOU, LHHFFADYSA-N

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

State-of-the-art indexing augments content richness and brings information from across disciplines into focus

Indexing the full article text body brings the complete information landscape into focus

Additional indexing based on 4 market-leading databases grants access to chemistry across disciplines



And augments Reaxys content richness:

- ~**300K** compounds every year
- **Multiple** Reaxys index terms per source

Antiviral activity of Bignoniaceae species occurring in the state of Minas Gerais (Brazil): Cited 6 times
Part 1
Brandao; Kroon; Dos Santos; +3 others - Letters in Applied Microbiology, 2010, vol. 51, # 4, p. 469 - 476
Abstract ▾ Index Terms ▲ Full Text ↗

Index terms

Author keyword: antiviral activity, Bignoniaceae, EMCV, HSV-1, in vitro assays, plant extracts, VACV
Compendex Terms: Antiviral activities, Bignoniaceae, EMCV, HSV-1, In-vitro assays, Plant extract, VACV
Compendex Terms: Assays, Bromine compounds, Ethanol
EMTREE drug term: aciclovir, alpha2a interferon, natural product, plant extract
EMTREE medical term: animal cell, antiviral activity, article, Bignoniaceae, Brazil, controlled study, cytopathogenic effect, cytotoxicity, ethnopharmacology, fruit, Herpes simplex virus 1, in vitro study, Murine encephalomyelitis virus, nonhuman, plant leaf, plant stem, Vaccinia virus, Vero cell
Species index: Bignoniaceae, Encephalomyocarditis virus, Human herpesvirus 1, Murinae, Vaccinia virus
Reaxys Index Terms: antiviral agent

- **Compendex**: Technology & Engineering
- **EMBASE**: Biomedicine & Pharmacology
- **GeoBase**: Geosciences & Environment
- **MedLine**: Life Sciences & Medicine

Filters and Analysis are interactive for fast filtering and evaluation of results

The image displays two side-by-side screenshots of a 'Filters and Analysis' interface, illustrating how selecting an index term highlights corresponding records in other filters.

Left Screenshot: The 'Index Terms (List)' filter is expanded, showing a list of terms with their respective counts and progress bars. The 'total synthesis' term is selected, indicated by an orange square and a progress bar.

Index Term	Count
stereoselectivity	44
enantioselectivity	24
total synthesis	18
oxidation reaction	18
enantiomer excess	11
catalysed reaction	11
catalyst	10

Right Screenshot: The 'Index Terms (List)' filter is expanded, and the 'total synthesis' term is selected. An orange arrow points from the 'total synthesis' term to the 'Authors' filter, where the 'weinreb, steven m' author is highlighted, indicating that the selected index term highlights corresponding records in other filters.

Index Term	Count
stereoselectivity	44
enantioselectivity	24
total synthesis	18
oxidation reaction	18
enantiomer excess	11
catalysed reaction	11
catalyst	10

Authors:

Author	Count
weinreb, steven m	2
nakata, tadashi	1
kroutil, wolfgang	0
cha, jin soon	0
oishi, takeshi	0
nakamura, kaoru	0

Selected index term highlights corresponding records in other filters

Search Examples

Find melting point of nicotinic acid

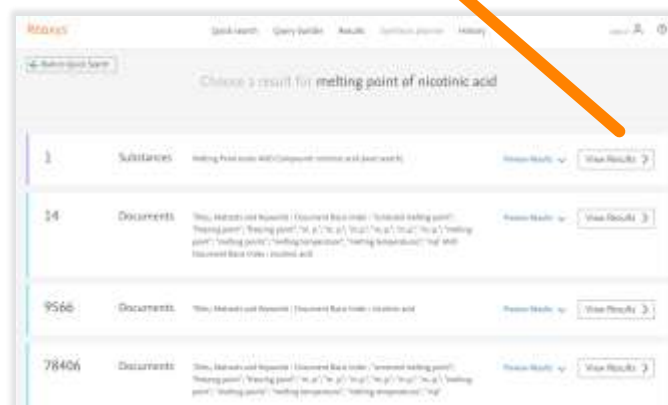
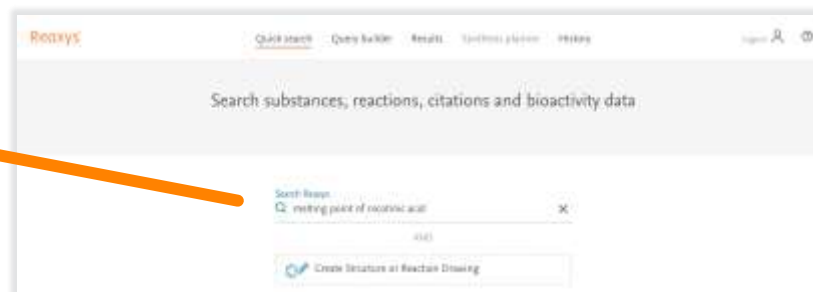
A vast number of simple properties can very quickly be found when the property field and the substance name are entered in **Quick search**.

1. Enter query.

Use prepositions but not truncation or Boolean/proximity operators so that Reaxys searched in **Substance records**.

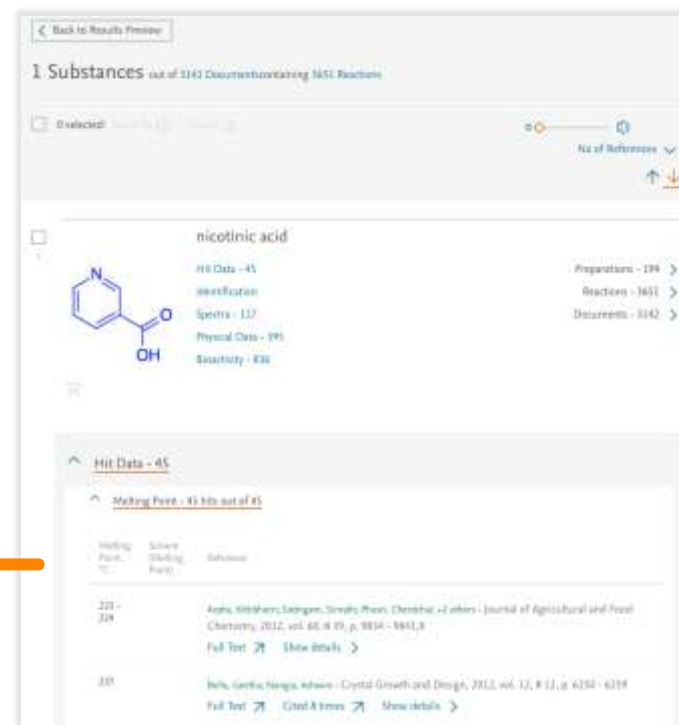
2. Browse options

3. Choose View Results (Substances)

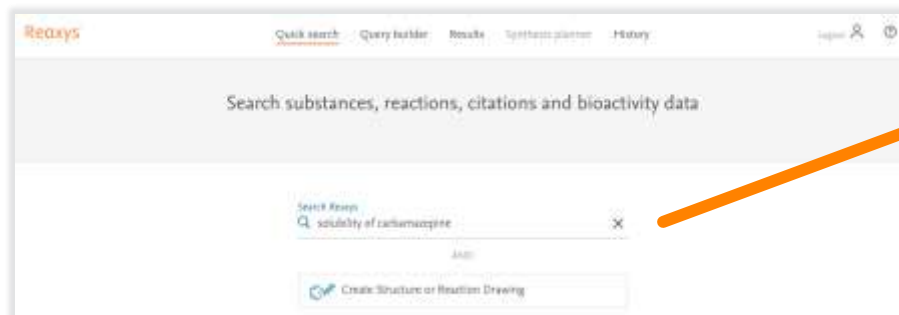


4. Click Hit Data, then Melting Point.

Note that only the first 2 of the 45 entries are shown here.



Find solubility of carbamazepine

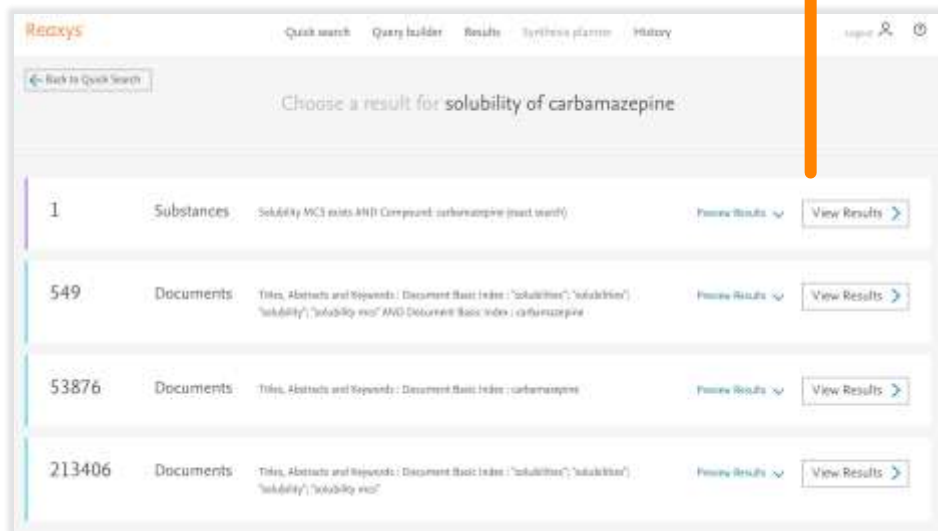


1. Enter query.

2. Browse options.

Note that the property has been recognized through the Solubility (MultiComponentSystem) field.

3. Click View Results (Substances).



4. Click Hit Data, then Solubility.

Note that there are 107 data points that report the solubility of carbamazepine – many in different solvents/conditions. Rather than perform further searches it is easier simply to browse through the list.

Options carbamazepine

Hit Data - 107

Identification

Spectra - 120

Physical Data - 306

Bioactivity - 1203

Preparations - 54

Reactions - 157

Documents - 1338

Hit Data - 107

Solubility (MCS) - 107 hits out of 107


Solubility	Saturation	Temperature	Solvent	Ratio of	Reference
g/L		(MCS), °C	(MCS)	Solvents	
0.164919	in pure solvent		water		Muswal, Musrat; Chat, Oyar; Ahmad; Jabeen, Saraga; +4 others - RSC Advances, 2015, vol. 5, # 10, p. 7696 - 7712

Full Text Show details

Search substances, reactions and documents

in Reaxys, PubChem, eMolecules and LabNetwork

Search Reaxys

 preparation of carbamazepine



AND



Create Structure or Reaction Drawing


Choose a result for preparation of carbamazepine

100

Reactions

Product(s) :  as drawn

Preview Results 

View Results 

5416

Documents

Titles, Abstract, Keywords : preparation, carbamazepine

Preview Results 

View Results 

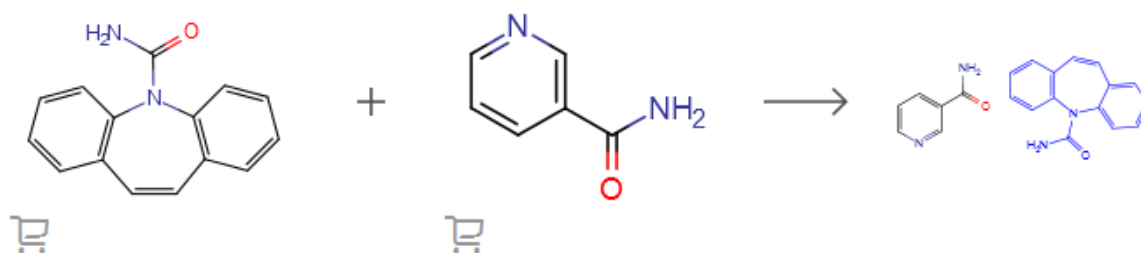
100 Reactions out of 55 Documents containing 127 Substances


☐ 0 selected: [Limit To](#)  [Exclude](#)  [Export](#) 

Reaxys Ran



1




[Show All Details](#)  [Find Similar Reactions](#) 

Yield

Conditions

Reference

In dimethyl sulfoxide

[Experimental Procedure](#) 

Zaworotko, Michael J.; Moulton, Brian; Rodriguez-Hornedo, Nair
- US2003/224006, 2003, A1

Location in patent: Page 9

[Full Text](#)  [Show details](#) 


Searching Reaxys2016 – *Structure drawing*


Create Structure or Reaction Drawing

Click Create Structure or Reaction Drawing to open the MarvinJS Structure Editor.

Structure drawing tools.
Hover over with mouse to
see a description.

Structure editing tools.
Hover over with mouse
to see a description.

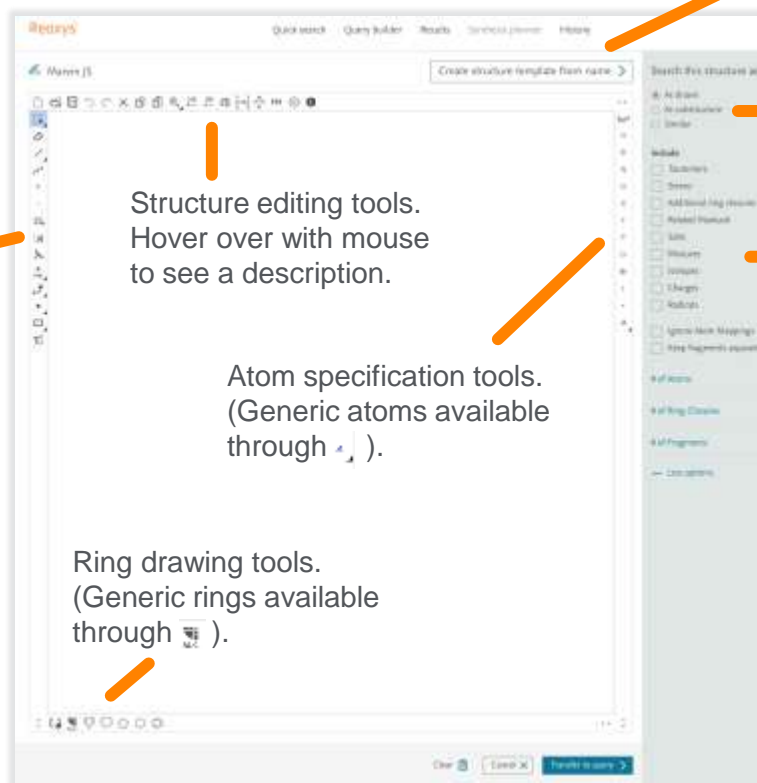
Atom specification tools.
(Generic atoms available
through ).

Ring drawing tools.
(Generic rings available
through ).

Enter substance name and
Reaxys builds the structure for
you. Then modify as needed.

Check type of search
required.

Check options as required.
Note: check **Salts and
Mixtures** to additionally
search for these classes of
substances (often required
for substances in pharma
and agriculture).

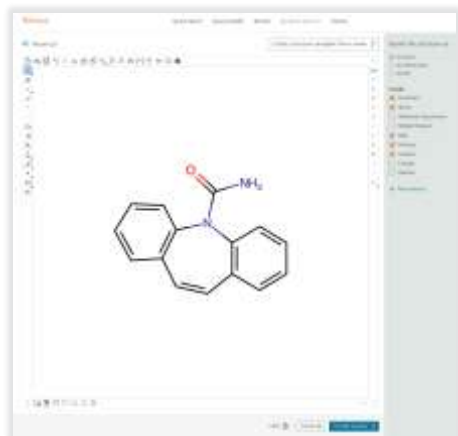


Searching Reaxys2016 – *Structure drawing*

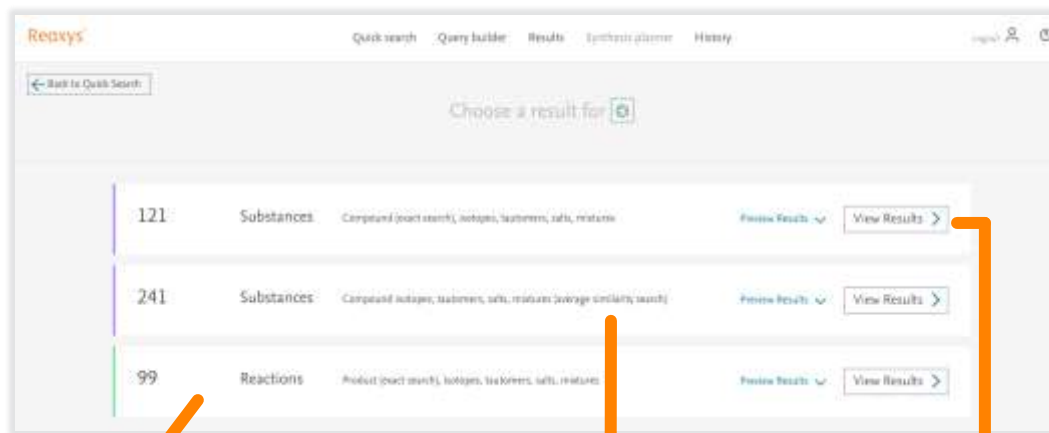
Create Structure or Reaction Drawing

If you enter in Search Reaxys: carbamazepine (i.e., the text term), Reaxys performs an exact search of the substance (gives 4 **Substance Records**), and a keyword search (gives 53,876 **Document Records**). However, many **Substance Records** have the exact structure as a component and when these substances are of interest it is necessary to perform initially a structure search.

Create the Structure Template from Name (carbamazepine), and check required boxes in the right-hand panel. Click Transfer to Query, and then click Search.



Because of the more general way the query was entered, Reaxys provides more general Options in the results list.



121	Substances	Compound (exact search), isotopes, tautomers, salts, mixtures	Preview Results ▾	View Results >
241	Substances	Compound isotopes, tautomers, salts, mixtures (average similarity search)	Preview Results ▾	View Results >
99	Reactions	Product (exact search), isotopes, tri-ketones, salts, mixtures	Preview Results ▾	View Results >

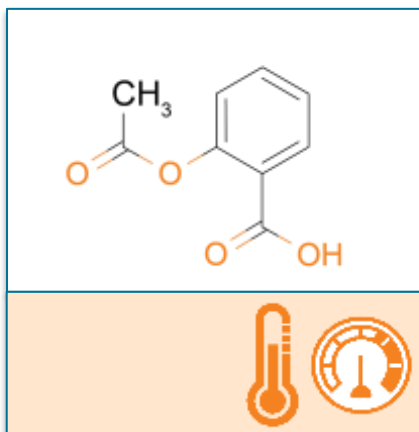
This results set gives **Reaction records** in which the searched substances are prepared.

This results set additionally includes **Substance records** that have closely related structures.

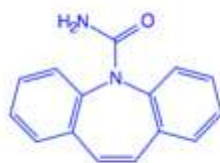
This results set includes **Substance records** that contain salts and mixtures.

Substances: A lot of data on properties

Substances may have information in many property fields, e.g., the substance carbamazepine has data in ~3,000 fields and sub-fields.



>100 M Substance records with **>500 M** excerpted facts on their **properties**: physical, chemical, spectral, ecological, bioactivity and more



carbamazepin

Identification

Spectra - 120

Physical Data - 306

Bioactivity - 1203

Other Data - 1430

Preparations - 54 >

Reactions - 157 >

Documents - 1338 >

^ Spectra - 120

- ✓ Raman Spectroscopy - 9
- ✓ UV/VIS Spectroscopy - 40
- ✓ Mass Spectrometry - 30
- ✓ IR Spectroscopy - 24
- ✓ Fluorescence Spectroscopy - 3
- ✓ NMR Spectroscopy - 14

^ Physical Data - 306

- ✓ Liquid/Solid Systems (MCS) - 6
- ✓ Interatomic Distances and Angles - 4
- ✓ Further Information - 1
- ✓ Solubility (MCS) - 107
- ✓ Transport Phenomena (MCS) - 2
- ✓ Association (MCS) - 14
- ✓ Optics - 4
- ✓ Crystal Phase - 20
- ✓ Crystal System - 8
- ✓ Melting Point - 29

^ Bioactivity - 1203

- ✓ Pharmacological Data - 1154
- ✓ Ecotoxicology - 49

^ Other Data - 1430

- ✓ Abiotic Degradation, Hydrolysis - 3
- ✓ Abiotic Degradation, Photolysis - 14
- ✓ Transport and Distribution - 13
- ✓ Biodegradation - 5
- ✓ Exposure Assessment - 3
- ✓ Concentration in the Environment - 94
- ✓ Use - 1293
- ✓ Bioaccumulation, Biomagnification and Biomonitoring - 2
- ✓ Quantum Chemical Calculations - 3

Substances: Content (Mass Spectrometry)

One of the fields is **Mass Spectrometry**, which contains information in the **Description** sub-field and the relevant Reference(s).



Source of Description
text: **indexers**

Source of index
terms: **indexers**

^ <u>Mass Spectrometry - 30</u>	
Description (Mass Spectrometry)	Reference
liquid chromatography mass spectrometry (LCMS), tandem mass spectrometry, electrospray ionisation (ESI), spectrum	<p>Su, Lijuan; Khunjar, Wendell O.; Aga, Diana S. - Rapid Communications in Mass Spectrometry, 2014, vol. 28, # 11, p. 1265 - 1272</p> <p>Full Text ↗ Cited 3 times ↗ Show details ></p> <p>Hou, Mei-Ling; Lin, Chi-Hung; Lin, Lie-Chwen; +1 other - Journal of Pharmacology and Experimental Therapeutics, 2015, vol. 355, # 1, p. 125 - 134</p> <p>Full Text ↗ Show details ></p>

Source of bibliographic
data: **authors**

liquid chromatography mass spectrometry (lcms) (559884)
liquid secondary ion mass spectrometry (lsims) (608)
lrms (51)
lsims (liquid secondary ion mass spectrometry) (1989)
m (9)
maldi (1)
maldi (matrix assisted laser desorption ionization) (55758)
maldi-tof (matrix assisted laser desorption ionization - time of flight) (46524)
mass (10)
mass ion kinetic energy (mike) (220)
mass spectrometry (1293)
metastable ions (228)
ms (570)
multiphoton ionization (mpi) (65)
negative chemical ionization (1632)
negative ion spectroscopy (29915)
negative secondary ions (456)

A complete list of the different systematic terms entered in the **Description** (Mass Spectrometry) field is displayed through the querylet, available through **Query builder**. Some of the terms (with current numbers of substances) are shown here.

Terms in Description sub-fields **are** searched by **Search Reaxys** and by querylets.

Substances: Content (Ecotoxicology)

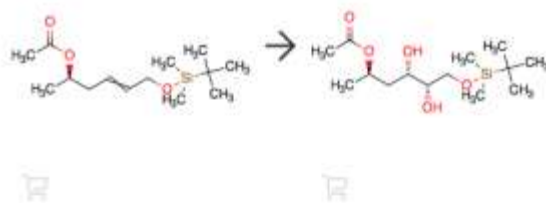
Classification of data
is done by **indexers**

Effect (Ecotoxicology)	Endpoint of Effect (Ecotoxicology)	Species or Test-System (Ecotoxicology)	Sex	Route of Application	Concentration (Ecotoxicology)	Kind of Dosing (Ecotoxicology)	Exposure Period (Ecotoxicology)	Method (Ecotoxicology)	Further Details (Ecotoxicology)	Type (Ecotoxicology)	Value of Type (Ecotoxicology)	Results	Metabolite (Ecotoxicology)	Reference
toxic to algae		Dunaliella tertiolecta			5000 - 80000 µg/l	title comp. solution prepared in 100percent acetone		test species (50000 cells/ml) inoculated in test tubes containing title comp.; maintained at 25 deg C. with a 16:8-hour light:dark photoperiod with continual mixing at 150 rpm; cell density assessed at ca. 0-96 h on a hemocytometer; ASTM 1996		EC50	> 80000 µg/l			DeLorenzo, Marie E.; Fleming, Jessica - Archives of Environmental Contamination and Toxicology, 2008, vol. 54, # 2, p. 203 - 210 Full Text ↗ Cited 60 times ↗ Show details >

Source of data: **authors**

All data here are related to information provided by authors in the original document. Thus, the data are **not** searched by **Search Reaxys**, but it is searched by the **Ecotoxicology** querylet (and by the **Substance Basic Index** querylet).

Reactions: Experimental procedure



Find Similar Reactions >

Yield

Conditions

Reference

86%

With AD-mix- α ; methanesulfonamide In water; tert-butyl alcohol at 0°C for 24h Sharpless asymmetric dihydroxylation
Experimental Procedure ^

Reddy, D. Kumar; Shekhar; Prabhakar; +5 others - Bioorganic and Medicinal Chemistry Letters, 2011, vol. 21, # 3, p. 997 - 1000

Full Text ↗ Cited 15 times ↗ Show details >

Source of reaction type and name: **indexers**

Names and types of reactions are entered by indexers. These are searched by **Search Reaxys** and by the **Reaction Type** and **Reaction Basic Index** querylets.

Compound 11

To a solution of tert-butylalcohol and water (10:10 mL) was added AD-mix- α (4.70g) and MeSO₂NH₂ (30mg, 0.31 mmol) and stirred at room temperature until both phases are clear, and then cooled to 0°C. To this solution the olefin (10, 0.9 g, 3.36 mmol) was added at once and the heterogeneous slurry is stirred vigorously at 0°C for about 24 h. After completion the reaction, the reaction was quenched at 0°C by addition of sodium sulfite (1 g) and then warmed to room temperature and stirred for 30 min. The reaction mixture was poured into water (30 mL) and extracted into EtOAc (3 x 40 mL). The combined organic layer was washed with brine (30 mL), and dried over anhydrous Na₂SO₄. The solvent was removed under reduced pressure to yield the crude diol which was purified over silica gel column chromatography (7/3 v/v ethyl acetate/hexane) to afford diastereomer 11 as clear liquid (860g, 86percent). [α]_D²⁵: -39.5 (c 0.25, CHCl₃). IR (Neat): ν 3435, 2925, 1716, 1643, 1378, 1267 cm⁻¹. ¹H NMR (300MHz, CDCl₃): δ 5.12 (ddq, j = 12.1, 6.8, 4.2 Hz, 1H), 3.67 (dd, j = 5.0, 2.4 Hz, 2H), 3.64-3.60 (m, 1H), 3.42-3.24 (m, 1H) 3.07 (br s, OH), 2.63 (br s, OH), 2.04 (s, 3H), 1.76 (ddd, j = 14.1, 11.1, 3.0 Hz, 1H), 1.62 (ddd, j = 14.3, 10.0, 2.8 Hz, 1H), 1.28 (d, j = 6.2 Hz, 3H), 0.9 (s, 9H), 0.08 (s, 6H). ¹³C NMR (75MHz, CDCl₃): δ 170.6, 67.8, 67.6, 66.9, 39.9, 29.9, 29.5, 25.6, 21.2, 19.4, -2.9, -3.6. ESIMS: m/z 329 [M+Na]⁺.

Source of data: **authors**

Text in **Experimental Procedures** is author-related. This text is searched by the **Reaction Basic Index** querylet.

Superhydrophobic surfaces (hysteresis)

1. Enter query.

Note that you don't know the number and types of answers you get, so initially try a simple search on a couple of concepts.

Search Reaxys

×

2. Look carefully at the option given.

Note that surface/surfaces are searched and that the proximity operator NEAR (searched terms are in either order and within a maximum of 4 words) has been applied. If you wish to broaden the search enter: superhydrophobic* surface*; in this case the AND operator is applied (and over 6,700 **Document records** are obtained).

Reaxys

Quick search Query builder Results Synthesis planner History

← Back to Quick Search

Choose a result for superhydrophobic surfaces

3758 Documents

Titles, Abstracts and Keywords Document Basic Index : superhydrophobic NEAR Document Basic Index : surface; surface

Preview Results

View Results

3. Use Index Term filter.

Check the box, then click **Apply**.
344 more precise answers are obtained.

Reaxys

Quick search Query builder Results Synthesis planner History

← Back to Results Preview

3758 Documents with 377 Substances, 309 Reactions

0 selected

Relevance

☐ Mimicking natural superhydrophobic surfaces and grasping the wetting process: A review on recent progress in preparing superhydrophobic surfaces

Cited 276 times

Yany Gao; Barthome - Advances in Colloid and Interface Science, 2011, vol. 169, # 2, p. 80 - 100

Abstract Index Terms Full Text

Filters and Analysis

Apply

Index Terms (List)

☐ Contact angle with compound 1,795

☐ Hydrophobic surface 676

☐ Roughness 467

☒ Surface 544

☐ Nanoparticle 116

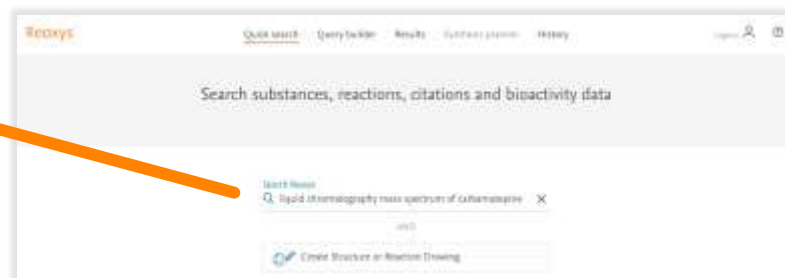
☐ Hydrophilic surface 294

☐ Scanning electron microscopy 293

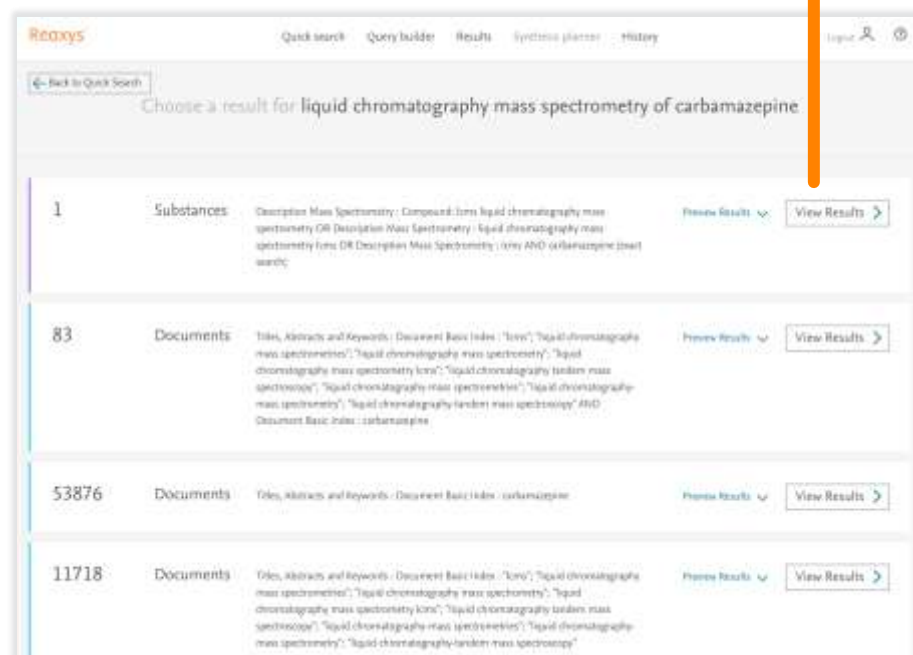
+ More

Find liquid chromatography mass spectrum (information) for carbamazepine

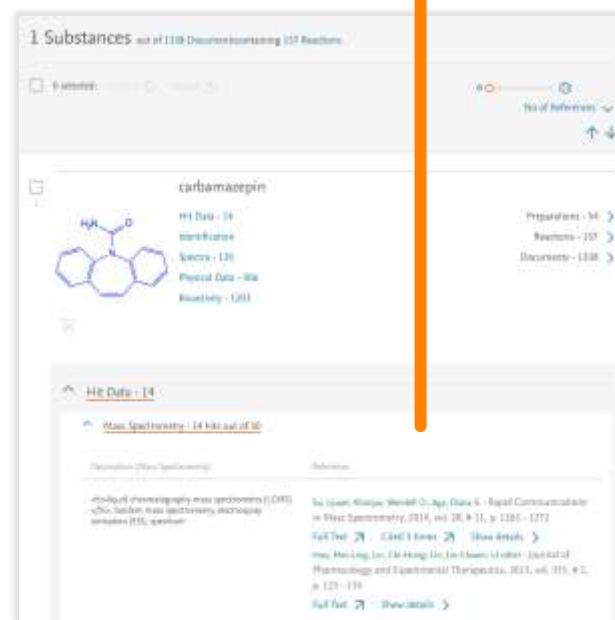
1. Enter query.
Note that 'lcms of carbamazepine' gives the same result.



2. Browse options.
Note that the property has been recognized through the Description Mass Spectrometry sub-field.
3. Click View Results (Substances).



4. Click Hit Data, then Mass Spectrometry.
Note that only the first of the 14 Hit Data entries are shown here.



Find substance through its properties

Identify an unknown substance isolated from a **natural product** ^③. Experimental results indicate that the substance has **30 carbon atoms** ^① and an **optical rotation of 75-85°** ^②. Has it been tested for **antimicrobial** activity ^④?

In **Query builder** drag the Molecular Formula, Optical Rotatory Power, Isolation from Natural Product, and Substance Basic Index querylets into the main working screen and enter data as shown.



^①

⋮ Molecular Formula 



eg.C₆H₅COOH
C₃₀* 


Look up

^③


⋮ Isolation from Natural Product Exist  

^②


⋮ Optical Rotatory Power Exist  

is 


Type (Optical Rotatory Power)

is 


Concentration (Optical Rotatory Power)

= 


Length of Path, cm

is 


Solvent (Optical Rotatory Power)

= 

Optical Rotatory Power, deg
75-85

= 

Wavelength (Optical Rotatory Power), nm

= 

Temperature (Optical Rotatory Power), °C

^④

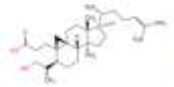
⋮ Basic Indexes 

is 

Substance Basic Index
antimicrobi*

Find substance through its properties

One of the substances found is dikamaliartane B, which contains specific hits in the fields (parts of the fields are shown).



dikamaliartane B

Hit Data - 8
Identification
Physical Data - 6
Spectra - 14
Bioactivity - 14

Hit Data - 8

- Optical Rotatory Power - 1 hits out of 3
- Pharmacological Data - 1 hits out of 14
- Isolation from Natural Product - 6 hits out of 6

Molecular Formula: C₃₀H₄₈O₃

Optical Rotatory Power - 1 hits out of 3

Type: (Optical Rotatory Power)	Concentration: (Optical Rotatory Power)	Length: of Path, cm	Solvent: (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength: (Optical Rotatory Power), nm	Temperature: (Optical Rotatory Power), °C	Reference
[alpha]	0.049 g/100ml		methanol	83.7	589	25	Kunert, Olaf; Sreekanth, Gandhe; Babu, Gummadi Sreedhar; +6 others - Chemistry and Biodiversity, 2009, vol. 6, # 8, p. 1185 - 1192 Full Text Cited 15 times Show details


Pharmacological Data - 1 hits out of 14

Effect: (Pharmacological Data)	Endpoint of Effect: (Pharmacological Data)	Species or Test-System: (Pharmacological Data)	Results	Comment: (Pharmacological Data)	Metabolite: (Pharmacological Data)	Reference
<no>antimicrobial</no>		Candida albicans ATCC 25923	no effect			Kunert, Olaf; Sreekanth, Gandhe; Babu, Gummadi Sreedhar; +6 others - Chemistry and Biodiversity, 2009, vol. 6, # 8, p. 1185 - 1192

Isolation from Natural Product - 6 hits out of 6


Isolation from Natural Product:	Reference:
Bud exudates of <i>Gardenia urvillei</i> (Rubiaceae); collected in the dry forest at the surroundings Noumea, South Province of New Caledonia, in August 2007	Mai, Hoang Linh; Greflier, Philippe; Prost, Elise; +7 others - Phytochemistry, 2016, vol. 122, p. 191 - 202 Full Text Show details
bank of <i>Coussarea macrophylla</i> (Mart.) Muell.Arg. (Rubiaceae); collected in a tropical damp forest near the village Santa Ana, Provincia de Sucumbios, district Cachalet, Ecuador	Giladoni, Gianluca; Chiriboga, Ximena; Vita Final, Paola; +1 other - Chemistry and Biodiversity, 2015, vol. 12, # 6, p. 946 - 954 Full Text Show details
apical buds of <i>Gardenia obtusifolia</i> ; collected from Khonkaen Province, Thailand, December 2009	Nuanyai, Thaneeuan; Sappapan, Ruengrit; Vilakan, Tirayut; +1 other - Chemical and Pharmaceutical Bulletin, 2011, vol. 59, # 3, p. 385 - 387 Full Text Cited 10 times Show details

Complex substance search

Choose a result for 1H NMR AND 

2

Substances

Structure :  as drawn; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals AND Property : 1H NMR

[Preview Results](#) 

[View Results](#) 

9328842

Substances

Property : 1H NMR

[Preview Results](#) 

[View Results](#) 

Thank you for your attention

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