Reaxys

ELSEVIER

Introduction to Reaxys 2017

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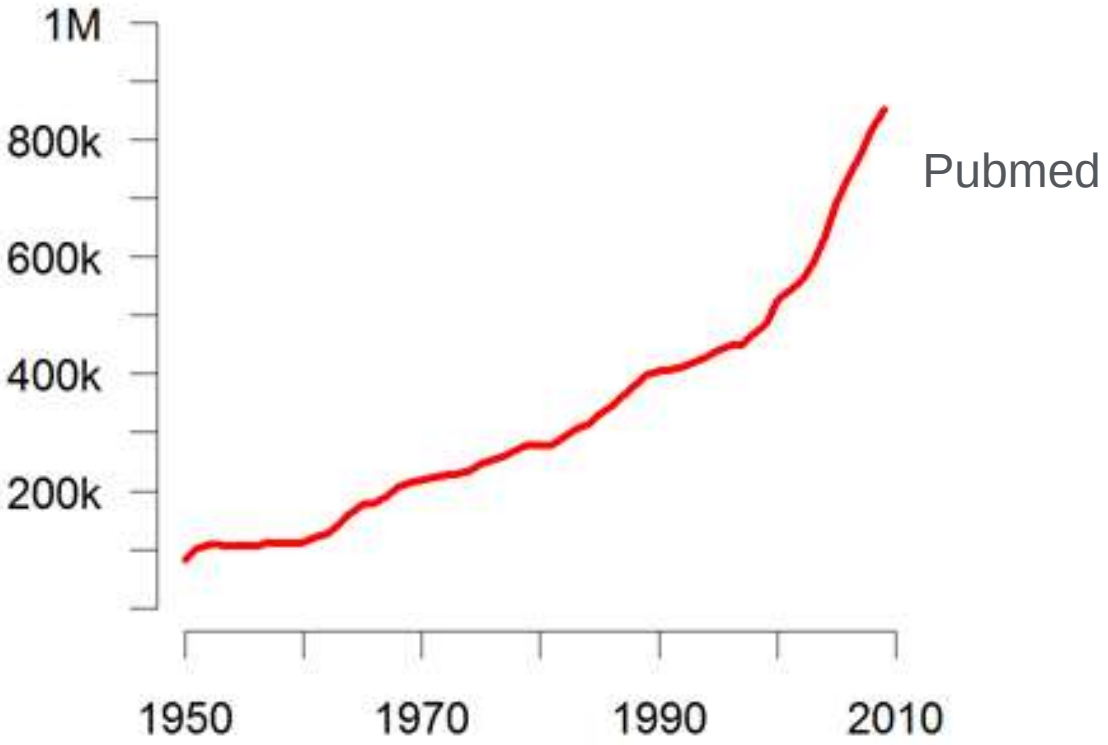
Number of scientific publications grows exponentially



... 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"

How Much Is Too Much? Information Overload in Disease and Drug Research
Frank White III, PhD, Director of Solution Marketing, Life Sciences, Elsevier R&D Solutions, Rdmag.com

Time spent on literature searching

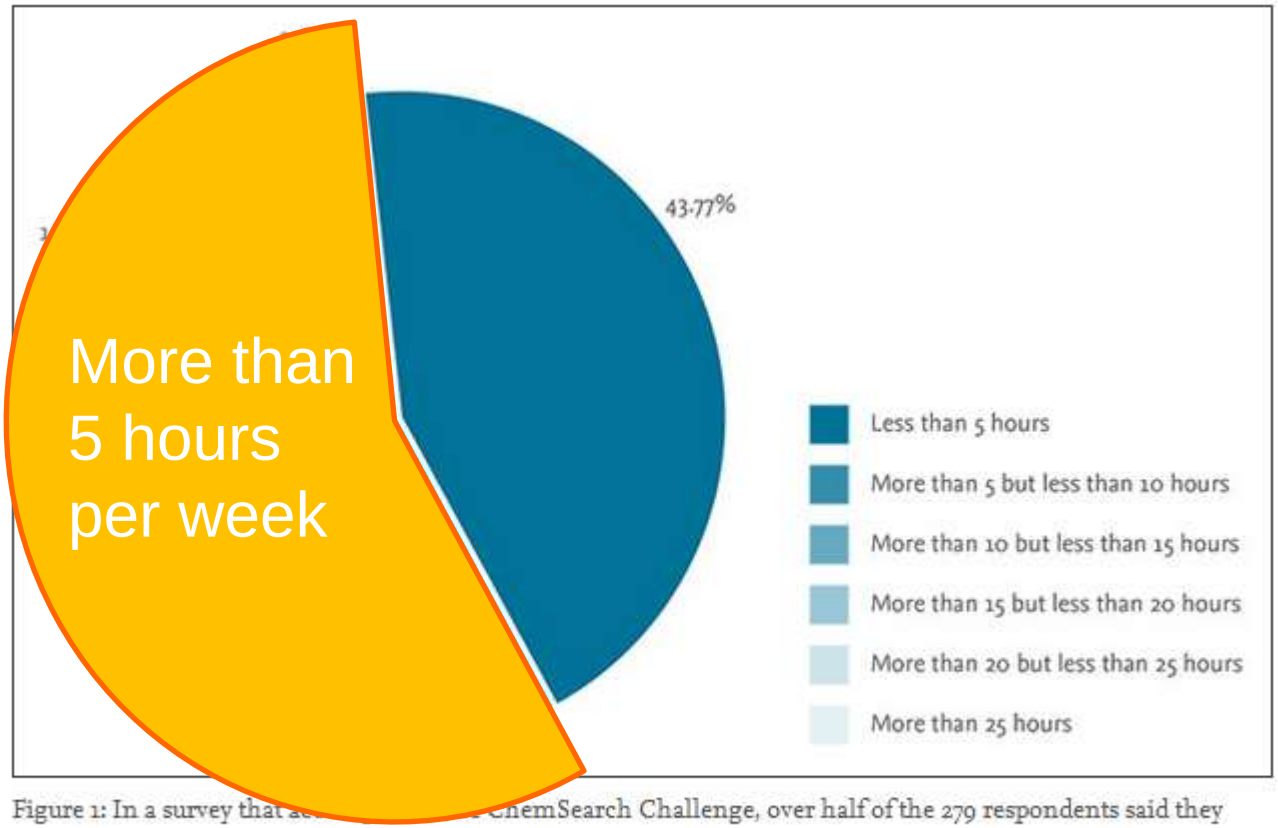


Figure 1: In a survey that ac… ChemSearch Challenge, over half of the 279 respondents said they spend more than five hours a week on data and literature retrieval, and over a quarter spend more than 10 hours a week on this task.

What do researchers search for (Life Science) ?

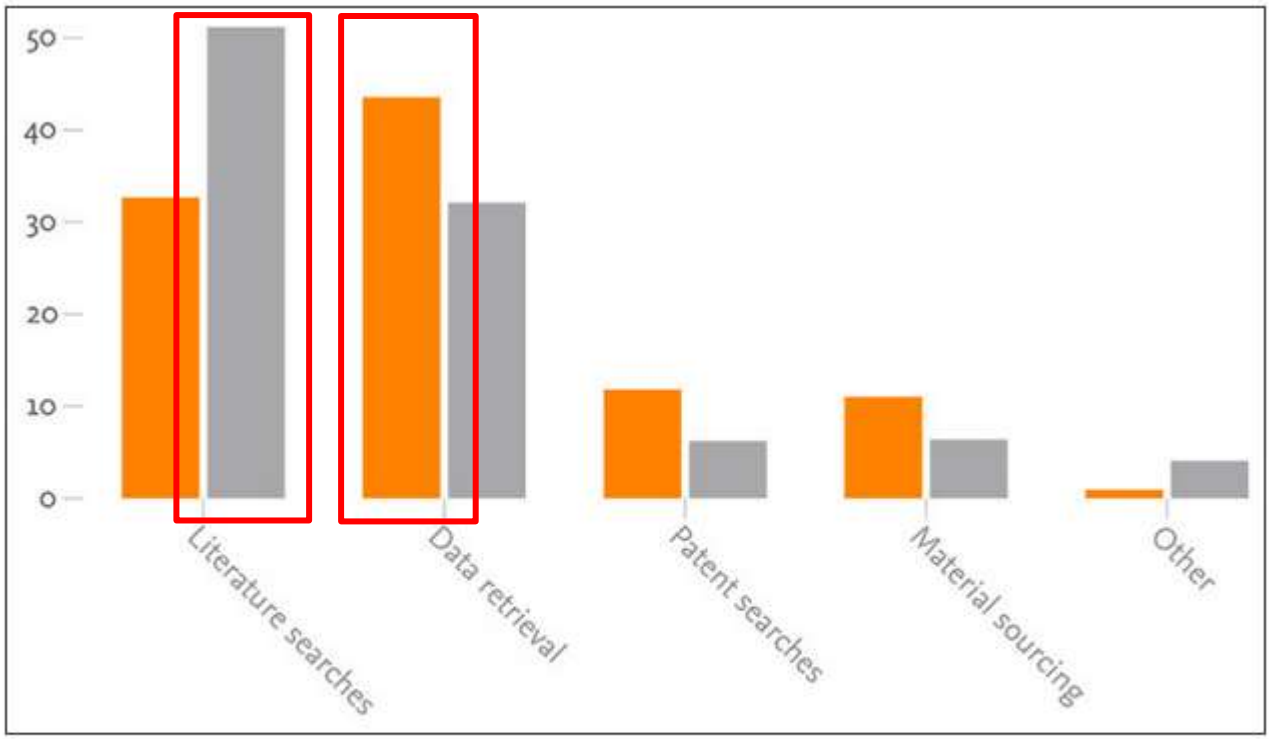


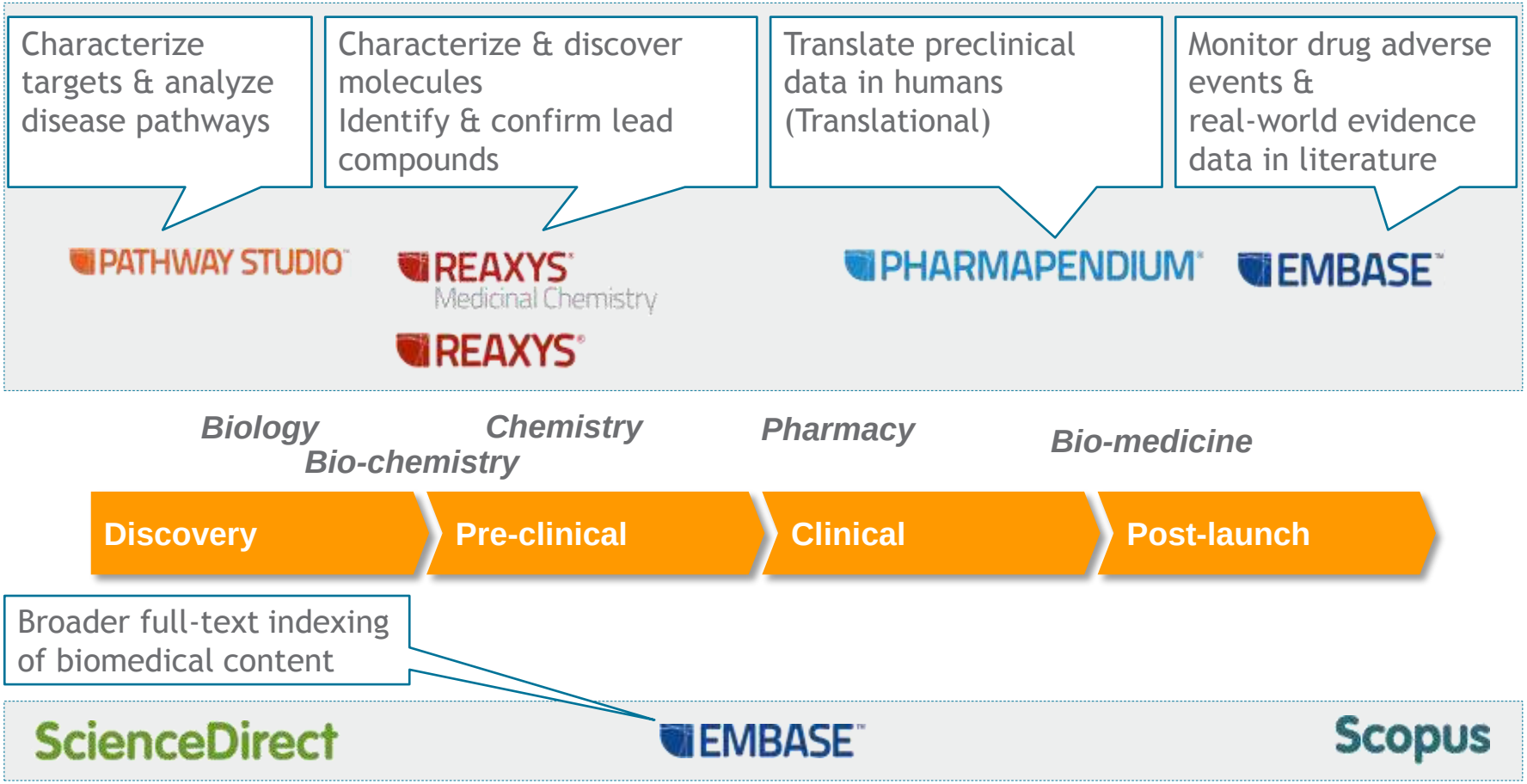
Figure 2: In the ChemSearch Challenge survey, 33 percent of the respondents' queries focused on literature, while 43 percent focused on data. However, in terms of time spent, the opposite is true; respondents reported that 51 percent of their time was spent was literature searches and 32 percent on data retrieval.

What sort of info they search

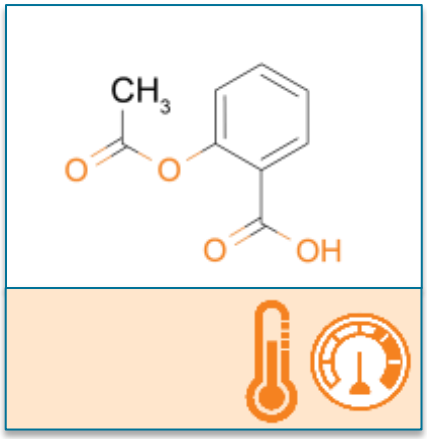
Time spent on searching

Serving the life sciences space

ADDRESSING KEY CHALLENGES ACROSS THE R&D VALUE CHAIN



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

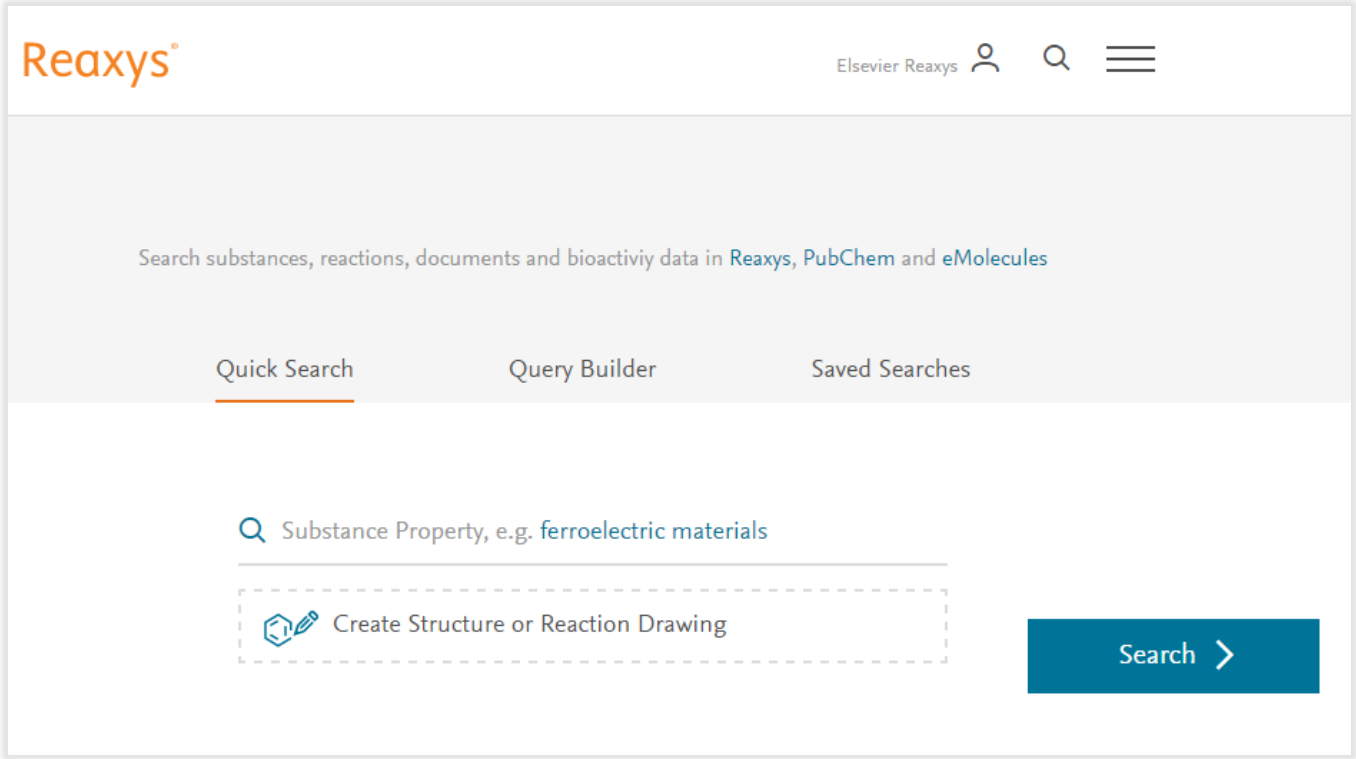
Chemistry fundamentals

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

Uses across disciplines

What does Reaxys2017 look like?

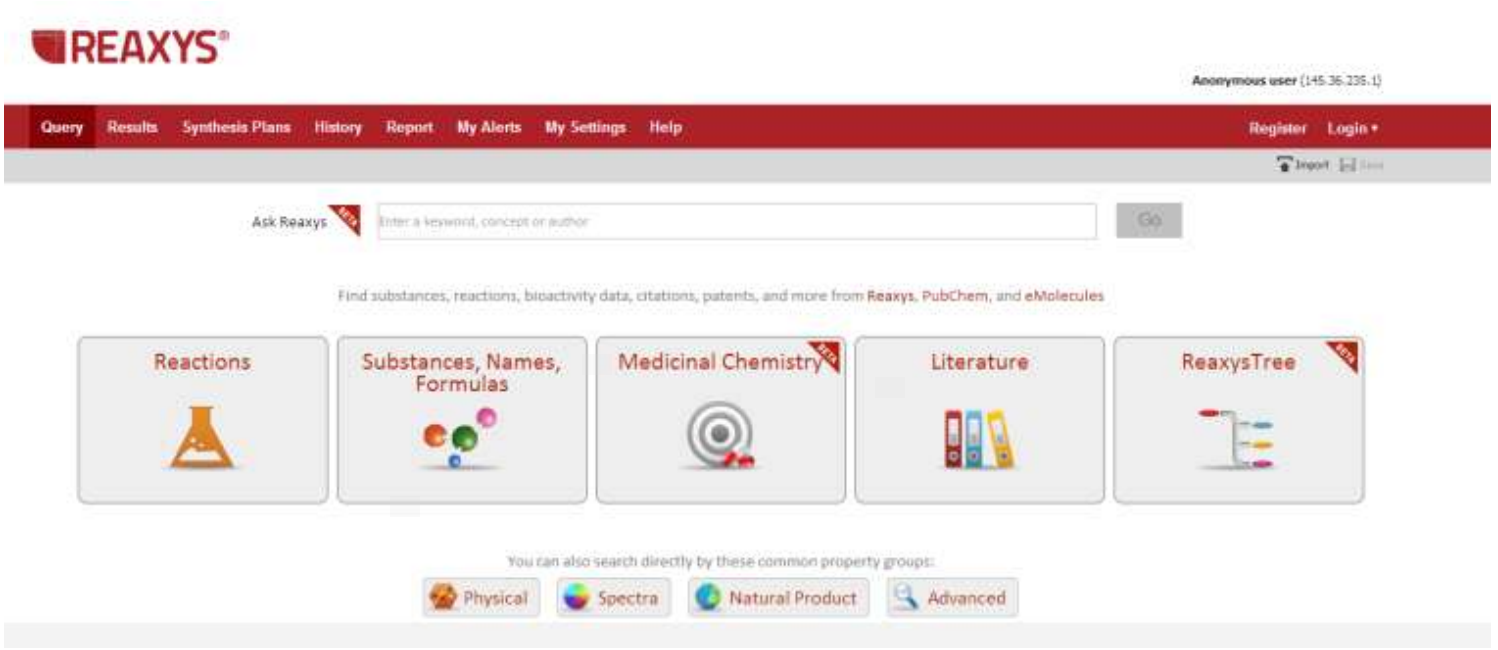
A clean, streamlined user interface fits to how YOU search and grants access to unparalleled content



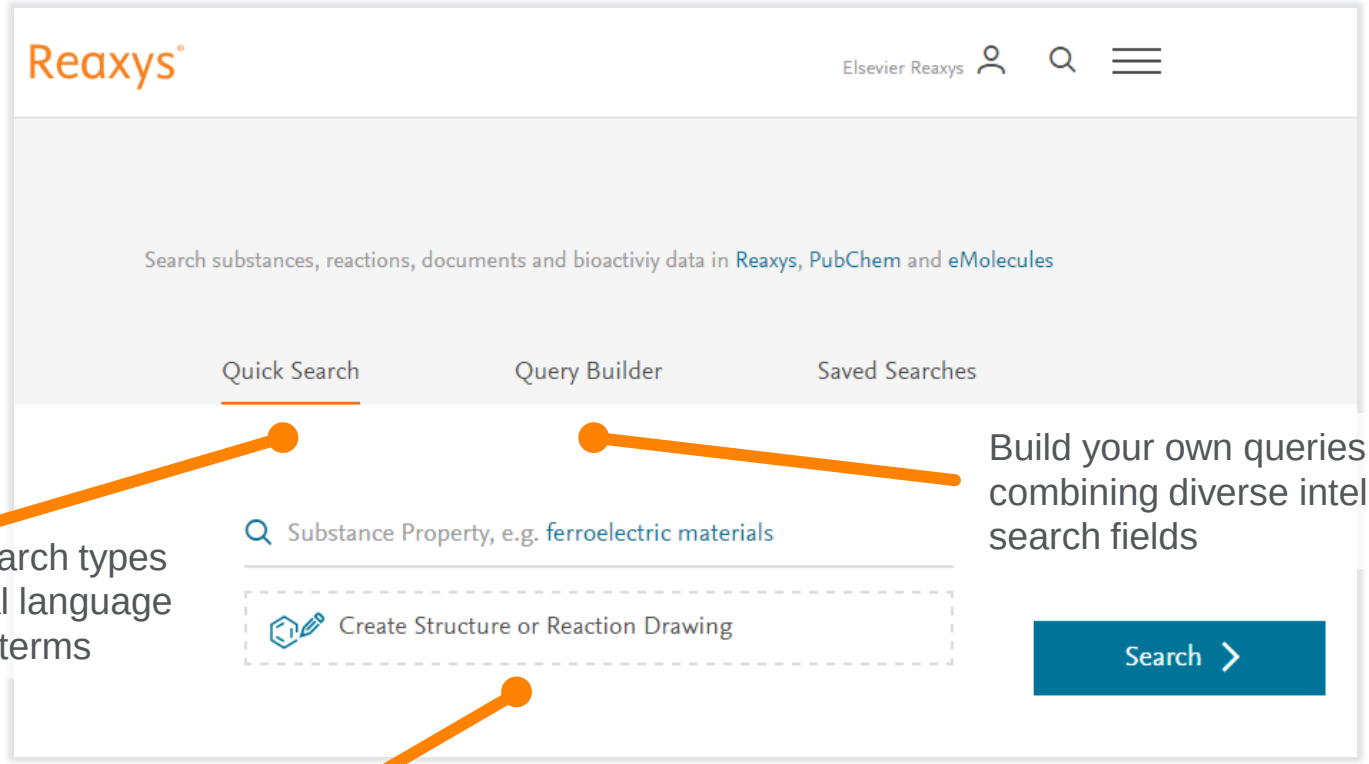
Old interface

SEARCH

REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION



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

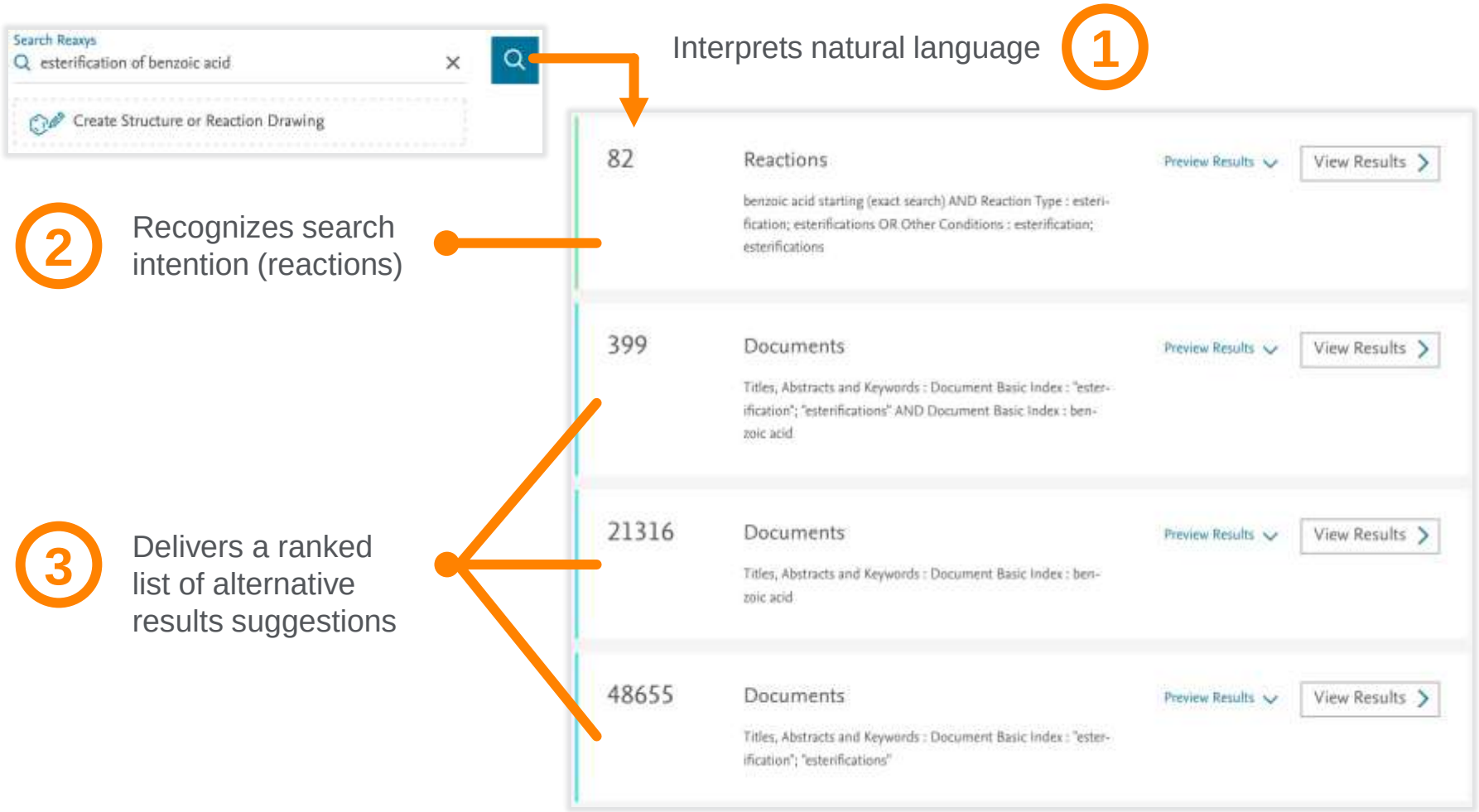


Common search types using natural language and familiar terms

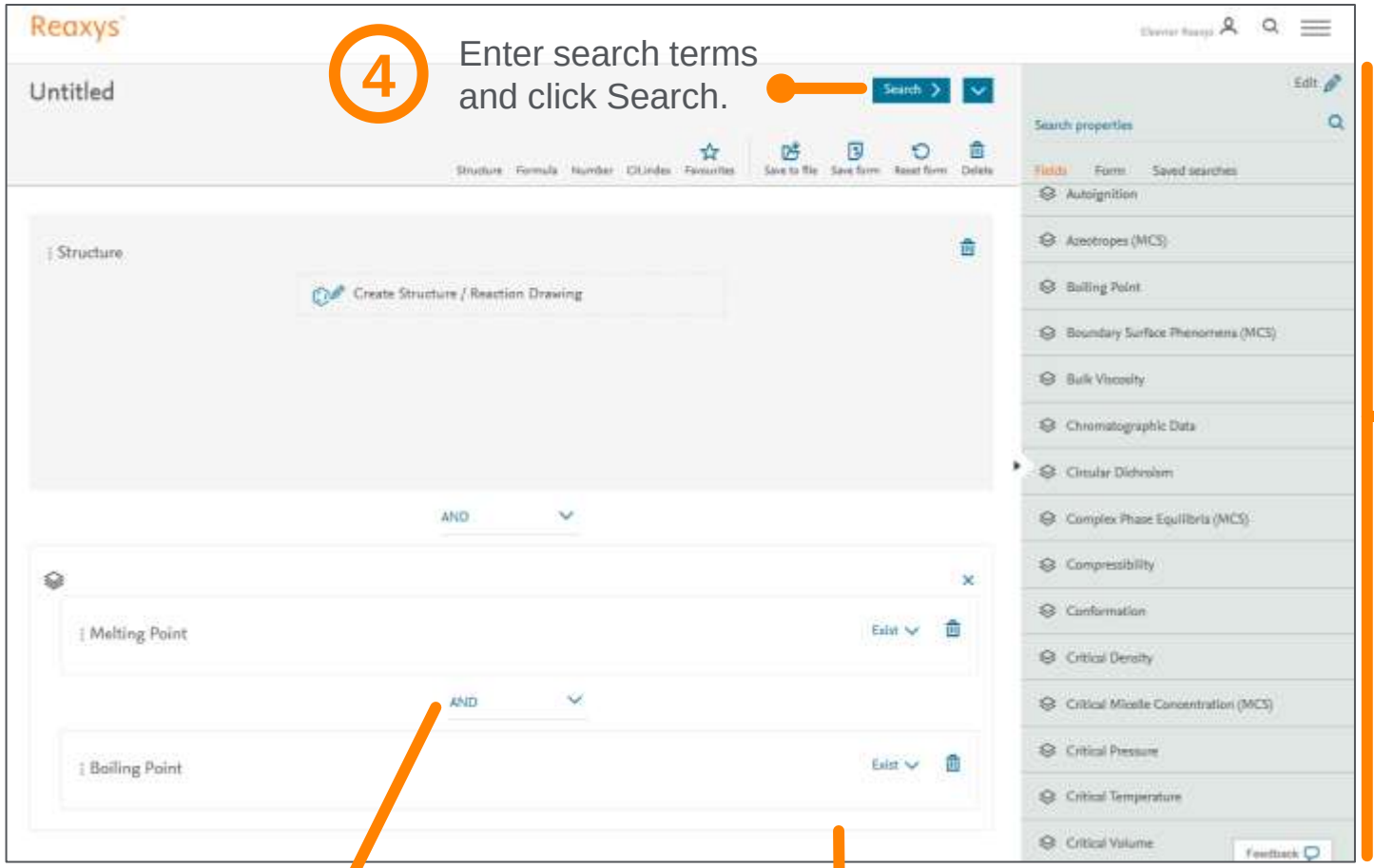
Build your own queries by combining diverse intelligent search fields

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

Quick Search recognizes search intention and lists alternative hitsets



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



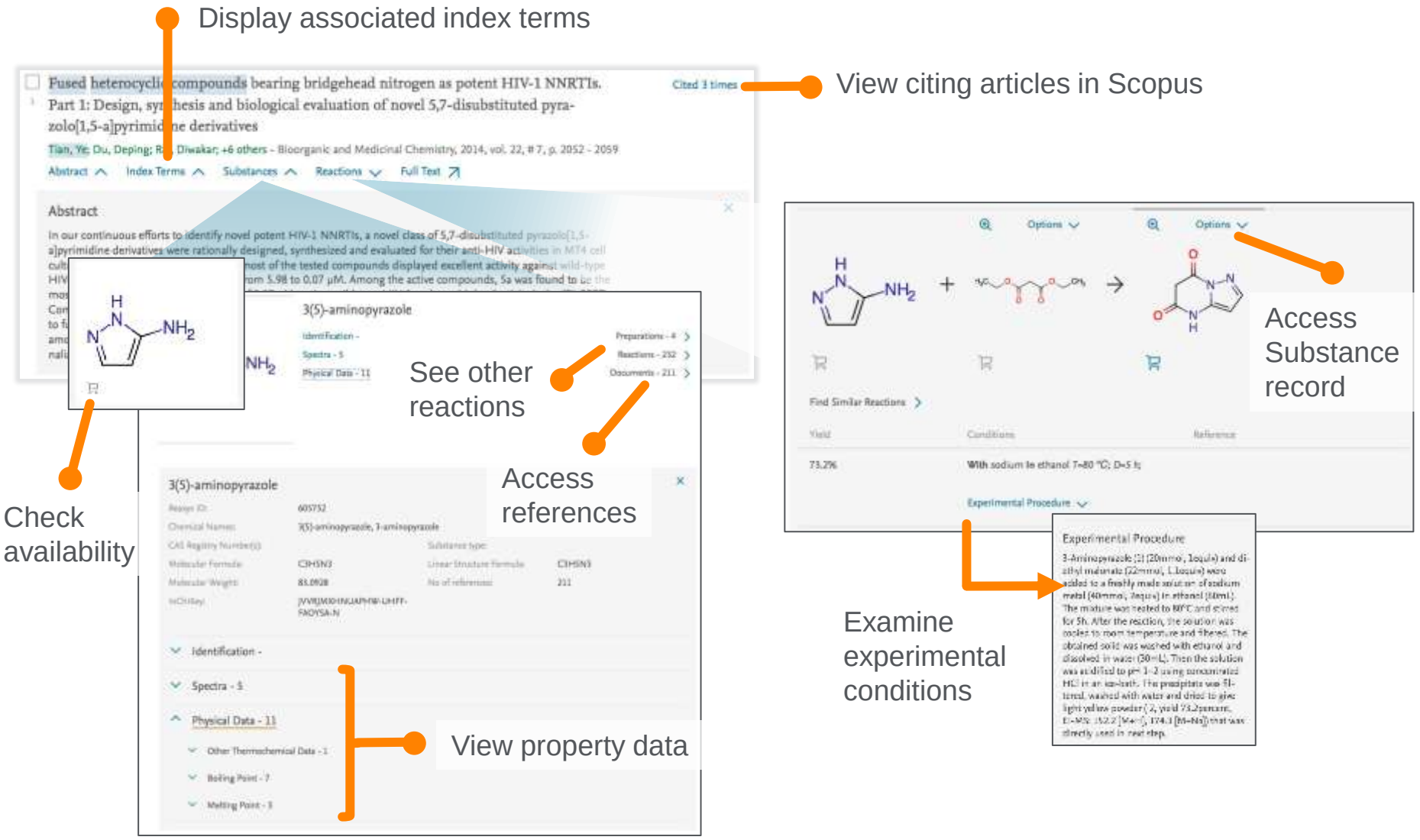
4 Enter search terms and click Search.

1 Search Querylets

2 Drag and drop them into a query

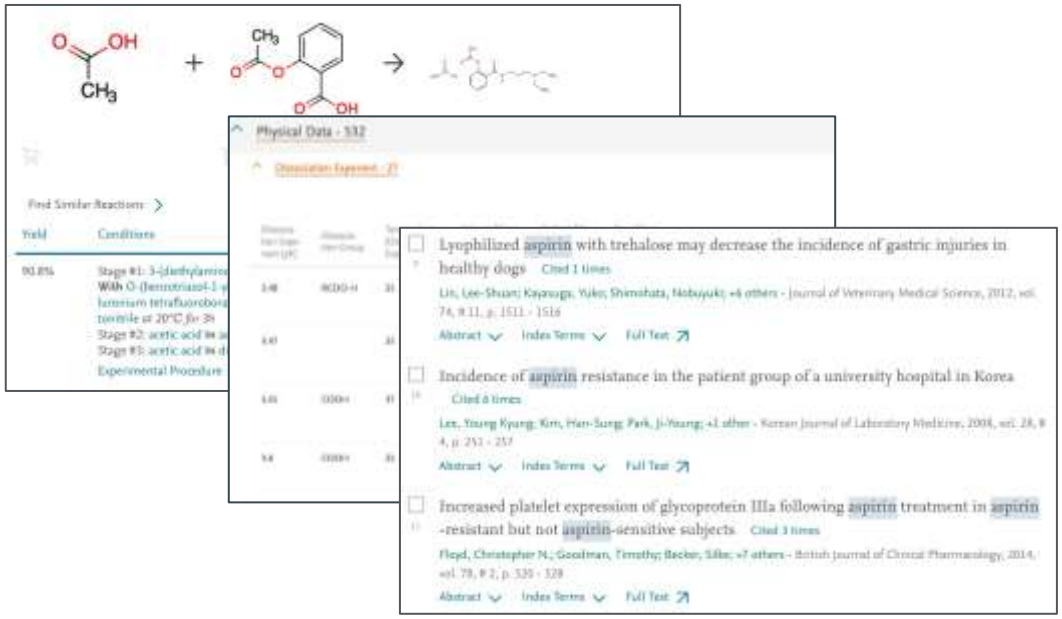
3 Combine them with operators

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



What is unique about Reaxys2016?

Reaxys2016 aims to deliver **immediate access to information**



While the philosophy of other solutions is to **deliver lists of references** that may be relevant to a query

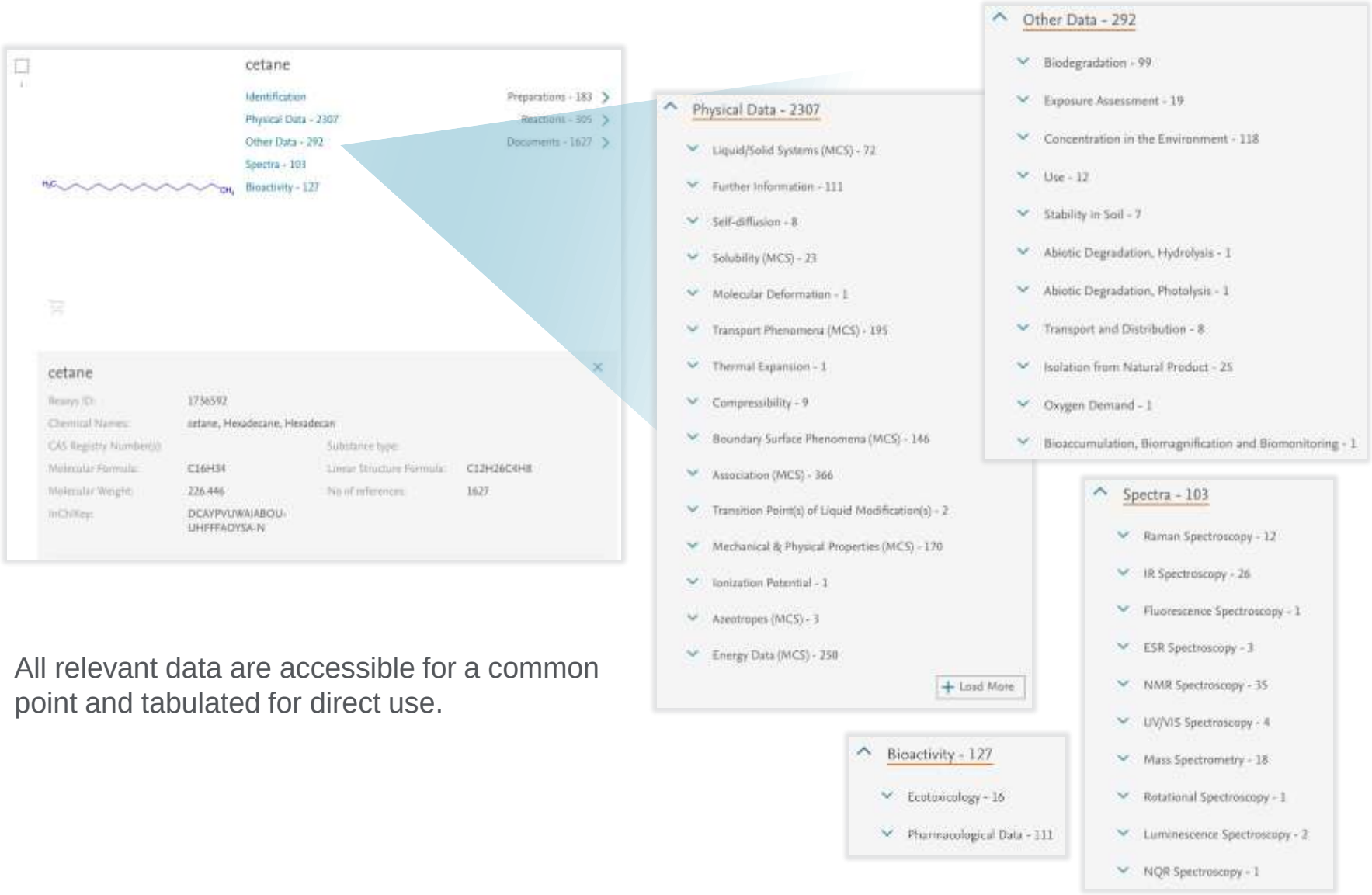
Reaxys strives to **deliver relevant answers on the spot:**

- 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?

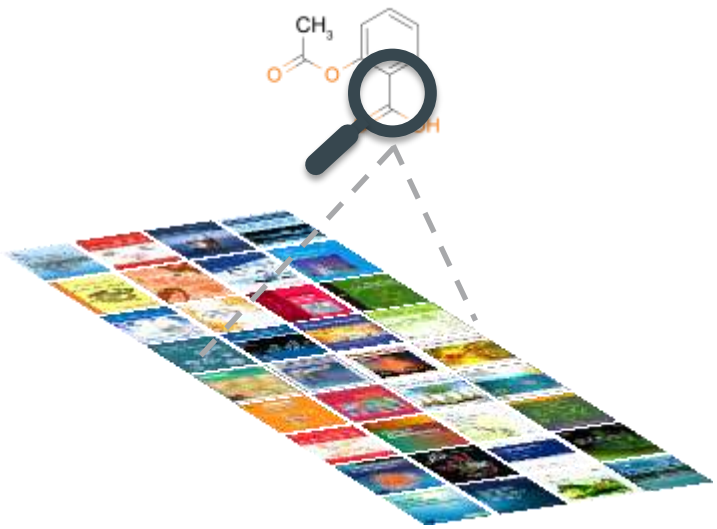
Excerpted data are standardized, normalized and collated into one record for quick and easy access



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


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

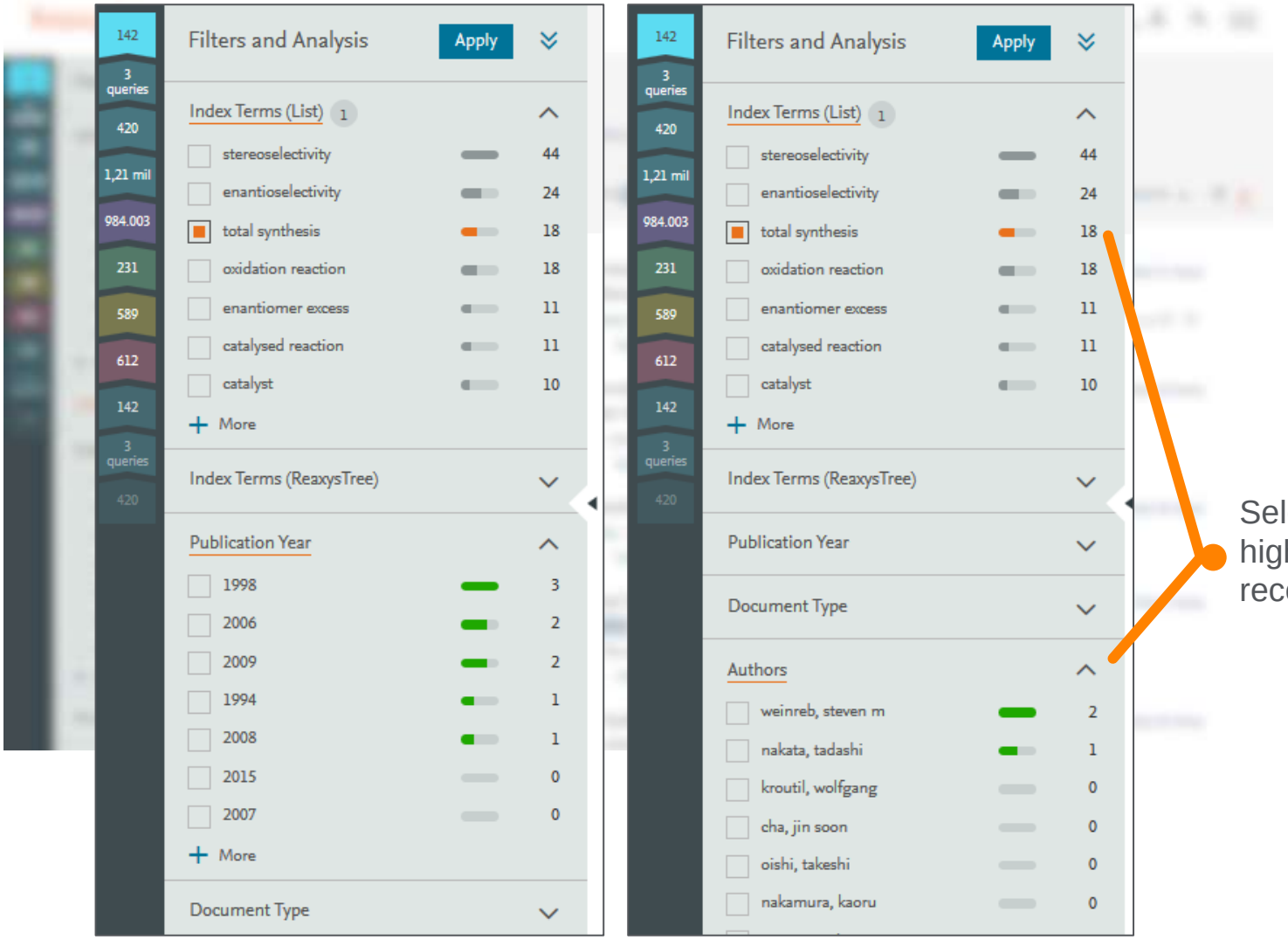
Author keyword: antiviral activity, Bignoniaceae, EMCV, HSV-1, in vitro assays, plant extracts, VACV
Compendex Terms: Antiviral activities, Bignoniaceae, EMCV, HSV-1, In-vitro assays, Plant extract, VACV
Compendex Terms: Assays, Bromine compounds, Ethanol
EMTREE drug term: aciclovir, alpha2a interferon, 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

And augments Reaxys content richness:

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

- **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



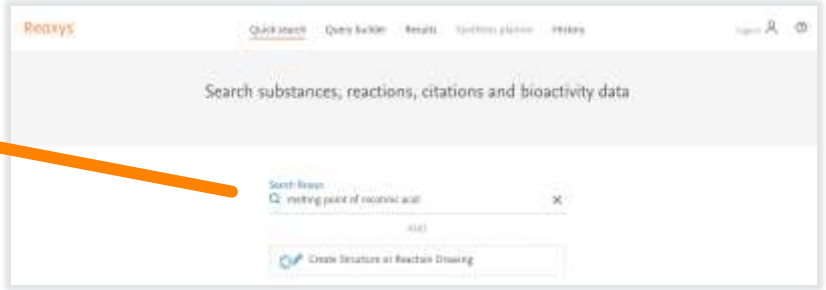
Selected index term highlights corresponding records in other filters

Search Examples

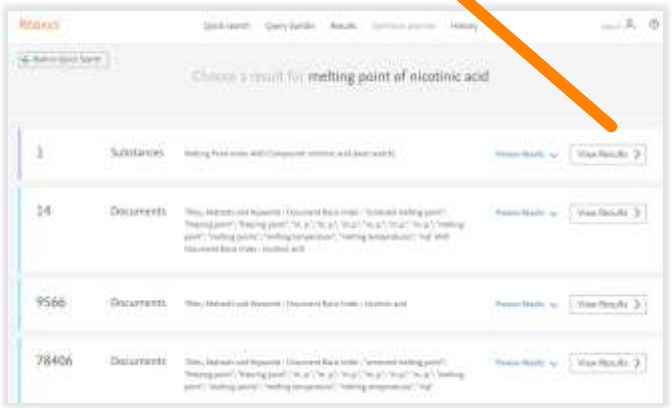
Find melting point of nicotinic acid

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**.

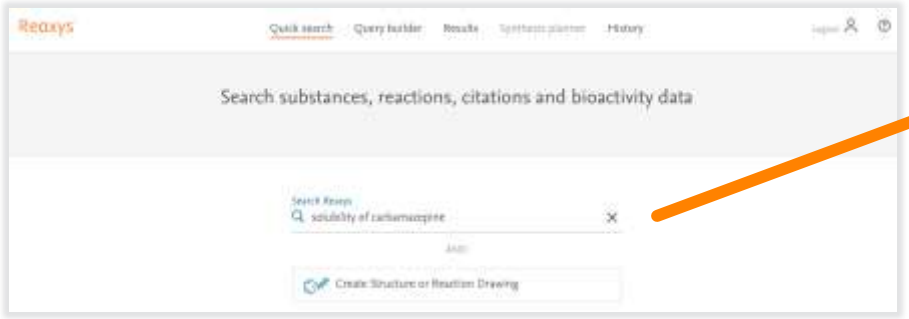


2. **Browse options**
3. **Choose View Results (Substances)**



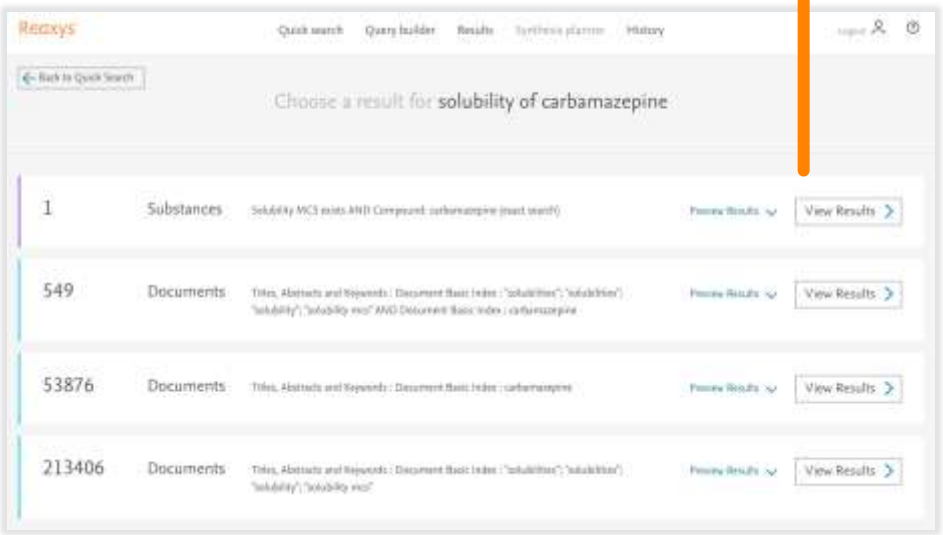
4. **Click Hit Data, then Melting Point.**
   Note that only the first 2 of the 45 entries are shown here.

Find solubility of carbamazepine

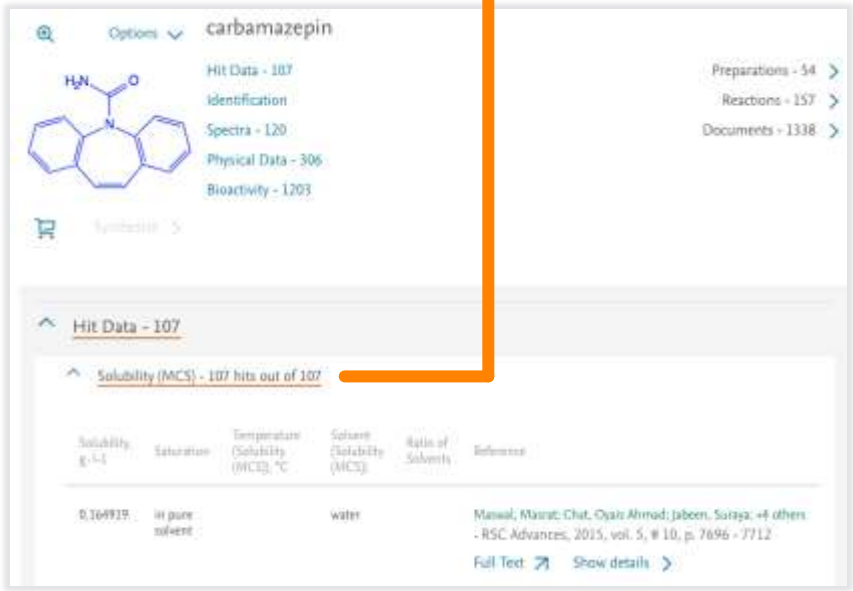


1. **Enter query.**

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.



Search substances, reactions and documents

in Reaxys, PubChem, eMolecules and LabNetwork

Search Reaxys

preparation of carbamazepine

AND

Create Structure or Reaction Drawing

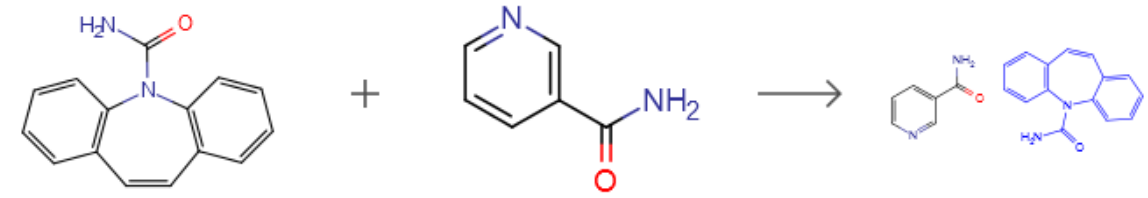
Choose a result for preparation of carbamazepine

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



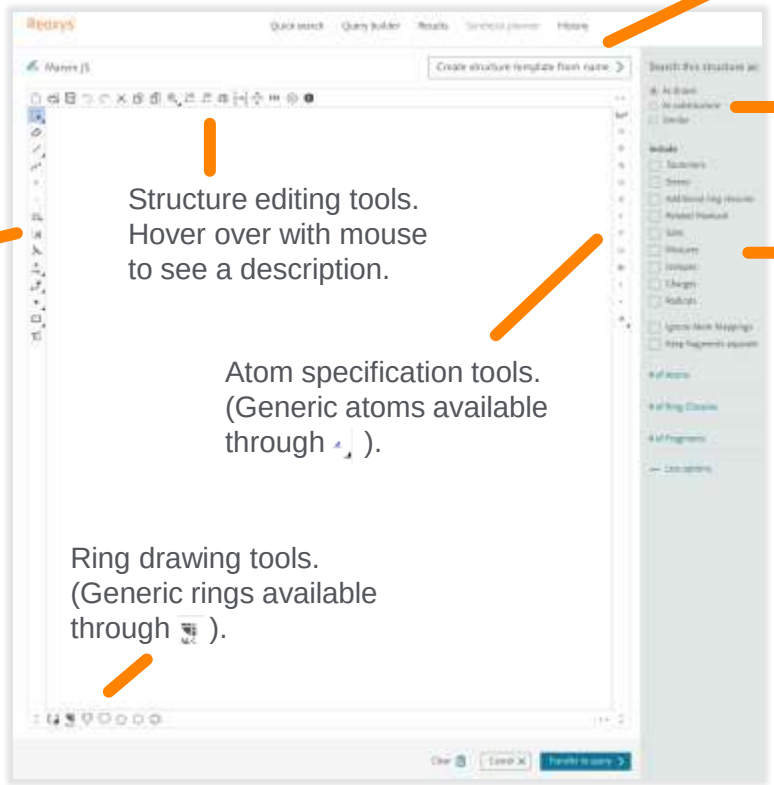
Show All Details Find Similar Reactions

Yield	Conditions	Reference
	In dimethyl sulfoxide	Zaworotko, Michael J.; Moulton, Brian; Rodriguez-Hornedo, Nair - US2003/224006, 2003, A1 Location in patent: Page 9
	Experimental Procedure	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.



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).

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

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

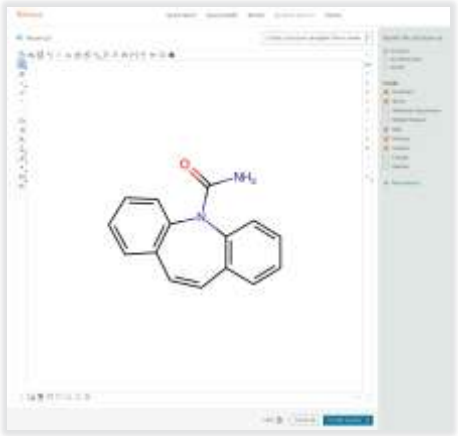
Atom specification tools. (Generic atoms available through).

Ring drawing tools. (Generic rings available through).

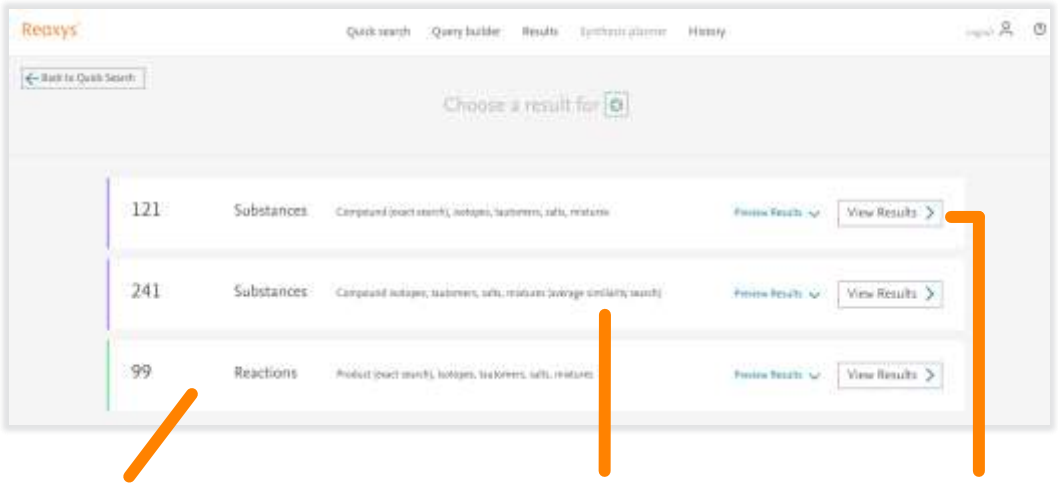
Searching Reaxys2016 – *Structure drawing*

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.



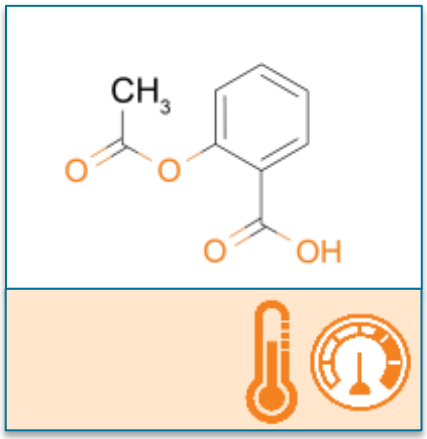
This results set gives **Reaction records** in which the searched substances are prepared.

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

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

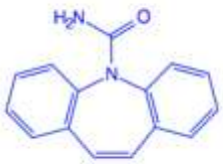
Substances: A lot of data on properties

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

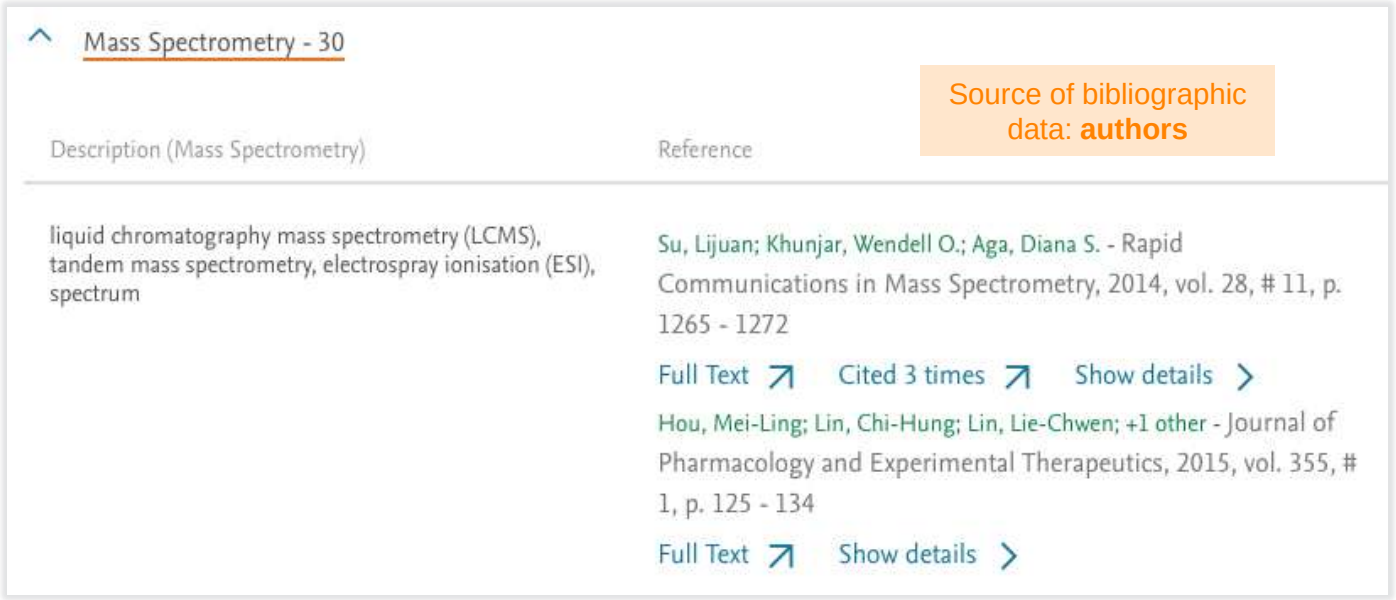
Physical Data - 306
- Liquid/Solid Systems (MCS) - 6
- Interatomic Distances and Angles - 4
- Further Information - 1
- Solubility (MCS) - 107
- Transport Phenomena (MCS) - 2
- Association (MCS) - 14
- Optics - 4
- Crystal Phase - 20
- Crystal System - 8
- Melting Point - 29

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**

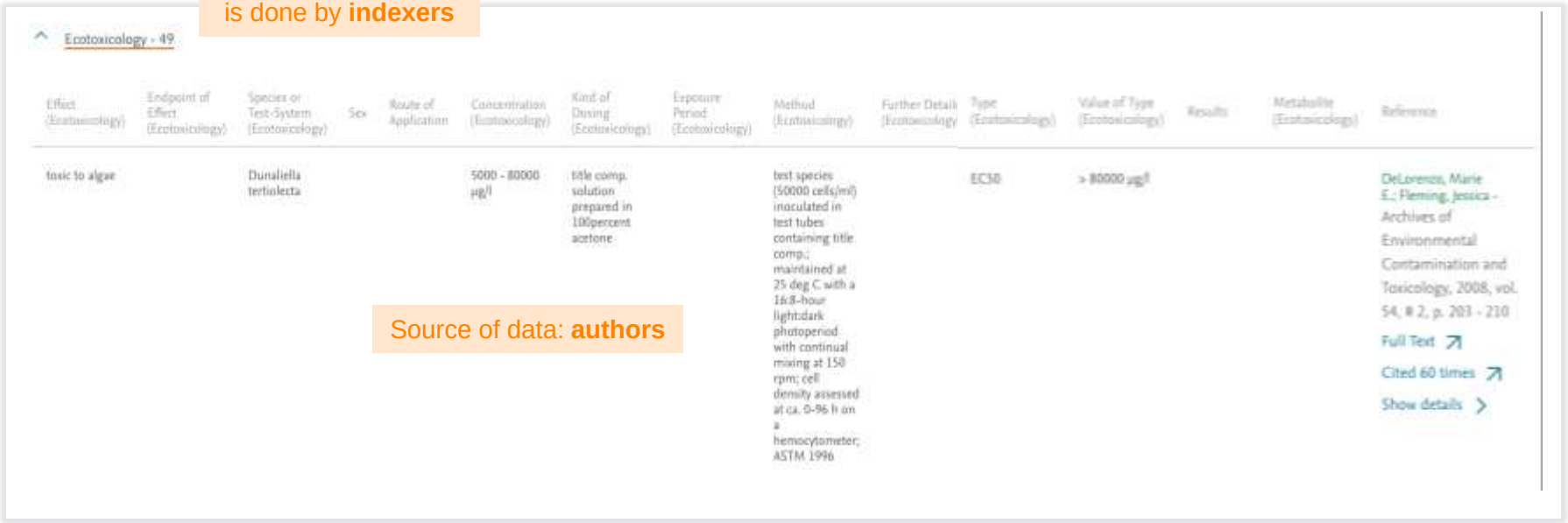
liquid chromatography mass spectrometry (lcms) (559884)
liquid secondary ion mass spectrometry (lsims) (608)
lrms (51)
lsims (liquid secondary ion mass spectrometry) (1989)
m (9)
maldi (1)
maldi (matrix assisted laser desorption ionization) (55758)
maldi-tof (matrix assisted laser desorption ionization - 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)

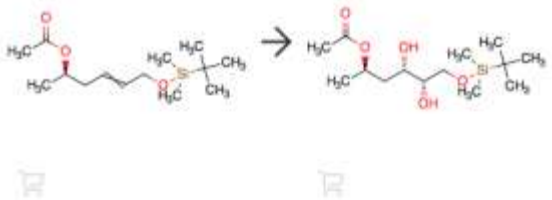
Classification of data is done by **indexers**



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

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 0oC. To this solution the olefin (10, 0.9 g, 3.36 mmol) was added at once and the heterogeneous slurry is stirred vigorously at 0oC for about 24 h. After completion the reaction, the reaction was quenched at 0oC 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): υ 3435, 2925, 1716, 1643, 1378, 1267cm-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 = 6.2Hz, 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 reaction type and name: **indexers**

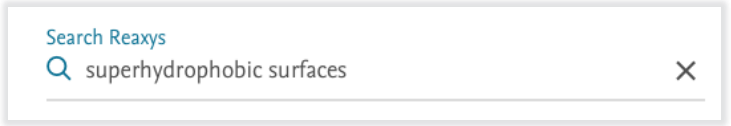
Names and types of reactions are entered by indexers. These are searched by **Search Reaxys** and by the **Reaction Type** and **Reaction Basic Index** querylets.

Source of data: **authors**

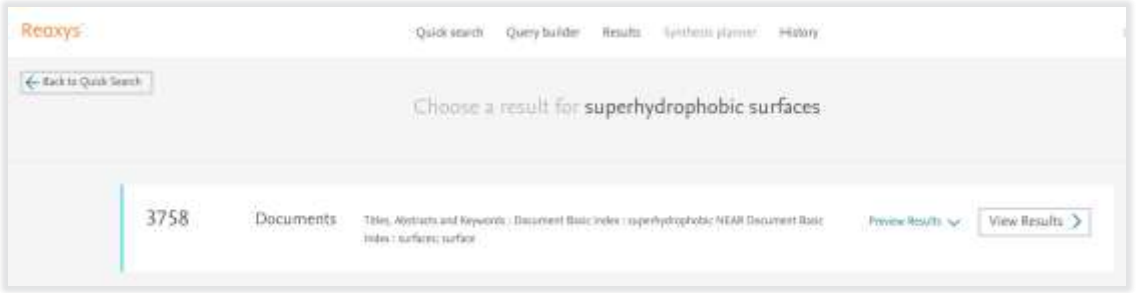
Text in **Experimental Procedures** is author-related. This text is searched by the **Reaction Basic Index** querylet.

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.



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).

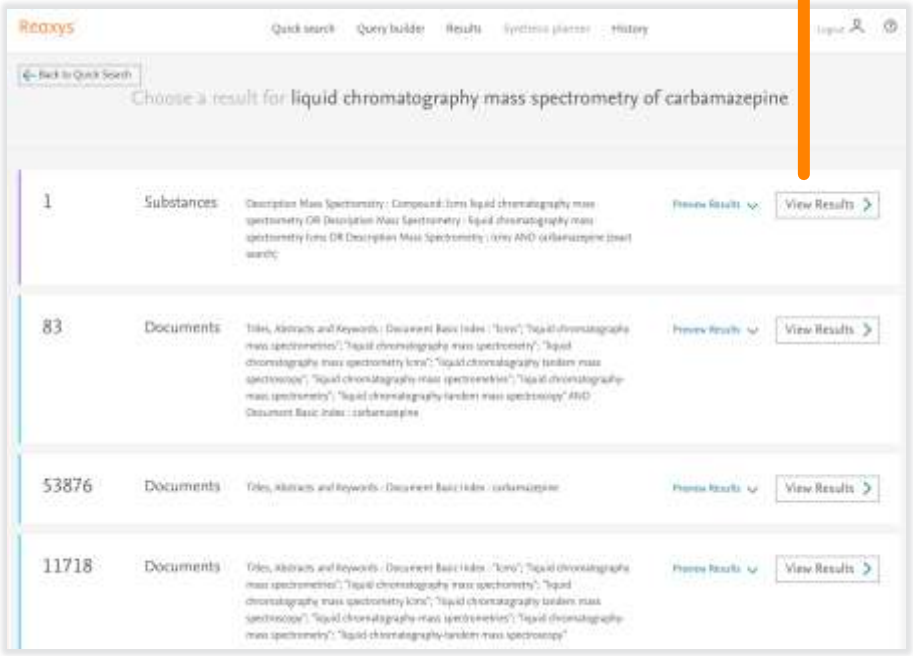


3. **Use Index Term filter.**
Check the box, then click **Apply**. 344 more precise answers are obtained.

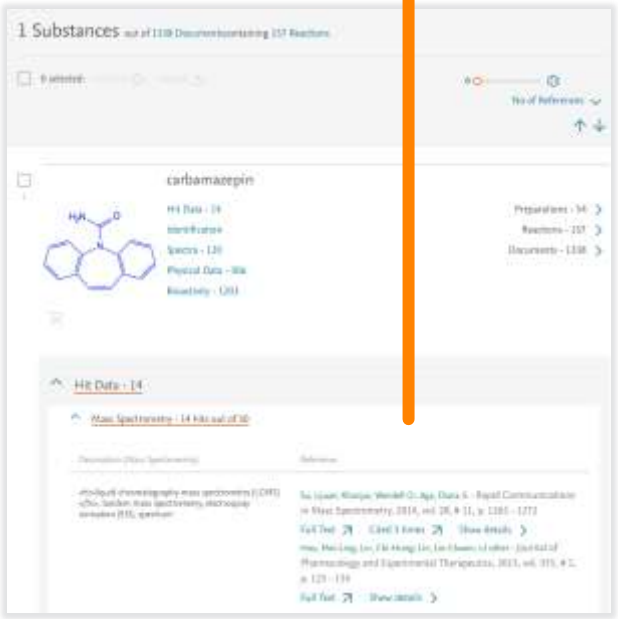
Find liquid chromatography mass spectrum (information) for carbamazepine

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

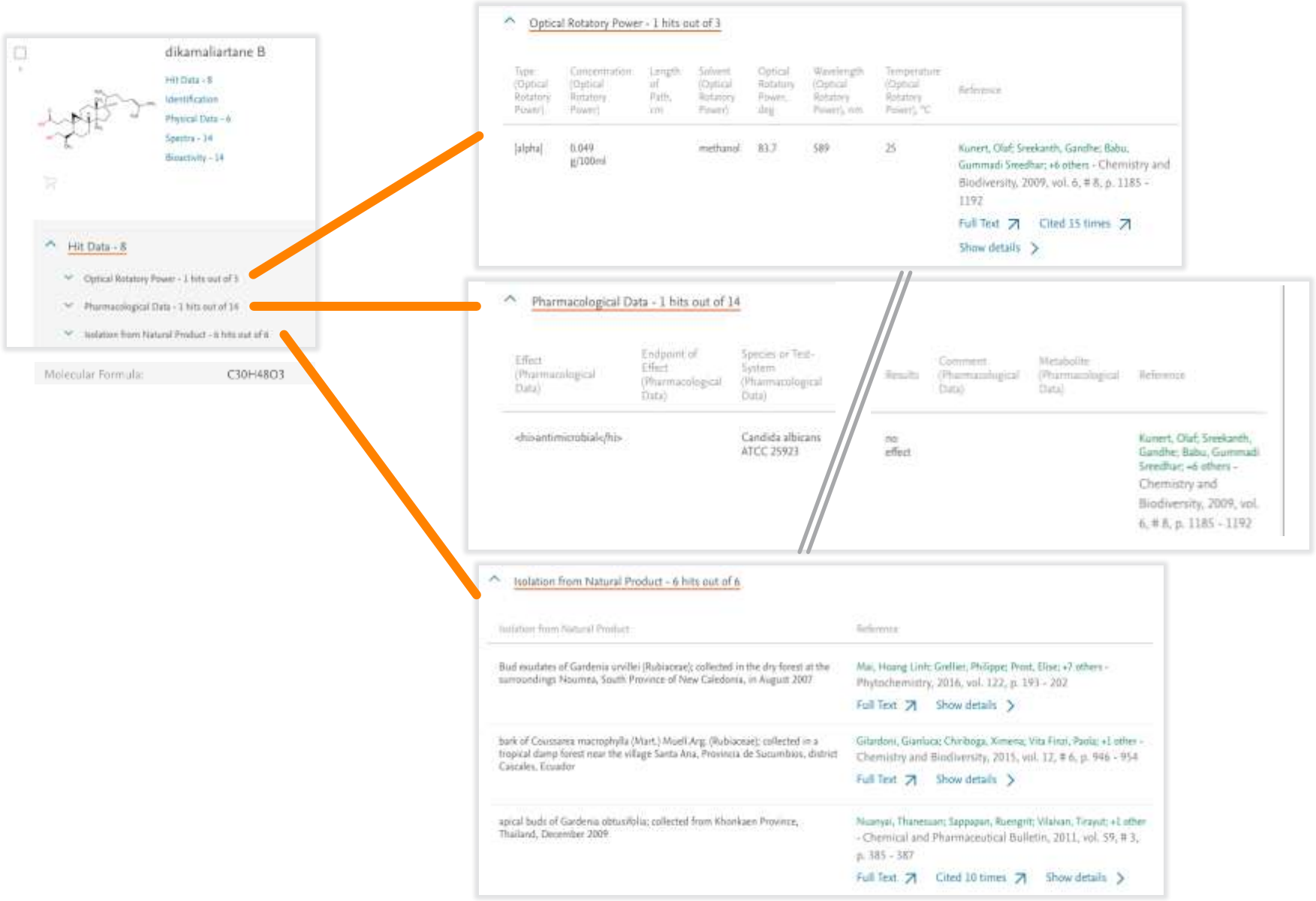
(4)

Basic Indexes

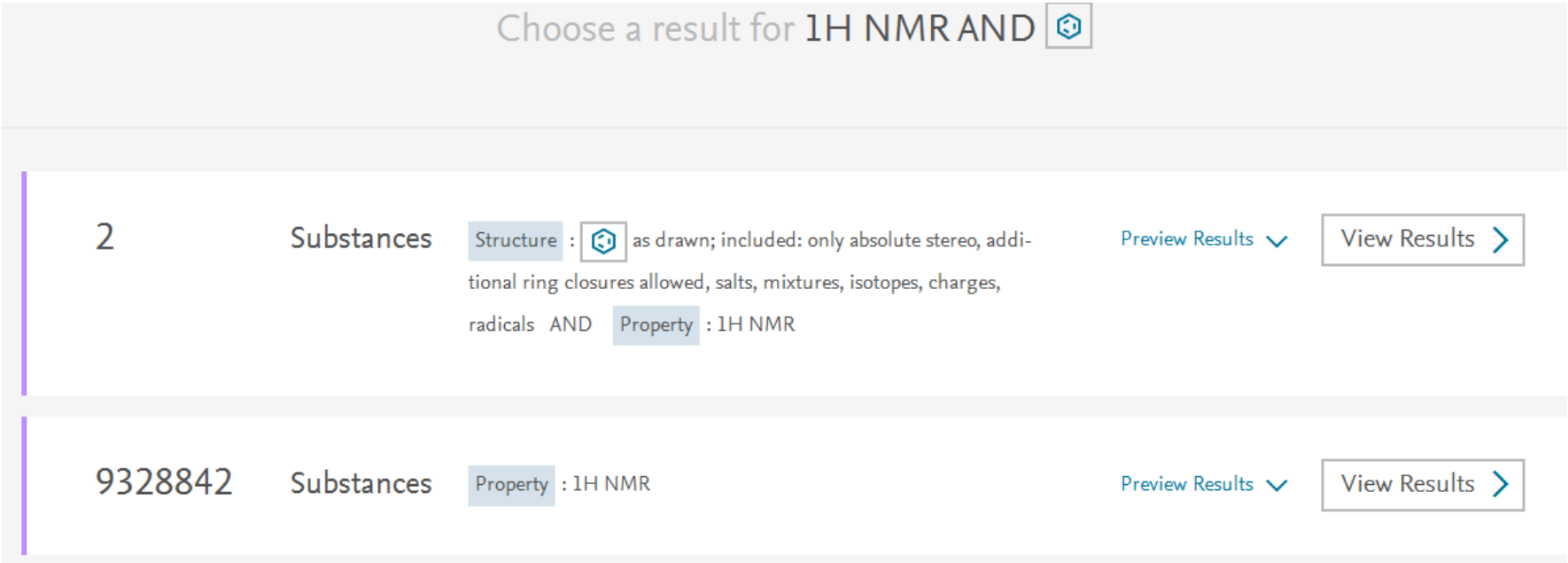
is		Substance Basic Index antimicrobi*

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).



Complex substance search



Thank you for your attention

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