

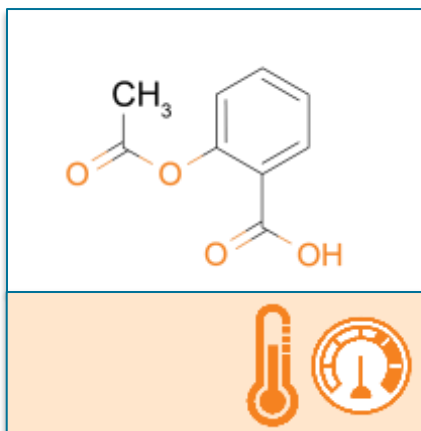
# Reaxys



## Introduction to Reaxys2016

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# Reaxys is a powerful allround research solution for facts and literature



**>90 M Substance records** with **>500 M** excerpted facts on their **properties**: physical, chemical, spectral, ecological, bioactivity

**Chemistry fundamentals**



**>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...

**Uses across disciplines**

# What does Reaxys2016 look like?

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

The screenshot shows the Reaxys search interface. At the top left is the Reaxys logo. At the top right are the Elsevier Reaxys logo, a user profile icon, a search icon, and a menu icon. Below the header is a search bar with the text "Search substances, reactions, documents and bioactivity data in Reaxys, PubChem and eMolecules". Below the search bar are three tabs: "Quick Search" (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 callout lines point from text boxes to the interface: one from the left text box to the "Quick Search" tab, one from the right text box to the "Query Builder" tab, and one from the bottom text box to the "Create Structure or Reaction Drawing" option.

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

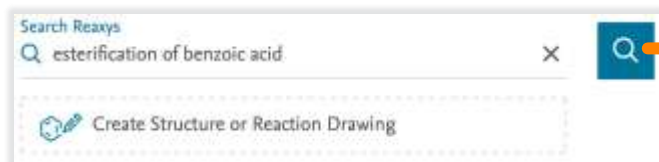
Search >

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



Interprets natural language

1

2

Recognizes search intention (reactions)

3

Delivers a ranked list of alternative results suggestions

82	Reactions	benzoic acid starting (exact search) AND Reaction Type : esterification; esterifications OR Other Conditions : esterification; esterifications	Preview Results ▾	View Results >
399	Documents	Titles, Abstracts and Keywords : Document Basic Index : "esterification"; "esterifications" AND Document Basic Index : benzoic acid	Preview Results ▾	View Results >
21316	Documents	Titles, Abstracts and Keywords : Document Basic Index : benzoic acid	Preview Results ▾	View Results >
48655	Documents	Titles, Abstracts and Keywords : Document Basic Index : "esterification"; "esterifications"	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 left, the Reaxys logo is visible. The main workspace is titled 'Untitled' and contains a 'Structure' section with a 'Create Structure / Reaction Drawing' button. Below this, there is a query builder area with an 'AND' operator and two query cards: 'Melting Point' and 'Boiling Point'. On the right side, there is a 'Search properties' panel with a list of querylets, including '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'. A 'Feedback' button is at the bottom right of the list. The interface is annotated with four numbered orange circles and lines:

- 1** Search Querylets (points to the right-hand list)
- 2** Drag and drop them into a query (points to the 'Boiling Point' query card)
- 3** Combine them with operators (points to the 'AND' operator)
- 4** Enter search terms and click Search. (points to the 'Search' button at the top right)

# 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. Cited 3 times

1 Part 1: Design, synthesis and biological evaluation of novel 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives

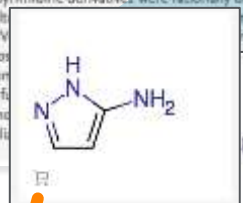
Tian, Ye Du, Deping; Rao, Dhwanir; +6 others - Bioorganic and Medicinal Chemistry, 2014, vol. 22, # 7, p. 2052 - 2059

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

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 culture. Most of the tested compounds displayed excellent activity against wild-type HIV-1 with IC<sub>50</sub> values ranging from 5.98 to 0.07 μM. Among the active compounds, 5a was found to be the most potent.



Check availability

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, 3-aminopyrazole

CAS Registry Number(s): 100000000

Molecular Formula: C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>

Molecular Weight: 81.0808

isChiral: No

Substance type: Organic

Linear Structure Formula: C<sub>4</sub>H<sub>5</sub>N<sub>3</sub>

No. of references: 211

Identification -

Spectra - 5

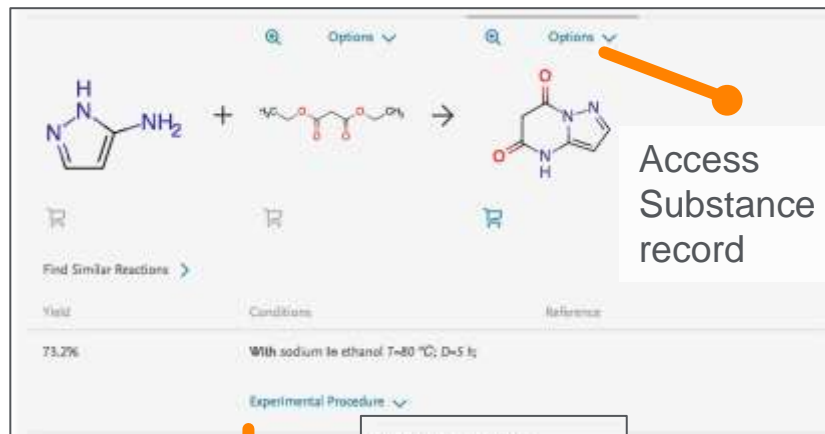
Physical Data - 11

Other Thermochemical Data - 1

Boiling Point - 7

Melting Point - 5

View property data



Reaction scheme showing the synthesis of 3(5)-aminopyrazole from 3-aminopyrazole and diethyl malonate, catalyzed by sodium in ethanol.

Yield: 73.2%

Conditions: With sodium in ethanol T=80 °C; D=5 h

Reference:

Experimental Procedure

Access Substance record

Examine experimental conditions

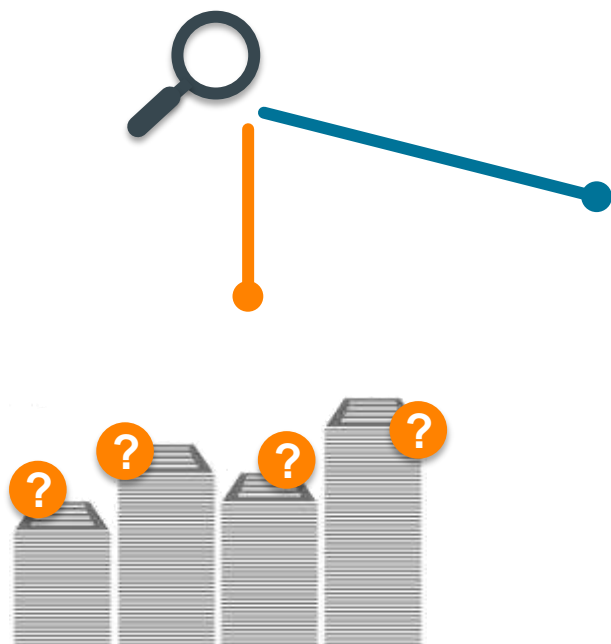
Experimental Procedure

3-Aminopyrazole (1) (20mmol, 1.0eq) and diethyl malonate (22mmol, 1.1eq) were added to a freshly made solution of sodium metal (40mmol, 1.0eq) 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 (500mL). 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 in a vacuum oven. The product was purified by column chromatography (silica gel, 10% MeOH in CH<sub>2</sub>Cl<sub>2</sub>) to give 3(5)-aminopyrazole (3) as a light yellow powder (3), yield 73.2% (mmol). E<sub>n</sub>-MS: 152.2 [M+], 174.1 [M+H]<sup>+</sup> that was directly used in next step.

What is unique about Reaxys2016?



# Reaxys2016 aims to deliver immediate access to information



The screenshot displays a chemical reaction between acetic acid and salicylic acid to form aspirin. Below the reaction, a table titled "Find Similar Reactions" lists experimental conditions and yields. To the right, a "Physical Data" window is open, and a list of references is shown, including articles on aspirin's effects on dogs, resistance in patients, and platelet expression.

Yield	Conditions
93.8%	Stage #1: 3-(diethylamino)ethyl N-(3-dimethylamino)propyl carbodiimide cross-linked agarose resin Stage #2: acetic acid in water Stage #3: acetic acid in water Experimental Procedure

Physical Data - 332

Classification Experiment - 27

Yield	Conditions	Relevance	Classification	Experiment
93.8%	Stage #1: 3-(diethylamino)ethyl N-(3-dimethylamino)propyl carbodiimide cross-linked agarose resin Stage #2: acetic acid in water Stage #3: acetic acid in water Experimental Procedure	1.00	ACID-H	33
93.8%	Stage #1: 3-(diethylamino)ethyl N-(3-dimethylamino)propyl carbodiimide cross-linked agarose resin Stage #2: acetic acid in water Stage #3: acetic acid in water Experimental Procedure	0.60	ACID-H	33
93.8%	Stage #1: 3-(diethylamino)ethyl N-(3-dimethylamino)propyl carbodiimide cross-linked agarose resin Stage #2: acetic acid in water Stage #3: acetic acid in water Experimental Procedure	0.40	ACID-H	33

Lyophilized aspirin with trehalose may decrease the incidence of gastric injuries in healthy dogs. Cited 1 times  
Lin, Lee-Shuan; Kazuaga, Yuki; Shimahata, Nobuyuki; et al. - Journal of Veterinary Medical Science, 2012, vol. 74, no. 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-Yeung; et al. - Korean Journal of Laboratory Medicine, 2008, vol. 28, no. 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  
Flepl, Christopher N.; Goodman, Timothy; Becker, Silke; et al. - British Journal of Clinical Pharmacology, 2014, vol. 78, no. 2, p. 325 - 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

**cetane**

- Identification
- Physical Data - 2307
- Other Data - 292
- Spectra - 103
- Bioactivity - 127

Preparations - 183 >  
Reactions - 305 >  
Documents - 1627 >

CCCCCCCCCCCCCCCCCC

**cetane**

Beary ID:	1736592		
Chemical Name(s):	cetane, Hexadecane, Hexadecan		
CAS Registry Number(s):	Substance type:		
Molecular Formula:	E16H34	Linear Structure Formula:	C12H26C4H8
Molecular Weight:	226.446	No. of references:	1627
InChIKey:	DCAYPVUWAIABOU-LHFFADYSA-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

[+ Load More](#)

**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

**Bioactivity - 127**

- Ecotoxicology - 16
- Pharmacological Data - 311

**Spectra - 103**

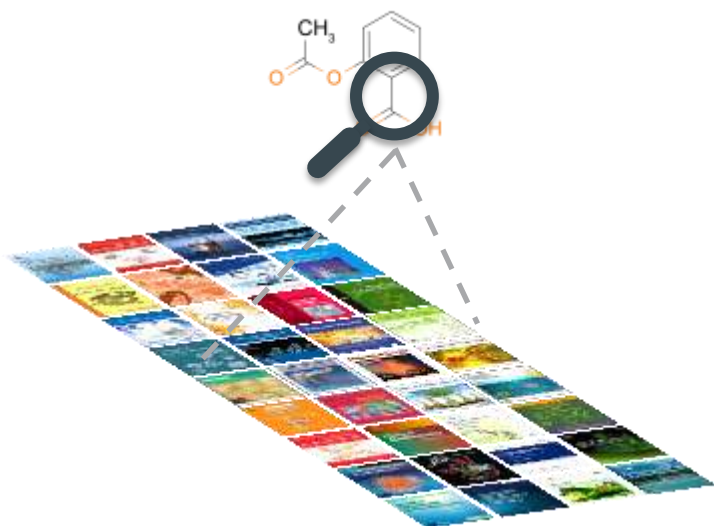
- Raman Spectroscopy - 12
- IR Spectroscopy - 26
- Fluorescence Spectroscopy - 1
- ESR Spectroscopy - 3
- NMR Spectroscopy - 35
- UV/VIS Spectroscopy - 4
- Mass Spectrometry - 18
- Rotational Spectroscopy - 1
- Luminescence Spectroscopy - 2
- NQR Spectroscopy - 1

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

142  
3 queries  
420  
1,21 mil  
984.003  
231  
589  
612  
142  
3 queries  
420

Filters and Analysis Apply ⌵

Index Terms (List) 1 ⌵

<input type="checkbox"/>	stereoselectivity	<span>▬</span>	44
<input type="checkbox"/>	enantioselectivity	<span>▬</span>	24
<input checked="" type="checkbox"/>	total synthesis	<span>▬</span>	18
<input type="checkbox"/>	oxidation reaction	<span>▬</span>	18
<input type="checkbox"/>	enantiomer excess	<span>▬</span>	11
<input type="checkbox"/>	catalysed reaction	<span>▬</span>	11
<input type="checkbox"/>	catalyst	<span>▬</span>	10
<span>+</span> More			

Index Terms (ReaxysTree) ⌵

Publication Year ⌵

<input type="checkbox"/>	1998	<span>▬</span>	3
<input type="checkbox"/>	2006	<span>▬</span>	2
<input type="checkbox"/>	2009	<span>▬</span>	2
<input type="checkbox"/>	1994	<span>▬</span>	1
<input type="checkbox"/>	2008	<span>▬</span>	1
<input type="checkbox"/>	2015	<span>▬</span>	0
<input type="checkbox"/>	2007	<span>▬</span>	0
<span>+</span> More			

Document Type ⌵

142  
3 queries  
420  
1,21 mil  
984.003  
231  
589  
612  
142  
3 queries  
420

Filters and Analysis Apply ⌵

Index Terms (List) 1 ⌵

<input type="checkbox"/>	stereoselectivity	<span>▬</span>	44
<input type="checkbox"/>	enantioselectivity	<span>▬</span>	24
<input checked="" type="checkbox"/>	total synthesis	<span>▬</span>	18
<input type="checkbox"/>	oxidation reaction	<span>▬</span>	18
<input type="checkbox"/>	enantiomer excess	<span>▬</span>	11
<input type="checkbox"/>	catalysed reaction	<span>▬</span>	11
<input type="checkbox"/>	catalyst	<span>▬</span>	10
<span>+</span> More			

Index Terms (ReaxysTree) ⌵

Publication Year ⌵

Document Type ⌵

Authors ⌵

<input type="checkbox"/>	weinreb, steven m	<span>▬</span>	2
<input type="checkbox"/>	nakata, tadashi	<span>▬</span>	1
<input type="checkbox"/>	kroutil, wolfgang	<span>▬</span>	0
<input type="checkbox"/>	cha, jin soon	<span>▬</span>	0
<input type="checkbox"/>	oishi, takeshi	<span>▬</span>	0
<input type="checkbox"/>	nakamura, kaoru	<span>▬</span>	0

Selected index term highlights corresponding records in other filters

# Three flexible integration points fit to your workflow

WEB

## Web Interface

The **database is maintained by Elsevier** and augmented with expertly curated content

Data are accessed from a **web browser** using a powerful User Interface maintained by Elsevier

The interface and presentation of results are optimized for specific end users

API

## Application Programming Interface

The **database is maintained by Elsevier** and augmented with expertly curated content

Data are accessed from **internal systems** and integrated with existing tools, such as electronic lab notebooks

Enables **streamlined use of Reaxys content** and seamless integration for a wide range of applications

FF

## Reaxys Flatfile

Expertly curated content of Reaxys is delivered to customer in easily implemented format and **stored internally**

**Data are integral component of internal systems environment** and access by standing tools and workflows

Enables **data mining and processing**, as well as integration with other internal or external sources