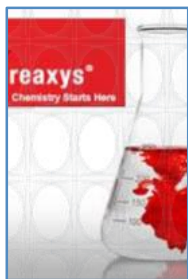




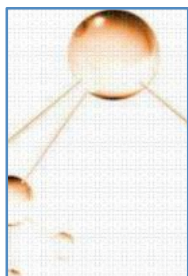
# Reaxys



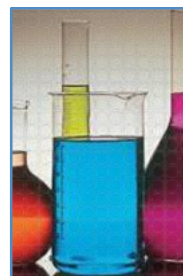
Reaxys dona accés a la major col·lecció de dades de propietats físiques i químiques i de reaccions de compostos orgànics, inorgànics i organometàl·lics. Són dades experimentals, no extrapolades o calculades.



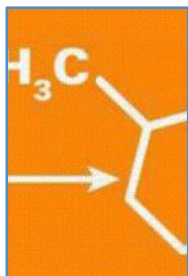
Ofereix funcionalitats com el planificador de rutes de síntesi, la generació de l'estructura química a partir del nom del compost i diferents filtres per a refinar els resultats de cerca.



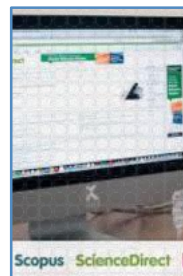
Es pot cercar per estructura, subestructura, text i propietat.



Permet fer cerques de substàncies i de les seves propietats, de reaccions, incloses les de més d'un pas, de rutes de síntesi i d'autors i bibliografia.



La fitxa de cada substància o reacció corresponent a la substància o reacció, incloent la informació bibliogràfica.



És un sistema integrat amb la base de dades Scopus i el portal de revistes ScienceDirect.

**Reaxys** dona informació química des de 1771 i inclou bases de dades de diferents tipus:

Base de dades de  
substàncies:

>78 milions de substàncies  
orgàniques, inorgàniques i  
organometàliques.

Base de dades de reaccions  
químiques:

>40,7 milions de reaccions  
d'una o varies etapes.

Base de dades de propietats:

> 500 milions de propietats  
experimentals de diferents  
camps temàtics

Base de dades bibliogràfica:

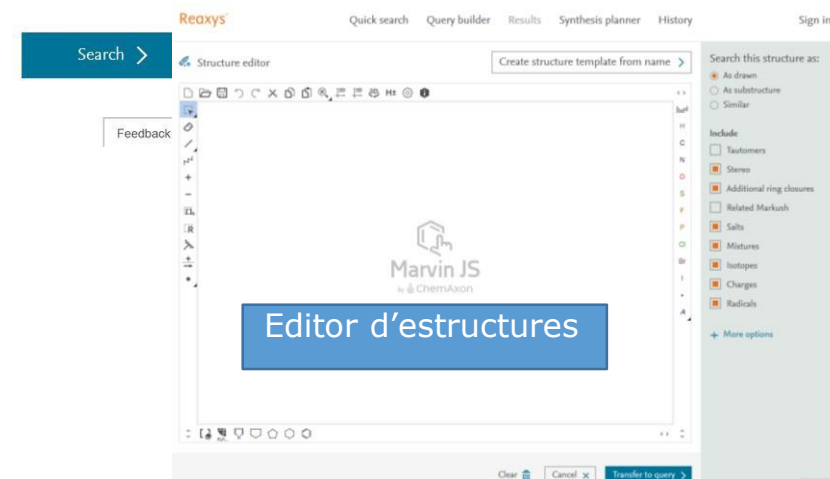
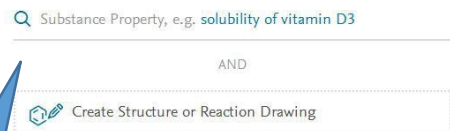
> 46 milions de registres  
provinents de uns 16.000  
títols de revistes i de  
patents de les oficines més  
importantes.

## Quick Search



Permet cercar:

- Substàncies
- Reaccions
- Propietats
- Bibliografia



A la cerca de text es pot utilitzar llenguatge natural. Els termes de cerca poden ser truncats a l'esquerra, la dreta i al mig, mitjançant \*

Cerca estructural per buscar substàncies i reaccions

## Query Builder

Cerca propietats pel seu nom

Reaxys

Quick search Query builder Results Synthesis planner History

Elsevier Reaxys

Search >

Import Save Reset form Delete

Structure Molecular Formula CAS RN Doc. Index

Search properties

Fields Forms History

Reaxys

PubChem

eMolecules

LabNetwork

Structure

Drag & Drop to build a query

Search properties

Fields Forms History

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

Pharmacological Data

Ecotoxicology

More +

Permet cercar:

- Substàncies
- Reaccions
- Propietats
- Bibliografia

Tria la base de dades per veure les propietats disponibles

# Query Builder

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sign in ?

Search Substances > ▾

Import Save Reset form Delete Structure Molecular Formula CAS RN Doc. Index

Melting Point Find any Hide fields ^ ×

= Melting Point, °C 200-250

is Solvent (Melting Point)

AND

Boiling Point Find any Hide fields ^ ×

> Boiling Point, °C 300

Pressure (Boiling Point), Torr 760

Search properties

Fields Forms History

Reaxys ^

Basic Indexes ▾

Identification ▾

Physical Properties ^

☞ Melting Point ⋮

☞ Boiling Point 📄 ⋮

☞ Sublimation ⋮

☞ Refractive Index ⋮

☞ Density ⋮

☞ Adsorption ⋮

More +

Spectra ▾

Pharmacological Data ▾

Toxicology Feedback ?

S'utilitzen els operadors  
booleans (AND, OR, NOT i  
PROXIMITY) per buscar  
més d'una propietat alhora

Les propietats que volem  
cercar s'arrosseguen a la  
zona de treball des de la  
barra lateral

Reaxys® Quick search Query builder Results Synthesis planner History Sign in ⓘ

← Back to Quick Search

Choose a result for amoxicillin

19	Substances	Structure :  as drawn	Preview Results ▾	View Results
74,510	Documents	Titles, Abstract, Keywords : amoxicillin	Preview Results ▾	View Results >

Quan s'utilitza Quick Search hi ha l'opció de previsualitzar els resultats

Els resultats depenen del tipus de terme utilitzat per fer la cerca. Aquí s'ha introduït el nom de una substància i els resultats són substàncies (cerca estructural) i bibliografia

Reaxys® Quick search Query builder Results Synthesis planner History Sign in ⓘ

← Back to Quick Search

Choose a result for preparation of amoxicillin

54	Reactions	Product(s) :  as drawn	Preview Results ▾	View Results >
6,486	Documents	Titles, Abstract, Keywords : preparation, amoxicillin	Preview Results ▾	View Results >
74,510	Documents	Titles, Abstract, Keywords : amoxicillin	Preview Results ▾	View Results >
8,126,202	Documents	Titles, Abstract, Keywords : preparation	Preview Results ▾	View Results >

Aquí s'ha cercat una frase i dona reaccions i documents

Fitxa d'una substància amb  
totes les propietats,  
reaccions i bibliografia

The screenshot shows the Reaxys interface for the search results of benzophenone. On the left, there is a sidebar with a 'Filters and Analysis' section containing various filter options like 'By Structure', 'Substances Classes', 'Molecular Weight', etc. The main content area displays the chemical structure of benzophenone, its molecular formula (C<sub>13</sub>H<sub>10</sub>O), and a list of properties such as 'Hit Data - 5', 'Spectra - 701', 'Preparations - 3,054', etc. Below this, there are two expanded sections: 'Hit Data - 5' and 'Boiling Point - 4 hits out of 61'. The 'Hit Data' section shows a table with columns for 'Melting Point, °C' and 'Reference', with one entry: 236 - 238, referencing Zhang, Gui-Sheng; Yang, De-Hong; Chen, Mi-Feng; +1 other - Synthetic Communications, 1998, vol. 28, # 12, p. 2221 - 2225. The 'Boiling Point' section shows a table with columns for 'Boiling Point, °C', 'Pressure (Boiling Point), Torr', and 'Reference', with three entries: 306, 305.47, and 305.9, all at 760 Torr, with references to Kalamar et al. (1967), Dow Chem. Co. (1955), and Burriel; Marti (1931).

Opcions per filtrar o  
analitzar els resultats

El camp Hit Data dóna  
les dades concretes de  
les propietats que  
s'han cercat



The screenshot shows the Reaxys interface with search results for 162 reactions. On the left, a sidebar contains filters such as 'By Structure', 'Yield', 'Reagent/Catalyst', 'Solvent', 'Catalyst Classes', 'Solvent Classes', 'Product Availability', 'Reactant Availability', 'Reaction Classes', 'Document Type', and 'Publication Year'. The main area displays '162 Reactions out of 117 Documents containing 2 Substances'. Below this, there are two reaction cards. The first card shows a chemical reaction with a yield of 55%. Below the reaction, there is a table with columns for 'Yield', 'Conditions', and 'Reference'. The 'Reference' column contains the citation: 'Rehman, Hajira; Qadir, Abdul; Ali, Zulfiqar; +4 others - Asian Journal of Chemistry, 2016, vol. 28, # 2, p. 343 - 346'. There are links for 'Full Text' and 'Show details'. A 'Feedback' button is visible at the bottom right of the reaction card.

Fitxa d'una reacció amb totes les dades, inclosos el procediment experimental i la cita bibliogràfica

Es pot arribar al text complet

Amb l'ús dels filtres es poden ajustar els resultats



The screenshot shows the Reaxys search results page. On the left is a sidebar with 'Filters and Analysis' and a count of 6,486. The main area shows a list of 6,486 documents. The first document is 'Amoxicillin sodium potassium clavulanate for injection preparation, and its preparation method (by machine translation)' by North China Pharmaceutical Co., Ltd.; Gao, Renlong; Hu, Weiguo. The second is 'Preparation of amoxicillin intragastric buoyant sustained-release tablets and the dissolution characteristics' by Tokumura, Tadakazu; Machida, Yoshiharu. The third is 'Novel sodium amoxicillin preparations' by Gist-Brocades N.V. The fourth is 'Preparation and in vitro release of amoxicillin sustained-release tablets' by Ye, Bing; Liu, Zhong-Rong; Ji, Yuan-Qiao. Each document entry includes a checkbox, a title, authors, and options for Abstract, Front Page Info, Substances, and Full Text.

Llistat de documents ordenats per rellevància per defecte; però hi ha altres opcions

Accés a la primera pàgina, en el cas de les patents

Accés al text complet

Els autors estan enllaçats amb la informació de les seves publicacions a Scopus

Accés al resum

# Synthesis Planner

Reaxys® Quick search Query builder **Results** Synthesis planner History Sign in ⓘ

19 Filters and Analysis

By Structure ▾

Substances Classes ▾

Molecular Weight ▾

Availability ▾

Available Data ▾

Document Type ▾

Publication Year ▾

Back to Results Preview Database: Reaxys - 19 ▾

19 Substances out of 4,252 Documents containing 211 Reactions

0 selected: Options ▾

Synthesize

- > Manually
- > Autoplan

Spectra - 53

26787-78-0

Bioactivity - 4,062

Other Data - 994

Preparations - 20 >

Reactions - 162 >

Documents - 3,930 >

Add preparation - 19

Preparation

1

2

Cancel × Add 1 to plan >

A partir d'una substància es pot elaborar una ruta de síntesi, manualment o de forma automàtica (Autoplan)

Amb l'opció manual cal triar la reacció que ens interessa i afegir-la al pla de síntesi

# Synthesis Planner

The screenshot shows the Reaxys Synthesis Planner interface. At the top, there are navigation links: Quick search, Query builder, Results, Synthesis planner (selected), and History. On the right, there are links for Sign in and a help icon. The main area is titled "Synthesis plan 1" and includes options for Import, Save, and Export, along with Undo and Redo buttons. A central reaction scheme shows two starting materials reacting to form a product. A blue callout box on the left points to the reaction scheme with the text: "Aquí s'escull el Pla de síntesi que interessa". A red callout box on the right points to a context menu with the text: "Cadascuna de les etapes de reacció dóna l'opció de veure les condicions i procediment experimentals". The context menu includes: Show conditions, Hide preparation, Add preparations, and Remove preparation. A "Conditions" window is open at the bottom right, showing details for "Preparation - 1".

Yield	Conditions	Reference
	With triethyl amine hydrochloride In <i>N</i> -methyl-acetamide; dichloromethane Experimental Procedure ▾	Antibioticos - U54193918, 1980, A1 Full Text ↗ Show details >

# Synthesis Planner

Reaxys Quick search Query builder Results Synthesis planner History Sign in

Filters and Analysis

- By Structure
- Substances Classes
- Molecular Weight
- Availability
- Available Data
- Document Type

19 Substances out of 4,252 Documents containing 211 Reactions

0 selected: Options

26787-78-0

Bioactivity - 4,062 Preparations - 20

Other Data - 994 Reactions - 162

Spectra - 53 Documents - 3,930

Synthesize

- Manually
- Autoplan

L'opció Autoplan serveix per crear la ruta sintètica automàticament

Aquí es defineixen els paràmetres per generar la ruta o rutes de síntesi

Reaxys Quick search Query builder Results Synthesis planner History Sign in

Synthesis Planner Edit

Autoplan 1

Plan 1

Import Save Export

Undo Redo

Yield Conditions Reference

2 95%

1

Create plans by autoplan

Number of plans to create 5

Max. alternative branches 5

Max. number of steps 5

Stop searching if starting material is commercially available  Yes  No

Default yield for reactions without a given yield

Always show screen before creating autoplan

Create Plans

S'escull el Pla de síntesi amb el que es vol treballar

# Gravar i Exportar

Es pot gravar la cerca per  
repetir-la més endavant

Des del Query Builder:

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sign in

Import Save Reset form Delete Structure Molecular Formula CAS RN Doc. Index

Search

Chemical Name is Chemical Name amoxicillin

AND

Effect (PharmData) Find any Show fields

Search properties

Fields Forms History

- Sublimation
- Refractive Index
- Density
- Adsorption
- Spectra
- Pharmacological Data
  - Effect (PharmData)
  - Endpoint of Effect (PharmData)
  - Species or Test-System (PharmData)
  - Sex (PharmData)
  - Route of Application (PharmData)
  - Concentration (PharmData)

Des de l'Historial:

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sign in

History

Recent Saved

Reaxys

4,252 Documents	Today 17:09	Query Builder: in documents -	Edit Query Save Alert View
54 Reactions	Today 17:03	Quick Search: "preparation of amoxicillin"	View

# Gravar i Exportar

Des del Synthesis planner:

The screenshot displays the Reaxys Synthesis Planner interface. At the top, there are navigation tabs: Quick search, Query builder, Results, Synthesis planner (selected), and History. A 'Sign in' button is also present. The main area shows 'Plan 1' with an 'Export' button highlighted by a red arrow. Below the plan, a reaction scheme is visible, showing a multi-step synthesis starting from a starting material and proceeding through two steps (labeled 2 and 1) to a final product. A blue callout bubble points to the 'Export' button with the text: "Es pot gravar la ruta de síntesi".

An 'Export reactions' dialog box is open on the right side of the screen. It has two tabs: 'Export reactions' (selected) and 'Export documents'. Under 'Export reactions', there is a 'Choose a format:' dropdown menu set to 'PDF/Print'. Below this, there are 'Additional options' with three checkboxes: 'Include structures' (checked), 'Include experimental procedure' (checked), and 'Include a description in the document' (unchecked). An 'Export' button is located at the bottom right of the dialog box. A blue callout bubble points to the dialog box with the text: "És possible exportar, en diferents formats, les reaccions i els documents".

# Exportar

Des de la pàgina de resultats d'una cerca de bibliografia:

The screenshot shows the Reaxys search results interface. At the top, there are navigation links: Quick search, Query builder, Results (underlined), Synthesis planner, and History. On the right, there are links for Sign in and a help icon. A left sidebar contains a 'From history' button and a 'Filters and Analysis' section with various filter categories like Index Terms, Publication Year, Document Type, etc. The main content area shows search results for '4,252 Documents with 20 Substances, 23,406 Reactions'. Below this, there are three search results listed with checkboxes and options for Abstract, Front Page Info, and Substances. A red arrow points from the 'Export' button in the search results area to an 'Export documents' dialog box. The dialog box has a title bar with a close button (X). It contains the following options: 'Choose a format:' set to 'PDF/Print'; 'Range:' set to 'All results - 4252' with a note 'The Export is limited to 1-1000 range.'; 'Export:' with radio buttons for 'All available data' (selected) and 'Hit data only'; and 'Additional options:' with checkboxes for 'Include structures', 'Include abstracts', 'Include reactions', 'Include Front page information', and 'Include a description in the document'. An 'Export >' button is at the bottom right of the dialog.



# Exportar

Des de la pàgina de resultats d'una cerca de substàncies:

The screenshot shows the Reaxys search results interface. On the left, a sidebar titled "Filters and Analysis" is visible. The main content area displays "19 Substances" with a table of results. A "Select action" dialog box is open over the first result, with the "Export" option selected. A red arrow points from this dialog to the "Export substances Reaxys" modal window. This modal window allows users to choose a format (PDF/Print), range (All results - 19), and export options (All available data, Identification data only, Hit data only, Choose specific data). Additional options include "Include structures" and "Include a description in the document".

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Sign in

Database: Reaxys - 19

19 Substances out of 4,252 Documents containing 211 Reactions

0 selected: Options

No of References

1 Oc1ccc(O)cc1 26787-78-0  
Bioactivity - 4,062 Preparations - 20  
Other Data - 994 Reactions - 162  
Documents - 3,930

2 Amoxicillin  
CC1(C)NC(=O)C2=CC=C(C=C2)C(=O)N1C C<sub>19</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S 365.41 24141054  
Bioactivity - 22

3 amoxicillin  
CC1(C)NC(=O)C2=CC=C(C=C2)C(=O)N1C C<sub>19</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S 365.41 5485834 38083-36-2  
Identification Bioactivity - 2  
Physical Data - 1 Other Data - 3

Export substances Reaxys

Choose a format: PDF/Print

Range: All results - 19

Export:  
 All available data  
 Identification data only  
 Hit data only  
 Choose specific data

Additional options:  
 Include structures  
 Include a description in the document

Export

# Exportar

Des de la pàgina de resultats d'una cerca de reaccions:

The screenshot displays the Reaxys search results page. On the left is a sidebar with filters and analysis options, including 'By Structure', 'Yield', 'Reagent/Catalyst', 'Solvent', 'Catalyst Classes', 'Solvent Classes', 'Product Availability', 'Reactant Availability', 'Reaction Classes', and 'Document Type'. The main area shows '211 Reactions out of 4,252 Documents containing 19 Substances'. An 'Export' button is highlighted with a red arrow pointing to an 'Export reactions' dialog box. The dialog box contains the following options:

- Choose a format: PDF/Print
- Range: All results - 211
- Export:  All available data,  Identification data only,  Hit data only
- Additional options:  Include structures,  Include experimental procedure,  Include a description in the document

The 'Export' button at the bottom right of the dialog box is also highlighted.



**Moltes gràcies!**



**Us ha estat útil?**  
**Ajudeu-nos a millorar**  
**[bit.ly/2s05WCQ](https://bit.ly/2s05WCQ)**

