



UNIVERSITAT DE
BARCELONA

CRAI Biblioteca
Física i Química

CRAI

Centre de Recursos per a
l'Aprenentatge i la Investigació

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.



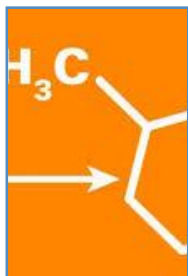
Ofereix funcionalitats com el planificador de rutes de síntesi, la generació de l'estructura química a partir del nom del compost i diferents filtres per a refinar els resultats de cerca.



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 conté agrupada tota la informació 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
organometàl·liques.

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

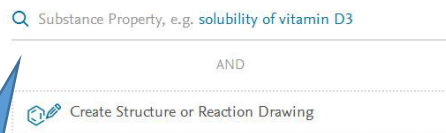
Base de dades bibliogràfica:

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

Quick Search

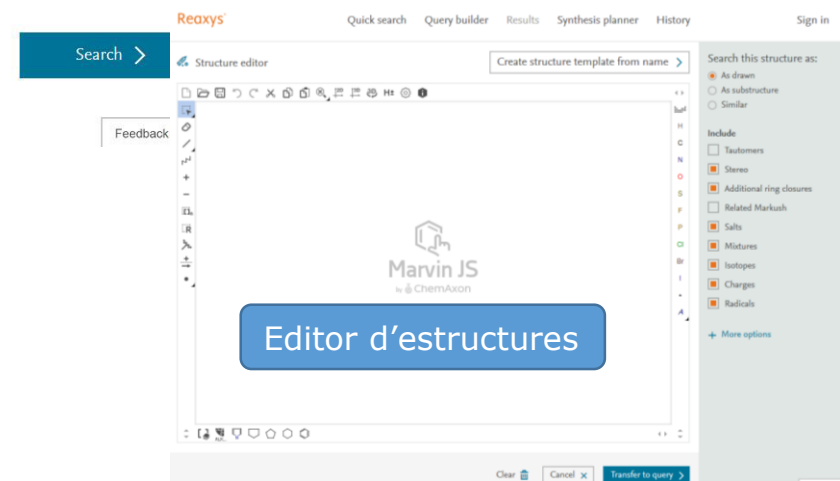
Permet cercar:

- 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

Permet cercar:

- Substàncies
- Reaccions
- Propietats
- Bibliografia

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

Basic Indexes

Identification

Physical Properties

Spectra

Pharmacological Data

Ecotoxicology

More +

Drag & Drop to build a

Tria la base de dades per veure les propietats disponibles

Query Builder

The screenshot shows the Reaxys Query Builder interface. At the top, there are navigation links: Quick search, Query builder (highlighted), Results, Synthesis planner, History, and Sign in. Below the navigation is a toolbar with icons for Import, Save, Reset form, and Delete. A search bar labeled 'Search Substances' is also present. The main area contains two query clauses:

- Melting Point**: Find any. Operators: = (Melting Point, °C, 200-250) and is (Solvent (Melting Point)).
- Boiling Point**: Find any. Operators: > (Boiling Point, °C, 300) and > (Pressure (Boiling Point), Torr, 760).

An 'AND' operator is shown between the two clauses. On the right, a sidebar titled 'Search properties' lists various property categories: Basic Indexes, Identification, Physical Properties, Melting Point, Boiling Point, Sublimation, Refractive Index, Density, Adsorption, Spectra, Pharmacological Data, and Cytotoxicology. The 'Boiling Point' property is highlighted in the sidebar.

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

Resultats

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

Resultats: Substàncies

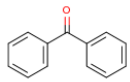
Fitxa d'una substància amb
totes les propietats,
reaccions i bibliografia

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

52 Filters and Analysis

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

benzophenone
C₁₃H₁₀O 182.222 1238185 119-61-9



Hit Data - 5 Spectra - 701 Preparations - 3,054
Identification Bioactivity - 747 Reactions - 14,279
Physical Data - 1,222 Other Data - 128 Documents - 12,958

Hit Data - 5

Melting Point - 1 hits out of 85

Melting Point, °C	Reference
236 - 238	Zhang, Gui-Sheng; Yang, De-Hong; Chen, Mi-Feng; +1 other - Synthetic Communications, 1998, vol. 28, # 12, p. 2221 - 2225 Full Text ↗ Cited 33 times ↗ Show details >

Boiling Point - 4 hits out of 61

Boiling Point, °C	Pressure (Boiling Point), Torr	Reference
306	760	Kalamar et al. - Chemické Zvesti, 1967, vol. 21, p. 350,355,356 str., 1967, vol. 67, # 116737 Full Text ↗ Show details >
305.47	760	Dow Chem. Co. - Adv. Chem. Series 15, Phys. Prop. Chem. Co 1955, p. 354 Full Text ↗ Show details >
305.9	760	Burriel; Marti - Anales de la Real Sociedad Española de Ciencias 1931. vol. 29. n. 89.119 Feedback 🗨

Opcions per filtrar o
analitzar els resultats

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

Resultats: Reaccions

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

162 Filters and Analysis

- By Structure
- Yield
- Reagent/Catalyst
- Solvent
- Catalyst Classes
- Solvent Classes
- Product Availability
- Reactant Availability
- Reaction Classes
- Document Type
- Publication Year
- Single step reactions only

162 Reactions out of 117 Documents containing 2 Substances

0 selected: Limit To Exclude Export Reaxys Ranking

1

Find Similar Reactions >

Yield	Conditions	Reference
55%	Stage #1: amoxicillin; p-toluenesulfonyl chloride In water at 20°C ; pH=8 - 9 Torr Stage #2: With hydrogencchloride In water ; pH=2 - 3 Torr	Rehman, Hajira; Qadir, Abdul; Ali, Zulfiqar; +4 others - Asian Journal of Chemistry, 2016, vol. 28, # 2, p. 343 - 346 Full Text Show details

Experimental Procedure

2

Feedback

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

Resultats: Bibliografia

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

6,486 Filters and Analysis

- Index Terms (List) ▾
- Index Terms (ReaxysTree) ▾
- Publication Year ▾
- Document Type ▾
- Authors ▾
- Patent Assignee ▾
- Journal Title ▾
- Substance Classes ▾
- Reaction Classes ▾

6,486 Documents with 9,906 Substances, 12,529 Reactions

0 selected: Limit To Exclude Export

Relevance ▾ ↑ ↓

1 Amoxicillin sodium potassium clavulanate for injection preparation, and its preparation method (by machine translation)
 North China Pharmaceutical Co.,Ltd.; Gao, Renlong; Hu, Weiguang
 Patent Family Members: CN105343067 A
 Abstract ▾ Front Page Info ▾ Full Text ↗

2 Preparation of amoxicillin intragastric buoyant sustained-release tablets and the dissolution characteristics
 Tokumura, Tadakazu; Machida, Yoshiharu - Journal of Controlled Release
 Abstract ▾ Index Terms ▾ Full Text ↗

3 Novel sodium amoxicillin preparations
 Gist-Brocades N.V. - US4607029, 1986, A1
 Patent Family Members: PT70225 A; LU81753 A1; IE791875 L; BE879174 A1; DK413279 A; ...
 Abstract ▾ Front Page Info ▾ Substances ▾ Full Text ↗

4 Preparation and in vitro release of amoxicillin sustained-release tablets
 Ye, Bing; Liu, Zhong-Rong; Ji, Yuan-Qiao - Chinese Journal of Antibiotics, 2003, vol. 28, # 9, p. 534 - 536
 Abstract ▾ Index Terms ▾ 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

Database: Reaxys - 19

19 Substances out of 4,252 Documents containing 211 Reactions

0 selected: Options

Synthesize

- Manually
- Autoplan

Synthesize > 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 x 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

Reaxys[®] Quick search Query builder Results Synthesis planner History Sign in ?

Synthesis Planner Edit

Synthesis plan 1 Import Save Export Undo Redo

Synthesis plan 1

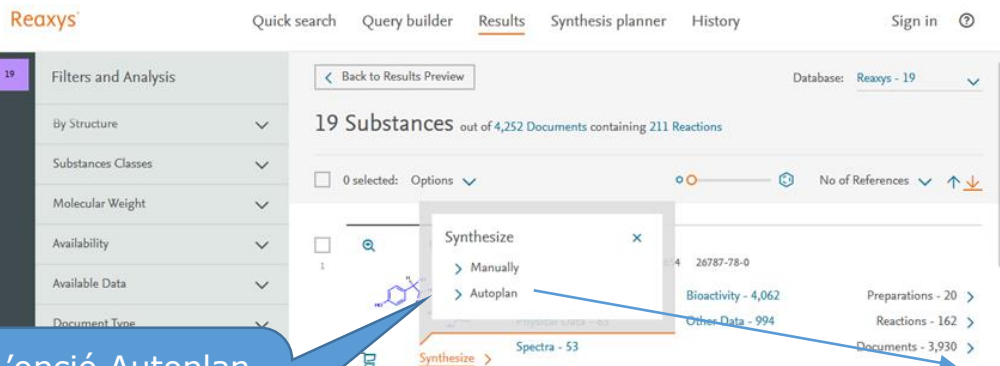
Aquí s'escull el Pla de síntesi que interessa

Cadascuna de les etapes de reacció dóna l'opció de veure les condicions i procediment experimentals

- Show conditions
- Hide preparation
- + Add preparations
- Remove preparation

Yield	Conditions	Reference
	With triethyl amine hydrochloride In N-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

Reactions - 162

Other Data - 994

Documents - 3,930

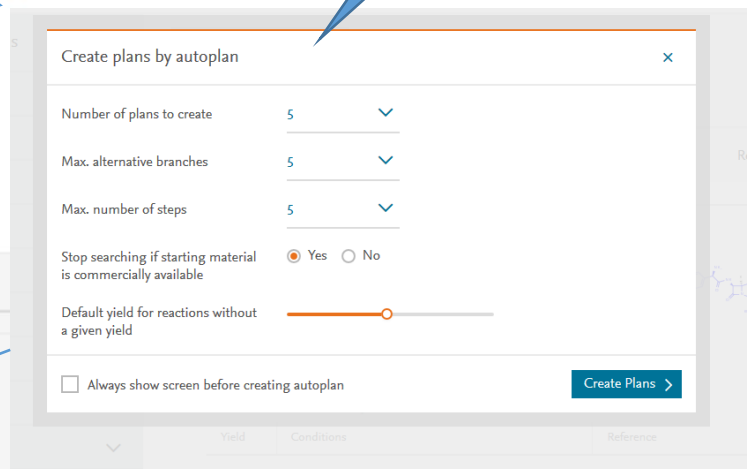
Spectra - 53

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



Create plans by autoplan

Number of plans to create: 5

Max. alternative branches: 5

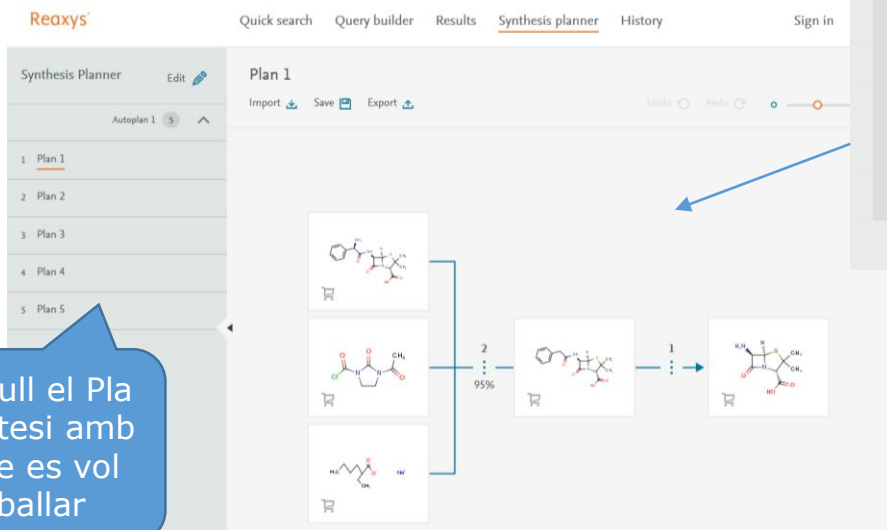
Max. number of steps: 5

Stop searching if starting material is commercially available: Yes No

Default yield for reactions without a given yield: [Slider]

Always show screen before creating autoplan

Create Plans >



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

Synthesis Planner Edit

Autoplan 1

Plan 1

Import Save Export

Undo Redo

Plan 1

Plan 2

Plan 3

Plan 4

Plan 5

Chemical reaction scheme showing the synthesis of a complex molecule from starting materials.

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

Gravar i Exportar

Des del Query Builder:

Es pot gravar la cerca per
repetir-la més endavant

Reaxys[®] 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[®] 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. On the right, there are links for Sign in and a help icon. The main area shows a reaction plan for 'Plan 1' with an 'Export' button. A red arrow points from this button to an 'Export reactions' dialog box. The dialog box has two tabs: 'Export reactions' (selected) and 'Export documents'. Under 'Export reactions', there is a 'Choose a format:' dropdown set to 'PDF/Print'. Below that, 'Additional options' are listed: 'Include structures' (checked), 'Include experimental procedure' (checked), and 'Include a description in the document' (unchecked). An 'Export >' button is at the bottom right of the dialog. A blue callout bubble on the left says 'Es pot gravar la ruta de síntesi' (The synthesis route can be saved). Another blue callout bubble at the bottom right says 'És possible exportar, en diferents formats, les reaccions i els documents' (It is possible to export, in different formats, the reactions and the 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 options: Quick search, Query builder, Results (highlighted), 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' menu 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'. An 'Export' button is visible in the toolbar. An 'Export documents' dialog box is open, showing options for format (PDF/Print), range (All results - 4252), and export type (All available data or Hit data only). Additional options include checkboxes for including structures, abstracts, reactions, front page information, and document descriptions. A red arrow points from the 'Export' button in the main interface to the dialog box.

Exportar

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

The screenshot shows the Reaxys interface with search results for 19 substances. 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' dialog box, which is also open. The 'Export substances Reaxys' dialog shows the following settings:

- 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

The main search results table is partially visible, showing the following entries:

Substance	Chemical Formula	MW	Pub ID	DOI	Bioactivity	Preparations	Reactions	Documents
1	[Chemical Structure]	26787-78-0			Bioactivity - 4,062	Preparations - 20	Reactions - 162	Documents - 3,930
2	Amoxicillin	C ₁₉ H ₁₉ N ₃ O ₅ S	365.41	24141054	Bioactivity - 22			
3	amoxicillin	C ₁₉ H ₁₉ N ₃ O ₅ S	365.41	5485834	38083-36-2	Identification	Bioactivity - 20	Other Data - 3

Exportar

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

The screenshot shows the Reaxys search results interface. On the left is a sidebar with filters and analysis options. The main area displays search results for 211 reactions. An 'Export' button is highlighted with a red arrow pointing to an 'Export reactions' dialog box. The dialog box allows users to choose a format (PDF/Print), set the range (All results - 211), and select export options (All available data, Identification data only, Hit data only). Additional options include including structures, experimental procedure, and a description in the document.

Reaxys Quick search Query builder Results Synthesis planner History Sign in

Database: Reaxys - 211

211 Reactions out of 4,252 Documents containing 19 Substances

0 selected: Limit To Exclude Export

Options

Synthesize

Find Similar Reactions

Yield	Conditions	R
55%	Stage #1: amoxicillin; p-toluenesulfonyl chloride In water at 20°C ; pH=8 - 9 Torr Stage #2: With hydrogencchloride In water ; pH=2 - 3 Torr	R A 3 F

Experimental Procedure

Export reactions

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

Export



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Moltes gràcies!



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