

OBTENCION DE INFORMACION QUIMICA MEDIANTE REAXYS

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FACULTAD DE QUIMICA
JUNIO 2011

Reactions **Substances and Properties** Text, Authors and more

Generate structure from name ← insertar por nombre

Double click this frame and draw structure query

Área de estructuras

- As drawn
 - Substructure:
 - on heteroatoms
 - on all atoms
- Include tautomers
 - Ignore stereo
 - No salts
 - No mixtures
 - No isotopes
 - No additional rings
 - Further options**

Variantes de búsqueda

←

Search

Properties (Form-based) **Properties (Advanced)**

- Substance Data
- Bibliographic Data

Área de opciones

Búsqueda por nombre

Se hace clic al botón

Se escribe el nombre

Reaxys

https://www.reaxys.com/reaxys/secured/start.do

Anonymous user (132.248.103.247)

Query Results Synthesis Plans History My Alerts My Settings Help Info Register Login

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query

Please enter a chemical identifier and then click "Submit"

is vancomycin

Chemical Name: aspirin
InChI-Key: BSYNRYMUTXBXSQ-UHFFFAOYSA-N
CAS-No: 50-78-2
Smiles: CC(=O)OC1=C(C=CC=C1)C(O)=O

Submit Cancel

Further options

COPY TO REACTIONS TAB CLEAR

Properties (Form-based) Properties (Advanced)

Search

Substance Data
Bibliographic Data

Clear Query Load Query/Batch Save Query

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- La correlación de nombres con estructuras no es exhaustiva, por lo que muchas veces no va a aparecer la estructura, en este caso buscamos el número de registro de CA (RN) y se introduce en el campo, esto lo podemos hacer usando
- <http://scholar.google.com.mx/>

El compuesto es transferido a la ventana de búsqueda

The screenshot shows the Reaxys web interface. At the top, there is a navigation bar with tabs for "Reactions", "Substances and Properties", and "Text, Authors and more". Below this, there is a search input field labeled "Generate structure from name". The main content area displays a chemical structure query window. On the left, there is a chemical structure of a complex molecule with various functional groups. Below the structure, there is a "By name search in Reaxys" section with "COPY TO REACTIONS TAB" and "CLEAR" buttons. On the right, there are search options: "As drawn", "Substructure:" (with radio buttons for "on heteroatoms" and "on all atoms"), and a list of checkboxes: "Include tautomers", "Ignore stereo", "No salts", "No mixtures", "No isotopes", "No additional rings", and "Further options". A "Search" button is highlighted with a red box. At the bottom, there are "Clear Query", "Load Query/Batch", and "Save Query" buttons. The footer contains contact information and copyright details.

reaxys®

Anonymous user (132.248.103.247)

Query Results Synthesis Plans History My Alerts My Settings Help Info Register Login

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query

As drawn
Substructure:
 on heteroatoms
 on all atoms

Include tautomers
 Ignore stereo
 No salts
 No mixtures
 No isotopes
 No additional rings
 Further options

By name search in Reaxys COPY TO REACTIONS TAB CLEAR

Properties (Form-based) Properties (Advanced)

Substance Data
 Bibliographic Data

Clear Query Load Query/Batch Save Query

Search

Ventana de busqueda

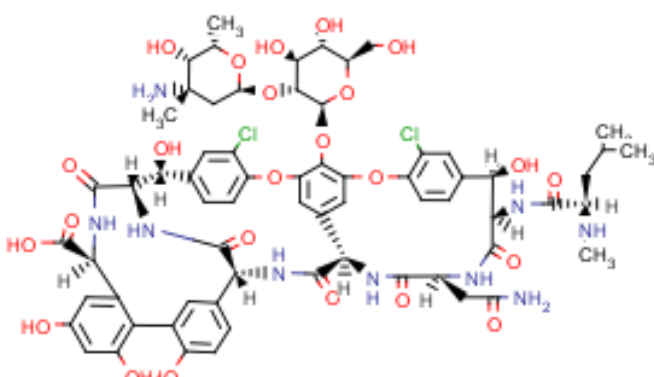
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Se pueden activar o desactivar opciones adicionales

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query



By name search in Reaxys

As drawn
Substructure:
 on heteroatoms
 on all atoms

Include tautomers
 Ignore stereo
 No salts
 No mixtures
 No isotopes
 No additional rings

Further options

Include related Markush
 Keep Fragments separate
 No charges
 No radicals

(type values in fields e.g. 3-5)

of Atoms
 # of Fragments
 # of Ring Closures

Properties (Form-based) Properties (Advanced)

Se manda la búsqueda

El sistema hace la búsqueda

The screenshot displays the Reaxys web application interface. At the top, the browser address bar shows the URL <https://www.reaxys.com/reaxys/secured/start.do>. The Reaxys logo is visible in the top left corner, and the user is identified as "Anonymous user (132.248.103.247)" in the top right. A navigation menu includes "Query", "Results", "Synthesis Plans", "History", "My Alerts", "My Settings", "Help", and "Info".

The main content area is titled "Substances and Properties" and contains a search input field with the placeholder text "Generate structure from name". Below this is a large drawing area with the instruction "Double click this frame and draw structure query". A "Search" button is located at the bottom right of this area.

A "Search Progress" dialog box is overlaid on the interface, indicating that the search is complete. It displays "Search finished." and "51 hits found." with a progress bar at 100%. Below the progress bar, there is a "Loading..." indicator and a list of search filters:

- Include related Markush
- Keep Fragments separate
- No charges
- No radicals

Below the filters, there are input fields for "(type values in fields e.g. 3-5)":

- # of Atoms
- # of Fragments
- # of Ring Closures

At the bottom of the main interface, there are buttons for "Clear Query", "Load Query/Batch", and "Save Query".

Nos muestra los resultados con formula y datos disponibles.

Reaxys

https://www.reaxys.com/reaxys/secured/paging.do?performed=true&action=restore

Query → 51 substances

Create Alert

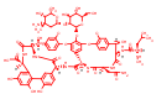
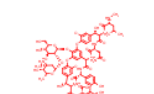
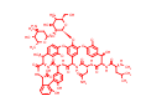
51 substances out of 733 citations

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Availability
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Substances (Grid) Substances (Table) Citations

Limit to Output Print Zoom in Zoom out Hide Sort by No of References

Structure	Chemical Name	N° of preparations All Preps All Reactions	Available Data	N° of ref.	Boiling Point
 Synthesize Show Details	Vancomycin Abbott vancomycin Vancoin Vanco VCM Van Vancomycin	7 prep out of 77 reactions.	Identification Physical Data (29) Spectra (16) Bioactivity/ECOTOX (3791) Use/Application (88) Natural Product (1)	429	
 Synthesize Show Details	VCM vancomycin Vancomycin Va-30 VAN	2 prep out of 21 reactions.	Identification Physical Data (21) Spectra (3) Bioactivity/ECOTOX (818) Use/Application (5)	115	
 Synthesize Show Details	vancomycin	no reactions.	Identification Bioactivity/ECOTOX (584)	62	

Podemos analizar
Datos físicos
Biológicos, espectros
Etc.

Los podemos ver en forma de estructuras

Reaxys

https://www.reaxys.com/reaxys/secured/paging.do?performed=true&action=context&workflowId=1308156189324&workflowStep=0&tabIndex=0&viewNumber=0&openFactID=undefined

Create Alert

51 substances out of 733 citations

Substances (Grid) Substances (Table) Citations

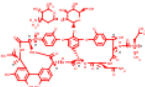
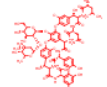
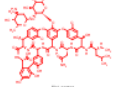
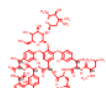
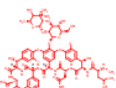
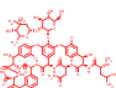
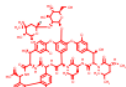
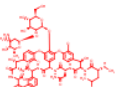
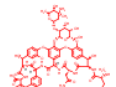
go to Page Page 1 of 6

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Availability
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Substances (Grid) Substances (Table) Citations

Limit to Output Print Zoom in Zoom out Sort by No of References

<input type="checkbox"/> 1  Synthesize	<input type="checkbox"/> 2  Synthesize	<input type="checkbox"/> 3  Synthesize
<input type="checkbox"/> 4  Synthesize	<input type="checkbox"/> 5  Synthesize	<input type="checkbox"/> 6  Synthesize
<input type="checkbox"/> 7  Synthesize	<input type="checkbox"/> 8  Synthesize	<input type="checkbox"/> 9  Synthesize

Show 9 results per page

51 substances out of 733 citations go to Page Page 1 of 6

Substance 1: Identification (29), Physical Data (29), Spectra (16), Bioactivity/Ecotox (3791), Use/Application (88), Natural Product (1)

Substance 2: Identification (21), Physical Data (21), Spectra (3), Bioactivity/Ecotox (818), Use/Application (5)

Substance 3: Identification (584), Bioactivity/Ecotox (584)

Substance 4: Identification (140), Bioactivity/Ecotox (140), Use/Application (371)

Substance 5: Identification (1), Spectra (1), Bioactivity/Ecotox (29), Use/Application (4)

Substance 6: Identification (3), Physical Data (3), Spectra (2), Bioactivity/Ecotox (18)

Substance 7: Identification (1), Spectra (1), Bioactivity/Ecotox (27)

Substance 8: Physical Data (24), Bioactivity/Ecotox (3), Use/Application (1)

Substance 9: Physical Data (18)

Se pueden ver como citas

The screenshot shows the Reaxys website interface. On the left, there is a sidebar with various filters such as 'Number of Fragments', 'Physical Data', 'Spectroscopic Data', 'Bioactivity', 'Natural Product', 'Availability', 'Document Type', 'Authors', 'Patent Assignee', 'Journal Title', and 'Publication Year'. The main content area displays a table of search results. The table has columns for 'Title of the Document', 'Authors', 'Year', 'Source', and 'Times cited'. There are three entries visible, each with a checkbox on the left. The first entry is selected. A blue arrow points from the text 'Haciendo clic podemos ver las referencias originales' to the 'Full Text' link in the 'Source' column of the first entry.

	Title of the Document	Authors	Year	Source	Times cited
<input checked="" type="checkbox"/>	Synthesis and antibacterial activity study of a novel class of cationic anthraquinone analogs	Zhang, Jianjun; Redman, Nathan; Litke, Anthony Phillip; Chan, Ka Yee; Chang, Cheng-Wei Tom; Zeng, Jia; Zhan, Jixun	2011	Bioorganic and Medicinal Chemistry, 2011 , vol. 19, # 1 p. 498 - 503 Full Text View citing articles	
▼ Title/Abstract ▼ Show All Reactions (26) ▼ Show All Substances (42) ▼ Hit Substances in this article (1 out of 42)					
<input type="checkbox"/>	Design, synthesis and antibacterial activity of 3-methylenepyrrolidine formyl hydroxyamino derivatives as novel peptide deformylase inhibitors	Shi, Wei; Ma, Haikun; Duan, Yuejiao; Yang, Liping; Hu, Wenhao; Aubart, Kelly; Fang, Yuhong; Zonis, Rimma	2011	Bioorganic and Medicinal Chemistry Letters, 2011 , vol. 21, # 3 p. 1060 - 1063 Full Text View citing articles	
▼ Title/Abstract ▼ Show All Reactions (138) ▼ Show All Substances (51) ▼ Hit Substances in this article (1 out of 51)					
<input type="checkbox"/>	PHTHALANILATE COMPOUNDS AND METHODS OF USE	UNIVERSITY OF NOTRE DAME DU LAC; MOBASHERY, Shahriar; HESEK, Dusan; CHANG, Mayland	2011	Patent: WO2011/26107 A1, 2011 ; Patent Family: WO2011/26107 A1; Full Text	
▼ Title/Abstract ▼ Front page Information ▼ Show All Reactions (261) ▼ Show All Substances (285) ▼ Hit Substances in this article (1 out of 285)					
<input type="checkbox"/>	Triterpenoid saponins from <i>Symplocos lancifolia</i>	Acebey-Castellon, Ivone Lucia; Voutquenne-Nazabadioko, Laurence; Roseau, Nathalie; Bouthagane, Naima; Muhammad, Dima; Lavaud.	2011	Journal of Natural Products, 2011 , vol. 74, # 2 p. 163 - 168 Full Text	