

# Conozca Reaxys

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# Reaxys

Reaxys es la nueva herramienta de Elsevier desarrollada especialmente para investigadores de las áreas de química, bioquímica y farmacología.

Reaxys promueve la descubierta y la innovación integrando la investigación de propiedades de sustancias y reacciones con la planificación de síntesis químicas.

- Consulte procedimientos experimentales y rendimientos de reacciones químicas en segundos
- Analice las propiedades físicas, farmacéuticas y de toxicidad de los compuestos extraídas de los artículos científicos y de patentes
- Desarrolle la mejor estrategia de síntesis con la exclusiva herramienta de síntesis de Reaxys



# Reaxys - Contenido

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Reaxys reúne el contenido más relevante de la literatura científica y de patentes en química orgánica, inorgánica y órgano metálica a través de las consagradas bases de datos

- **CrossFire Beilstein** – química orgánica
- **CrossFire Gmelin** – química inorgánica y órgano metálica
- **Patent Chemistry Database**



# Facilidad de búsqueda

The screenshot displays the Reaxys search interface. At the top left is the Reaxys logo. A navigation bar contains links for Query, Results, Synthesis Plans, History, My Settings, Help, Register, and Login. Below this, there are tabs for Reactions, Substances and Properties, and Text, Authors and more. A main search area includes a 'Generate structure from name' button and a large text input field with the instruction 'Double click this frame and draw reaction query'. A red arrow points from this instruction to a modal dialog box. The dialog box has a title 'Please enter a chemical identifier and then click "Submit"' and a close button. It contains a text input field with 'aspirin' entered, and three example identifiers: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKJCCW', and 'Example 3: 50-78-2'. There are 'Submit' and 'Cancel' buttons in the dialog. To the right of the main search area is a 'Search as / by' section with radio buttons for 'Product', 'Starting material', 'Any role', 'Reagent/ Catalyst', 'As drawn', and 'Substructure:'. The 'Substructure' section has sub-options for 'on heteroatoms' and 'on all atoms'. Further right is a list of checkboxes for search filters: 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No additional rings', 'Keep Fragments separate', and 'Ignore Atom Mappings'. At the bottom right of the main search area is a 'Search' button. At the bottom left are 'Clear Query', 'Load Query', and 'Save Query' buttons. The footer contains contact information and a copyright notice: 'Contact Us | Support | About Reaxys | Terms and Conditions | Privacy Policy Copyright © 2008 All rights reserved.'

Please enter a chemical identifier and then click "Submit"

aspirin

Example 1: aspirin  
Example 2: BSYNRYMUTXBXSQ-WXRBYKJCCW  
Example 3: 50-78-2

Submit  
Cancel

Search as / by

Product  
 Starting material  
 Any role  
 Reagent/ Catalyst  
 As drawn  
 Substructure:  
 on heteroatoms  
 on all atoms

Ignore stereo  
 No isotopes  
 No charges  
 No radicals  
 No additional rings  
 Keep Fragments separate  
 Ignore Atom Mappings

Search

Clear Query Load Query Save Query

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Interfaz intuitiva: búsquedas por nombre, diseño del compuesto o reacción, número CAS o InChi-Key

# Recursos inteligentes para filtrar y ordenar resultados

Query Results Synthesis Plans History My Settings Help Logout

Query 24 reactions 2 reactions Limited by hits

Ordene los resultados por:  
- Reaxys-Ranking: reacciones más detalladas  
- Reacciones de mayor rendimiento

2 reactions out of 4 citations go to Page Page 1 of 1

Filter by:  
Yield  
Record Type  
Reagent/Catalyst  
Solvent  
Reaction Type  
No. of Steps  
Document Type  
Authors  
Patent Assignee  
Journal Title  
Publication Year

Reactions Citations

Limit to Selection Output Sort by Reaxys-Ranking

Yield Conditions References

1

243.3 g **With** aq. hydrazine hydrate **in** tetrahydrofuran; methanol  
T=10 - 20°C; Reduction cyclization;

**Katayama, Masato**  
Bioscience, Biotechnology, and Biochemistry, **2000**, vol. 64, # 4 p. 808 - 815  
Title/Abstract Full Text Scopus

74%

**With** Zn; AcOH **in** methanol; CH<sub>2</sub>Cl<sub>2</sub>  
Heating;

**Siu, Jason; Baxendale, Ian R.; Ley, Steven V.**  
Organic and Biomolecular Chemistry, **2004**, vol. 2, # 2 p. 160 - 167  
Title/Abstract Full Text Scopus

**in** benzene  
969212;  
Show Experimental Procedure

**Hoffmann-La Roche Inc.**  
Patent: US3976639, 1976  
Title/Abstract Full Text

2

**Multi-step reaction with 2 steps**  
1: 1.) Triton B, 2.) Zn, CaCl<sub>2</sub> / 1.) Me<sub>2</sub>SO, 95 deg C, 1 h, 2.) H<sub>2</sub>O, reflux  
2: 92 percent / RuCl<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub> / toluene / 6 h / Heating  
View Scheme

**Tsuji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuharu; Watanabe, Yoshihisa**  
Journal of the Chemical Society, Chemical Communications, **1986**, # 21 p. 1575 - 1576  
Title/Abstract Full Text Scopus

Producto comercialmente disponible

Enlace para informaciones comerciales

Rx-ID: 8619391

Rx-ID: 18555314

Filtros para los resultados

# Recursos inteligentes para filtrar y ordenar resultados

Filter by:

**Yield**

<input type="checkbox"/> >95 - 100	2
<input type="checkbox"/> >85 - 90	1
<input type="checkbox"/> >75 - 80	4
<input type="checkbox"/> >70 - 75	1

More

Limit to Exclude

**Record Type**

<input type="checkbox"/> full reaction	162
<input type="checkbox"/> has preparation	118
<input type="checkbox"/> half reaction	26
<input type="checkbox"/> has multi-step	1

Limit to Exclude

**Reagent/Catalyst**

<input type="checkbox"/> water	13
<input type="checkbox"/> 10 percent human plasma	12
<input type="checkbox"/> oh-	9
<input type="checkbox"/> methanol	9

More

Limit to Exclude

**Solvent**

<input type="checkbox"/> h2o	32
<input type="checkbox"/> acetonitrile	20
<input type="checkbox"/> methanol	18
<input type="checkbox"/> dioxane	18

More

Limit to Exclude

**Reaction Type**

<input type="checkbox"/> hydrolysis	2
<input type="checkbox"/> complexation	2
<input type="checkbox"/> substitution	1
<input type="checkbox"/> acetylation	1

More

Limit to Exclude

**No. of Steps**

<input type="checkbox"/> 1	187
<input type="checkbox"/> 2	1

Limit to Exclude

**Document Type**

<input type="checkbox"/> journal	108
<input type="checkbox"/> patent	58
<input type="checkbox"/> book review / secondary ref.	2

Limit to Exclude

**Authors**

<input type="checkbox"/> abordo, evelyn a.	1
<input type="checkbox"/> aboul-fadl, tarek	1
<input type="checkbox"/> abraham j.	1
<input type="checkbox"/> abuhijleh, a. latif	1

More

Limit to Exclude

**Patent Assignee**

<input type="checkbox"/> abraham j.	1
<input type="checkbox"/> alfatec-pharma gmbh	1
<input type="checkbox"/> antognazza, patrizia	1
<input type="checkbox"/> ashton, paul	1

More

Limit to Exclude

Journal Title

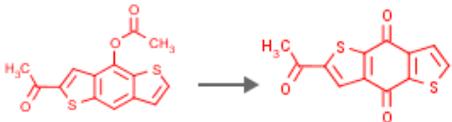
Publication Year



# La mejor fuente para investigar reacciones químicas

Reactions Citations

Limit to Selection Output Sort by

Yield	Conditions	
<input type="checkbox"/> 1	 <p>Rx-ID: 5168182</p>	<p><b>With</b> HOAc, CrO<sub>3</sub> 1 h; Yield given;</p> <p><b>With</b> chromium(VI) oxide in acetic acid 1 h; 10773376; 506007; <a href="#">Hide Experimental Procedure</a></p>
45%		<p><b>Chao, Yu-Hua; Kuo, Sheng-Chu; Wu, Chun-Hsiung; Lee, Chun-Yann; Mauger, Anthony; et al.</b> Journal of Medicinal Chemistry, <b>1998</b>, vol. 41, # 23 p. 4658 - 4661 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Scopus</a></p> <p><b>University of North Carolina at Chapel Hill</b> <b>Patent:</b> US6337346, <b>2002</b> <a href="#">Title/Abstract</a> <a href="#">Full Text</a></p>

**Example 1**  
2-Acetyl-4,8-dihydrobenzo[1,2-b:4,5-b']dithiophene-4,8-dione (9)  
To a stirring mixture of acetyl chloride (5.1 g, 65 mmol) and AlCl<sub>3</sub> (8.7 g, 65 mmol) in 1,2-dichloroethane (200 ML) under N<sub>2</sub> was added dropwise a solution of 4-acetoxybenzo[1,2-b:4,5-b']dithiophene (7)7a (8 g, 32.3 mmol) in 1,2-dichloroethane (90 ML)..  
After stirring for 4 h, this solution was poured into dilute HCl and the aqueous layer was extracted with CHCl<sub>3</sub> three times..  
The combined extracts were washed with saturated NaHCO<sub>3</sub> and water, dried over anhydrous MgSO<sub>4</sub>, and concentrated under reduced pressure to give 7.5 g of the crude intermediate 4-acetoxy-2-acetylbenzo[1,2-b:4,5-b']dithiophene (8).  
To a suspension of crude 8 (7.5 g) in HOAc (30 ML) was added CrO<sub>3</sub> (5.7 g, 57 mmol)..  
After stirring for 1 h, i-PrOH (20 ML) and CHCl<sub>3</sub> (300 ML) were added and stirred for 30 min..  
The resulting solution was poured into ice water, and the aqueous layer was extracted with CHCl<sub>3</sub> three times..  
The combined extracts were dried over anhydrous MgSO<sub>4</sub> and concentrated under reduced pressure..  
The residue was purified by column chromatography (silica gel, CHCl<sub>3</sub>) to give 9 (mp 223-225 .deg. C.) in a 45percent yield. IR (KBr) 1650, 1670 (C=O) cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.67 (s, 3H, CH<sub>3</sub>), 7.68 (d, J=5.1 Hz, 1H, H-7), 7.74 (d, J=5.1 Hz, 1H, H-6), 8.12 (s, 1H, H-3); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ 26.9 (C-2-CH<sub>3</sub>), 126.9 (C-7), 129.4 (C-3), 134.3 (C-6), 170.0 (C-4), 174.4 (C-8), 190.7 (C-2-C=O); MS m/z 262 (M<sup>+</sup>); Anal. (C<sub>12</sub>H<sub>6</sub>O<sub>3</sub>S<sub>2</sub>) C, H.

| 2 |  |  |

1. Reacciones similares, pero con condiciones diferentes son extraídas de diversos artículos científicos y patentes y después reunidas en una única tabla
2. Los textos con procedimientos de reacciones patentadas son exhibidos para inmediata validación de las condiciones

De un artículo científico

De una patente

Reaxys - Microsoft Internet Explorer
Internet

# Beneficios para la química medicinal

Evite procedimientos de laboratorio dispendiosos para a validación de datos calculados

- Reaxys contiene datos experimentales extraídos de la literatura científica:
- Puntos de fusión / ebullición, solubilidad
- Coeficiente de partición octanol/water logP
- Constantes de disociación pKa

Datos de bioactividad y toxicidad, por ejemplo:

- Inhibición / concentración efectiva (e.g. IC/EC50)
- Constantes de unión / disociación (K<sub>i</sub>/k<sub>d</sub>)

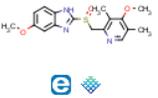
Evite el trabajo de coleta manual de informaciones usando el recurso “Substance Profiles“ y obtenga todos los datos de una sustancia en un único registro



# Evite procedimientos de laboratorio dispendiosos

Substances (Grid) Substances (Table) Citations 1 substances out of 480 citations go to No.  Page 1

Limit to Selection  Sort by Molweight

Structure	Chemical Name	Available Data
	5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole 5-methoxy-2-[[4-methoxy-3,5-dimethyl-pyridin-2-yl)-methylsulfinyl]benzimidazole 2-[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole rac-omeprazole	Identification (70) Physical Data (41) Spectra (26) Bioactivity/ECotox (658) Use/Application (746)

Structure/Compound Data

**Reaxys Registry Number:** 3628192  
**CAS Registry Number:** 73590-58-6 119141-88-7 119141-89-8 131959-78-9 326602-80-6  
**Chemical Name:** 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole, (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole, 5-methoxy-2-[[4-methoxy-3,5-dimethyl-pyridin-2-yl)-methylsulfinyl]benzimidazole, 2-[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole, rac-omeprazole  
**Type of Substance:** heterocyclic

**Molecular Formula:** C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S  
**Linear Structure Formula:** C<sub>17</sub>H<sub>19</sub>SN<sub>3</sub>O<sub>5</sub>  
**Molecular Weight:** 345.422  
**InChi Key:** SUBDBMMJZJVOS-LILDPLRNC

- Identification
- Physical Data
  - Melting Point (4)
  - Conformation (2)
  - Crystal Property Description (1)
  - Crystal Phase (1)
  - Crystal System (1)
  - Space Group (1)
  - Density of the Crystal (1)
  - Optics (1)
  - Optical Rotatory Power (3)
  - Electrochemical Behaviour (2)
  - Dissociation Exponent (7)
  - Electrochemical Characteristics (2)
  - Solubility (MCS) (2)
- Partition octan-1-ol/water (MCS) (3)
- Energy Data (MCS) (3)
- Adsorption (MCS) (1)
- Association (MCS) (6)
- Spectra
  - NMR Spectroscopy (8)
  - IR Spectroscopy (7)
  - Mass Spectrometry (1)
  - UV/VIS Spectroscopy (10)
- Bioactivity/ECotox
  - Pharmacological Data (681)
  - Ecotoxicology (1)
  - Abiotic Degradation, Hydrolysis (7)
  - Abiotic Degradation, Photolysis (1)
  - Use/Application

Pharmacological Data (797)

Effect	Species or Test-System	Sex	Route of Application	Concentration	Method	Further Details	Type	Value of Type	Results	Comment	Reference
enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20α-hydroxysteroid dehydrogenase	IC50	29 μmol/l			Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484-493 Title/Abstract Full Text Scopus

## Valores experimentales para:

- Solubilidad
- Coeficiente de partición octanol/water logP
- Exponente de disociación pK<sub>a</sub>
- Datos de bioactividad (ex: IC/EC, Ki/Kd)
- Datos toxicológicos

## Datos farmacológicos (bio-ensayos)

Type	Value of Type
IC50	29 μmol/l

# Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

▼ Identification	▼ Enthalpy of Vaporization (1)	▲ Spectra
▲ Physical Data	▼ Heat Capacity Cp (1)	▼ NMR Spectroscopy (16)
▼ Melting Point (5)	▼ Other Thermochemical Data (3)	▼ IR Spectroscopy (3)
▼ Boiling Point (17)	▼ Electrochemical Behaviour (5)	▼ Mass Spectrometry (4)
▼ Refractive Index (8)	▼ Dissociation Exponent (5)	▼ Raman Spectroscopy (1)
▼ Density of the Liquid (7)	▼ Further Information (1)	▼ Other Spectroscopic Methods (1)
▼ Conformation (1)	▼ Solubility (MCS) (1)	▼ Bioactivity/ECOTOX
▼ Electrical Moment (2)	▼ Liquid/Vapour Systems (MCS) (2)	▲ Use/Application
▼ Ionization Potential (1)	▼ Azeotropes (MCS) (1)	▼ Use (1)
▼ Vapour Pressure (1)	▼ Liquid/Liquid Systems (MCS) (9)	▲ Natural Product
▼ Mechanical Properties (1)	▼ Mechanical & Physical Properties (MCS) (2)	▼ Derivative (23)
▼ Transport Data (1)	▼ Transport Phenomena (MCS) (1)	▼ Purification (1)
	▼ Energy Data (MCS) (4)	
	▼ Association (MCS) (12)	



Los números representan el número de resultados encontrados en esta búsqueda para cada propiedad



# Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

## ▲ NMR Spectroscopy (22)

Description	Nucleus	Solvents	Frequency	Original Text	Reference
CPMAS (Cross Polarization Magic-Angle Spinning) Solid phase	<sup>13</sup> C			20.5+/-0.5 ppm; 19.8 (+/-0.5 ppm) ppm	<b>SCICONCEPT GMBH</b> <b>Patent:</b> WO2008/37289 , 2008 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>
CPMAS (Cross Polarization Magic-Angle Spinning) Solid phase	<sup>13</sup> C				<b>SCICONCEPT GMBH</b> <b>Patent:</b> WO2008/37289 , 2008 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>
Chemical shifts	<sup>1</sup> H	CDCl <sub>3</sub>	300MHz		<b>Rastrelli, Federico; Bagno, Alessandro</b> Journal of Magnetic Resonance, <b>2006</b> , vol. 182, # 1 p. 29 - 37 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Scopus</a>
	<sup>1</sup> H	CDCl <sub>3</sub>		<sup>1</sup> H NMR (CDCl <sub>3</sub> ), 2.37 (s, 3H), 5.83 (s, 2H), 7.12 (m, 1H), 7.34 (m, 1H), 7.62 (m, 1H), 7.72 (d, 2H), 8.05 (dd, 1H)	<b>Ashton, Paul; Cynkowska, Grazyna; Cynkowski, Tadeusz; Smith, Thomas J.</b> <b>Patent:</b> US2003/170286 , 2003 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <b>Control Deliver Systems, Inc.</b> <b>Patent:</b> US2005/164994 , 2005 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>
	<sup>1</sup> H	CDCl <sub>3</sub>		<sup>1</sup> H NMR (CDCl <sub>3</sub> ): 8.21 (1H,dd); 7.66 (1H,dt); 7.42 (3H,m); 7.20 (3H,m); 5.40 (2H, s), 2.25 (3H,s)	<b>Del Soldato, Piero</b> <b>Patent:</b> US2004/23890 , 2004 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>
	<sup>1</sup> H		200MHz	<sup>1</sup> H NMR (200 MHz) (CDCl <sub>3</sub> ): 8.10 (2H, m); 7.7 (1H, t); 7.56(2H, d); 7.48 (1H, t); 7.30(1H, d); 5.74 (2H, s); 5.43 (2H, s); 2.20 (3H, s)	<b>Del Soldato, Piero; Benedini, Francesca; Antognazza, Patrizia</b> <b>Patent:</b> US2004/23933 , 2004 <a href="#">Title/Abstract</a> <a href="#">Full Text</a>
Spectrum	<sup>1</sup> H	tetradeuteriomethanol			<b>Leo, Gregory C.; Krikava, Aaron; Caldwell, Gary W.</b> Analytical Chemistry, <b>2003</b> , vol. 75, # 8 p. 1954 - 1957 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Scopus</a>

# Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

▲ Pharmacological Data (1775)									
Effect	Species or Test-System	Sex	Route of Application	Concentration	Method	Type	Value of Type	Results	Reference
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on COX-2 expression induced by ox-LDL			cells pre-incubated with title comp. signif. reduced COX-2 expression induced by ox-LDL; fig.	<b>Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng</b> Journal of Cardiovascular Pharmacology, <b>2008</b> , vol. 51, # 1 p. 32 - 37 <a href="#">Title/Abstract Full Text</a> <a href="#">Scopus</a>
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on ICAM-1 expression induced by ox-LDL			title comp. almost completely suppressed ICAM-1 expression induced by ox-LDL; title comp. alone had no effect on ICAM-1 expression in unstimulated cells; fig.	<b>Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng</b> Journal of Cardiovascular Pharmacology, <b>2008</b> , vol. 51, # 1 p. 32 - 37 <a href="#">Title/Abstract Full Text</a> <a href="#">Scopus</a>
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on ICAM-1 expression induced by ox-LDL detd. by using western blot			title comp. almost completely suppressed ICAM-1 expression induced by ox-LDL; fig.	<b>Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng</b> Journal of Cardiovascular Pharmacology, <b>2008</b> , vol. 51, # 1 p. 32 - 37 <a href="#">Title/Abstract Full Text</a> <a href="#">Scopus</a>

# Beneficios para los químicos medicinales

## Actividad

Encontrar sustancias con determinadas propiedades o drogas con ciertos efectos

Comprender los efectos de una droga e interacciones droga-objetivo biológico

Analizar resultados de búsquedas para encontrar nuevas sustancias con estructuras similares

Encontrar sustancias separadas de los productos naturales

## Beneficios de Reaxys

Búsqueda por propiedad o efecto de la sustancia

Investiga bioactividad (efectos, blancos, especies, etc.)

Exporta sustancias y sus datos para planillas y analiza sus relaciones

Campo de Datos  
"Isolation from natural product"



# Herramienta para planificación de síntesis

The screenshot displays a chemical synthesis planning tool interface. At the top, there are buttons for 'Undo', 'Open', 'Save', and 'Copy plan to new page'. The 'Synthesis representation' is set to 'Left to Right'. The main area shows a reaction scheme with three steps: Step 1 (2,4-dimethylphenylacetic acid to 2,4-dimethylphenylacetyl chloride), Step 2 (2,4-dimethylphenylacetyl chloride to 2,4-dimethylphenylacetic acid, 94.7% yield), and Step 3 (2,4-dimethylphenylacetic acid to 2,4-dimethylphenylacetyl chloride). A red box highlights the 'Synthesize' button for Step 3, with a red arrow pointing to the 'Add' button in the filter panel below. The filter panel includes options for Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, and No. of Steps. The bottom right shows a table of references for the selected reaction.

Step	Yield	Conditions	References
2	94.7%	in CH <sub>2</sub> Cl <sub>2</sub>	<b>Koul, Surrinder; Koul, Jawahir Lal; Singh, Budh; Kapoor, Munish; Parshad, Rajinder; Manhas, Kuldeep S.; Taneja, Subhash C.; Qazi, Ghulam N.</b> Tetrahedron: Asymmetry, <b>2005</b> , vol. 16, # 15 p. 2575 - 2592 Title/Abstract Full Text Scopus
3	82%	With SOCl <sub>2</sub> in toluene T=90°C; 4 h;	<b>Bellucci, Giuseppe; Berti, Giancarlo; Bianchini, Roberto; Vecchiani, Sandra</b> Gazzetta Chimica Italiana, <b>1988</b> , vol. 118, # 6 p. 451 - 456 Title/Abstract Full Text
		With thionyl chloride in benzene 3 h; Heating;	<b>Rao, Ch Prasad; Srimannarayana, G; Sundaramurthy, V</b> Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chem Title/Abstract Full Text Scopus
		With SOCl <sub>2</sub> T=90°C; 3 h;	<b>Gualtieri, Fulvio; Conti, Gabriele; Dei, Silvia; Giovannoni, Maria Paola; Nan</b> Journal of Medicinal Chemistry, <b>1994</b> , vol. 37, # 11 p. 1704 - 1711 Title/Abstract Full Text Scopus

161 reactions out of 117 citations go to Page 1 of 18

Sort by Reaxys-Ranking

Hide Details

Yield Conditions References

CC1=CC=C(C=C1)C(C)C(=O)Cl >> CC1=CC=C(C=C1)C(C)C(=O)O

Rx-ID: 1062590

Done Internet

Seleccione la mejor ruta entre diversas publicaciones para optimizar su estrategia de síntesis.

# Compare estructuras y sus datos

**reaxys**

**Output Substance Results**

**Output**  Substance Grid  Substance Details Table  Substance Citations Table

**to**  PDF/Print  XML  Microsoft Word  Microsoft Excel  Literature Management Systems (e.g. ReferenceManager, EndNote etc.)

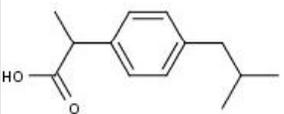
RD File  SD/Molfile  Smiles

Include the following headline

**Output range**  All Hits  Selected hits  Range:  e.g. 1, 2-5, 10

**Output contains**  include Structures  All available data  Identification data only  Select data

Exporte estructuras y sus datos en XLS, WORD, PDF

Structure	Reaxys RegNo	CAS Registry Number	Pharmacological Data: Effect	Species or Test-System	Method	Further Details	Type	Value of Type	References
	2049713	15687-27-1; 51146-56-6; 51146-57-7; 58560-75-1	enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1	enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20 $\alpha$ -hydroxysteroid dehydrogenase	IC50	29 $\mu$ mol/l	Journal; Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M.; Biochemical Pharmacology; vol. 75; 2; (2008); p. 484 - 493;

# Resumiendo

- Reaxys reduce el tiempo necesario para encontrar resultados relevantes
- Interfaces simples, poderosa herramienta de búsqueda y contenido indexado con foco en la síntesis química
- Extenso repositorio de propiedades químicas y datos experimentales de reacciones
- Información extraída de la literatura científica y de patentes



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