



Особенности и покрытие базы данных Reaxys.

Источники информации

Индексация

Извлечение данных

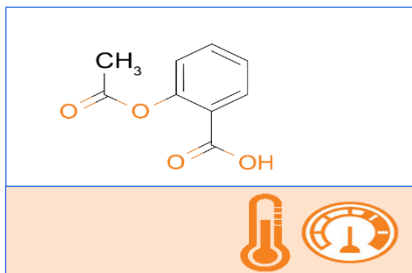
08,08,2019

Моисеев Алексей Александрович

a.Moiseev@elsevier.com +79251131255



Информационная система, построенная для отражения реального использования химических знаний



>105 Млн Записей соединений с
>500 Млн извлеченных фактов об их свойствах: физические, химические, спектральные, экологические, биоактивность



>41 Млн Записей реакций включают извлеченные данные об условиях проведения реакций, растворителях, катализаторах, выходе



Связь с



51.9 Млн записей Литературы из 16,000 периодических изданий описывая применения в области материалo-ведения, биомедицины, наук о Земле, технических и экологических наук, фармакологии...

Применение в различных дисциплинах

Reaxys источники для научного контента

16.000 titles

(journals, books and patents)

56+mio articles

(Elsevier, ACS, Nature-Springer, Blackwell, Taylor and Francis, etc)

1,5+mio patents

WPO, USPO, EPO [≈ mid 70's >]

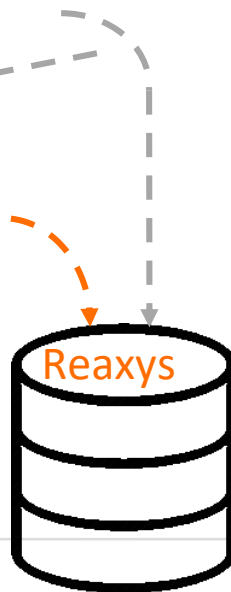
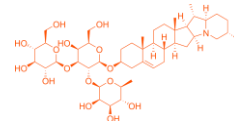
PO: JP, KR, CN, TW [2015 >]

380+k book chapters

Beilstein, Gmelin,



≈ 450 journals + PO
[manually excerpted]



Reaxys

Это обширные, хорошо проиндексированные данные под рукой

Реахус является крупнейшим хранилищем данных о свойствах веществ в мире.
Растворимость это только одно из **>500 полей данных для поиска** в Reaxys

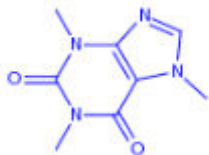
Melting point	Enthalpy of Formation	NMR Spectroscopy	Target
Boiling point	Enthalpy of Sublimation	IR Spectroscopy	Substance Effect
Sublimation	Flash Point	Mass Spectroscopy	Substance Action on Target
Refractive index	Gas Phase	UV/VIS Spectroscopy	Substance Dose
Density	Dissociation Energy	ESR Spectroscopy	Bioassay
Adsorption	Crystal System	NQR Spectroscopy	Animal Model
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Bound Surface Phenomena	Henry Constat	Fluorescence Spectroscopy	Measurement Parameter
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Circular Dichromism	Isoelectric Point	Bioaccumulation	Ecotoxicology Data
Complex Phase Equilibria	Kinematic Viscosity	Biomagnification	Dielectric Constant
Compressibility	Liquid Phase	Biodegradation	Dissociation Exponent
Conformation	Magnetic Data	Biodegradation in Soil	Dynamic Viscosity
Critical Density	Mechanical Properties	Oxygen Demand	Electrolytic Conductivity
Critical Micelle Concentration	Molecular Deformation	Uses	Enthalpy of Fusion
Critical Pressure	Optical Data	Isolation from Natural Prod.	Enthalpy of Vaporization
Critical Temperature	Thermochemical Data	Reaction Yield	Explosion Limits
Critical Volume	Solubility	Reaction Conditions	Interatomic Distance/Angle
Electrical Data	Solution Behavior	Reaction Type	Kinematic Viscosity
Electrical Moment	Sound Properties	Named Reaction	Liquid/Solid Systems
Electrochemistry Data	Static Dielectric Constant	Pharmacological Data	Liquid/Vapor Systems
Electron Binding	Surface Tension	Route of Administration	Metarotation
Energy Barriers	Transition Points	Concentration	
Energy Data	Transport Data		

Solubility

And many more...



Вы получаете данные непосредственно извлеченные данные



Physical Data - 766

✓ Melting Point - 43

✓ Sublimation - 2

✓ Refractive Index - 2

✓ Density - 9

✓ Adsorption (MCS) - 23

✓ Association (MCS) - 22

✓ Boundary Surface Phen

✓ Chromatographic Data

✓ Conformation - 1

✓ Crystal Phase - 7

✓ Crystal Property Descri

✓ Crystal System - 2

✓ Decomposition - 1

✓ Heat Capacity Cp - 2

✓ Heat Capacity Cp0 - 1

✓ Solubility (MCS) - 102

✓ Solution Behaviour (MCS) - 20

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS))	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
20.88		28	water		Singh, Neetu; Singh, Udai P.; Nikhil, Kumar; Roy, Partha; Singh, Hariji Full Text ↗ Details > Abstract >
	in pure solvent	25	methanol	Solubility: 1.23 g/100g solvent	Guo, Kun; Sadiq, Ghazala; Seaton, Colin; Davey, Roger; Yin, Qiuxiang Full Text ↗ Cited 42 times ↗ Details > Abstract >
	in pure solvent	25	ethanol	Solubility: 1.48 g/100g solvent	Guo, Kun; Sadiq, Ghazala; Seaton, Colin; Davey, Roger; Yin, Qiuxiang Full Text ↗ Cited 42 times ↗ Details > Abstract >
	in pure solvent	25	acetone	Solubility: 1.51 g/100g solvent	Guo, Kun; Sadiq, Ghazala; Seaton, Colin; Davey, Roger; Yin, Qiuxiang Full Text ↗ Cited 42 times ↗ Details > Abstract >

(s) - 7

1



Оптимальная стратегия поиска литературы.

Как быстро и эффективно найти и проанализировать литературу, включая патенты, по различным направлениям химии?

Какова оптимальная стратегия поиска литературы по данному соединению или классу соединений?

08.08.2019

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Поиск литературы. Поиск по ключевым словам

Reaxys®

Quick search

Query builder

Results

Synthesis planner

History ^{new}

Register >

Sign in ?

Search in:

Reactions >

Targets >

Substances >

Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Keywords

is	▼	<u>Keyword Basic Index</u>	🔍	✕
is	▼	Reaxys Index Terms	🔍	
is	▼	Biotechnology Terms	🔍	
is	▼	Compendex Terms	🔍	
is	▼	EMTREE Drug Term	🔍	
is	▼	Fluids Engineering Terms	🔍	
is	▼	EMTREE Medical Term	🔍	
is	▼	Species	🔍	
is	▼	GEObase Subject Index	🔍	
is	▼	Author Keywords	🔍	

Find search fields and forms

key

Reaxys ^

InChI Key

Keywords

PubChem ^

InChI Key

eMolecules ^

InChI Key

LabNetwork ^




InChI Key


Feedback



15,33 K Filters and Analysis

15,330 Documents with 235,476 Substances, 262,529 Reactions, 654 Targets

0 selected  Limit To  Exclude  Export

Sort by Publication Year ↓ 

Authors

<input type="checkbox"/>	lindsey, jonathan s	92
<input type="checkbox"/>	sessler, jonathan l	65
<input type="checkbox"/>	lee, chang-hee	51
<input type="checkbox"/>	ravikanth, mangalampalli	46
<input type="checkbox"/>	ciamician	39
<input type="checkbox"/>	osuka, atsuhiro	38
<input type="checkbox"/>	latos-grazynski, lechoslaw	38
<input type="checkbox"/>	+ More	

Common roasting defects in coffee: Aroma composition, sensory characterization and consumer perception
1 [Giacalone, Davide](#); [Degn, Tina Kreuzfeldt](#); [Yang, Ni](#); [Liu, Chujiao](#); [Fisk, Ian](#); [Münchow, Morten](#) - [Food Quality and Preference, **2019**, vol. 71, p. 463 - 474]
[Abstract](#) [Index Terms](#) [Substances 37](#) [Full Text](#)
[Hit Substances 1](#)

Competitive adsorption of CO₂/N₂/CH₄ onto coal vitrinite macromolecular: Effects of electrostatic interactions and oxygen functionalities
2 [Yu, Song](#); [Bo, Jiang](#); [Fengjuan, Lan](#) - [Fuel, **2019**, vol. 235, p. 23 - 38]
[Abstract](#) [Index Terms](#) [Substances 1](#) [Full Text](#)
[Hit Substances 1](#)

Kohn–Sham energy decomposition for molecules in a magnetic field
3 [Reimann, Sarah](#); [Borgoo, Alex](#); [Austad, Jon](#); [Tellgren, Erik I.](#); [Teale, Andrew M.](#); [Helgaker, Trygve](#); [Stopkowicz, Stella](#) - [Molecular Physics, **2019**, vol. 117, # 1, p. 97 - 109]
[Abstract](#) [Index Terms](#) [Substances 1](#) [Full Text](#)
[Hit Substances 1](#)

Synthesis of new TiO₂/porphyrin-based composites and photocatalytic studies on methylene blue degradation
4 [Min, Kyeong Su](#); [Kumar, Rangaraju Satish](#); [Lee, Jeong Hoon](#); [Kim, Kang Seok](#); [Lee, Seung Geol](#); [Son, Young-A.](#) - [Dyes and Pigments, **2019**, vol. 160, p. 37 - 47]
[Abstract](#) [Index Terms](#) [Substances 17](#) [Reactions 13](#) [Full Text](#)
[Hit Substances 1](#)

[Feedback](#)

PATENT SEARCHING USING THE LITERATURE SEARCH FORM

The screenshot shows the Reaxys search results page. The top navigation bar includes 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History'. The user is identified as 'Alexey Moiseev'. The search results are displayed in a list format with filters on the left. The results include:

- 1** Common roasting defects in coffee: Aroma composition, sensory characterization and consumer perception
Giacalone, Davide; Degr, Tina Kreuzfeldt; Yang, Ni; Liu, Chujiao; Fisk, Ian; Münchow, Morten - [Food Quality and Preference, 2019, vol. 71, p. 463 - 474]
Abstract | Index Terms | Substances (37) | Full Text | Hit Substances (1)
- 2** Competitive adsorption of CO₂/N₂/CH₄ onto coal vitrinite macromolecular: Effects of electrostatic interactions and oxygen functionalities
Yu, Song; Bo, Jiang; Fengjuan, Lan - [Fuel, 2019, vol. 235, p. 23 - 38]
Abstract | Index Terms | Substances (1) | Full Text | Hit Substances (1)
- 3** Kohn-Sham energy decomposition for molecules in a magnetic field
Reimann, Sarah; Borgoo, Alec; Austad, Jørn; Tellgren, Erik I.; Teale, Andrew M.; Helgaker, Trygve; Stopkowitz, Stella - [Molecular Physics, 2019, vol. 117, # 1, p. 97 - 109]
Abstract | Index Terms | Substances (1) | Full Text | Hit Substances (1)
- 4** Synthesis of new TiO₂/porphyrin-based composites and photocatalytic studies on methylene blue degradation
Min, Kyeong Su; Kumar, Rangaraju Satish; Lee, Jeong Hoon; Kim, Kang Seok; Lee, Seung Geol; Son, Young-A. - [Dyes and Pigments, 2019, vol. 160, p. 37 - 47]
Abstract | Index Terms | Substances (17) | Reactions (33) | Full Text | Hit Substances (1)

Patent: US6147080 A1, 2000 ; (granted)
Patent: US2005/9844 A1, 2005 ; (published application)
Patent: US1996-34288P (pre-published application number)
Patent: US-109128 (pre-published application number no date)

wo2013091285a1 ->>>> wo2013*91285
20110281878 ->>>> *2011*281878
US6147080 ->>>> Direct



(IPC) A61K* -

препараты для медицины, стоматологии или косметики.

◇ Patents: Secondary IPC is A61K* 🔍 ✕

OR

◇ Patents: Secondary IPC is A61K* 🔍 ✕

Filters

Limit to >

Exclude >

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

Document Type ▲

article 243,174

patent 138,648

conference paper 975

report 576

letter 350

review 318

note 99

[View more](#)

384,382 Documents with 4,523,504 Substances, 7,501,904 Reactions, 45,970 Targets

0 selected [Limit To](#) [Exclude](#) [Export](#)

- 1** The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents
[Sofer, Zdeněk](#); [Luxa, Jan](#); [Bouša, Daniel](#); [Sedmidubský, David](#); [Lazar, Petr](#); [Hartman, Tomáš](#); [Hardtdegen, Hilde](#); [Pt](#)
Chemie - International Edition, 2017, vol. 56, # 33, p. 9891 - 9896[*Angew. Chem.*, 2019, vol. 129, p. 10023 - 10023]
[Abstract](#) ▾ [Index Terms](#) ▾ [Substances](#) 4 ▾ [Reactions](#) 2 ▾ [Full Text](#) ↗
- 2** Design, synthesis, and evaluation of new series of Imperatorin analogs with potential vas
[Hou, Ya-Jing](#); [Wang, Cheng](#); [Wang, Tao](#); [Huang, Li-Min](#); [Lin, Yuan-Yuan](#); [He, Huai-Zhen](#) [*Journal of Asian Natural*
vol. 21, # 1, p. 43 - 50]
[Abstract](#) ▾ [Index Terms](#) ▾ [Substances](#) 14 ▾ [Reactions](#) 8 ▾ [Full Text](#) ↗
- 3** Synthesis and bioactivities of diamide derivatives containing a phenazine-1-carboxamide
[Zhu, Xiang](#); [Zhang, Min](#); [Yu, Linhua](#); [Xu, Zhihong](#); [Yang, Dan](#); [Du, Xiaoying](#); [Wu, Qinglai](#); [Li, Junkai](#) [*Natural Prod*
17, p. 2453 - 2460]
[Abstract](#) ▾ [Index Terms](#) ▾ [Substances](#) 62 ▾ [Reactions](#) 113 ▾ [Full Text](#) ↗



ELSEVIER

БЫСТРОЕ ОБЪЕДИНЕНИЕ ПОИСКОВЫХ ПОЛЕЙ ЛОГИКОЙ (OR,AND,NOT,NEXT)

Reaxys

Quick search


Query builder ^{New}

Results

Synthesis planner

History

Register >

Sign in 

Search in:





Reactions >





Targets >

Substances >




Documents >

 Import  Save  Reset form  Delete all

 Structure  Molecular Formula  CAS RN  Doc. Index

 Molecular Formula  Mo(10b)  

AND

 Density Find any Hide fields  

OR



AND



NOT



NEAR



NEXT

PROXIMITY

 Density, g·cm-3 

 Reference Temperature, °C 


 Measurement Temperature, °C 


 Type (Density) 


Find search fields and forms



Fields Forms History



Reaxys 



Basic Indexes 



Identification 



Physical Properties 

 Melting Point 

 Boiling Point 

 Sublimation 

 Refractive Index 

 Density 

Feedback 

ELSEVIER


Reaxys

LIFE SCIENCE SOLUTIONS

СОЗДАНИЕ ОПОВЕЩЕНИЙ


Можно создать оповещение для появления новых совпадений, о которых система вас будет оповещать по электронной почте.

Create Alert ×

Query: Quick Search: ""narlaprevir" "preparation"" AND 

Alert name: Name
alert1

Send alerts to: a.moiseev@elsevier.com ×

Frequency: After each update 

From databases: Reaxys

Create Alert >

Например, если появляются новые пути синтеза нужного вещества, Reaxys будет присылать Вам оповещение по электронной почте.



Reaxys®





ELSEVIER

Свойства веществ в Reaxys

Как быстро найти экспериментальные свойства химических соединений, включая физико-химические, механохимические, электрохимический и многие другие? Как найти соединения с заданными свойствами?



Reaxys

Это обширные, хорошо проиндексированные данные под рукой

Reaxys является крупнейшим хранилищем данных о свойствах веществ в мире.
Растворимость это только одно из **>500 полей данных для поиска** в Reaxys

Melting point	Enthalpy of Formation	NMR Spectroscopy	Target
Boiling point	Enthalpy of Sublimation	IR Spectroscopy	Substance Effect
Sublimation	Flash Point	Mass Spectroscopy	Substance Action on Target
Refractive index	Gas Phase	UV/VIS Spectroscopy	Substance Dose
Density	Dissociation Energy	ESR Spectroscopy	Bioassay
Adsorption	Crystal System	NQR Spectroscopy	Animal Model
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Autoignition	Heat Capacity	Luminescence Spectroscopy	Cells/Cell Lines
Bound Surface Phenomena	Henry Constat	Fluorescence Spectroscopy	Measurement Parameter
Viscosity	Ionization Potential	Exposure Assessment	Endpoint of Effect
Circular Dichromism	Isoelectric Point	Bioaccumulation	Ecotoxicology Data
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Electrochemistry Data	Static Dielectric Constant	Pharmacological Data	Liquid/Vapor Systems
Electron Binding	Surface Tension	Route of Administration	Metarotation
Energy Barriers	Transition Points	Concentration	
Energy Data	Transport Data		

Solubility

And many more...



Как найти соединения с заданными свойствами?

Reaxys[®]

Quick search

Query builder

Results

Synthesis planner

History

Andrey Khudoshin



Import Save Reset form Delete all



Molecular Formula

CAS RN



Doc. Index

Search Substances



Find search fields and forms



Fields

Forms

History

Sublimation Hide fields ^ x

= EQ

= EQ

AND

Melting Point Hide fields ^ x

= EQ

is EQ

AND

Substance Basic Index x

is EQ

Reaxys ^

Basic Indexes ^

Substance Basic Index

Reaction Basic Index

Document Basic Index

Identification v

Physical Properties ^

Melting Point

Boiling Point

Sublimation



ELSEVIER

Поиск веществ с необходимыми хроматографическими свойствами

◇ Chromatographic Data Find any Hide fields ^ ×

is	▼	Chromatographic data	
is	▼	Original string	

Chromatographic data Q Search ×

<input type="checkbox"/>	gpc (gel permeation chromatography)	499	
<input type="checkbox"/>	hplc (high performance liquid chromatography)	567,623	
<input type="checkbox"/>	ion chromatography	1,390	
<input type="checkbox"/>	lc (liquid chromatography)	266,210	
<input type="checkbox"/>	mplc (medium pressure liquid chromatography)	538	
<input type="checkbox"/>	paper chromatography	107	
<input type="checkbox"/>	partition chromatography	58	
<input type="checkbox"/>	sfc (supercritical fluid chromatography)	10,467	
<input type="checkbox"/>	tlc (thin layer chromatography)	532,633	
<input type="checkbox"/>	uplc (ultra performance liquid chromatography)	90,976	

Clear selected × Transfer >

Время удерживания

◇ Chromatographic Data Find any Hide fields ^ X

is	▼	electrophoresis	🔍
is	▼	Original string	🔍

Original string 1 X

<input type="checkbox"/> 'lb-ms (esi): c'lueiht mass: 482.18; observdm: 483.55 :[m	1	
<input type="checkbox"/> 'r 0.35 (25percent ethyl acetaie- peniane; faa, stains brown).	1	
<input type="checkbox"/> 'r =2.011 mins. (lcms condition 1)	1	
<input checked="" type="checkbox"/> 'retention time=1.52 min	1	⬆
<input type="checkbox"/> (6	⬆
<input type="checkbox"/> (1.20 min).	1	⬇
<input type="checkbox"/> ((rf=0.28 (70percent hexanes/24percent chcl3/5.9percent etoh/0.1percent nh4oh))	1	⬇
<input type="checkbox"/> (+) enantiomer, peak 1, rt 2.22 min	1	
<input type="checkbox"/> (+) enantiomer, peak 2, rt 1.09 min	1	
<input type="checkbox"/> (+)-(r,r)-8: 1.9 mm	1	

Состав элюента

◇ Chromatographic Data Find any Hide fields ^

is	▼	Chromatographic data	🔍
is	▼	eluent	🔍

eluent : methylene chloride / ethyl acetate 94/6 : rf : 0.25

eluent : methylene chloride : rf : 0.32

eluent : methylene chloride : rf : 0.41

eluent : methylene chloride : rf : 0.46

eluent : methylene chloride/ethyl acetate 94/6 : rf : 0.38

🔍 More suggestions for **eluent**



ELSEVIER

Химические реакции в Reaxys

-В какие реакции вступает заданное соединение? И в каких условиях (катализатор, растворитель, температура и др.) Как получить соединение или класс соединений? Как построить план синтеза данного соединения?

Как проверить доступность соединения

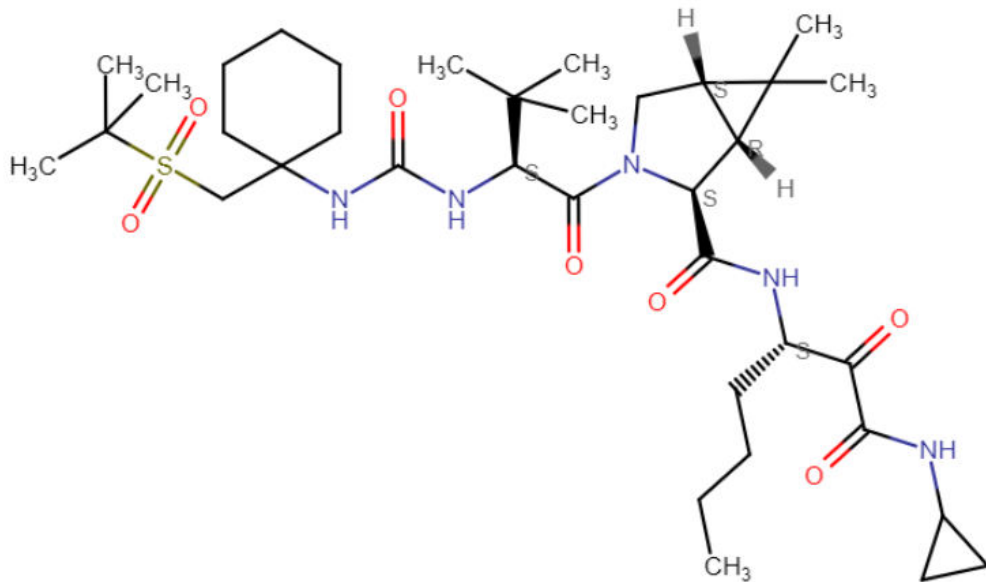


Разработка методики синтеза химических веществ (субстанций) в Reaxus

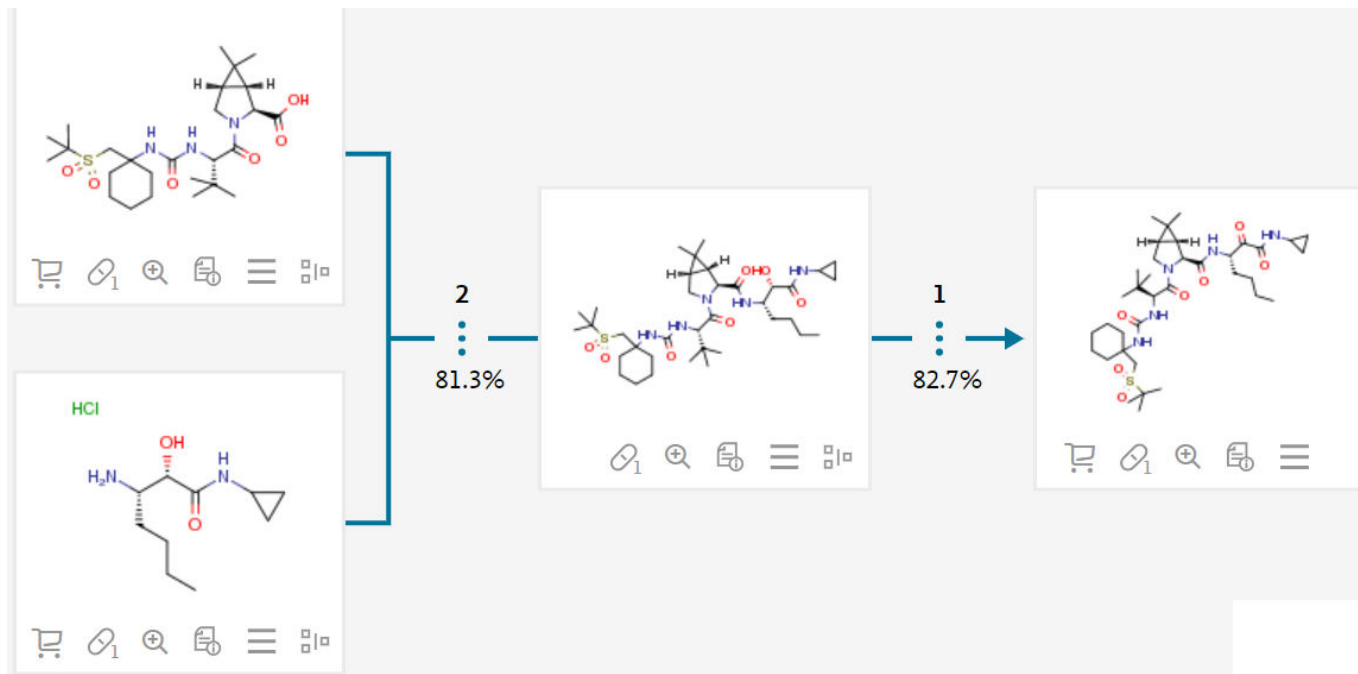
С помощью Reaxus можно решать задачу поиск оптимальных условий синтеза субстанций.

Допустим, Вас интересует данное соединение

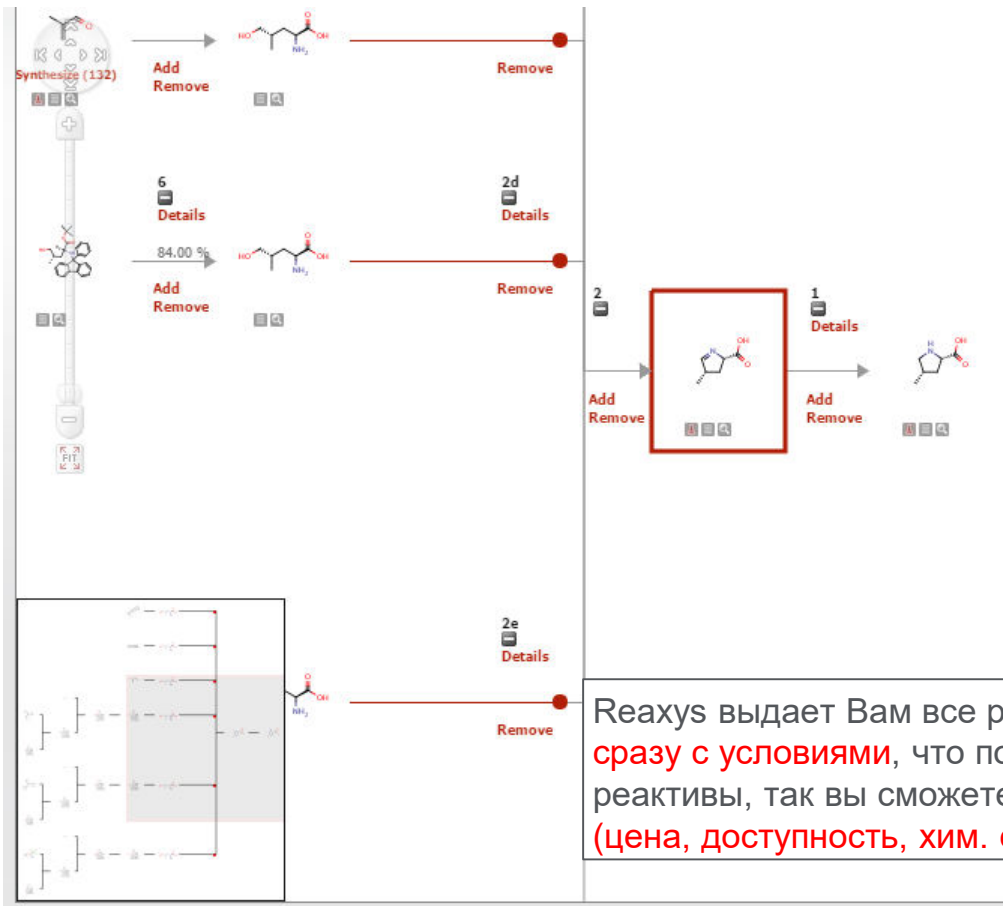
NARLAPREVIR



С помощью Reaxus можно гораздо эффективнее решать задачу поиск оптимальных условий синтеза субстанций.



Разработка методики синтеза химических веществ (субстанций)



Также за секунды Reaxys может **построить многостадийный план синтеза** из базовых соединений, что сэкономит время сотрудников и **позволит выбрать метод, в котором не образуются опасные побочные продукты.**

Reaxys выдает Вам все реакции синтеза заданного соединения **сразу с условиями**, что позволит сэкономить деньги на реактивы, так вы сможете **выбрать оптимальную методику (цена, доступность, хим. стабильность, токсичность и т.д.)**

ПОИСК РЕАКЦИЙ

Можно либо нарисовать схему реакции, нарисовать одну структуру, затем определить ее роль, ввести название химического вещества и определить его роль, либо использовать построитель молекулярных формул и определить его роль.

The screenshot displays the Reaxys search interface with the following sections:

- Structure:** Shows a chemical reaction scheme where benzamide reacts with an indole derivative in the presence of a catalyst (L) and reagents [O, F, Cl]. Below the scheme are buttons for PASTE, EDIT, and CLEAR, and a link to "Create Structure Template from Name".
- Filters:** A list of search criteria including:
 - As drawn
 - Substructure (selected)
 - on heteroatoms
 - on all atoms
 - Similarity
 - Include tautomers
 - Ignore stereo
 - No isotopes
 - No charges
 - No radicals
 - No ring closures
 - Ignore atom mappings
 - Align results with query (checked)
 - Keep fragments (separate selected, together unselected)
- Molecular Formula:** A search field with a "Lookup" button and a "Formula Builder" button.
- Identification:** A search field for "Chemical Name" with a dropdown menu set to "is" and a "Lookup" button.
- Show AND Buttons:** A section with radio buttons to select the role of the structure:
 - Product (selected)
 - Starting material
 - Reagent / Catalyst
 - Any role
- Reaction Data:** A table of reaction parameters with dropdown menus and input fields, each with a "Lookup" button:
 - Yield (numerical): =
 - Solvent (Reaction Details): is
 - Reagent/Catalyst: is
 - Time (Reaction Details) (h): =
 - Temperature (Reaction ...) (°C): =
 - Pressure (Reaction D... (Torr): =
 - Reaction Type: is
 - Reaction Basic Index: is

91
680

Filters and Analysis

- By Structure
- Measurement pX
- Highest Clinical Phases
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Availability in other databases
- Available Data

91 Substances

Substance Availability ×

- Accelrys' ACD
- CambridgeSoft ACX
- Labnetwork
- PharmaPendium
- Sigma Aldrich
- eMolecules

1,317 Reactions, 424 Targets

Reaxys - 680

Grid Heatmap

Sort by No of References ↓

0 selected

1

2

3

calcium O-acetylsalicylate

Identification

Druglikeness

Physical Data - 2

Other Data - 20

lysine Acetylsalicylate

$C_{26}H_{34}O_4 \cdot C_9H_{15}N_2O_2$ 326.349 5690287 62952-06-1

Preparations - 96 >

Reactions - 1,184 >

Targets - 418 >

Documents - 16,028 >

Preparations - 5 >

Reactions - 8 >

Documents - 90 >

Feedback



Дополнительную информацию о поставщике можно найти в этой вкладке.

На что уходит время? Ждем пока придут нужные реагенты!!!

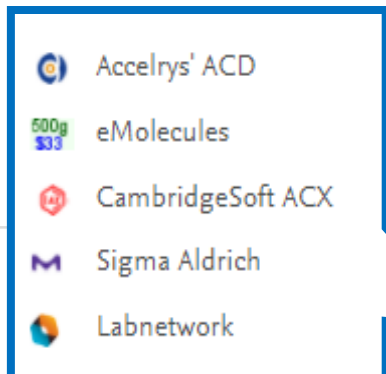
При планировании синтетической стратегии химики должны учитывать, как приобретать исходные материалы.

Три больших вопроса:

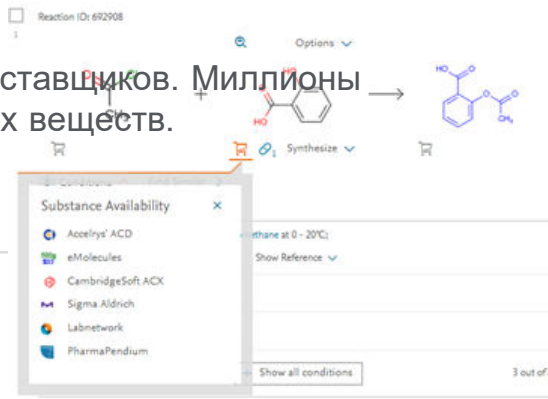
Есть ли этот материал на моем местном складе?

Есть ли материал присутствует на складе у любого поставщика?

Есть ли этот поставщик в моей системе покупки?



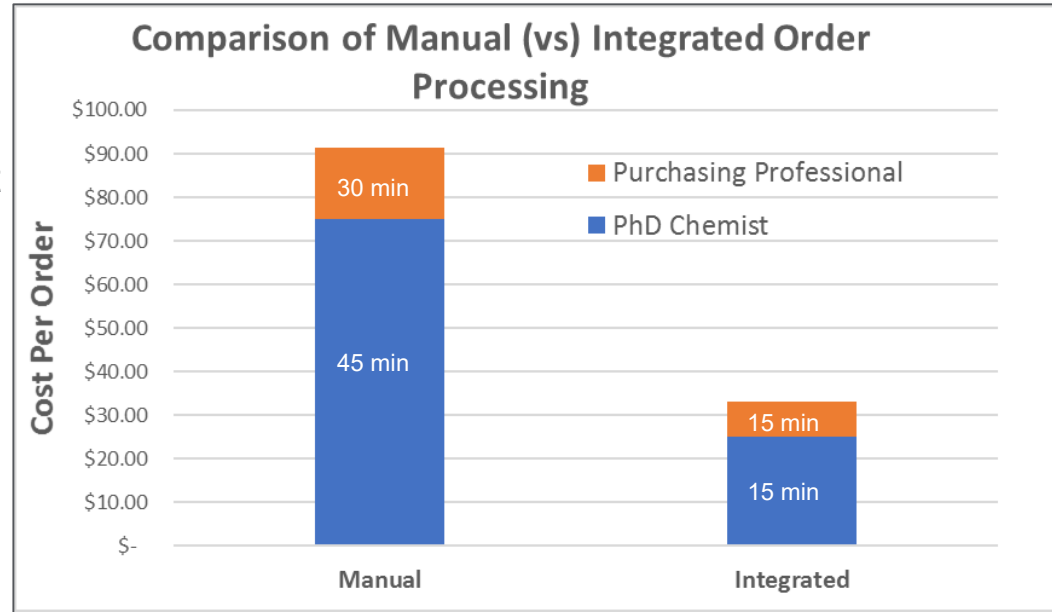
Тысячи поставщиков. Миллионы химических веществ.



In addition to reinforcing negotiated discounts, procurement integration reduces the order process cost.

Synthesis Project
Order
Cost

60% Less



Order Process Time Savings:

- Chemist saves 30 minutes per order
- Purchasing saves 15 minutes per order



ELSEVIER

Биологическая активность и медицинская химия в Reaxys

Как получить экспериментальные данные о биологической активности соединения и его производных? На какие биологические виды действует данное соединения? И какие соединения изучены на данном виде? Как оценить безопасность, активность и эффективность соединений?



Какие соединения, действующие на EGFR, могут быть использованы при заболевании Альцгеймера?

◇ Substance Basic Index ×

contains ▼ Substance Basic Index
Alzheimer 🔍

AND

◇ Affinity on target ×

◇ Target Name ×

is ▼ Target Name
egfr 🔍

AND

◇ Measurement pX ×

> ▼ Measurement pX
6 🔍

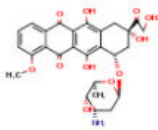
Какие соединения, действующие на EGFR, могут быть использованы при заболевании Альцгеймера?

72 Substances out of 537 Documents, containing 2,482 Reactions, 234 Targets Reaxys - 72

0 selected Limit To Exclude Export Sort by No of References Heatmap



1



doxorubicin

C₂₇H₂₉NO₁₁ 543.527 1445814 23214-92-8

[Hit Data - 4](#)

[Identification](#)

[Druglikeness](#)

[Bioactivity \(Hit Data\)](#)

[Bioactivity \(All\)](#)

[Physical Data - 141](#)

[Spectra - 198](#)

[Other Data - 4,448](#)

[Preparations - 56](#)

[Reactions - 292](#)

[Targets - 301](#)

[Documents - 13,217](#)

Hit Data - 4

Use - 4 hits out of 4,438

Show/Hide columns

Use Pattern	Reference
Alzheimer's Disease	NEXUSPHARMA INC. - WO2008/34039, 2008, A2 Full Text Details Abstract



Как найти вещества для которых изучено взаимодействие с биологическими видами Chlamydiae. Фильтр Biological species

Reaxys





Quick search Query builder Results Synthesis planner History

Alexey Moi...   



Search in: **Reactions** > **Targets** > **Substances** > **Documents** >



Find search fields and forms

   
Import Save Reset form Delete all

   
Structure Molecular Formula CAS RN Doc. Index

Reaxys 

 Biological Species 

 Biological Species 


Reaxys


Quick search Query builder Results Synthesis planner History


Alexey Moi...   


148


Filters

Index Terms (List) 



Index Terms (ReaxysTree) 

Publication Year 

Document Type 

Authors 

148 Documents with 881 Substances, 4,327 Reactions, 9 Targets

0   
Limit To Exclude Export

  Publication Year  

In vitro activity of omadacycline against chlamydia pneumoniae [Cited 1 times](#)

¹ [Kohlhoff, Stephan A.](#); [Huerta, Natalia](#); [Hammerschlag, Margaret R.](#) [Antimicrobial Agents and Chemotherapy, 2019, vol. 63, # 2, art. no. E01907-18]

[Abstract](#)  [Substances](#) **5**  [Full Text](#) 

Identification of chlamydial T3SS inhibitors through virtual screening against T3SS ATPase [Cited 4 times](#)

² [Grishin, Alexander V.](#); [Luyksaar, Sergey I.](#); [Kapotina, Lidiya N.](#); [Kirsanov, Dmitry D.](#); [Zayakin, Egor S.](#); [Karyagina, Anna S.](#); [Zigangirova, Naylia A.](#) [Chemical Biology and Drug Design, 2018, vol. 91, # 3, p. 717 - 727]



Вывод в виде тепловой карты

Heatmap settings

Value of X-axis: **Effects**

Value of Y-axis: **Substances**

Value of Cells: **Maximum of pX**

Show substances: Names Structure drawing

Display mode: Normal Full Screen

Always show settings

Apply



Navigator



ELSEVIER

Другие примеры использования Reaxys

- Как найти вещества извлекаемые из природных компонентов
- О применении Reaxys для поиска информации о минералах.
- Как найти соединения, используемые в качестве катодных материалов или ингибиторов коррозии.



Форма поиска натурального продукта

Reaxys®

Quick search

Query builder ^{New}

Results

Synthesis planner

History



Alexey Moiseev



Search in:

Reactions >

Targets >

Substances >

Documents >



Import



Save



Reset form



Delete all



Structure



Molecular Formula



CAS RN



Doc. Index

◇ Isolation from Natura...

Find any

Hide fields ^

is

chamomile



Find search fields and forms



Fields

Forms

History

Reaxys ^

Basic Indexes



Identification



Physical Properties



Spectra



MedChem



Other



◇ Isolation from Natural Product



◇ Use



◇ Exposure Assessment



◇ Concentration in the



Feedback



Reaxys®

LIFE SCIENCE
SOLUTIONS

◇ Isolation from Natural Product Find any Hide fields ^ ×

is



Isolation from Natural Product

camomile



17 Substances out of 569 Documents, containing 195 Reactions, 9 Targets

0 selected Limit To Exclude Export

Sort by No of References ↓ ▾

Grid Heatmap

1



spathulenol

$C_{15}H_{24}O$ 220.355 4671447 6750-60-3

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)

Physical Data - 37

Spectra - 39

Other Data - 111

Preparations - 15 >

Reactions - 19 >

Targets - 9 >

Documents - 406 >

^ Hit Data - 1

▾ Isolation from

9 Targets out of 26 Documents, 2 Substances, 15 Reactions

0 selected Limit To Exclude Export

Sort by Target Details ↑ ▾

Heatmap

2



Single protein

1 **Acetylcholinesterase (Wild)**

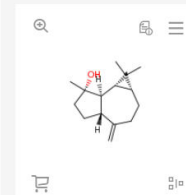
Synonyms: acetylcholinesterase

Show target details ▾

Substances - 10 >

Documents - 1 >

Most active substance:



inhibition rate=49.1%

Single protein

2 **Cannabinoid receptor 2 (Wild)**

Synonyms: cannabinoid receptor 2

Substances - 5 >

Documents - 1 >

Most active substance:



Форма поиска натурального продукта (yeast, Escherichia coli, cell ...)

The screenshot displays the Reaxys Query builder interface. At the top, the Reaxys logo is on the left, and navigation tabs for 'Quick search', 'Query builder' (highlighted with a 'New' badge), 'Results', 'Synthesis planner', and 'History' are in the center. On the right, the user name 'Alexey Moiseev' and icons for profile, notifications, and help are visible.

The main search area features a 'Search in:' dropdown with options for 'Reactions', 'Targets', 'Substances', and 'Documents'. Below this are utility buttons: 'Import', 'Save', 'Reset form', and 'Delete all'. On the right side of this bar are icons for 'Structure', 'Molecular Formula', 'CAS RN', and 'Doc. Index'.

The search query is displayed in a box: 'Isolation from Natural Product' with a 'Find any' button and a 'Hide fields' dropdown. The value 'Escherichia coli' is entered in the search field, with a 'Find' icon to its right.

On the right side of the interface is a sidebar titled 'Find search fields and forms' with a search icon. It contains a list of search fields: 'Fields', 'Forms', and 'History'. Under 'Fields', there is a list of categories: 'Reaxys', 'Basic Indexes', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Isolation from Natural Product', 'Use', 'Exposure Assessment', and 'Concentration in the'. A 'Feedback' button is located at the bottom of the sidebar.

Форма поиска натурального продукта

542

Filters and Analysis

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

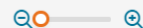
Available Data

Document Type

542 Substances out of 94,335 Documents, containing 28,875 Reactions, 1,688 Targets

 0 selected

Limit To Exclude Export

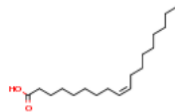


Sort by No of References ↓

Grid

Heatmap

1



cis-Octadecenoic acid

C₁₈H₃₄O₂ 282.467 1726542 112-80-1

Hit Data - 4

Identification

Druglikeness

Bioactivity (All)

Physical Data - 779

Spectra - 183

Other Data - 1,051

Preparations - 134 >

Reactions - 2,979 >

Targets - 198 >

Documents - 24,667 >



Hit Data - 4

Isolation from Natural Product - 4 hits out of 173

Show/Hide columns

Isolation from Natural Product

Reference

Escherichia coli rpoD40 (KY1411) mutant cells

Suzuki; Kondo; Makise; Mima; Sakamoto; Tshuchiya; Mizushima - [Biological and Pharmaceutical Bulletin, 1998, vol. 21, # 7, p. 657 - 661]

Full Text Cited 3 times Details Abstract

Escherichia coli dnaE486 (ME8680) mutant cells

Suzuki; Kondo; Makise; Mima; Sakamoto; Tshuchiya; Mizushima - [Biological and Pharmaceutical Bulletin, 1998, vol. 21, # 7, p. 657 - 661]

Full Text Cited 3 times Details Abstract

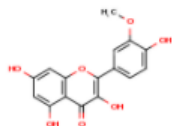
Какие соединения были найдены в тысячелистнике Yarrow?



◇ Isolation from Natural Product Find any Hide fields ^ ×

contains ▼ Isolation from Natural Product

Yarrow



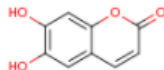
isorhamnetin
C₁₆H₁₂O₇ 316.267

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



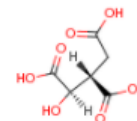
aesculetin
C₉H₆O₄ 178.144 152788

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



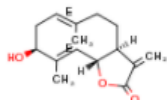
threo-D-isocitric acid
C₆H₈O₇ 192.125 1727947

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



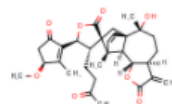
hanphyllin
C₁₅H₂₀O₃ 248.322 1623169

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)

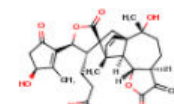


achillinin B
C₃₁H₃₈O₈ 538.638

Hit Data - 1

Identification

Druglikeness



C₃₀H₃₆O₈

Synthesize ▼

Options ▼ **achillinin C**
C₃₀H₃₆O₈ 524.611

Hit Data - 1

Identification

Druglikeness

Все вещества получаемые с помощью ферментации.

Reaxys®

Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

◇ Isolation from Natura... Find any Hide fields ^

is ferme*

Поиск применимости веществ в медицине и фармацевтике

Use Pattern 10

Q medic x x

<input type="checkbox"/>	medicago	18
<input checked="" type="checkbox"/>	medical	6,385
<input type="checkbox"/>	medicalconditions	1
<input type="checkbox"/>	medically	154
<input type="checkbox"/>	medicals	2
<input checked="" type="checkbox"/>	medicament	6,715
<input type="checkbox"/>	medicamental	11
<input type="checkbox"/>	medicamentary	10
<input type="checkbox"/>	medicamentns	1
<input checked="" type="checkbox"/>	medicamentosa	788
<input type="checkbox"/>	medicamentous	7
<input type="checkbox"/>	medicamentously	4
<input checked="" type="checkbox"/>	medicaments	796
<input type="checkbox"/>	medicamernt	1
<input type="checkbox"/>	medicanents	2



Вещества используемые в онкологии

Reaxys®

Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

◇ Use Find any Hide fields ^

is	▼	Laboratory Use and Handling	🔍
is	▼	oncol*	🔍

добычи и глубокой переработки углеводородного сырья

Use Pattern 1 Q processing × ×

<input checked="" type="checkbox"/> processing	1,349
<input type="checkbox"/> procession	7
<input type="checkbox"/> processivity	3
<input type="checkbox"/> processless	9
<input type="checkbox"/> processor	9

◇ Use Find any Hide fields ^ ×

is	▼	Laboratory Use and Handling	🔍
is	▼	Use Pattern processing	🔍

AND

◇ Use Find any Hide fields ^ ×

is	▼	Laboratory Use and Handling	🔍
is	▼	Use Pattern hydrocarbon\$	🔍

Use “cataly*”

◇ Use Find any Hide fields ^ X

is	▼	Laboratory Use and Handling	🔍
is	▼	cataly*	🔍

Какие соединения используются в качестве ингибиторов коррозии?

251 Substances out of 356,601 Documents, containing 531,983 Reactions, 610 Targets

0 selected Limit To Exclude Export

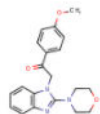
Use Find any Hide fields ^ X

is Laboratory Use and Handling

is Use Pattern (corros* NEAR inhib*) OR (anticorr*)

Sort by

1



Reaxys ID: 8160472

C₂₀H₂₁N₃O₃ 351.405 8160472

Hit Data - 1

Identification

Druglikeness

Other Data - 1

Hit Data - 1

Use - 1 hits out of 1

Use Pattern

Reference

corrosion inhibitor

Starchak; Anishchenko; Kuzina; Priimenko; Boiko; Chelyabieva; Tsybulya - Russian Journal of Applied Chemistry, 1997, vol. 70, # 5, p. 732 - 736

Full Text > Details > Abstract >

Определить неизвестное соединение X:

1. Элементный анализ показал следующее соотношение атомов C:F:N = 16:6:5
2. Угол оптического вращения раствора X с концентрацией 1 г на 100 г хлороформа при длине волны 589 нм при 20°C составляет -22.6 - -21.8
3. Какими дополнительными методами можно подтвердить предположение?

Определить неизвестное соединение X:

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

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

Find search fields and forms

Fields Forms History

Optical Rotatory Power Find any Hide fields ^ x

is	▼	Type (Optical Rotatory Power)	EQ
is	▼	Concentration (Optical Rotatory Power)	EQ
=	▼	Length of Path, cm	EQ
is	▼	Solvent (Optical Rotatory Power) chloroform	EQ
=	▼	Optical Rotatory Power, deg -22.6 - -21.8	EQ
=	▼	Wavelength (Optical Rotatory Power), nm	EQ
=	▼	Temperature (Optical Rotatory Power), °C	EQ

AND

Molecular Formula x

is	▼	Molecular Formula F6N5C16*	EQ
----	---	-------------------------------	----

Reaxys ^

Basic Indexes ▼

Identification ▼

Physical Properties ▼

Spectra ▼

MedChem ▼

Other ▼

Reactions ▼

Bibliography ▼

PubChem ▼

eMolecules ▼

LabNetwork ▼

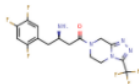
SigmaAldrich ▼

Structure

Определить неизвестное соединение X:



1

**sitagliptin**C₁₆H₁₅F₂N₃O 407.318 9962060 486460-32-6

Hit Data - 3

Identification

Druglikeness

Bioactivity (All)

Physical Data - 46

Spectra - 75

Other Data - 914

Preparations - 153 >

Reactions - 236 >

Targets - 68 >

Documents - 421 >



Hit Data - 3

Optical Rotatory Power - 3 hits out of 7

Show/Hide columns

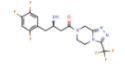
Type (Optical Rotatory Power)	Concentration (Optical Rotatory Power)	Length of Path, cm	Solvent (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength (Optical Rotatory Power), nm	Temperature (Optical Rotatory Power), °C	Location	Reference
alpha	0.92 g/100ml		chloroform	-22.4	589	25	Page/Page column 28	COUNCIL OF SCIENTIFIC and INDUSTRIAL RESEARCH; BARUA, Nabin Chandra; SAIKIA, Bishwajit; BORAH, Preetismita; BAISHYA, Gakul - WO2015/189862, 2015, A1 Full Text Details Abstract
[alpha]	1 g/100ml	1	chloroform	-22.6	589	25	supporting information	Zhou, Shengbin; Wang, Jiang; Chen, Xia; Acena, Jose Luis; Soloshonok, Vadim A.; Liu, Hong - Angewandte Chemie - International Edition, 2014, vol. 53, # 30, p. 7883 - 7886, Angew. Chem., 2014, vol. 126, # 30, p. 8017 - 8020 Full Text Details Abstract
[alpha]	1 g/100ml	10	chloroform	-22	589	25	supporting information	Davies, Stephen G.; Fletcher, Ai M.; Lv, Linlu; Roberts, Paul M.; Thomson, James E. - Tetrahedron Letters, 2012, vol. 53, # 24, p. 3052 - 3055 Full Text Cited 24 times Details Abstract



ELSEVIER

Определить неизвестное соединение X.

Какими дополнительными методами можно подтвердить предположение?



sitagliptin
 $C_{24}H_{35}F_7N_5O$ 407.318 9962060 486460-32-6

[Hit Data - 3](#) [Bioactivity \(All\)](#)
[Identification](#) [Physical Data - 46](#)
[Druglikeness](#) [Spectra - 75](#)

[Hit Data - 3](#)
[Optical Rotatory Power - 3 hits out of 7](#)

Type (Optical Rotatory Power)	Concentration (Optical Rotatory Power)	Length of Path, cm	Solvent (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength (Optical Rotatory Power), nm	Temperature (Optical Rotatory Power), °C
alpha	0.92 g/100ml		chloroform	-22.4	589	25
[alpha]	1 g/100ml	1	chloroform	-22.6	589	25

Spectra - 75

- ✓ NMR Spectroscopy - 49
- ✓ IR Spectroscopy - 6
- ✓ Mass Spectrometry - 18
- ✓ UV/VIS Spectroscopy - 2

Melting Point - 15

- ✓ Chromatographic Data - 7
- ✓ Crystal Property Description - 15
- ✓ Optical Rotatory Power - 7
- ✓ Partition octan-1-ol/water (MCS) - 2

Chemical shifts	1H		d(4)-methanol	400	1H NMR (CH_3OD , 400MHz): 1.37 (s, 9H), 2.61~3.00 (m, 4H), 3.92~4.30 (m, 5H), 4.93 (s, 1H), 4.95~5.12 (m, 1H), 5.22~5.35 (br, 1H), 6.83~6.95, (m, 1H), 7.02~7.12 (m, 1H)	Paragraph 0211
-----------------	----	--	---------------	-----	--	----------------

Melting Point, °C	Solvent (Melting Point)	Location
117.4		
118 - 120		Paragraph 0039; 0040

UV/VIS Spectroscopy - 2

Description (UV/VIS Spectroscopy)	Solvent (UV/VIS Spectroscopy)	Absorption Maxima (UV/VIS), nm
Spectrum	dimethyl sulfoxide	580



Определить неизвестное соединение Y:

1. Температура сублимации при атмосферном давлении составляет $\sim 56,5$ °C
2. Температура плавления 64 °C
3. Обнаружено, что данное соединение является стабильным (не разлагается) при нагревании до 2000 K
4. Элементный анализ показал отсутствие атомов C или O в соединении

Определить неизвестное соединение Y:

Reaxys[®]

Quick search

Query builder

Results

Synthesis planner

History

Andrey Khudoshin



Import Save Reset form Delete all



Molecular Formula

CAS RN

Doc. Index

Search Substances



Find search fields and forms



Fields

Forms

History

Sublimation Hide fields ^ x

= Sublimation, °C
55 - 57

= Pressure (Sublimation), Torr

AND

Melting Point Hide fields ^ x

= Melting Point, °C
63 - 65

is Solvent (Melting Point)

AND

Substance Basic Index x

is Substance Basic Index
stable

Reaxys ^

Basic Indexes ^

Substance Basic Index

Reaction Basic Index

Document Basic Index

Identification v

Physical Properties ^

Melting Point

Boiling Point

Sublimation

Определить неизвестное соединение Y:



uranium hexafluoride

F₆U 352.019 14965871 7783-81-5

[Hit Data - 11](#)

[Identification](#)

[Druglikeness](#)

[Bioactivity \(All\)](#)

[Physical Data - 451](#)

[Spectra - 115](#)

[Other Data - 66](#)

[Preparations - 208 >](#)

[Reactions - 485 >](#)

[Documents - 845 >](#)

[Sublimation - 1 hits out of 3](#)

[Hit Data - 11](#)

- ✓ [Melting Point - 2 hits out of 4](#)
- ✓ [Sublimation - 1 hits out of 3](#)
- ✓ [Use - 8 hits out of 13](#)

Melting Point, °C

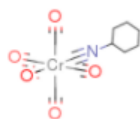
63.94

Sublimation, °C

56.54

Pressure (Sublimation), Torr

760



Cr(CNCy)(CO)₅

C₁₂H₁₁CrNO₅ 301.219 16967578 19706-05-9

[Hit Data - 3](#)

[Identification](#)

Melting Point, °C

65

[Druglikeness](#)

[Physical Data - 9](#)

[Sublimation - 1 hits out of 1](#)

Sublimation, °C

40 - 60

Pressure (Sublimation), Torr

0.1

[Preparations - 15 >](#)

[Reactions - 33 >](#)

[Documents - 15 >](#)

Определить сплав Z:

1. Сплав содержит железо
2. Сплав содержит кобальт
3. Температура плавления 1410-1450 °C

Определить сплав Z:

Search Substances

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

◇ Molecular Formula ×

is ▼ Molecular Formula
Ni?Fe?*

AND

◇ Melting Point Find any

= ▼ Melting Point, °C
1410 - 1450

is ▼ Solvent (Melting Point)

Reaxys ID: 26601394
CoCrFeNi 225.526 26601394

alloy

Hit Data - 2 Preparations - 1 >

CoCrFeNi

Identification Reactions - 1 >

Druglikeness Documents - 3 >

Physical Data - 7

^ Hit Data - 2

^ Melting Point - 2 hits out of 2 Show/Hide columns ▼

Melting Point, °C	Reference
1443.84	Vaidya; Trubel; Murty; Wilde; Divinski - Journal of Alloys and Compounds, 2016, vol. 688, p. 994 - 1001 Full Text Cited 1 times Details Abstract

Поиск информации о минералах

АНДАЛУЗИТ И ДРУГИЕ МИНЕРАЛЫ

Search Reaxys

"andalusite" × Find >

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

14 Substances out of 242 Documents, containing 56 Reactions, 0 Targets Reaxys - 14

0 selected Limit To Exclude Export Sort by No of References ↓ Grid Heatmap

Substance	Chemical Formula	Identification	Physical Data	Other Data	Preparations	Reactions	Documents
andalusite	Al_2O_5Si	SiAl ₂ O ₅ 162.046 16453029	Physical Data - 54 Spectra - 11	Other Data - 9	Preparations - 4	Reactions - 7	Documents - 93
kyanite	Al_2O_5Si	SiAl ₂ O ₅ 162.046 16452963	Physical Data - 26 Spectra - 14	Other Data - 6	Preparations - 3	Reactions - 11	Documents - 82
sillimanite	Al_2O_5Si	SiAl ₂ O ₅ 162.046 16453049	Physical Data - 34 Spectra - 10	Other Data - 8	Preparations - 5	Reactions - 15	

Filters: Limit to > Exclude >

- By Structure
- Measurement pX
- Highest Clinical Phases
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Availability in other databases
- Available Data
- Document Type
- Publication Year
- Patent Assignee
- LogP
- H Bond Donors

14 Preview



Поиск информации о минералах

СВОЙСТВА АНДАЛУЗИТА

andalusite

Identification

Druglikeness

Physical Data - 54

Melting Point - 1

Refractive Index - 5

Density - 2

Crystal Phase - 6

Crystal Property Description - 9

Crystal System - 1

Dielectric Constant - 2

Further Information - 12

Interatomic Distances and Angles - 1

Mechanical Properties - 1

Spectra - 11

Other Data - 9

Density - 2

Show/Hide columns

Density, g·cm ⁻³	Measurement Temperature, °C	Type (Density)	Reference
3.151	-158.16	crystallographic	Bryant, Pamela L.; Harwell, Chris R.; Wu, Katherine; Fronczek, Frank R.; Hall, Randall W.; Butler, Leslie G. [Journal of Physical Chemistry A, 1999, vol. 103, # 27, p. 5246 - 5252] Full Text ↗ Cited 45 times ↗ Details > Abstract >
3.1 - 3.2		crystallographic	Mark, H.; Rosbaud, P. [1926, vol. 54, p. 127 - 127] Full Text ↗ Details > Rosbaud, P. [Zeitschrift fuer Elektrochemie, 1926, vol. 32, p. 317 - 317]

Refractive Index - 5

Show/Hide columns

Refractive Index	Wavelength (Refractive Index), nm	Comment (Refractive Index)	Reference
			Mark, H.; Rosbaud, P. [1926, vol. 54, p. 127 - 127] Full Text ↗ Details > Rosbaud, P. [Zeitschrift fuer Elektrochemie, 1926, vol. 32, p. 317 - 317] Full Text ↗ Details > No author [Gmelin Handbuch, Gmelin Handbooks: Al: MVol.A1, 10, page 41 - 43] Full Text ↗ Details >
1.629	589.3	α	Mark, H.; Rosbaud, P. [1926, vol. 54, p. 127 - 127] Full Text ↗ Details > Rosbaud, P. [Zeitschrift fuer Elektrochemie, 1926, vol. 32, p. 317 - 317] Full Text ↗ Details > No author [Gmelin Handbuch, Gmelin Handbooks: Al: MVol.A1, 10, page 41 - 43] Full Text ↗ Details >
1.6328	589.3	β	Mark, H.; Rosbaud, P. [1926, vol. 54, p. 127 - 127] Full Text ↗ Details > Rosbaud, P. [Zeitschrift fuer Elektrochemie, 1926, vol. 32, p. 317 - 317] Full Text ↗ Details > No author [Gmelin Handbuch, Gmelin Handbooks: Al: MVol.A1, 10, page 41 - 43] Full Text ↗ Details >



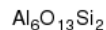
Поиск информации о минералах

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА

Temperature (Transition Point(s) of Crystalline Modification(s)), °C	Change of Modification	Reference
1600		<p>Norton, J. F.[Journal of the American Ceramic Society, 1925, vol. 8, p. 636 - 636] Full Text Details ></p> <p>No author[Gmelin Handbuch, Gmelin Handbook: AI: MVol.B2, 1, page 309 - 312] Full Text Details ></p>
1200 - 1300		<p>Vernadsky, W.[1889, vol. 12, p. 447 - 447] Full Text Details ></p> <p>Vernadsky, W.[1889, vol. 12, p. 447 - 447] Full Text Details ></p> <p>No author[Gmelin Handbuch, Gmelin Handbook: AI: MVol.B2, 1, page 309 - 312] Full Text Details ></p>
1400 - 1550	from andalusite to sillimanite	<p>No author[Gmelin Handbuch, Gmelin Handbook: AI: MVol.B2, 1, page 309 - 312] Full Text Details ></p> <p>Eitel, W.[Physikalisch-chemische Mineralogie und Petrologie in: Wissenschaftliche Forschungsberichte, Dresden-Leipzig 1925, Bd. 13, S. 43] Full Text Details ></p>

Поиск информации о минералах

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА В МУЛЛИТ



andalusite

mullite



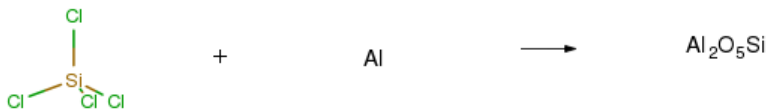
3 Conditions Find Similar Reaction ID: 26413460

Conditions	Yield	Reference
In neat (no solvent) heating (1073 - 1673 K); TEM;		Eberhard, E.,; Rahman, S, Hamid; Weichert, H.-T. [Zeitschrift fuer Kristallographie][1986, vol. 174, p. 44 - 46] Full Text Details
With aluminium(III) ion In neat (no solvent) absorbing of an Al-salt soln. by the powdered Al-silicate (if necessary under pressure); drying and heating up to transition temp.;;		Deutsche Ton- & Steinzeug-Werke Akt.-Ges. DE589556, 1931 Full Text Details
With Al⁽³⁺⁾ In neat (no solvent) absorbing of an Al-salt soln. by the powdered Al-silicate (if necessary under pressure); drying and heating up to transition temp.;;		No author [Gmelin Handbuch, Gmelin Handbook: Al: MVol.B2, 5, page 320 - 322] Full Text Details

3 out of 3

Поиск информации о минералах

ПОЛУЧЕНИЕ АНДАЛУЗИТА



andalusite



2 Conditions Find Similar Reaction ID: 26430724

Conditions	Yield	Reference
In neat (no solvent) in presence of water formation of prisms of andalusite (or cyanite) at red heat;;		Daubree, G. A. [Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences, 1854, vol. 39, p. 135 - 135] Full Text Details
In neat (no solvent) in presence of water formation of prisms of andalusite (or cyanite) at red heat;;		Meunier, S. [Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences, 1882, vol. 90, p. 1010 - 1010] Full Text Details
In neat (no solvent) in presence of water formation of prisms of andalusite (or cyanite) at red heat;;		No author [Gmelin Handbuch, Gmelin Handbook: Al: MVol.B2, 2, page 313 - 315] Full Text Details

Поиск информации о минералах

ПОИСК ЛИТЕРАТУРЫ ПО АНДАЛУЗИТУ

◇ Document Basic Index

1.00 K

Filters

Query

[Limit to >](#) [Exclude >](#)

Index Terms (List)

Index Terms (ReaxysTree)

Publication Year

Document Type

Authors

Patent Assignee

Journal Title

Substance Classes

Reaction Classes

1,597 Documents with 170 Substances, 4 Reactions, 0 Targets

0 selected [Limit To](#) [Exclude](#) [Export](#)

Sort by Publication Year [Heatmap](#)

Contrasting degrees of recrystallization of carbonaceous material in the Nelson aureole, British Columbia and Ballachulish aureole, Scotland, with implications for thermometry based on Raman spectroscopy of carbonaceous material [Cited 1 times](#)

¹ [Beysac, Oliver; Pattison, David R. M.; Bourdelle, Franck](#) [Journal of Metamorphic Geology, 2019, vol. 37, # 1, p. 71 - 95]

[Abstract](#) [Index Terms](#) [Substances 1](#) [Full Text](#) [↗](#)

Abstract hit:

{...Nelson aureole (garnet–staurolite–andalusite#x2013;sillimanite–K-feldspar sequence, ~550–650°C, 3.5–4.0 kbar) was developed in rocks that were...}

Metamorphic petrology of a high-T/low-P granulite terrane (Damara belt, Namibia) – Constraints from pseudosection modelling and high-precision Lu–Hf garnet-whole rock dating ²

[Jung, Stefan; Brandt, Soenke; Bast, Rebecca; Scherer, Erik E.; Berndt, Jasper](#) [Journal of Metamorphic Geology, 2019, vol. 37, # 1, p. 41 - 69]

[Abstract](#) [Index Terms](#) [Full Text](#) [↗](#)

Анализ вещественного состава

Molecular Formula ×

Molecular Formula Lookup × Formula Builder

Formula Builder ×

Molecular Formula: Use this Formula

	1A	2A	3B	4B	5B	6B	7B	8B	9B	10B	1B	2B	3A	4A	5A	6A	7A	8A	
1	H																		He
2	Li	Be											B	C	N	O	F	Ne	
3	Na	Mg											Al	Si	P	S	Cl	Ar	
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
6	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt										
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Metalloids

Nonmetals

Metals

Other Nonmetals

Halogens

Noble Gases

Alkali Metals

Alkaline Earth Metals

Lanthanoids

Actinoids

Transition Metals

Post Transition Metals

6 Carbon

C

Configuration [He] 2s² 2p²

Isotopes ¹²C ¹³C ¹⁴C

Density (kg/m³) 2670

12.0107

0 ▲ more element(s)
▼ with arbitrary count

Any more elements with any counts

Special groups:

Me **Et** **Ph**

Note: its also possible to enter

- ranges or enumerations defined via variables, e.g. Fe_xO_y x=2,3 y=2-4
- Arithmetic terms, e.g. C_nH_{2n+2} n=3,4,5

Анализ вещественного состава

160
Query

Filters

Limit to > Exclude >

- By Structure >
- Measurement pX >
- Highest Clinical Phases >
- Targets >
- Parameters >
- Substance Classes >
- Molecular Weight >
- Number of Fragments >
- Availability >
- Availability in other databases >
- Available Data >
- Document Type >
- Publication Year >
- Patent Assignee >
- LogP >
- H Bond Donors >
- H Bond Acceptors >
- Rotatable Bonds >
- TPSA >

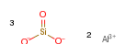
160 Substances out of 1,535 Documents, containing 403 Reactions, 0 Targets

Reaxys - 160

0 selected Limit To Exclude Export

Sort by No of References ↓ Grid Heatmap

1



3 2 Al³⁺

aluminum silicate
2Al⁽³⁺⁾3O₅⁽²⁻⁾ 282.214 14479534

Identification Documents - 688 >

Druglikeness

Other Data - 3

2

Al₆O₁₃Si₂

mullite

mullite
3Al₂O₃+2SiO₂=Al₆Si₂O₁₃ 426.052 16513662

Identification Physical Data - 313 Other Data - 8 Preparations - 140 >

Druglikeness Spectra - 44 Reactions - 169 >

Documents - 317 >

3

Al₂O₇Si₂

metakaolin
(Al₂O₃)₂(SiO₂)₂ 222.13 11341013

Identification Physical Data - 9 Other Data - 1 Preparations - 8 >

Druglikeness Spectra - 2 Reactions - 52 >

Documents - 162 >

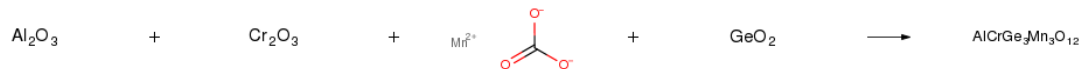
4

andalusite

andalusite
Al₂O₃ 101.961 14479534

Feedback

Получение вещества



1 Conditions Find Similar Reaction ID: 26074679

Conditions

In neat (no solvent) triturating MnCO₃, Cr₂O₃, Al₂O₃ and GeO₂, molding, heating on air for 2-25 h to 1200 °C;

Yield

Reference

Hrichova, R.
[Kristallografiya, 1973, vol. 18, p. 534 - 535][Kristallografiya, 1973, vol. 18, p. 847 - 848]
[Full Text](#) [Details](#)

No author
[Gmelin Handbuch, Gmelin Handbook: Mn: MVol.C3, 2.11.11.1.6, page 197 - 204]
[Full Text](#) [Details](#)

1 out of 1

**AUTOPLAN:**

АВТОМАТИЗИРУЕТ ПРОЦЕСС СОЗДАНИЯ ПЛАНА СИНТЕЗА ВЕЩЕСТВА

Plan 1

Import Save Export Undo Redo

Conditions

Preparation - 1

Conditions	Yield	Reference
In neat (no solvent) triturating MnCO ₃ , Cr ₂ O ₃ , Al ₂ O ₃ and GeO ₂ , molding, heating on air for 2-25 h to 1200 °C;		Hrichova, R. [Kristallografiya, 1973, vol. 18, p. 534 - 535][Kristallografiya, 1973, vol. 18, p. 847 - 848] Full Text Details >
		No author [Gmelin Handbuch, Gmelin Handbook: Mn: MVol.C3, 2.11.11.1.6, page 197 - 204] Full Text Details >

Feedback