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Особенности баз Reaxys и Reaxys Medicinal Chemistry и примеры решения исследовательских задач.

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направления химико-биологических решений Elsevier S&T
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План

- Особенности и покрытие базы данных Reaxys.
- Оптимальная стратегия поиска литературы.
- Свойства веществ в Reaxys
- Химические реакции в Reaxys
- Биологическая активность и медицинская химия в Reaxys
- Вопросы





Особенности и покрытие базы данных Reaxys.

Источники информации

Индексация

Извлечение данных

08,08,2019

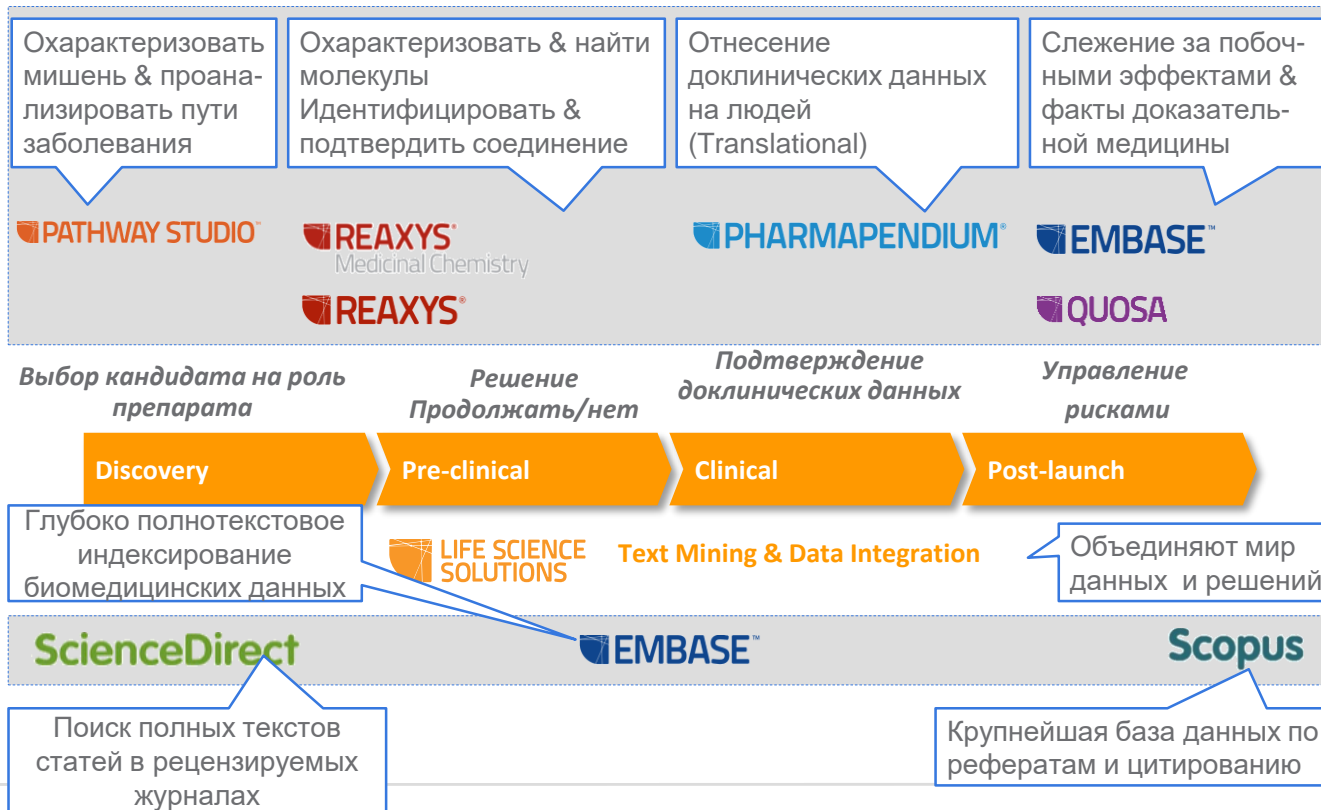
Моисеев Алексей Александрович

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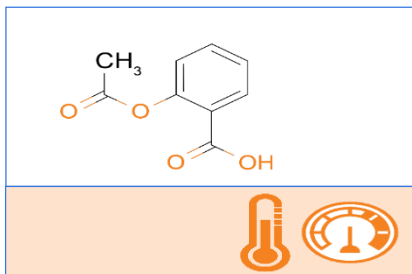
Решения в области life sciences

НАПРАВЛЕНИЯ И КЛЮЧЕВЫЕ ПРОБЛЕМЫ R&D



Продукты Elsevier охватывают всю цепочку "От геномов к лекарству in silico"

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 >]

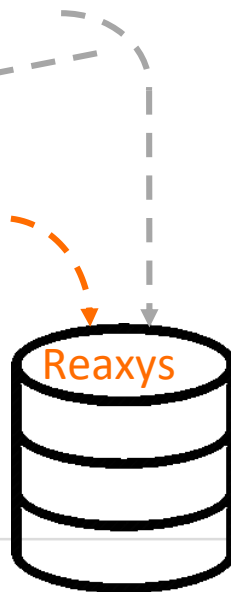
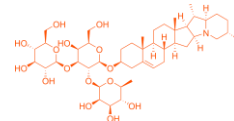
PO: JP, KR, CN, TW [2015 >]

380+k book chapters

Beilstein, Gmelin,



≈ 450 journals + PO
[manually excerpted]



Химия как принцип организации данных

Из экспериментальных данных статей из рецензируемых журналов и патентов

High-Affinity, Non-Nucleotide-Derived Competitive Antagonists of Platelet P2Y₁₂ Receptors

Younis Baqi,¹ Kerstin Atzler,¹ Meyren Klose,¹ Markus Gläsel,^{1,2} and Christa E. Müller^{1,3}
¹PharmCenter Bonn, Pharmaceutical Institute, Pharmaceutical Chemistry I, Pharmaceutical Sciences Bonn (PSB), University of Bonn, Am Rheinberg 4, D-53121 Bonn, Germany, ²Department of Experimental and Clinical Pharmacology and Toxicology, University of Freiburg, Albertstrasse 23, D-79104 Freiburg, Germany

Received March 16, 2009

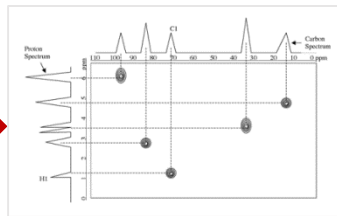
Anthraquinone derivatives related to the moderately potent, nonselective P2Y₁₂ receptor antagonist reactive blue 2 (6) have been synthesized and optimized with respect to P2Y₁₂ receptor affinity. A radioligand binding assay utilizing human blood platelet membranes and the P2Y₁₂ receptor-selective antagonist radioligand [³H]-propylthioadenosine-5'-adenylic acid (1,1-dichloro-1-[(phosphonoacetyl)-L-(phosphonyl) silylole] adenyloside ([³H]PSB-0413) was applied for compound testing. 1-Amino-2-methylanthraquinone derivatives bearing a (p-phenylamino)toluene substitution in the 8-position and an additional acidic function in the meta-position of the aniline ring showed high P2Y₁₂ receptor affinity. These new anthraquinone derivatives became accessible by a recently developed copper(I)-catalyzed Ullmann coupling reaction of 1-amino-2-methylanthraquinone derivatives with arylates in ethylenate buffer under microwave irradiation. The most potent compound

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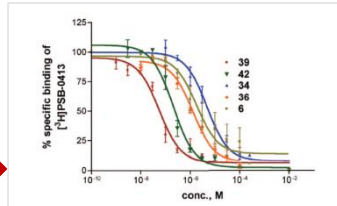
appears to be of paramount importance in regulating platelet function and, as a consequence, in controlling thrombotic diseases, which are the most common cause of morbidity and

irreversible inhibition, (iii) "drug resistance" in a high percentage of patients (up to 30%), (iv) moderate potency (therefore high doses are required), and (v) difficulties in storing and controlling the effects.

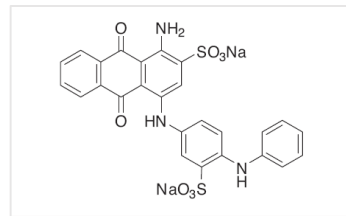
Therefore, it is highly desirable to develop P2Y₁₂ antagonists that are lacking the drawbacks associated with the standard P2Y₁₂ antagonists such as clopidogrel and other thienopyridine derivatives. Several groups have recently been developing competitive, reversible P2Y₁₂ antagonists that may be superior to clopidogrel and related drugs. Most approaches started from the adenosine nucleotides as lead structures, ADP,



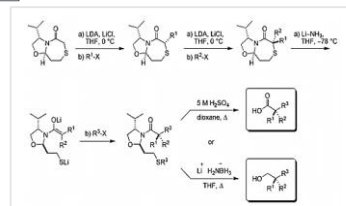
Физико-химические свойства



Фармакологические свойства



Химическая структура



Химический и биохимический синтез

- Физические свойства
- Спектры
- Биоактивность
- Природные материалы

Свойства химических соединений и их взаимодействия являются ключевыми для способа организации данных в базе данных.

Также индексируется информация о физико-химических и фармакологических свойствах.



Reaxys

Это обширные, хорошо проиндексированные данные под рукой

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Растворимость это только одно из **>500 полей данных для поиска** в Reaxys

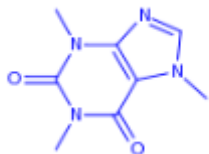
Melting point	Enthalpy of Formation	NMR Spectroscopy	Target
Boiling point	Enthalpy of Sublimation	IR Spectroscopy	Substance Effect
Sublimation	Flash Point	Mass Spectroscopy	Substance Action on Target
Refractive index	Gas Phase	UV/VIS Spectroscopy	Substance Dose
Density	Dissociation Energy	ESR Spectroscopy	Bioassay
Adsorption	Crystal System	NQR Spectroscopy	Animal Model
Association	Crystal Phase	Raman Spectroscopy	Organs/Tissue
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
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 (MC	Solvent (Solubility (MCS))	Comment (Solubility (MCS))	Reference
20.88		28	water		Singh, Neetu; Singh, Udai P.; Nikhil, Kumar; Roy, Partha; Singh, Harij 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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a.Moiseev@elsevier.com +79251131255



Поиск литературы. Поиск по ключевым словам

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Substances >

Documents >

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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 ^

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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  Heatmap 








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** 

[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
+ More		

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<http://www.reaxys.com>

PATENT SEARCHING USING THE LITERATURE SEARCH FORM

Reaxys

Quick search Query builder ^{New} Results Synthesis planner History Alexey Moiseev

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

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- Common roasting defects in coffee: Aroma composition, sensory characterization and consumer perception
1 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 (32) 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, Alec; Austad, Jon; 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)
- 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 Geok; Son, Young-A - [Dyes and Pigments, 2019, vol. 160, p. 37 - 47]
Abstract Index Terms Substances (17) Reactions (33) Full Text
Hit Substances (1)

Feedback



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

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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

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

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- 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*
Products, 2017, 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 Product*
Research, 2017, vol. 17, p. 2453 - 2460]
[Abstract](#)  [Index Terms](#)  [Substances](#) 62  [Reactions](#) 113  [Full Text](#) 



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

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Structure Molecular Formula CAS RN Doc. Index

Molecular Formula is Mo(10b)

AND

Density

OR
• AND
NOT
NEAR
NEXT
PROXIMITY

Find any Hide fields

= Density, g·cm-3

= Reference Temperature, °C

= Measurement Temperature, °C

is Type (Density)

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Physical Properties

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Sublimation

Refractive Index

Density

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alert1

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



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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

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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
Association	Crystal Phase	Raman Spectroscopy	Organs/Tissue
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
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...



Как найти соединения с заданными свойствами?

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Molecular Formula



CAS RN



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Fields

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Basic Indexes

◇ Substance Basic Index

◇ Reaction Basic Index

◇ Document Basic Index

Identification

Physical Properties

◇ Melting Point

◇ Boiling Point

◇ Sublimation

◇ 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



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

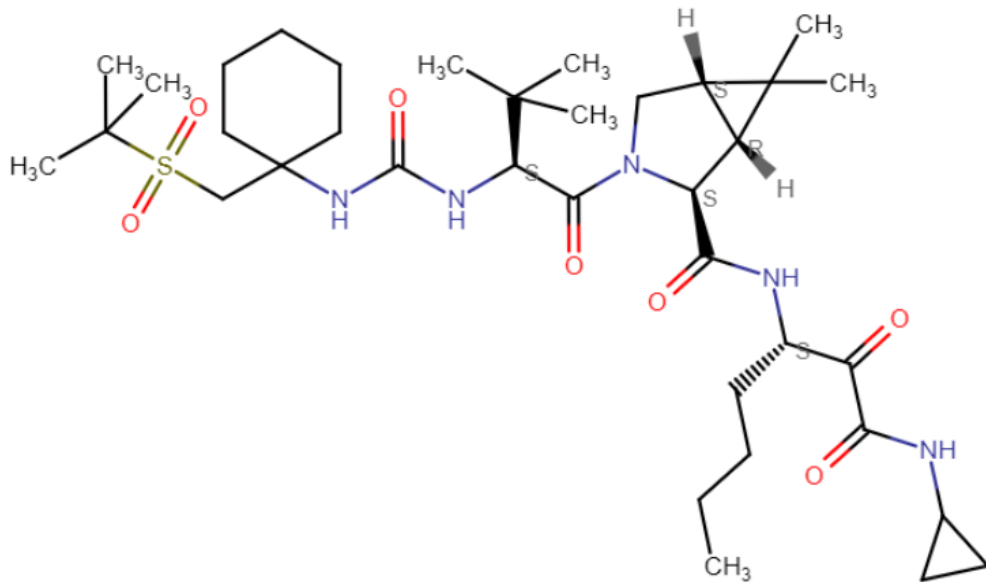


Разработка методики синтеза химических веществ (субстанций) в Reaxus

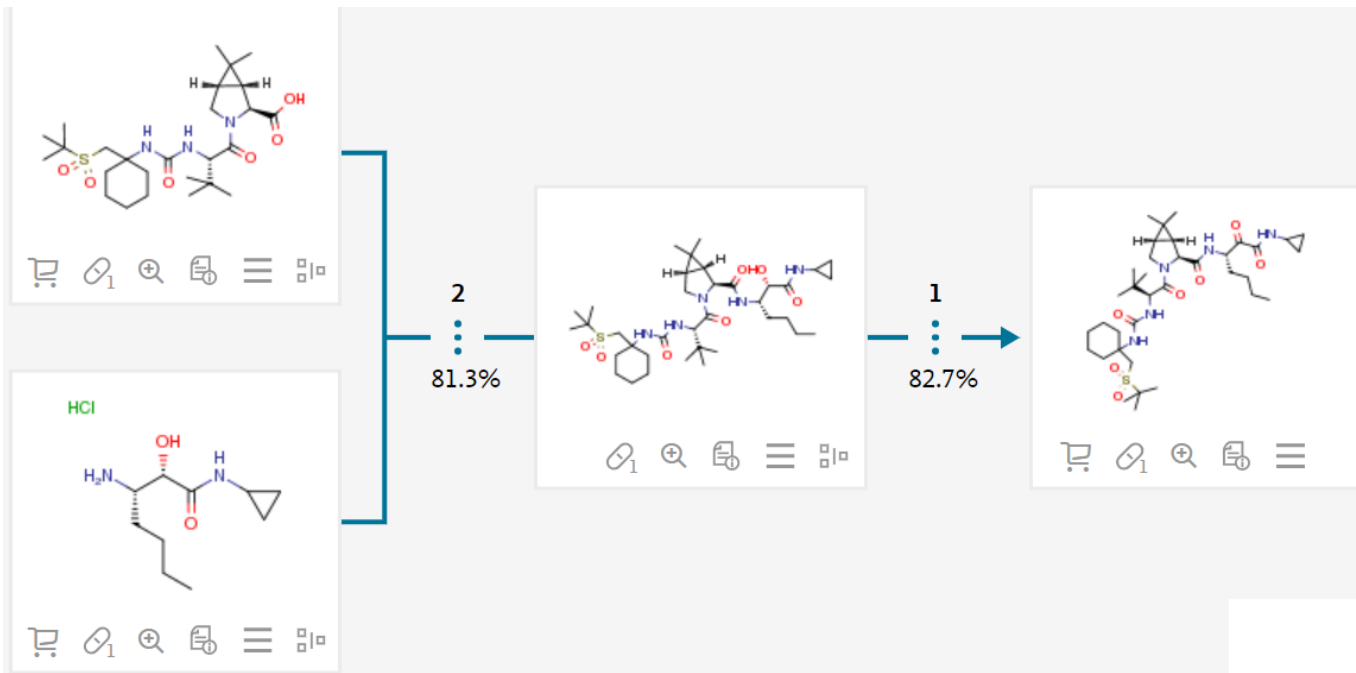
С помощью Reaxus можно решать задачу поиск оптимальных условий синтеза субстанций.

Допустим, Вас интересует данное соединение

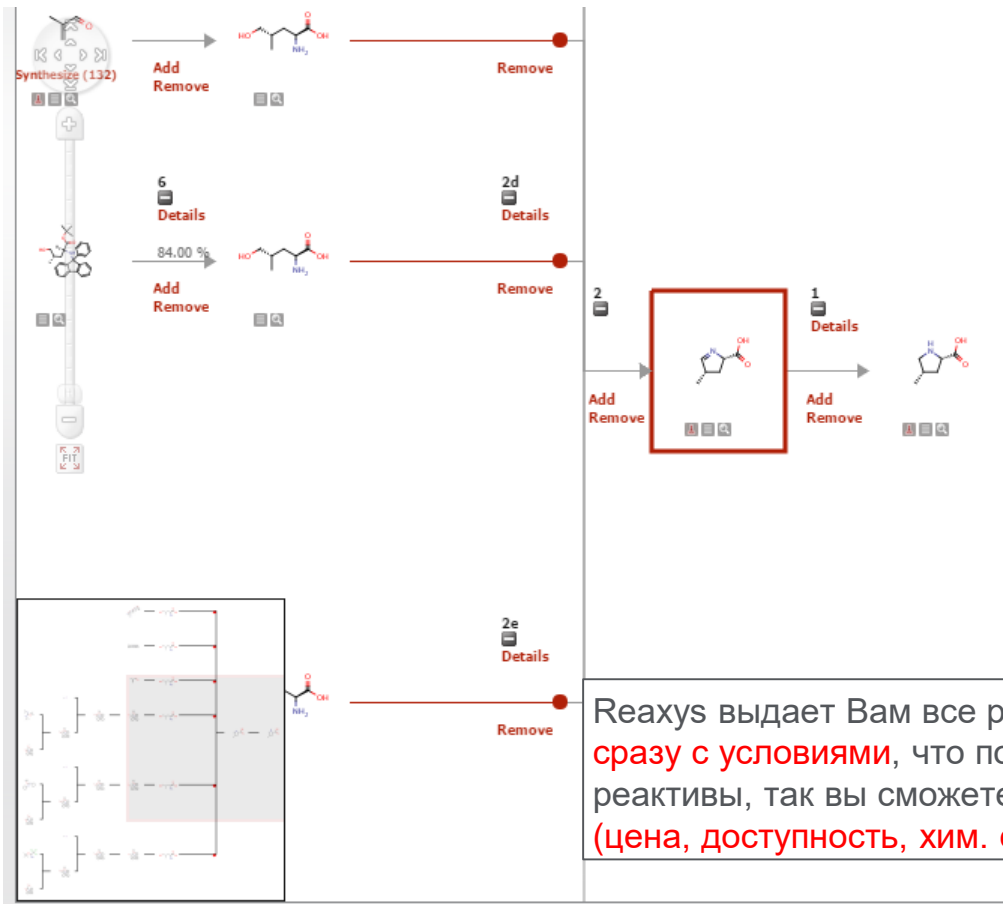
NARLAPREVIR



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



Разработка методики синтеза химических веществ (субстанций)



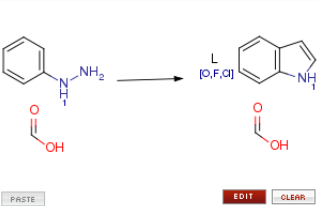
Также за секунды Reaxys может **построить многостадийный план синтеза** из базовых соединений, что сэкономит время сотрудников и **позволит выбрать метод, в котором не образуются опасные побочные продукты.**

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.

Structure



As drawn
 Substructure
 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
 Keep fragments
 separate together

CREATE STRUCTURE TEMPLATE FROM NAME

Molecular Formula

Molecular Formula Lookup

Identification

Chemical Name is Lookup

Show AND Buttons

Please select role Product Starting material Reagent / Catalyst Any role

Reaction Data

Yield (numerical)	=	<input type="text"/>	Lookup
Solvent (Reaction Details)	is	<input type="text"/>	Lookup
Reagent/Catalyst	is	<input type="text"/>	Lookup
Time (Reaction Details) (h)	=	<input type="text"/>	Lookup
Temperature (Reaction ... (°C)	=	<input type="text"/>	Lookup
Pressure (Reaction D... (Torr)	=	<input type="text"/>	Lookup
Reaction Type	is	<input type="text"/>	Lookup
Reaction Basic Index	is	<input type="text"/>	Lookup

Show AND Buttons

91 Substances

Substance Availability × 1,317 Reactions, 424 Targets Reaxys - 680

- Accelrys' ACD
- CambridgeSoft ACX
- Labnetwork
- PharmaPendium
- Sigma Aldrich
- 500g eMolecules

By Structure 0

Measurement pX 1

Highest Clinical Phases 1

Targets 1

Parameters 1

Substance Classes 1

Molecular Weight 2

Number of Fragments 2

Availability 2

Availability in other databases 2

Available Data 2

Document Type 2

Sort by No of References Grid Heatmap

Bioactivity (All) Spectra - 187 Preparations - 96 >

Physical Data - 560 Other Data - 3,709 Reactions - 1,184 >

Targets - 418 >

Documents - 16,028 >

Дополнительную информацию о поставщике можно найти в этой вкладке.

calcium O-acetylsalicylate

Identification Druglikeness Physical Data - 2 Other Data - 20

Preparations - 5 >

Reactions - 8 >

Documents - 90 >

lysine Acetylsalicylate

$C_{20}H_{24}O_4 \cdot C_9H_{11}N_2O_2$ 326.349 5690287 62952-06-1

Feedback

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 моей местном складе?

Есть ли материал присутствует на складе у любого поставщика?

Есть ли этот поставщик в моей системе покупки?

Reaction ID: 692908

Options

Synthesize

Substance Availability

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

500g \$33

3 out of

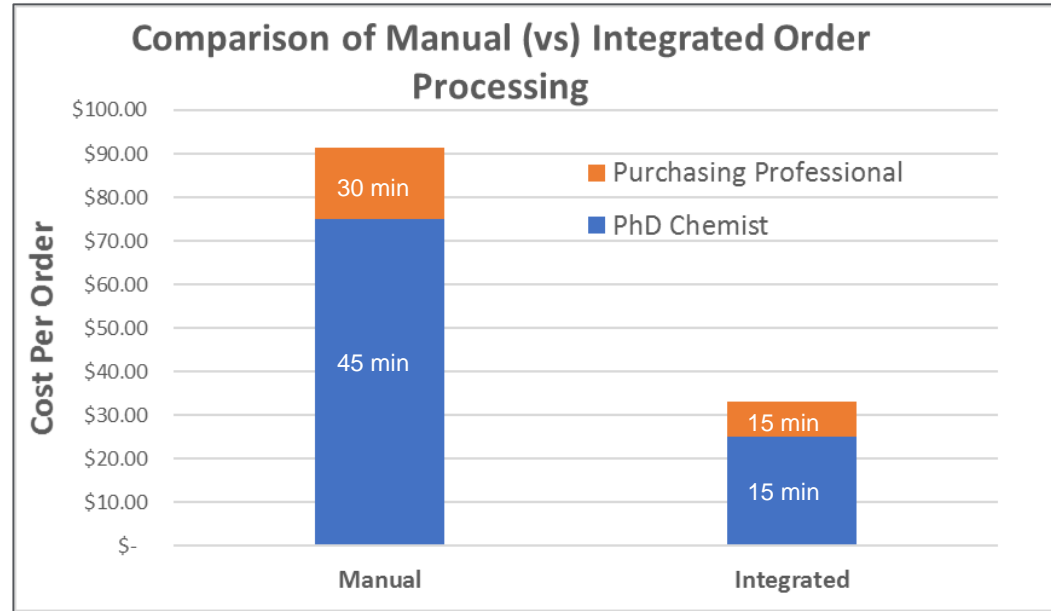
Reaction scheme showing a carboxylic acid reacting to form an ester.

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 ×

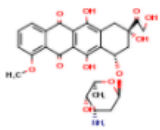
> ▼ Measurement pX
6 🔍

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

Bioactivity (Hit Data)

Spectra - 198

Preparations - 56 >

Identification

Bioactivity (All)

Other Data - 4,448

Reactions - 292 >

Druglikeness

Physical Data - 141

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 


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

C₁₅H₂₄O 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)

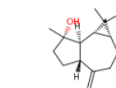
Synonyms: acetylcholinesterase

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 ...)

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 Escherichia coli

Find search fields and forms

Fields Forms History

Reaxys ^

Basic Indexes v

Identification v

Physical Properties v

Spectra v

MedChem v

Other ^

◇ Isolation from Natural Product

◇ Use

◇ Exposure Assessment

◇ Concentration in the

Feedback

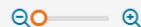
Форма поиска натурального продукта

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 ▼

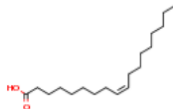
542 Substances out of 94,335 Documents, containing 28,875 Reactions, 1,688 Targets

 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](#)

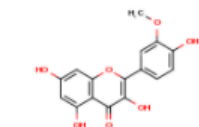
Какие соединения были найдены в тысячелистнике Yarrow?



◇ Isolation from Natural Product Find any Hide fields ^ x

contains ▼ Isolation from Natural Product

Yarrow



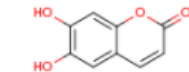
isorhamnetin
C₁₆H₁₂O₇ 316.267

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



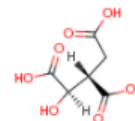
aesculetin
C₉H₆O₄ 178.144 152788

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



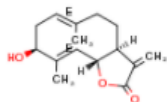
threo-D-isocitric acid
C₆H₈O₇ 192.125 1727947

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)



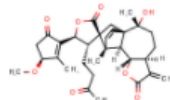
hanphyllin
C₁₅H₂₀O₃ 248.322 1623169

Hit Data - 1

Identification

Druglikeness

Bioactivity (All)

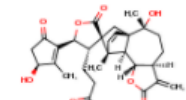


achillinin B
C₃₁H₃₈O₈ 538.638

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="button" value="↑"/>
<input type="checkbox"/>	medicamental	11	<input type="button" value="↑"/>
<input type="checkbox"/>	medicamentary	10	<input type="button" value="↓"/>
<input type="checkbox"/>	medicamentns	1	<input type="button" value="↓"/>
<input checked="" type="checkbox"/>	medicamentosa	788	<input type="button" value="↓"/>
<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 ^ ×

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

Какие соединения используются в качестве ингибиторов коррозии?

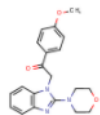
251 Substances out of 356,601 Documents, containing 531,983 Reactions, 610 Targets

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

◇ Use Find any Hide fields ^ ×

is	▼	Laboratory Use and Handling	
is	▼	Use Pattern	
		(corros* NEAR inhib*) OR (anticorr*)	

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

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

AND

Molecular Formula

is	Molecular Formula F6N5C16*
----	-------------------------------

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

MedChem

Other

Reactions

Bibliography

PubChem

eMolecules

LabNetwork

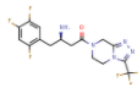
SigmaAldrich

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

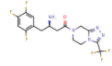
Type (Optical Rotatory Power)	Concentration (Optical Rotatory Power)	Length of Path, cm	Solvent (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength (Optical Rotatory Power), nm	Temperature (Optical Rotatory Power), °C	Location	Reference
alpha	0.92 g/100ml		chloroform	-22.4	589	25	Page/Page 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	¹ H NMR (CH ₃ OD, 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 $\sim 56,5$ °С
2. Температура плавления 64 °С
3. Обнаружено, что данное соединение является стабильным (не разлагается) при нагревании до 2000 К
4. Элементный анализ показал отсутствие атомов С или О 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

=

=

AND

Melting Point Hide fields ^ x

=

is

AND

Substance Basic Index Hide fields ^ x

is

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

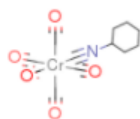
63.94

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)

alloy

Reaxys ID: 26601394
CoCrFeNi 225.526 26601394

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	Documents - 82

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

- 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

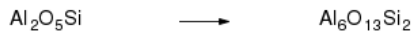
Transition Point(s) of Crystalline Modification(s)

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА
ANDALUSITE

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

Поиск информации о минералах

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА В МУЛЛИТ



andalusite

mullite



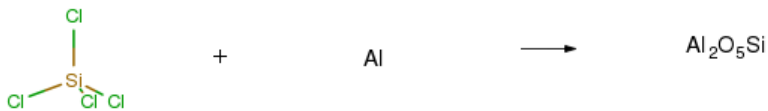
3 Conditions Find Similar Reaction ID: 26413460

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

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 ↓

- 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](#)

[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 [Cited 1 times](#)

[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

Transition Metals

Post Transition Metals

Actinoids

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

Filters

160 Query

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

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

Identification Documents - 688 >

Druglikeness

Other Data - 3

2

Al₆O₁₃Si₂

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 >

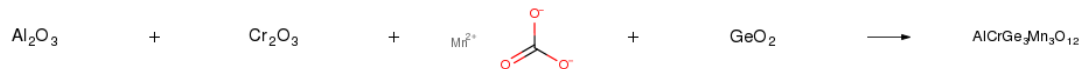
Druglikeness Spectra - 2 Reactions - 52 >

Documents - 162 >

andalusite

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

Reaction scheme diagram showing the synthesis of $\text{AlCrGe}_3\text{Mn}_3\text{O}_{12}$ from MnCO_3 , Al_2O_3 , Cr_2O_3 , and GeO_2 . The reactants are listed vertically on the left, and the product is shown in a box on the right, connected by a blue arrow. A vertical line with a '1' and three dots is positioned between the reactants and the product.

Conditions

Preparation - 1

Conditions	Yield	Reference
In neat (no solvent) triturating MnCO_3 , Cr_2O_3 , Al_2O_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

План

- Особенности и покрытие базы данных Reaxys.
- Оптимальная стратегия поиска литературы.
- Свойства веществ в Reaxys
- Химические реакции в Reaxys
- Биологическая активность и медицинская химия в Reaxys
- Вопросы

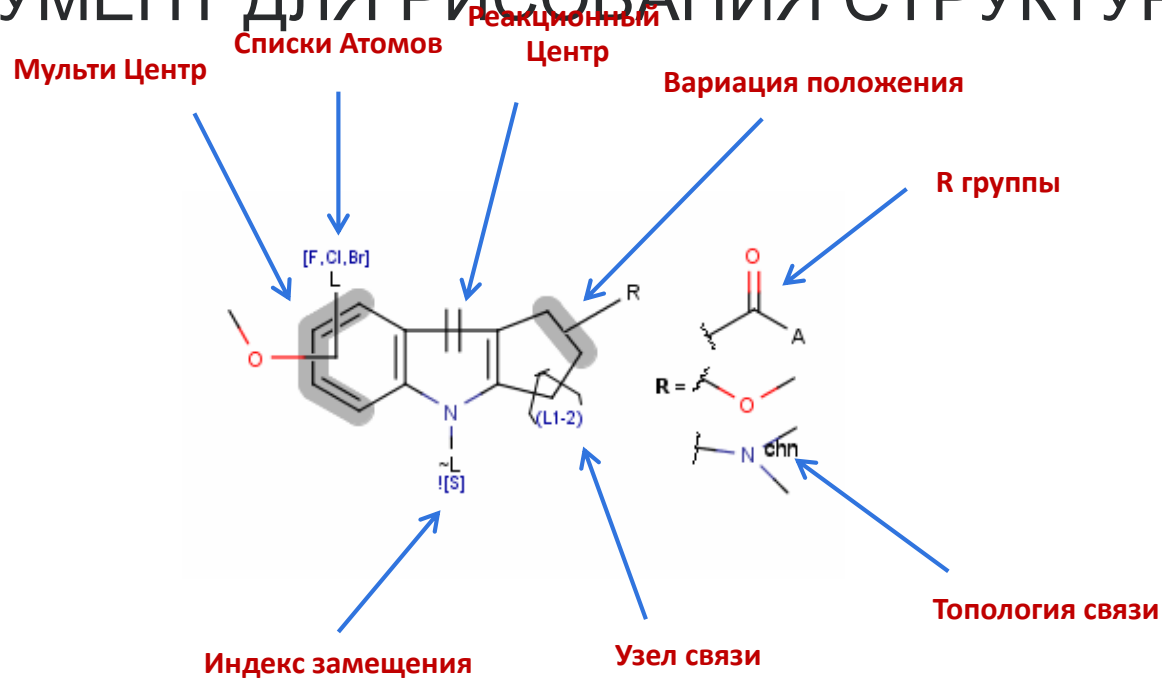


РИСОВАНИЕ СТРУКТУРЫ С ИСПОЛЬЗОВАНИЕМ MARVIN JS



MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ



MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ

The screenshot shows the Marvin JS software interface with the following annotations:

- Выбор** (Selection): Points to the selection tool icon in the top-left toolbar.
- Тип связей** (Bond type): Points to the bond type tool icon in the top-left toolbar.
- Повторяющиеся единицы** (Repeating units): Points to the s_{max} and s_{x-z} icons in the top-left toolbar.
- Селектор R-групп** (R-group selector): Points to the R selector icon in the top-left toolbar.
- Прикрепление R-Group** (R-group attachment): Points to the attachment icon in the top-left toolbar.
- Стрелка реакции/Мэппинг атомов** (Reaction arrow/Atom mapping): Points to the reaction arrow icon in the top-left toolbar.
- Общие шаблоны** (General templates): Points to the template icons in the bottom toolbar.
- Reaxys Generics**: Points to the Reaxys Generics icons in the bottom toolbar.
- показать/ убрать водороды** (Show/hide hydrogens): Points to the H^+ icon in the top toolbar.
- Список атомов (таблица Менделеева)** (List of atoms (Mendeleev table)): Points to the periodic table icon on the right side.
- Основные атомы** (Basic atoms): Points to the list of basic atoms (R, A, H, C, N, O, S, F, P, Cl, Br) on the right side.

MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ

The screenshot displays the Marvin JS software interface. On the left is a vertical toolbar with drawing tools like lines, polygons, and rings. A central drawing area contains a watermark for 'Marvin JS by ChemAxon'. On the right, several panels are open: 'Reaxys Group Generics' with 'Acyclic' and 'Cyclic' tabs, 'Abbreviated groups' with a search box containing 'fmoq' and an 'FMOQ' button, and a 'Periodic table' window. A vertical list of elements (R, A, H, C, N, O, S, F, P, Cl, Br) is on the far right. Blue arrows point from the drawing area to the 'Abbreviated groups' panel and from the 'Periodic table' panel to the 'Abbreviated groups' panel.

Reaxys Group Generics

Acyclic Cyclic

ACY ACH

Carb Hetero

ABC ABH AHC AHH

Alkyl Alkoxy

AYL AYH AOX AOH

Alkyl

ALK ALH

Alkenyl

AEL AEH

Abbreviated groups

fmoq Expand

FMOQ Ok

Periodic table

1	2											13	14	15	16	17	18		
H	He											B	C	N	O	F	Ne		
Li	Be											Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
Fr	Ra	#	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fl	Uup	Lv	Uus	Uuo		
Atom list	*	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
NOT list	#	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr			

Ok

MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТЫ

Marvin.js - Google Chrome
https://www.reaxys.com/reaxys/js/sre_5_4_2_01/child_marvin_js.html

Нажмите на атом или связь, он будет выделен в зеленый, затем щелкните правой кнопкой мыши

Нажмите на атом или связь свойств чтобы найти дополнительные варианты

Chemical structure: C1=CC=C2C(=C1)N(C2)C3CCCCC3

Property panels shown:

- Bond properties**
 - Type: single
 - Topology: undefined
 - Reacting center: undefined, in ring, in chain
- Bond properties**
 - Type: double
 - Topology: undefined
 - Reacting center: undefined
- Atom properties**
 - Change to: Element
 - Basic: Total H (H), Implicit H (h), Bond orders (v), Connections (X), Ring count (R), Smallest ring size (r)
 - Advanced: Ring bond (rb), Substitutions (s), Unsaturated (u), Aromaticity (a/A)

УРЯ

ПОИСК ВЕЩЕСТВ

Нажмите на редактор структуры, чтобы выбрать редактор по выбору. Java Free Marvin PS является предпочтительным редактором

Можно выполнить точный поиск, поиск по субструктуре или подобию

Используйте эти функции, чтобы исключить ненужные вещества

The screenshot shows the Marvin JS chemical structure editor. The main workspace contains the Marvin JS logo and the text "by ChemAxon". The interface includes a top toolbar with various editing tools, a left sidebar with additional tools, and a right sidebar with search options. A search panel is open on the right, showing search criteria and exclusion options.

Structure editor ChemAxon's MarvinJS

Create structure template from name

Search this structure as:

- As drawn
- As substructure
- Similar

Tautomers

Stereo

Additional ring closures

Related Markush

Salts

Mixtures

Isotopes

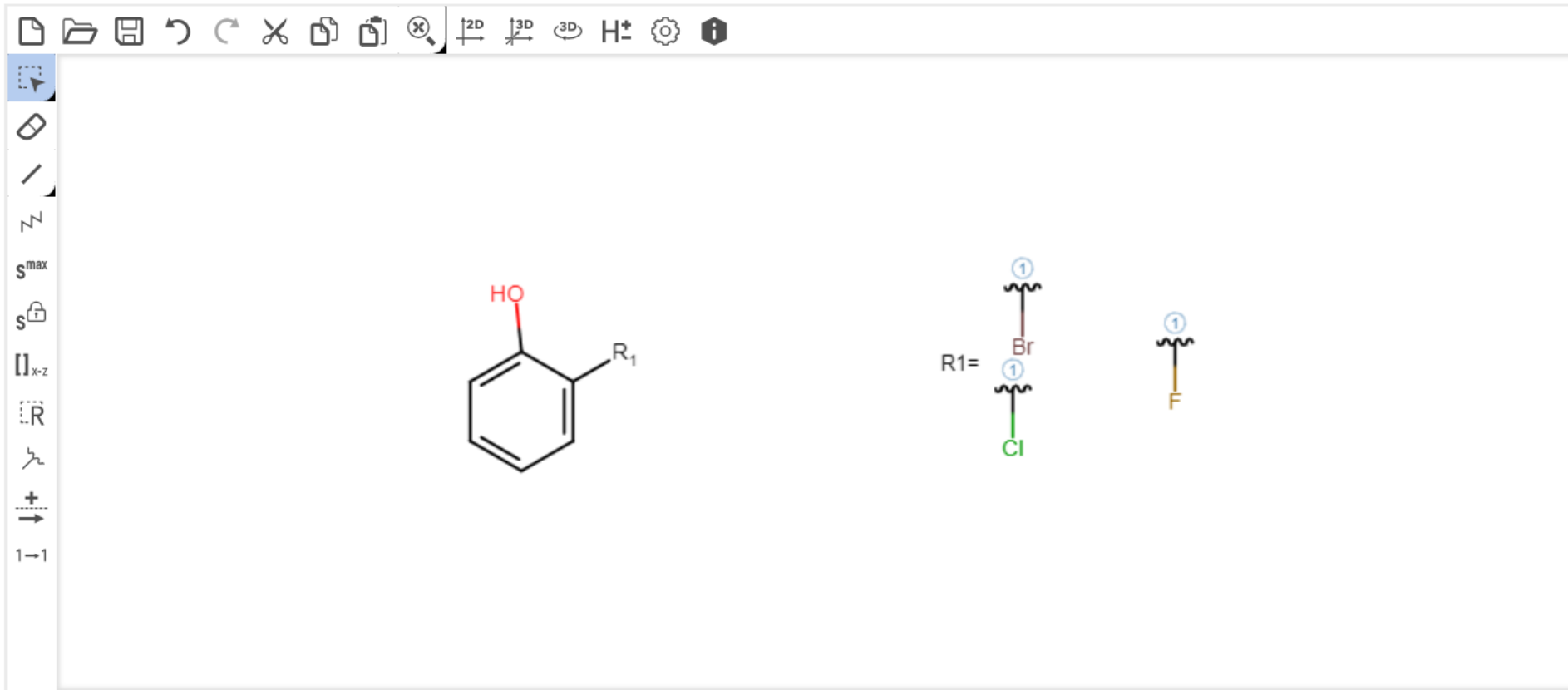
Charges

Radicals

+ More options

В большинстве случаев можно создать структуру из названия

Пример использования smart R-group



Structure editor

Create structure template from name >

$\text{H}_2\text{N}-\text{ARY}$ + $\text{ARY}-\text{B}(\text{OH})_2$ →

Search this structure as:

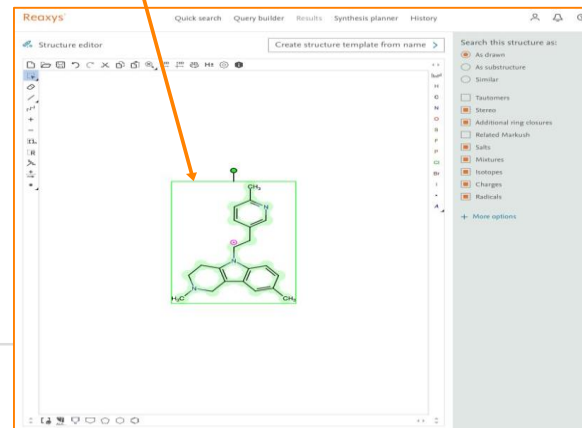
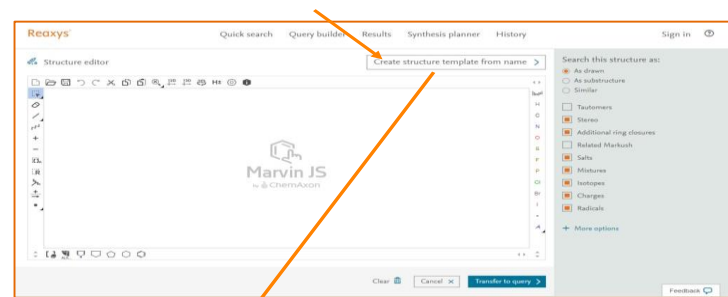
- As drawn
- As substructure
- Similar

- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

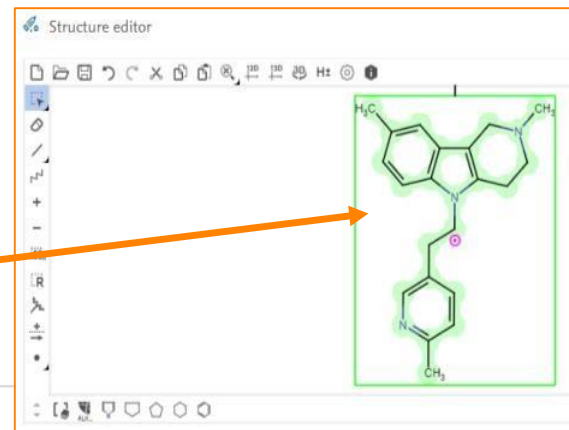
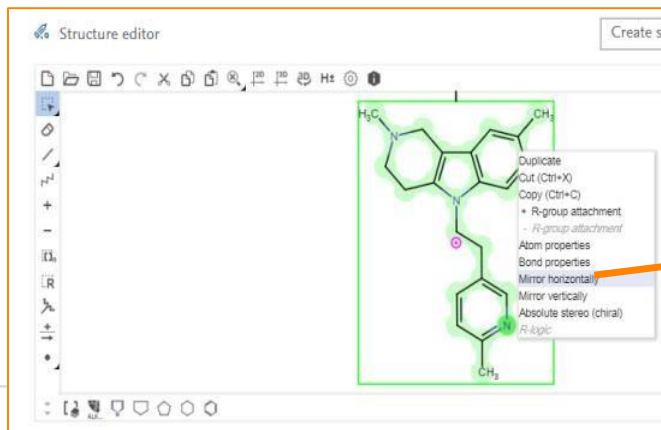
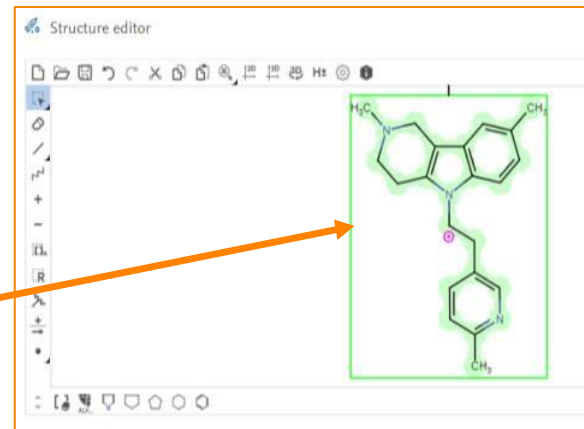
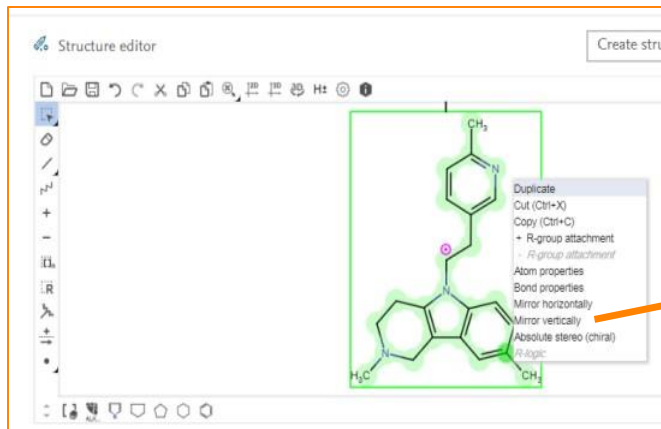
+ More options

Clear Cancel X Transfer to query >

стратегия синтеза аналогов димебона Dimebon



Чтобы изменить ориентацию структуры, щелкните правой кнопкой мыши на любом атоме и выберите «Отразить по вертикали» или «Отразить по горизонтали». Нужный участок структуры или вся структура должны быть выделены



Вы можете отрегулировать размер структуры, прокручивая вверх или вниз.

Удалите две метильные группы из верхних колец, нажав C и нажав Delete на клавиатуре.

Reaxys

Quick search Query builder Results Synthesis planner History

Structure editor

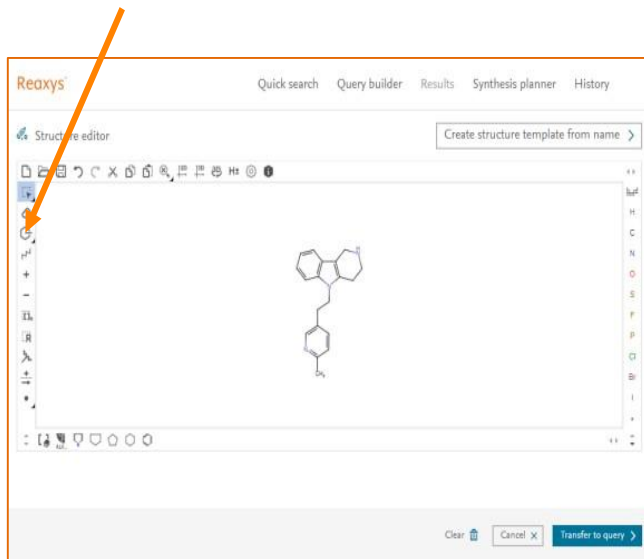
Create structure template from name >

Clear Cancel Transfer to query >

Задайте позиции плавающих связей

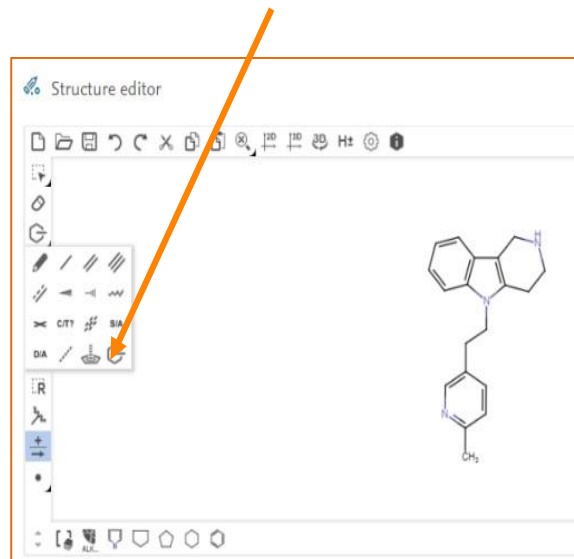
Открыть панель инструментов

a . Click here to open the tool panel.



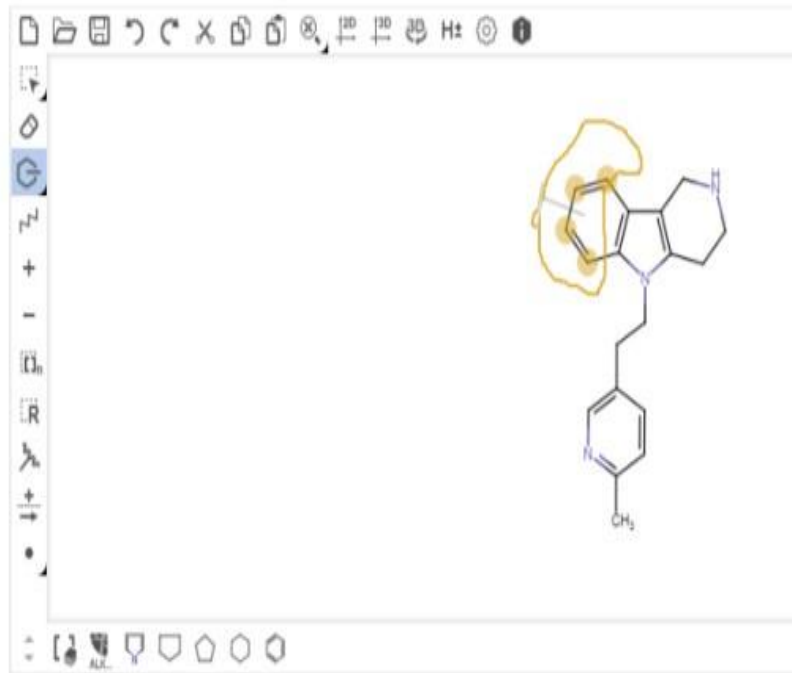
Открыть инструмент позиционирования плавающих связей

b . Select the position variation bond.

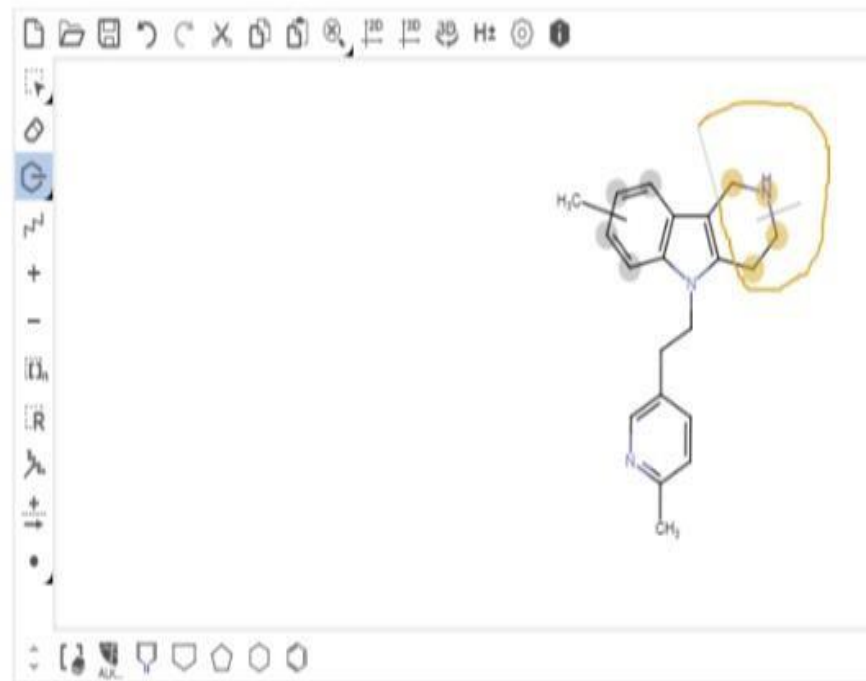


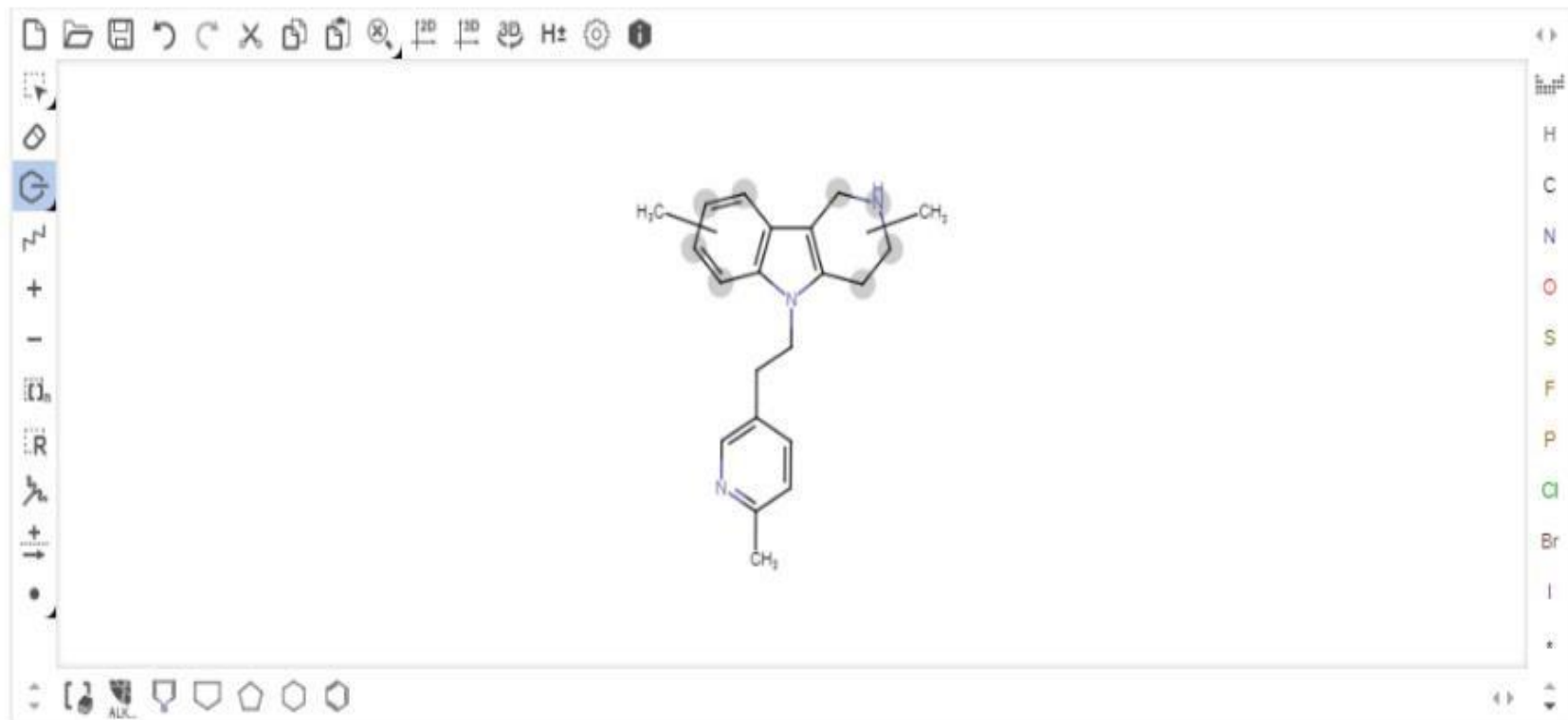
Выберите атомы для включения, нарисовав линию

Structure editor



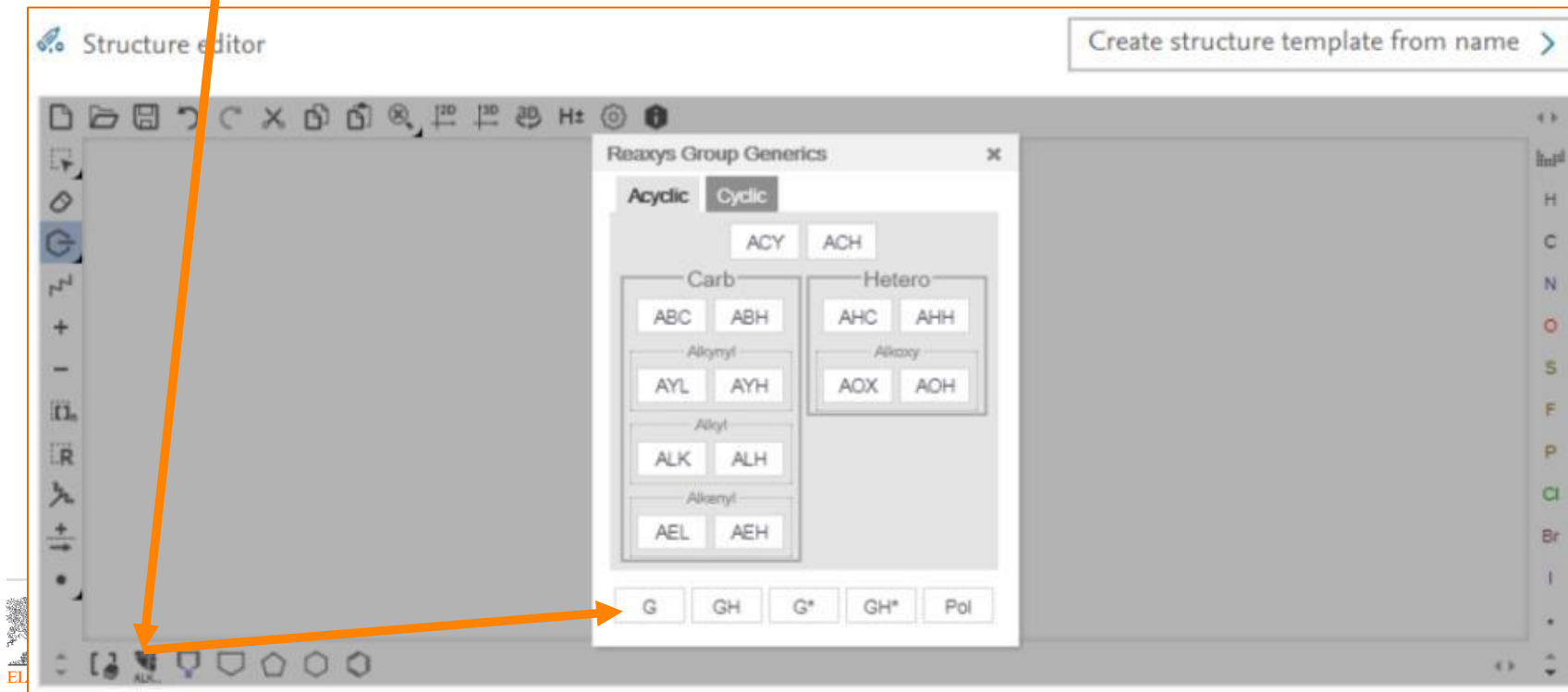
Structure editor





Откройте диалоговое окно Group Generics с помощью кнопки на нижней панели. Выберите G

Это позволяет добавлять любую группу в качестве запроса в связи с изменением позиции.



Добавьте стрелку реакции на левой панели, чтобы в запросе ваша структура

The screenshot shows a chemical structure editor window titled "Structure editor". The main workspace contains a chemical structure consisting of a complex fused ring system (indole-like) connected via a two-carbon chain to a pyridine ring with a methyl group (CH₃). A black arrow points from the left towards the pyridine ring. On the left side of the editor, there is a vertical toolbar with various icons; the bottom-most icon, representing a reaction arrow, is highlighted with a blue selection bar. An orange arrow from the text above points to this icon. At the top right of the editor, there is a button labeled "Create structure template from name >". On the right side, a panel titled "Search this structure as:" contains several search options: "As drawn" (selected with a radio button), "As substructure", "Similar", "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", and "Radicals". At the bottom of this panel is a "+ More options" link. At the bottom of the editor window, there are three buttons: "Clear" with a trash icon, "Cancel" with an "X" icon, and "Transfer to query" with a right-pointing arrow.

Нажмите find

Click **Transfer to query**

and then **Find**

The screenshot shows the Reaxys search interface. At the top, there are navigation tabs: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". On the right side of the top bar, there are icons for user profile, notifications, and a search icon. Below the top bar, there is a search input field with the placeholder text "Search for" and a search icon. To the left of the search field is an "Import" button. To the right of the search field is a blue "Find" button with a right-pointing arrow. An orange arrow points from the top right towards the "Find" button. Below the search bar, there is a search result snippet: "Documents, e.g. publications about quasicrystals". Below this, there is a chemical structure query. The query is labeled "AND" and shows two chemical structures. The first structure is a complex heterocyclic system with a methyl group (H₃C) and a methyl group (CH₃) attached to a nitrogen atom. The second structure is a pyridine ring with a methyl group (CH₃) attached to the nitrogen atom. An arrow points from the second structure to the first, indicating a search for documents containing both structures. At the bottom left of the search result area, there is a small "As drawn" label.

Исследуйте реакции вокруг определенных связей

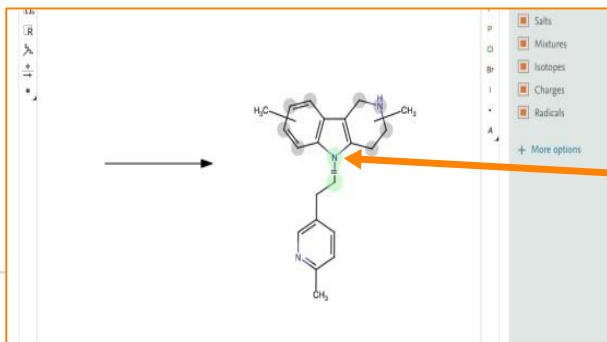
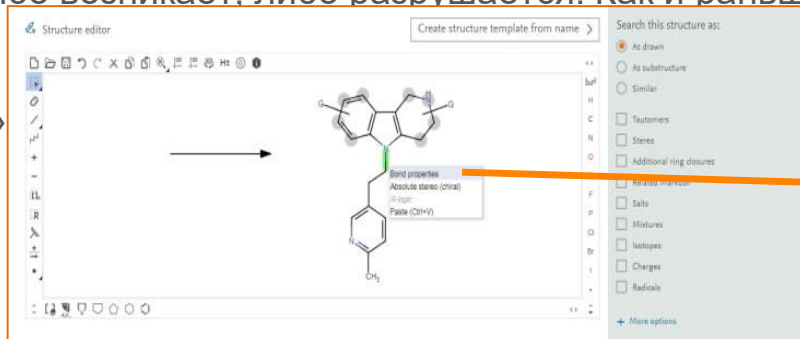
The screenshot displays the Reaxys search interface. At the top, there are navigation tabs: "Quick search", "Query builder", "Results", "Synthesis planner", and "History". Below these is a search bar with the text "Search for" and a "Find" button. A search result is shown: "Documents, e.g. publications about quasicrystals". The main content area features a chemical structure query. The query is a complex molecule consisting of a quinine-like core (a quinoline ring fused to a quinuclidine bicyclic system) with a methyl group (H₃C) on the quinoline ring and a methyl group (CH₃) on the quinuclidine nitrogen. This core is connected via a methylene bridge (-CH₂-) to a 4-methylpyridine ring. A large orange arrow points from the top right towards the methylene bridge in the chemical structure. The text "AND" is positioned above the structure, and "X" is to the right. Below the structure, it says "As drawn".

Щелкните правой кнопкой мыши на связи и выберите свойства связи. Нажмите на выпадающее меню

для Recting center и определите его как make или break. Это позволит искать те реакции, в которых эта

связь либо возникает, либо разрушается. Как и раньше, перенесите это в свой запрос и нажмите

«Найти»



Чтобы найти реакции, в которых связь не задействована, откройте структуру запроса и выберите Не центр в раскрывающемся

The screenshot shows a chemical software interface with a 'Bond properties' dialog box. The dialog box has the following fields:

- Type: single
- Topology: undefined
- Reacting center: make or break - |
- Stereo search: undefined

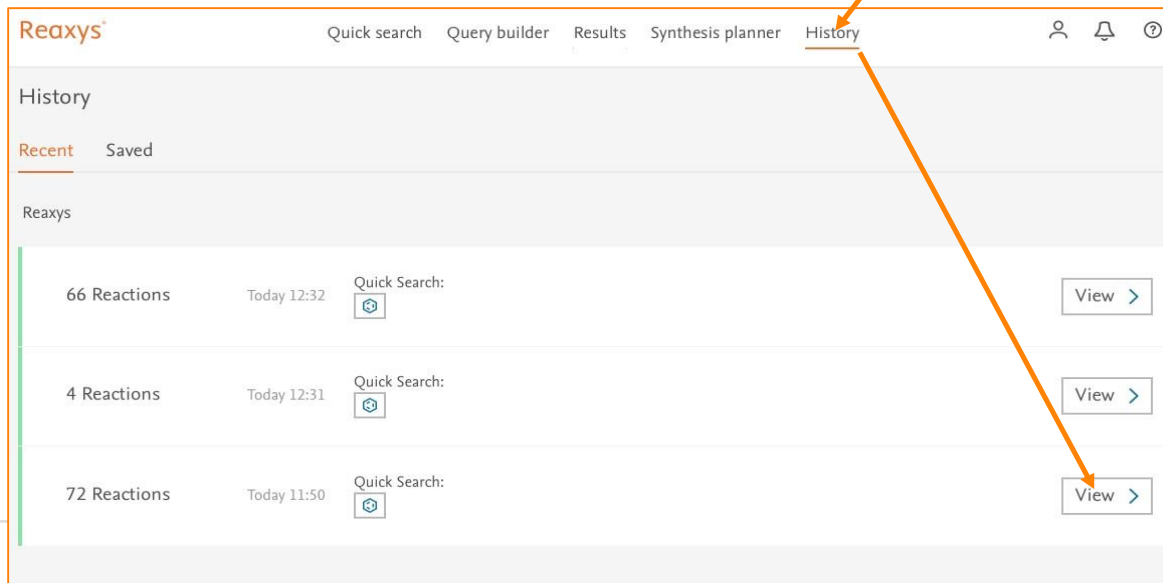
The 'Reacting center' dropdown menu is open, showing the following options:

- center - #
- make or break - ||
- change - |
- make and change - |||
- Not center - X** (highlighted)




An orange arrow points from the text 'выберите Не центр в раскрывающемся' to the 'Not center - X' option.

Фильтрация результатов для конкретных промежуточных продуктов или реагентов.

View for the first set of results.



The screenshot shows the Reaxys interface with the 'History' tab selected. The page displays a list of search results under the 'Recent' filter. Each result entry includes the number of reactions, the time of the search, a 'Quick Search' icon, and a 'View >' button. An orange arrow points from the 'History' menu item to the 'View >' button for the first result.

Reactions	Time	Quick Search	Action
66 Reactions	Today 12:32	Quick Search: 	View >
4 Reactions	Today 12:31	Quick Search: 	View >
72 Reactions	Today 11:50	Quick Search: 	View >

Откройте меню «Параметры» для данного реагента и выберите «Использовать как фильтр». Это автоматически добавит в фильтр по

Reaction ID: 29081541

Options

- Find Similar
- View details
- Copy structure to query
- Copy reaction to query
- Use as filter
- Open in database

Conditions

Yield

80%

55%

52%

With potassium hydroxide in 1-methyl-pyrrolidin-2-one at 100°C;

Experimental Procedure

With potassium hydroxide in diethylene glycol dimethyl ether at 120°C; for 42h; Product distribution / selectivity;

Experimental Procedure

With sodium ethanolate; sodium in dimethyl sulfoxide at 90 - 95°C;

References

MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1
Location in patent: Page/Page column 27
Full Text Details Abstract

MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1
Location in patent: Page/Page column 25-26
Full Text Details Abstract

MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1
Location in patent: Page/Page column 28; 29
Full Text Details Abstract

Ivachtchenko, Alexandre V.; Frolov, Eugene S.; Mitkin, Oleg D.; Kysil, Volodymyr M.; Khvat, Alexander V.; Okun, Ilya M.; Tkachenko, Sergey E. - Medicinal Chemistry Letters, 2009, vol. 19, # 12, p. 3183 -

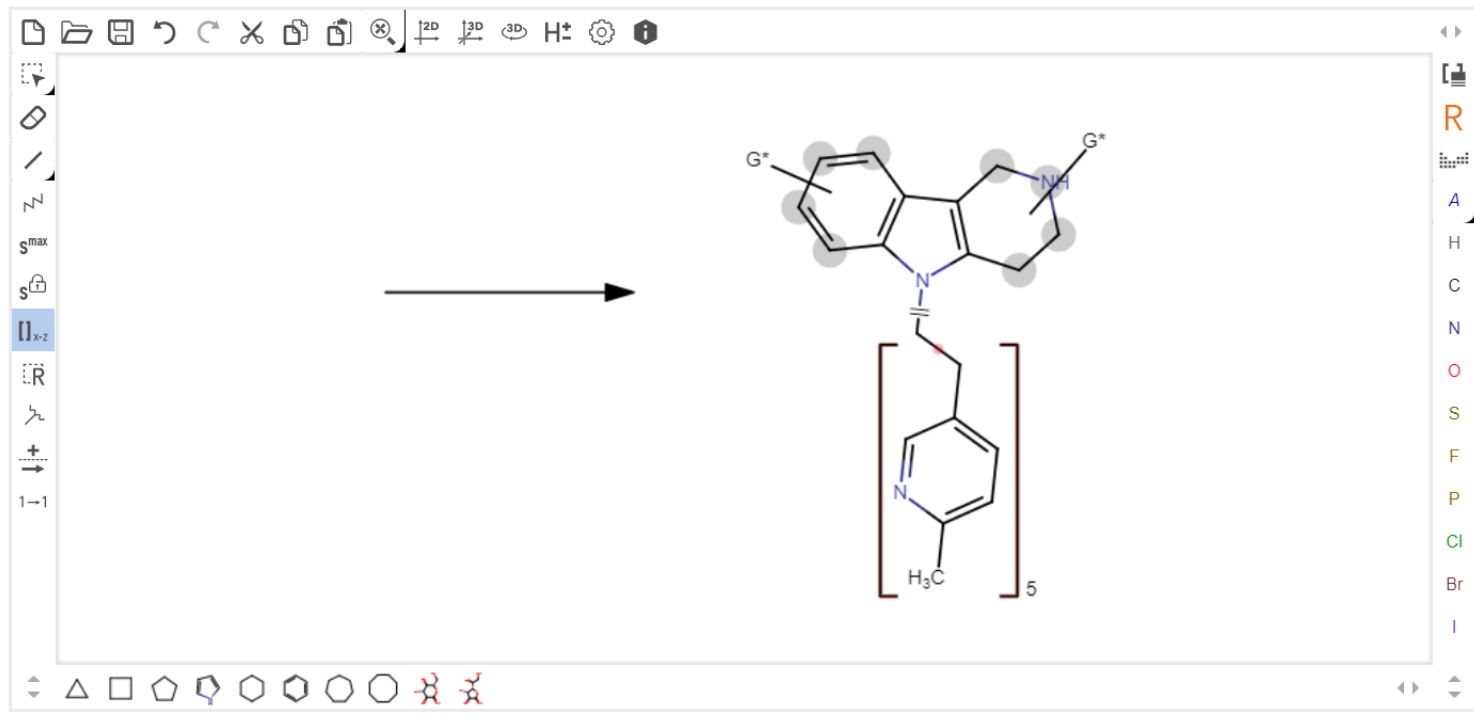
Выберите Exclude (Исключить), чтобы просмотреть все реакции, которые не включают выбранную структуру в качестве реагента. Выберите

Limit to to «ограничить», чтобы просмотреть все реакции, которые включают выбранную структуру в качестве реагента.

The screenshot displays the Reaxys web interface. On the left, the 'Filters and Analysis' sidebar is visible, with the 'Limit to >' and 'Exclude >' buttons highlighted by an orange oval. Below these buttons, the 'By Structure' filter is active, showing a chemical structure of 4-methyl-2-vinylpyridine. The main content area shows a reaction with ID 29081341, involving the reaction of 4-methyl-2-vinylpyridine with a substituted indole derivative to form a complex product. Below the reaction, there is a table of conditions and references.

Yield	Conditions	References
80%	With potassium phosphate in isobutyramide at 100°C; for 24h; inert atmosphere; Experimental Procedure >	MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1 Location in patent: Page/Page column 27 Full Text > Details > Abstract >
55%	With potassium hydroxide in 1-methyl-pyrrolidin-2-one at 100°C; Experimental Procedure >	MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1 Location in patent: Page/Page column 25-26 Full Text > Details > Abstract >
52%	With potassium hydroxide in diethylene glycol dimethyl ether at 120°C; for 42h; Product distribution / selectivity; Experimental Procedure >	MEDIVATION NEUROLOGY, INC. - WO2009/111540, 2009, A1 Location in patent: Page/Page column 28; 29 Full Text > Details > Abstract >
	With sodium ethanolate; sodium in dimethyl sulfoxide at 90 - 95°C;	Ivachtchenko, Alexandre V.; Frolov, Eugene B.; Mitkin, Oleg D.; Kyvil, Volodymyr M.; Khat, Alexander V.; Okun, Ilya M.; Tkachenko, Sergey E. - Medicinal Chemistry Letters, 2009, vol. 19, # 12, p. 3183 - Show Less >

Повторяющиеся фрагменты



Поиск плана синтеза crystal system

Search in:

Reactions >

Targets >

Substances >

Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Crystal System

Find any

Hide fields ^

is

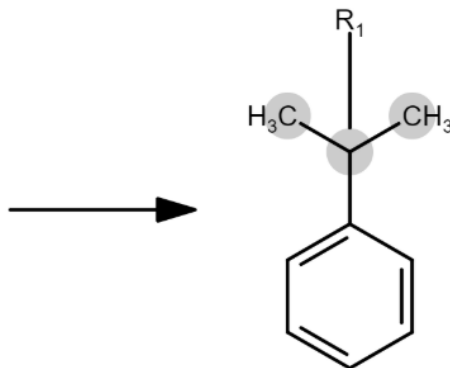
▼

trigonal|



AND

Structure



As drawn

crystal system, crystal phase, crystal properties...

◇ Crystal System Find any Show fields ▾ (Crystal System) ✕

AND

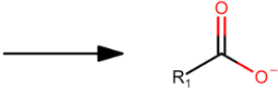
◇ Crystal Phase Find any Show fields ▾ (Description, Temperature, °C) ✕

AND

◇ Crystal Property Desc... Find any Show fields ▾ (Colour & Other Properties, Point group) ✕

AND

◇ Structure ✕

→ 

As drawn

Квантово-химические расчеты

Reaxys®

Quick search Query builder Results Synthesis planner History

Register > Sign in

362,72 K
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
- Potential Bonds

362,718 Substances out of 5,262,974 Documents, containing 8,405,783 Reactions, 21,591 Targets

0 selected
Limit To Exclude Export Preparations

Sort by No of References Grid Heatmap

1
H2N-OH
hydroxylamine
H₃NO 33.0299 3587190 7803-49-8



Hit Data - 110
Identification
Druglikeness

Bioactivity (All)
Physical Data - 65
Spectra - 23

Other Data - 197

Preparations - 386 >
Reactions - 1,966 >
Targets - 42 >
Documents - 142,901 >

Hit Data - 110

Quantum Chemical Calculations - 110 hits out of 110

Show/Hide columns

Calculated Properties	Method (Quantum Chemical Calculations)	Reference
Atom distances, angles	Electron correlation and CI calcn.	DeFrees, Douglas J.; Radhavachari, Krishnan; Schlegel, H. Bernhard; Pople, John A. <i>Journal of the American Chemical Society</i> , 1982, vol. 104, # 21, p. 5576 - 5580 Full Text Details Abstract Boche, Gernot; Bosold, Ferdinand; Lohrenz, John C. W. <i>Angewandte Chemie</i> , 1994, vol. 106, # 11, p. 1228 - 1230 Full Text Details Abstract Musin; Lin <i>Journal of Physical Chemistry A</i> , 1998, vol. 102, # 10, p. 1808 - 1814 Full Text Cited 26 times Details Abstract Knak Jensen; Csizmadia <i>Journal of Molecular Structure: THEOCHEM</i> , 1999, vol. 459, # 1-3, p. 287 - 294 Full Text Cited 3 times Details Abstract Del Bene, Janet E.; Elguero, Jose <i>Journal of Physical Chemistry A</i> , 2007, vol. 111, # 13, p. 2517 - 2526 Full Text Cited 8 times Details Abstract Ren, Yi; Geng, Song; Wei, Xi-Guang; Wong, Ning-Bew; Li, Wai-Kee <i>Journal of Physical Chemistry A</i> , 2011, vol. 115, # 11, p. 2522 - 2528 Full Text Cited 1 time Details Abstract

Feedback

Экспорт полной записи в PDF.

Теплопроводность оксида алюминия..

Reaxys

1500 - 1800	from α -Al ₂ O ₃ to β -Al ₂ O ₃			Goldschmidt, V. M.; Barth, T.; Lunde, G. ; Skr. Nor. Vidensk. - Akad., Kl. 1: Mat. - Naturvidensk. Kl.; nb. 7; (1925); p. 39, View in Reaxys ; vol. Af: MVol.B1; 2.9.1, page 78 - 80 ; (from Gmelin), View in Reaxys
Transport Data (92)				
Description (Transport Data)	Comment (Transport Data)	References		
Thermal conductivity	0.164 W/(m ² K); T = 298 K; Solid	Kim, Jieun; Lee, Doohwan ; Chemistry of Materials; vol. 28; nb. 8; (2016); p. 2786 - 2794, View in Reaxys		
Thermal conductivity	thermal conductivity = 6.3 J/(m ² *K)	Wang, Wei-Li; Bi, Jian-Qiang; Sun, Kang-Ning; Du, Ming; Long, Na-Na; Bai, Yu-Jun ; Journal of the American Ceramic Society; vol. 94; nb. 8; (2011); p. 2304 - 2307 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 35.7 J/(m ² *K); 25 Deg C	Hostasa, Jan; Pabst, Willi; Matejcek, Jiri ; Journal of the American Ceramic Society; vol. 94; nb. 12; (2011); p. 4404 - 4409 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 5.4 J/(m ² *K); 298 K	Bakshi, Srinivas R.; Balani, Kantesh; Agarwal, Arvind ; Journal of the American Ceramic Society; vol. 91; nb. 3; (2008); p. 942 - 947 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 26 J/(m ² *K)	Shi, Rui-Xia; Yin, Yan-Sheng; Li, Jia; Wang, Dong-Zhi ; Materials Research Bulletin; vol. 43; nb. 10; (2008); p. 2544 - 2553 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 30 J/(m ² *K)	Osborne; Norton ; Journal of Materials Science; vol. 33; nb. 15; (1998); p. 3859 - 3865, View in Reaxys ; Sim; Ramanan; Ismail; Seetharamu; Goh ; Thermochimica Acta; vol. 430; nb. 1-2; (2005); p. 155 - 165, View in Reaxys ; Zhou, Wenying; Qi, Shuhua; An, Qunli; Zhao, Hongzhen; Liu, Nailiang ; Materials Research Bulletin; vol. 42; nb. 10; (2007); p. 1863 - 1873 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 39 J/(m ² *K)	Manisha; Basu, Bikramjit ; Journal of the American Ceramic Society; vol. 90; nb. 6; (2007); p. 1858 - 1865 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 37 J/(m ² *K); 298 K	Takeuchi; Kato; Hanada; Koizumi; Aose ; Journal of Physics and Chemistry of Solids; vol. 66; nb. 2-4; (2005); p. 521 - 525 ; (from Gmelin), View in Reaxys		
Thermal conductivity	thermal conductivity = 25.9 J/(m ² *K); 25 Deg C	Smith, David S.; Fayette, Sylvain; Grandjean, Sylvie; Martin, Christian; Telle, Rainier; Tonnesen, Thorsten ; Journal of the American Ceramic Society; vol. 86; nb. 1; (2003); p. 105 - 111 ; (from Gmelin), View in Reaxys		

Прогнозный ретросинтез

- Мы использовали наши данные для сотрудничества с некоторыми ведущими мировыми учеными в области хеминформатики, такими как профессор Марк Уоллер, для разработки возможности прогнозного ретросинтеза и доведения ее до наших клиентов. Очень скоро исследователи и химики смогут спросить ReaxysAI о том, как сделать молекулу



Reaxus предлагает своим клиентам лучший в своем классе AI. Нужно синтезировать молекулу? Спросите у Reaxus AI как!

Одна из наиболее цитируемых работ в области прогнозирующего ретросинтеза стала возможной благодаря партнерству между Elsevier и профессором Марком Уоллером, и мы предлагаем это нашим клиентам.



Инструмент ретросинтеза, разработанный в сотрудничестве с профессором Марком Уоллером, расширит синтез малых органических молекул прогностическим моделированием ранее неопубликованных синтетических путей.

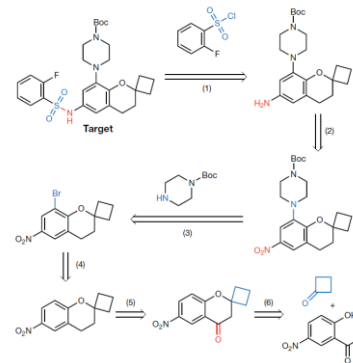
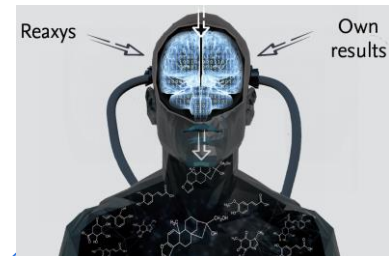
<https://www.nature.com/articles/nature25978.pdf>



Система решает задачи ретросинтеза для почти в два раза большего числа молекул



В тридцать раз быстрее, чем традиционные компьютерные методы



Прогнозирующий ретросинтез: переосмысление химии и изменение синтетических маршрутов

Harvard
Business
Review

DATA

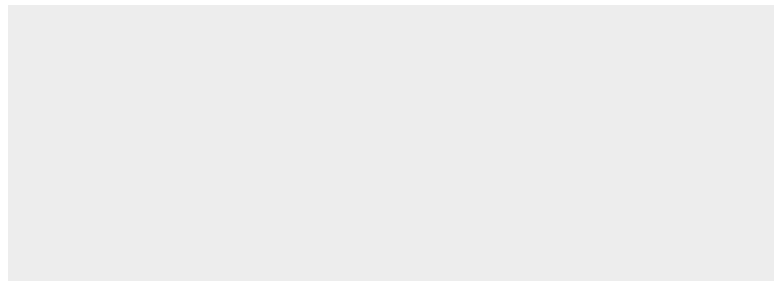
If Your Data Is Bad, Your Machine Learning Tools Are Useless

by Thomas C. Redman

APRIL 02, 2018



ALAN SCHEIN PHOTOGRAPHY/GETTY IMAGES



соотношение правильных / неправильных прогнозов

Extended Data Table 1 | Metrics for the supervised neural network policies

Policy	# rules	Coverage	Matching rules/mol ^b	Accuracy ^a	top10Acc ^a	top50Acc ^a
Expansion	301,671	0.79	46,175	0.310	0.633	0.725
Rollout	17,134	0.52	321	0.501	0.891	0.964

Top10Acc/top50Acc is the ratio of correct/incorrect predictions if we allow the system to make 10 or 50 predictions.

^aAccuracy is calculated on the molecules covered by the respective rulebase.

^bMatching rules/mol corresponds to the branching factor.





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Вопросы?

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Спасибо за внимание!

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