



ELSEVIER

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

Моисеев Алексей Александрович
Директор по развитию и обслуживанию клиентов
направления химико-биологических решений Elsevier S&T
a.Moiseev@elsevier.com +79251131255



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

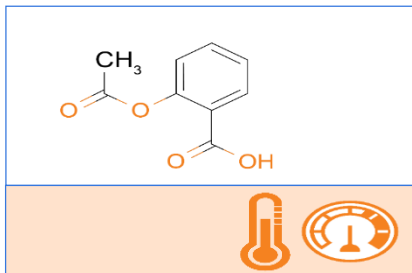
a.Moiseev@elsevier.com +79251131255



Решения в области life sciences

НАПРАВЛЕННЫМИ НА КЛЮЧЕВЫЕ ПРОБЛЕМЫ R&D





>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
материало-ведения, биомедицины,
наук о Земле, технических и
экологических наук, фармакологии...

**Применение в
различных
дисциплинах**

Основные принципы химии

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 >]

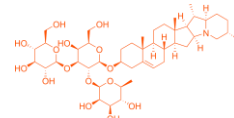
PO: JP, KR, CN, TW [2015 >]

380+k book chapters

Beilstein, Gmelin,



≈ 450 journals + PO
[manually excerpted]

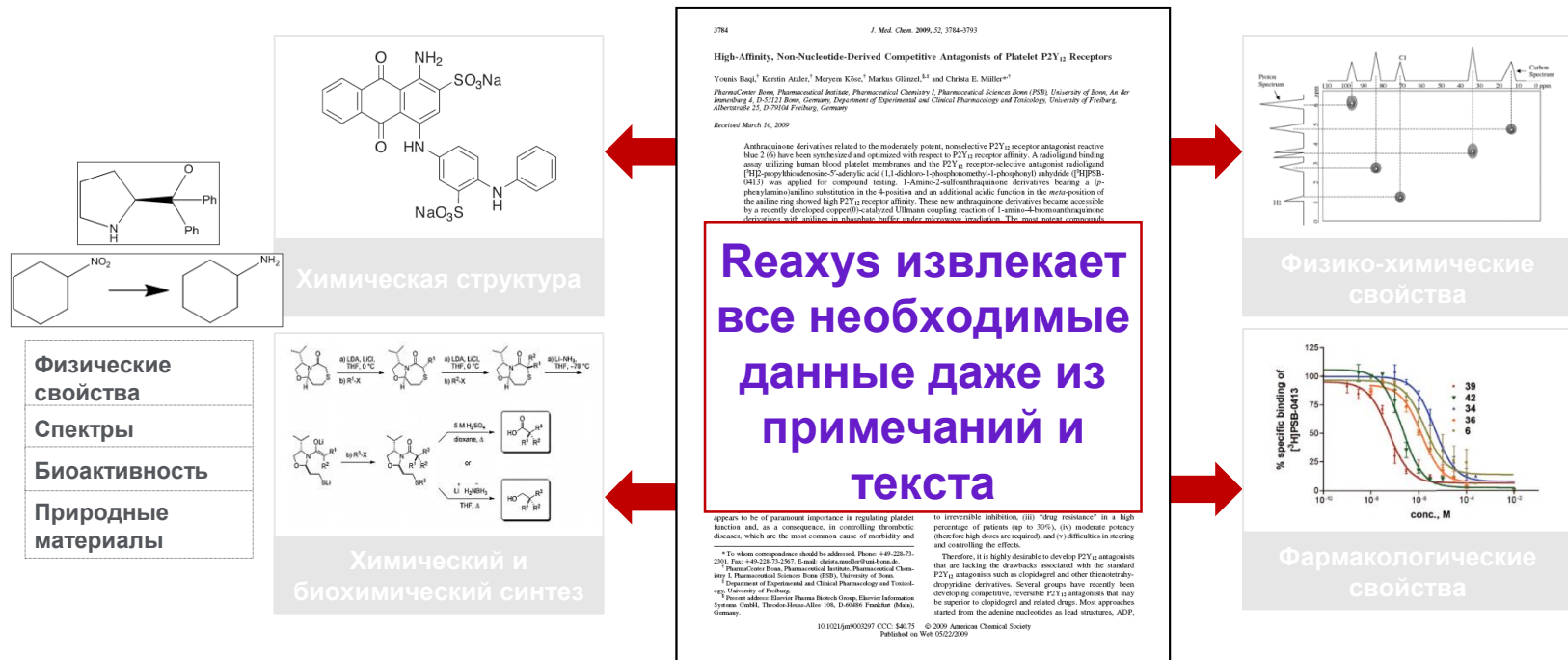


Reaxys



Химия как принцип организации данных

Из экспериментальных данных статей из рецензируемых журналов и патентов



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

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

Melting point

Boiling point
Sublimation
Refractive index
Density
Adsorption
Association
Autoignition
Bound Surface Phenomena
Viscosity
Circular Dichromism
Complex Phase Equilibria
Compressibility
Conformation
Critical Density
Critical Micelle Concentration
Critical Pressure
Critical Temperature
Critical Volume
Electrical Data
Electrical Moment
Electrochemistry Data
Electron Binding
Energy Barriers
Energy Data

Enthalpy of Formation
Enthalpy of Sublimation
Flash Point
Gas Phase
Dissociation Energy
Crystal System
Crystal Phase
Heat Capacity
Henry Constat
Ionization Potential
Isoelectric Point
Kinematic Viscosity
Liquid Phase
Magnetic Data
Mechanical Properties
Molecular Deformation
Optical Data
Thermochemical Data
Solubility
Solution Behavior
Sound Properties
Static Dielectric Constant
Surface Tension
Transition Points
Transport Data

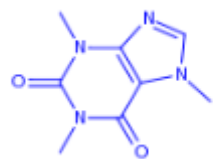
Solubility

NMR Spectroscopy
IR Spectroscopy
Mass Spectroscopy
UV/VIS Spectroscopy
ESR Spectroscopy
NQR Spectroscopy
Raman Spectroscopy
Luminescence Spectroscopy
Fluorescence Spectroscopy
Exposure Assessment
Bioaccumulation
Biomagnification
Biodegradation
Degradation in Soil
Oxygen Demand
Uses
Isolation from Natural Prod.
Reaction Yield
Reaction Conditions
Reaction Type
Named Reaction
Pharmacological Data
Route of Administration
Concentration

Target
Substance Effect
Substance Action on Target
Substance Dose
Bioassay
Animal Model
Organs/Tissue
Cells/Cell Lines
Measurement Parameter
Endpoint of Effect
Ecotoxicology Data
Dielectric Constant
Dissociation Exponent
Dynamic Viscosity
Electrolytic Conductivity
Enthalpy of Fusion
Enthalpy of Vaporization
Explosion Limits
Interatomic Distance/Angle
Kinematic Viscosity
Liquid/Solid Systems
Liquid/Vapor Systems
Metarotation

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, Harij (s) - 7 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 >



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

Моисеев Алексей Александрович

a.Moiseev@elsevier.com +79251131255



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	▼	Keyword Basic Index	🔍	✕
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 🗨



15,330

Filters and Analysis

Index Terms (List)

Index Terms (ReaxysTree)

Publication Year

Document Type

Authors

☐ lindsey, jonathan s 92☐ sessler, jonathan l 65☐ lee, chang-hee 51☐ ravikanth,
mangalampalli 46☐ ciamician 39☐ osuka, atsuhiro 38☐ latos-grazynski,
lechoslaw 38

More

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 perception¹ [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 functionalities² [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 field³ [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 degradation⁴ [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](#) <https://www.reaxys.com>

PATENT SEARCHING USING THE LITERATURE SEARCH FORM

Reaxys

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

15,330 €

Filters and Analysis

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

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 (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, Alex; Austad, Jørn; Tellgren, Erik I.; Teale, Andrew M.; Helgaker, Trygve; Stopkiewicz, 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 (37) 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



Reaxys®

LIFE SCIENCE
SOLUTIONS

(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

- ☐ 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](#); [Pl](#)
[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](#) ↗



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 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)

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.



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

Boiling point
Sublimation
Refractive index
Density
Adsorption
Association
Autoignition
Bound Surface Phenomena
Viscosity
Circular Dichromism
Complex Phase Equilibria
Compressibility
Conformation
Critical Density
Critical Micelle Concentration
Critical Pressure
Critical Temperature
Critical Volume
Electrical Data
Electrical Moment
Electrochemistry Data
Electron Binding
Energy Barriers
Energy Data

Enthalpy of Formation
Enthalpy of Sublimation
Flash Point
Gas Phase
Dissociation Energy
Crystal System
Crystal Phase
Heat Capacity
Henry Constat
Ionization Potential
Isoelectric Point
Kinematic Viscosity
Liquid Phase
Magnetic Data
Mechanical Properties
Molecular Deformation
Optical Data
Thermochemical Data
Solubility
Solution Behavior
Sound Properties
Static Dielectric Constant
Surface Tension
Transition Points
Transport Data

Solubility

NMR Spectroscopy
IR Spectroscopy
Mass Spectroscopy
UV/VIS Spectroscopy
ESR Spectroscopy
NQR Spectroscopy
Raman Spectroscopy
Luminescence Spectroscopy
Fluorescence Spectroscopy
Exposure Assessment
Bioaccumulation
Biomagnification
Biodegradation
Degradation in Soil
Oxygen Demand
Uses
Isolation from Natural Prod.
Reaction Yield
Reaction Conditions
Reaction Type
Named Reaction
Pharmacological Data
Route of Administration
Concentration

Target
Substance Effect
Substance Action on Target
Substance Dose
Bioassay
Animal Model
Organs/Tissue
Cells/Cell Lines
Measurement Parameter
Endpoint of Effect
Ecotoxicology Data
Dielectric Constant
Dissociation Exponent
Dynamic Viscosity
Electrolytic Conductivity
Enthalpy of Fusion
Enthalpy of Vaporization
Explosion Limits
Interatomic Distance/Angle
Kinematic Viscosity
Liquid/Solid Systems
Liquid/Vapor Systems
Metarotation

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



Doc. Index

Search
Substances



Find search fields and forms



Fields

Forms

History

Reaxys

Basic Indexes

◇ Substance Basic Index

◇ Reaction Basic Index

◇ Document Basic Index

Identification

Physical Properties

◇ Melting Point

◇ Boiling Point

◇ Sublimation

◇ Sublimation



Find any

Hide fields



=



Sublimation, °C

55 - 57



=



Pressure (Sublimation), Torr



AND

◇ Melting Point



Find any

Hide fields



=



Melting Point, °C

63 - 65



is



Solvent (Melting Point)



AND

◇ Substance Basic Index



is



Substance Basic Index

stable



Поиск веществ с необходимыми хроматографическими свойствами

◇ Chromatographic Data

☐ Find any

Hide fields ^

×

is

▼

Chromatographic data

🔍

is

▼

Original string

🔍

Chromatographic data		Search	×
☐	gpc (gel permeation chromatography)	499	
☐	hplc (high performance liquid chromatography)	567,623	
☐	ion chromatography	1,390	
☐	lc (liquid chromatography)	266,210	⬆
☐	mplc (medium pressure liquid chromatography)	538	⬆
☐	paper chromatography	107	▼
☐	partition chromatography	58	▼
☐	sfc (supercritical fluid chromatography)	10,467	
☐	tlc (thin layer chromatography)	532,633	
☐	uplc (ultra performance liquid chromatography)	90,976	
		Clear selected ×	Transfer >

Время удерживания

◇ Chromatographic Data

☐ Find any

Hide fields ^

×

is	▼	electrophoresis	
is	▼	Original string	

Original string 1

×

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

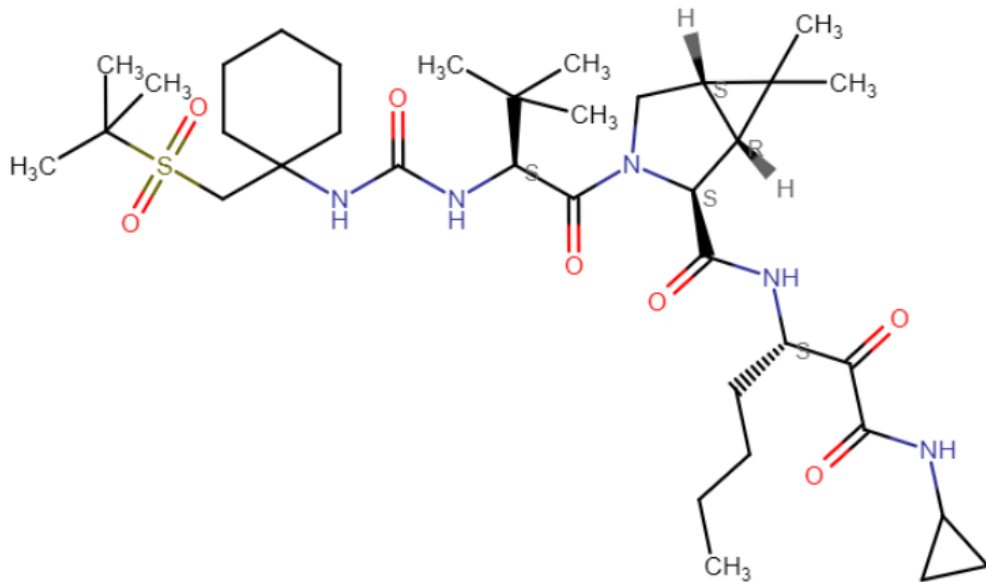


Разработка методики синтеза химических веществ (субстанций) в Reaxys

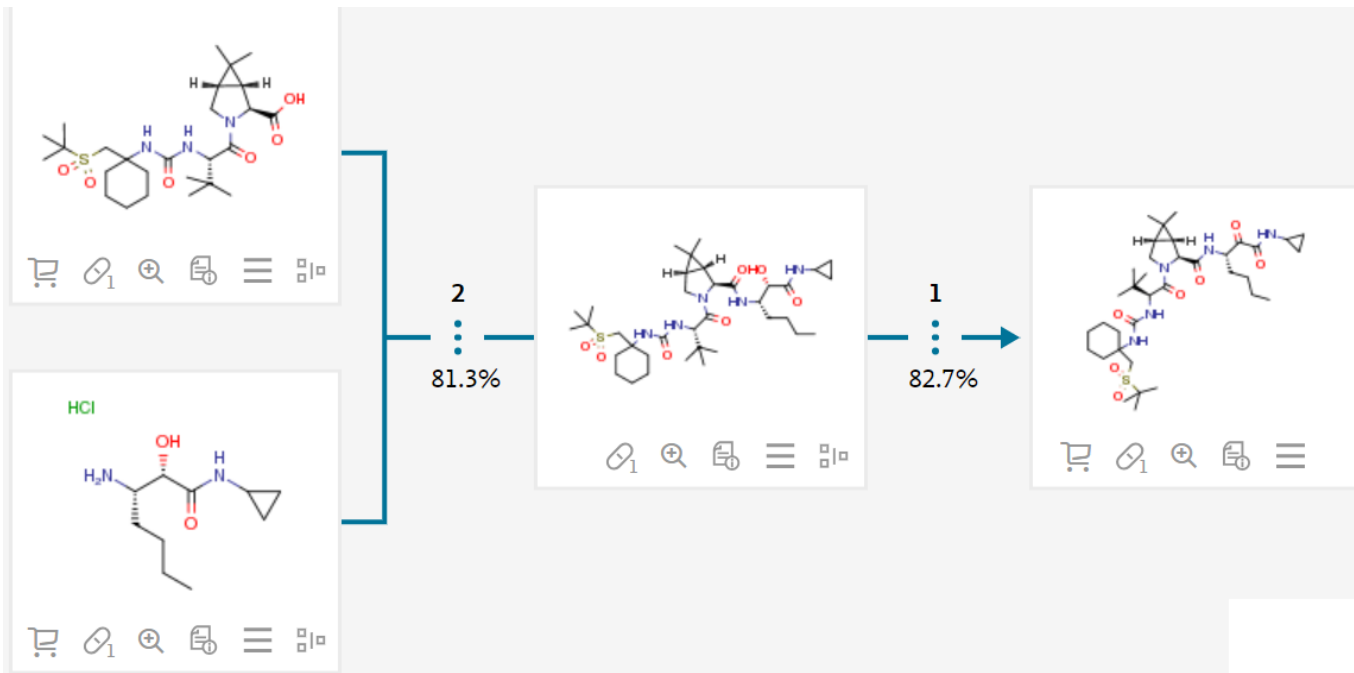
С помощью Reaxys можно решать задачу поиск оптимальных условий синтеза субстанций.

Допустим, Вас интересует данное соединение

NARLAPREVIR



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



Synthesizer (132)

Add Remove

6

Details

84.00 %

Add Remove

2d

Details

Remove

2e

Details

Remove

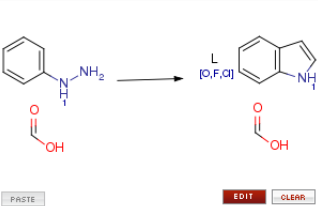
Reaxus выдает Вам все реакции с **сразу с условиями**, что позволит сразу с реактивы, так вы сможете **выбрать** (цена, доступность, хим. стабильность)

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

Identification

Chemical Name is

Show AND Buttons

Please select role ☒ Product ☐ Starting material ☐ Reagent / Catalyst ☐ Any role

Reaction Data

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

Show AND Buttons



ELSEVIER

Reaxys®

91 Substances

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

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 ↓

Bioactivity (All) Spectra - 187 Preparations - 96 >

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

Targets - 418 >

Documents - 16,028 >

calcium O-acetylsalicylate

Identification Druglikeness Physical Data - 2 Other Data - 20

lysine Acetylsalicylate

C6H8O4 * C6H7N2O2 326.349 5690287 62952-06-1

Feedback

Дополнительную информацию о поставщике можно найти в этой вкладке.

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

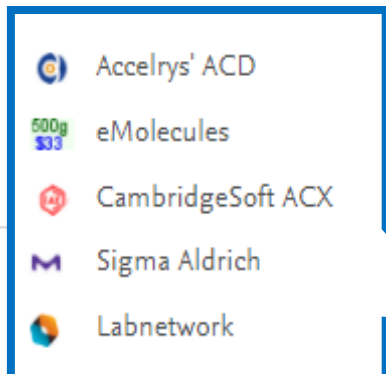
При планировании синтетической стратегии химии должны учитывать, как приобретать исходные материалы.

Три больших вопроса:

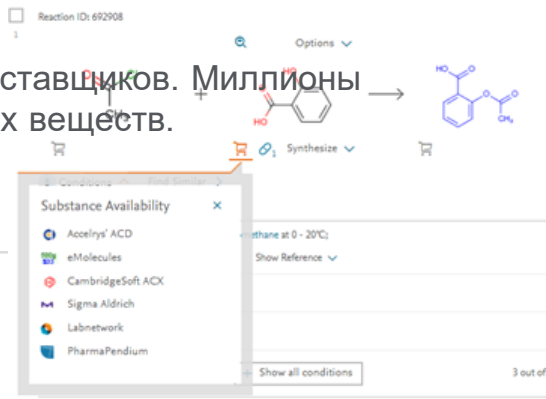
Есть ли этот материал на моей местном складе?

Есть ли материал присутствует на складе у любого поставщика?

Есть ли этот поставщик в моей системе покупки?



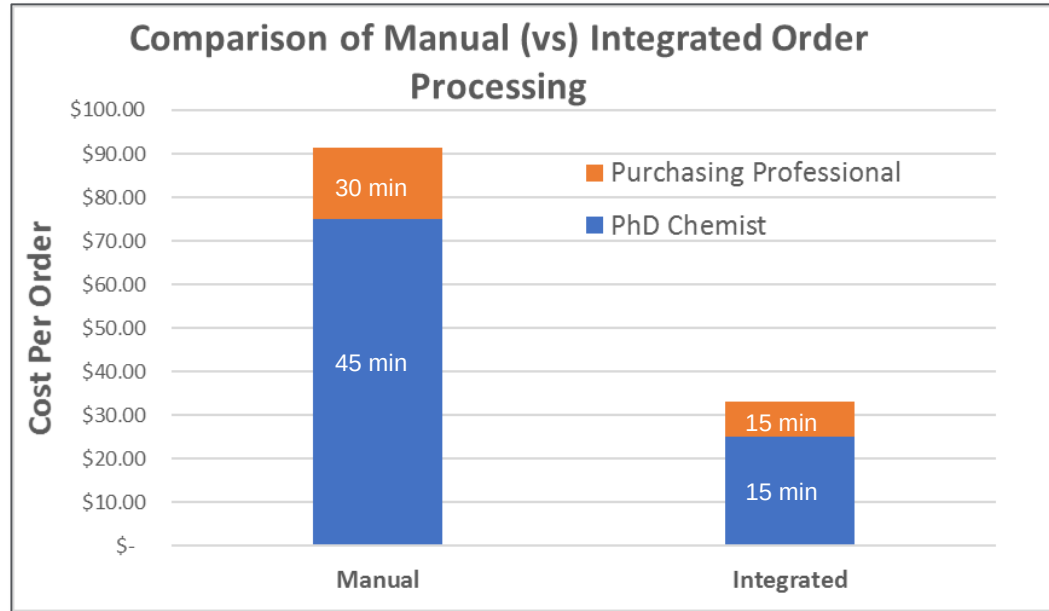
Тысячи поставщиков. Миллионы химических веществ.



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

Eq

AND

◇ Affinity on target

◇ Target Name

is

Target Name

egfr

Eq

AND

◇ Measurement pX

>

Measurement pX

6

Eq

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

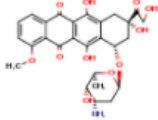
Export

☐ ☐

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](#)


ELSEVIER

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

Q biological species



Import



Save



Reset form



Delete all



Structure



Molecular Formula



CAS RN



Doc. Index

◇ Biological Species

is



chlamydiae



Reaxys ^

◇ Biological Species



Reaxys®

Quick search

Query builder

Results

Synthesis planner

History

Alexey Moi...



Alerts

148

Filters

Limit to >

Exclude >

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 ↓ >

Heatmap



☐ 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

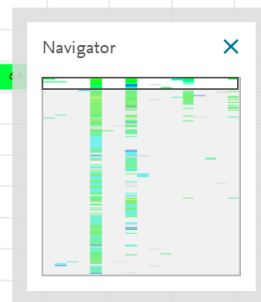
Value of Cells: Maximum of pX

Show substances:
☒ Names
☐ Structure drawing

Display mode:
☐ Normal
☒ Full Screen

☒ Always show settings

Apply





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

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

◇ Isolation from Natural Product ☐ Find any Hide fields ^ x

is ☐ Isolation from Natural Product
camomile ☐

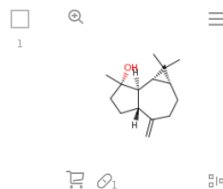
☐

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

☐ 0 selected Limit To Exclude Export

☐ Sort by No of References ↓ v

Grid ☐ Heatmap ☐



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 ↑ v

Heatmap ☐



Single protein

1 **Acetylcholinesterase (Wild)**

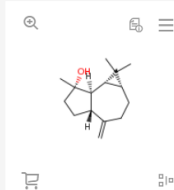
Synonyms: acetylcholinesterase

Show target details v

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 Natural Product

Find any is Escherichia coli

Hide fields

Feedback

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

LIFE SCIENCE SOLUTIONS

ELSEVIER

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

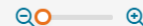
542 Substances out of 94,335 Documents, containing 28,875 Reactions, 1,688 Targets

☐ 0 selected

Limit To

Exclude

Export



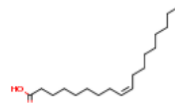
Sort by No of References ↓

Grid

Heatmap

☐

1



cis-Octadecenoic acid

$C_{18}H_{33}O_2$ 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 >

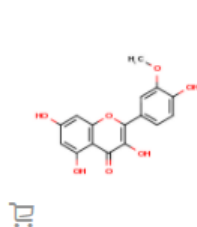
Какие соединения были найдены в тысячелистнике Yarrow?



◇ Isolation from Natural Product ☐ Find any Hide fields ^ x

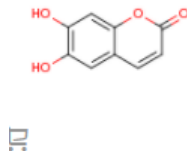
contains ▼ Isolation from Natural Product

Yarrow 



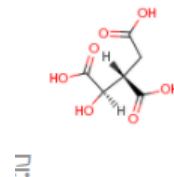
isorhamnetin
 $C_{16}H_{12}O_7$ 316.267

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)
[Bioactivity \(All\)](#)



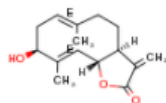
aesculetin
 $C_9H_6O_4$ 178.144 152788

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)
[Bioactivity \(All\)](#)



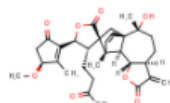
threo-D-isocitric acid
 $C_6H_8O_7$ 192.125 1727947

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)
[Bioactivity \(All\)](#)



hanphyllin
 $C_{15}H_{20}O_3$ 248.322 1623169

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)
[Bioactivity \(All\)](#)

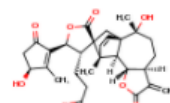


achillinin B
 $C_{31}H_{38}O_8$ 538.638

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)



Options ▼



achillinin C
 $C_{30}H_{36}O_8$ 524.611

[Hit Data - 1](#)
[Identification](#)
[Druglikeness](#)

 C30H36O8
[Synthesize ▼](#)

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

×

×

☐	medicago	18
☒	medical	6,385
☐	medicalconditions	1
☐	medically	154
☐	medicals	2
☒	medicament	6,715
☐	medicamental	11
☐	medicamentary	10
☐	medicamentns	1
☒	medicamentosa	788
☐	medicamentous	7
☐	medicamentously	4
☒	medicaments	796
☐	medicamernt	1
☐	medicanents	2



3,686 of 6,465



Go to page >

Clear selected ×

Transfer >

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	
☒	processing	1,349	
☐	procession	7	
☐	processivity	3	
☐	processless	9	
☐	processor	9	

◇ Use	☐ Find any	Hide fields ^	×
is	▼	Laboratory Use and Handling	Eq
is	▼	Use Pattern processing	Eq

AND

◇ Use	☐ Find any	Hide fields ^	×
is	▼	Laboratory Use and Handling	Eq
is	▼	Use Pattern hydrocarbons	Eq

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

◇ Use

Find any

Hide fields ^

×

is

▼

Laboratory Use and Handling

🔍

is

▼

Use Pattern

(corros* NEAR inhib*) OR (anticorr*)

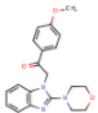
🔍

○ — ○

Sort by I

☐

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

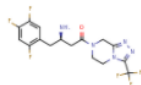
SigmaAldrich

Structure

Определить неизвестное соединение X:



1



sitagliptin

C₁₆H₁₅F₈N₅O 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

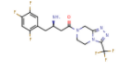
Optical Rotatory Power - 3 hits out of 7

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, Gukul - 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

Определить неизвестное соединение X.

Какими дополнительными методами можно подтвердить предположение?



Chemical structure of sitagliptin: C1=CC=C(C=C1)C(=O)N[C@@H](C2=CC=CC=C2)C(=O)N3C=CC(=C3)C

sitagliptin
C₁₄H₁₅F₃N₃O 407.318 9962060 486460-32-6

Hit Data - 3
Identification
Druglikeness

Bioactivity (All)
Physical Data - 46
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 $\sim 56,5^{\circ}\text{C}$
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



Search Substances



Find search fields and forms



Fields

Forms

History

Reaxys

Basic Indexes

◇ Substance Basic Index

◇ Reaction Basic Index

◇ Document Basic Index

Identification

Physical Properties

◇ Melting Point

◇ Boiling Point

◇ Sublimation

◇ Sublimation

Find any

Hide fields



=



Sublimation, °C
55 - 57



=



Pressure (Sublimation), Torr



AND

◇ Melting Point

Find any

Hide fields



=



Melting Point, °C
63 - 65



is



Solvent (Melting Point)



AND

◇ Substance Basic Index



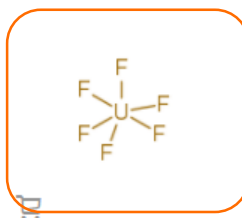
is



Substance Basic Index
stable



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

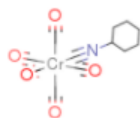
63.94

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
Ni₂Fe₂*

AND

◇ Melting Point Find any
Melting Point, °C
= 1410 - 1450
is Solvent (Melting Point)

Reaxys ID: 26601394
CoCrFeNi 225.526 26601394

alloy

CoCrFeNi

Hit Data - 2
Identification
Druglikeness
Physical Data - 7

Preparations - 1 >
Reactions - 1 >
Documents - 3 >

^ 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 ②

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

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
1															
andalusite															
<chem>SiAl2O5</chem> 162.046 16453029															
Identification		Physical Data - 54		Other Data - 9		Preparations - 4		Reactions - 7		Documents - 93					
Druglikeness		Spectra - 11													
andalusite															
☐ 2															
kyanite															
<chem>SiAl2O5</chem> 162.046 16452963															
Identification		Physical Data - 26		Other Data - 6		Preparations - 3		Reactions - 11		Documents - 82					
Druglikeness		Spectra - 14													
kyanite															
☐ 3															
sillimanite															
<chem>SiAl2O5</chem> 162.046 16453049															
Identification		Physical Data - 34		Other Data - 8		Preparations - 5		Reactions - 15		Documents - 93					
Druglikeness		Spectra - 10													
sillimanite															



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.; Hanwell, 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 Handbook: 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 Handbook: 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 Handbook: Al: MVol.A1, 10, page 41 - 43] Full Text ↗ Details >



Поиск информации о минералах

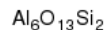
Transition Point(s) of Crystalline Modification(s)

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА
ANDALUSITE

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

Поиск информации о минералах

ПРЕВРАЩЕНИЯ АНДАЛУЗИТА В МУЛЛИТ



andalusite



mullite



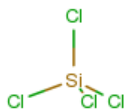
3 Conditions Find Similar Reaction ID: 26413460

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



+

Al



Al₂O₅Si

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 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  

1.60 K

Query

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 ▾ [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](#)

[Beyssac, 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

Other Nonmetals

Halogens

Noble Gases

Metals

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

[Al+3].[O-]([O-])OP(=O)([O-])[O-]

aluminum silicate

$2\text{Al}^{3+} + 3\text{O}_3\text{Si}^{2-}$

282.214 14479534

Identification

Druglikeness

Other Data - 3

Documents - 688

2

$\text{Al}_6\text{O}_{13}\text{Si}_2$

mullite

$3\text{Al}_2\text{O}_3 + 2\text{SiO}_2 = \text{Al}_6\text{Si}_2\text{O}_{13}$

426.052 16513662

Identification

Druglikeness

Physical Data - 313

Spectra - 44

Other Data - 8

Preparations - 140

Reactions - 169

Documents - 317

3

$\text{Al}_2\text{O}_7\text{Si}_2$

metakaolin

$(\text{Al}_2\text{O}_3)(\text{SiO}_2)_2$

222.13 11341013

Identification

Druglikeness

Physical Data - 9

Spectra - 2

Other Data - 1

Preparations - 8

Reactions - 52

Documents - 162

andalusite

Al_2SiO_5

258.012 11341013

Identification

Druglikeness

Physical Data - 9

Spectra - 2

Other Data - 1

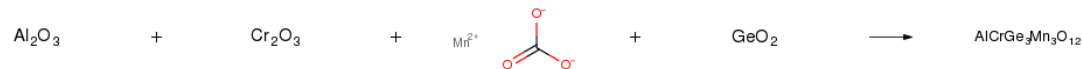
Preparations - 8

Reactions - 52

Documents - 162

Feedback

Получение вещества



1 Conditions Find Similar Reaction ID: 26074679

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

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

План

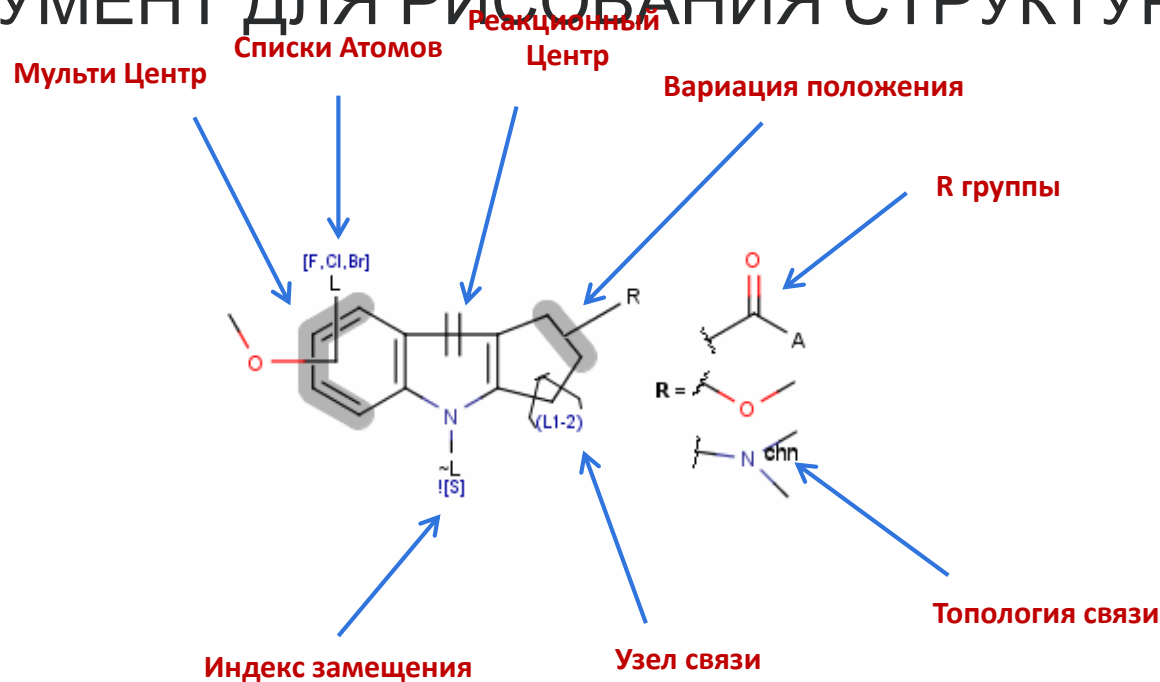
- Особенности и покрытие базы данных Reaxys.
- Оптимальная стратегия поиска литературы.
- Свойства веществ в Reaxys
- Химические реакции в Reaxys
- Биологическая активность и медицинская химия в Reaxys
- Вопросы



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 web 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 icons in the top-left toolbar.
- Повторяющиеся единицы** (Repeating units): Points to the repeat unit icon in the top-left toolbar.
- Селектор R-групп** (R-group selector): Points to the R-group selector icon in the top-left toolbar.
- Прикрепление R-Group** (R-group attachment): Points to the R-group 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-left toolbar.
- Reaxys Generics**: Points to the Reaxys Generics icon in the bottom-left 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 sidebar.
- Основные атомы** (Main atoms): Points to the main atoms list on the right sidebar.

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ



MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУКЦИЯ

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

Bond properties

- Type: single
- Topology: undefined
- Reacting center: undefined

Bond properties

- Type: single
- Topology: undefined
- Reacting center: undefined

Bond properties

- Type: double
- Topology: undefined
- Reacting center: undefined

Atom properties

Change to: Element

Basic **Advanced**

- Total H (H):
- Implicit H (h):
- Bond orders (v):
- Connections (X):
- Ring count (R): <not set>
- Smallest ring size (r):
- Ring bond (rb): <not set>
- Substitutions (s): <not set>
- Unsaturated (u): <not set>
- Aromaticity (a/A): <not set>

Chemical structure diagram showing a bicyclic system with highlighted atoms and bonds.

УРА

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

ПОИСК ВЕЩЕСТВ

Можно выполнить
точный поиск, поиск по
субструктуре или
подобию

Используйте
эти функции,
чтобы
исключить
ненужные
вещества

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

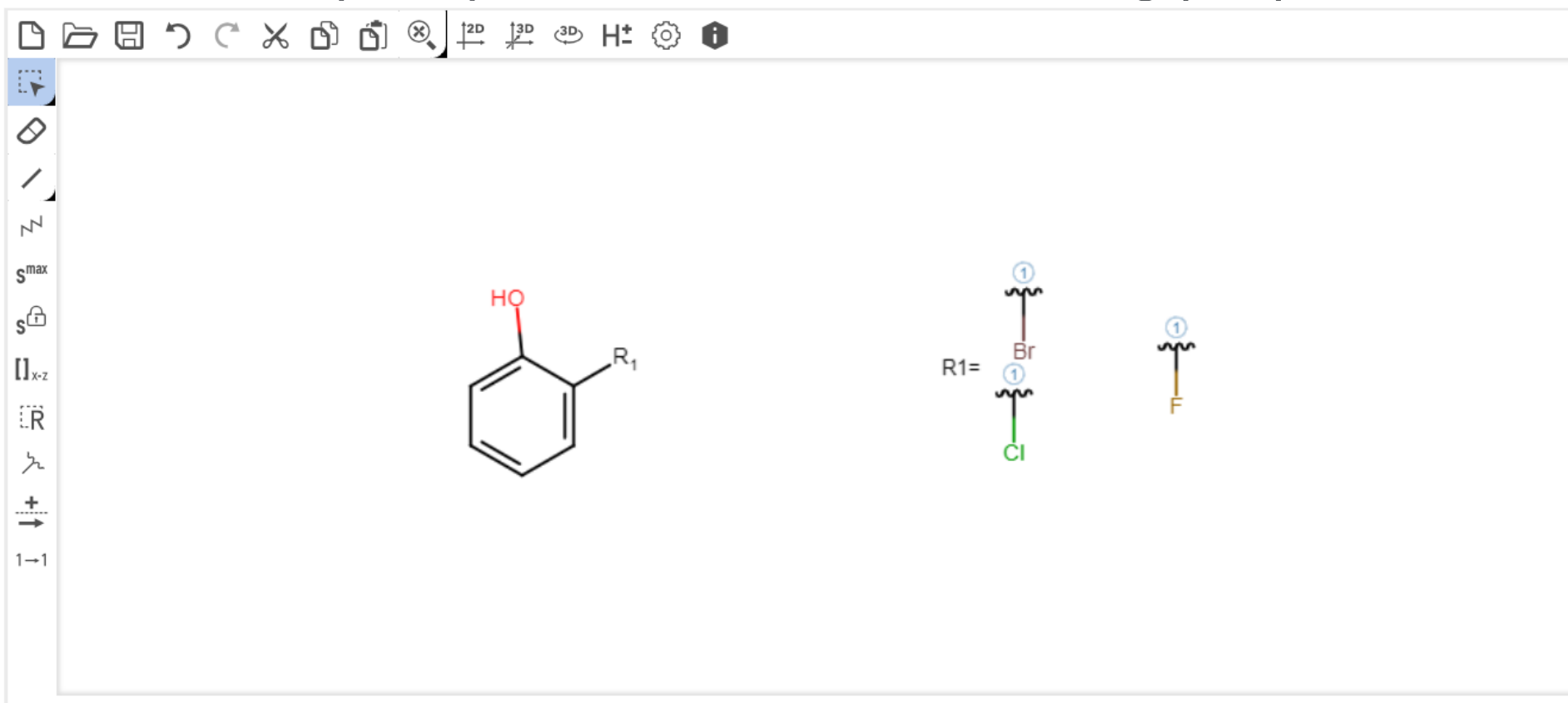
☒ Radicals

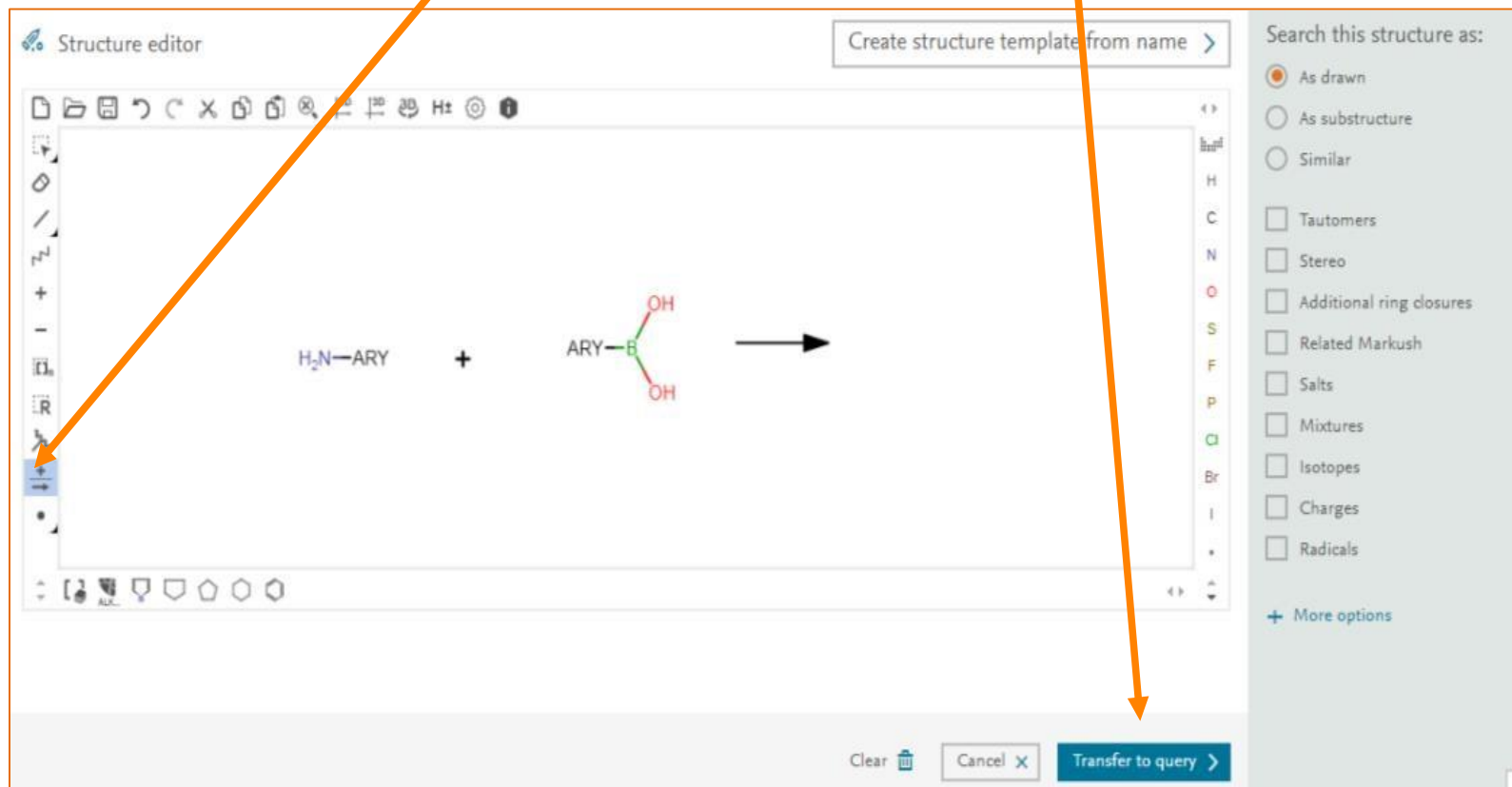
+ More options

В большинстве случаев можно создать структуру из названия

Marvin JS
by ChemAxon

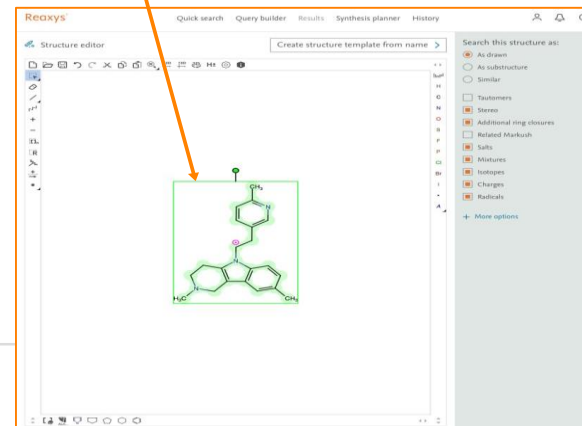
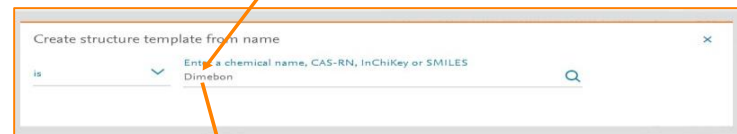
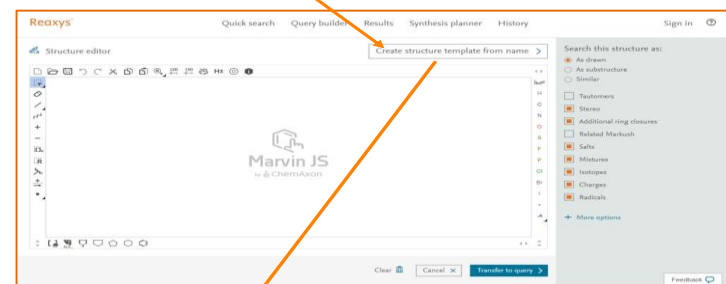
Пример использования smart R-group



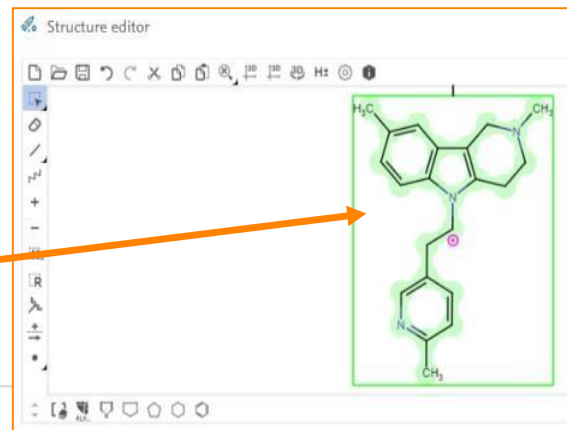
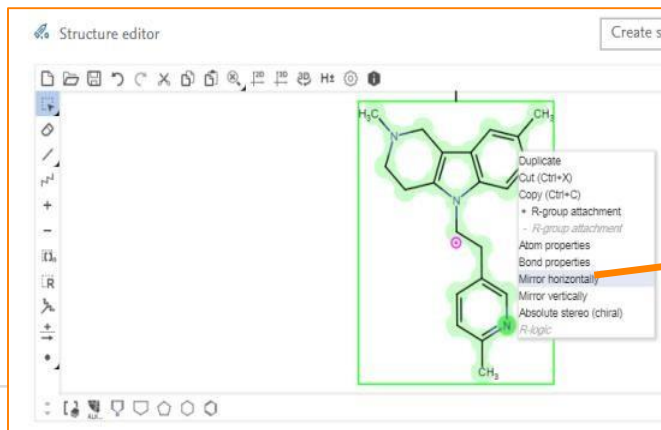
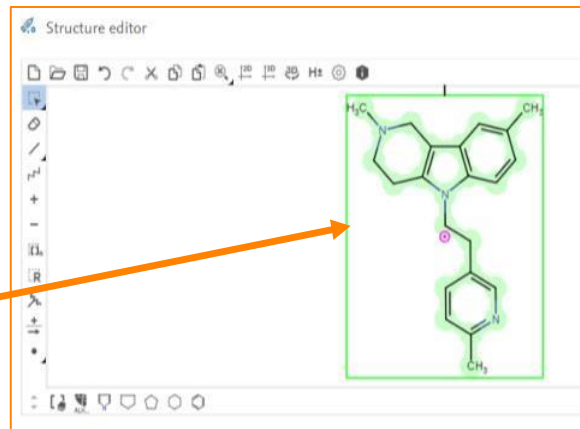
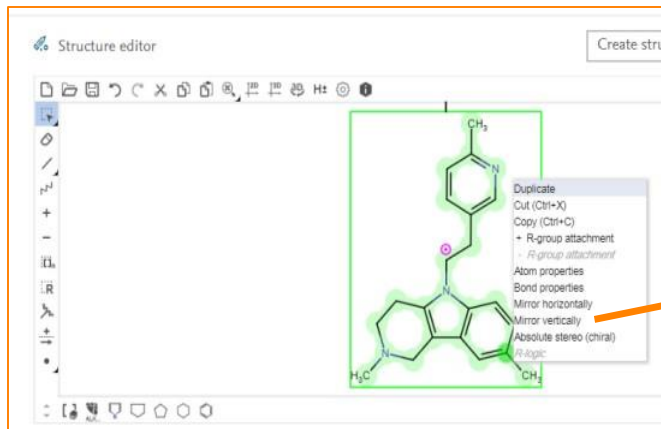


стратегия синтеза аналогов димебона

Dimebon

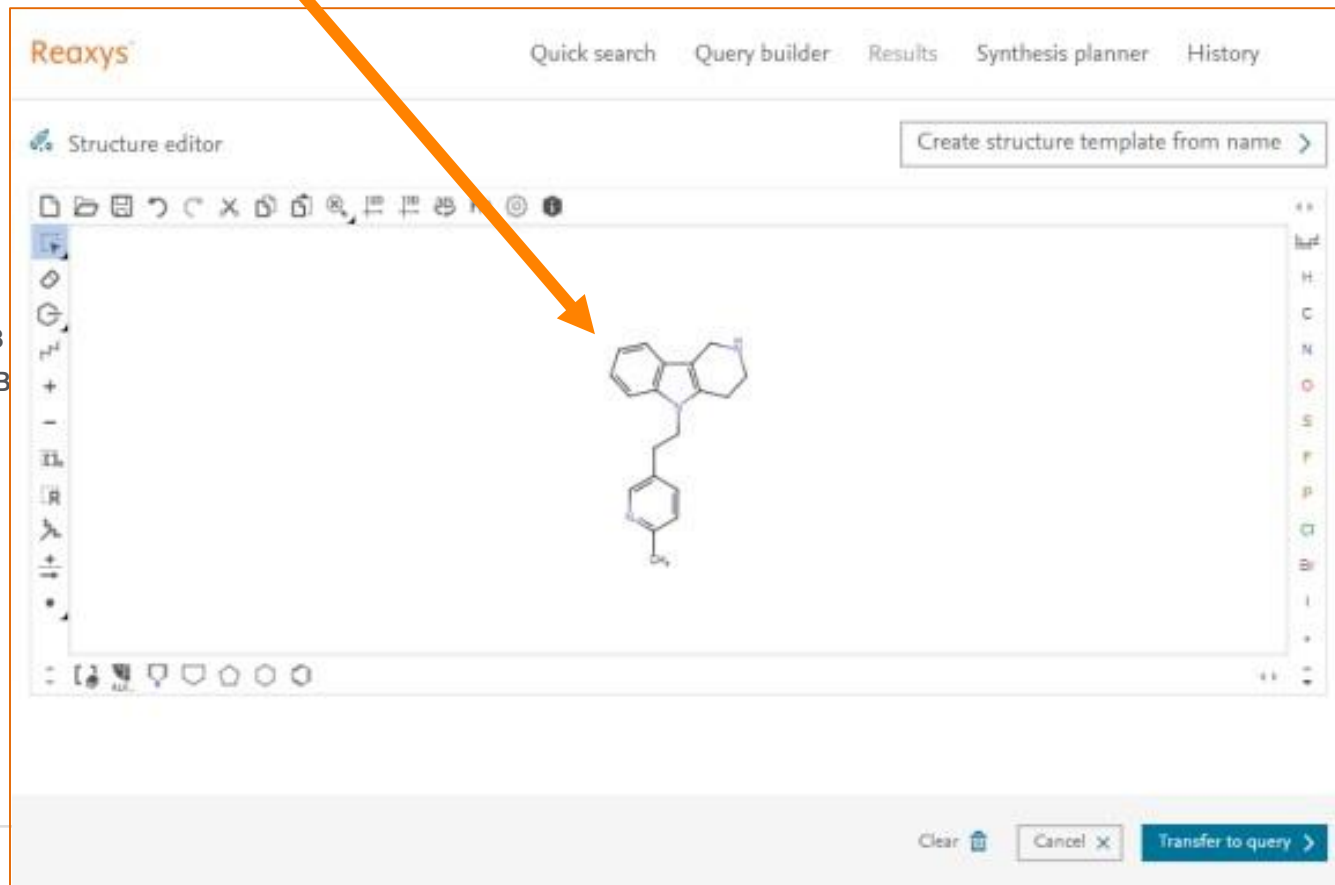


Чтобы изменить ориентацию структуры, щелкните правой кнопкой мыши на любом атоме и выберите «Отразить по вертикали» или «Отразить по горизонтали». Нужный участок структуры или вся структура должны быть выделены



Вы можете отрегулировать размер структуры, прокручивая вверх или вниз.

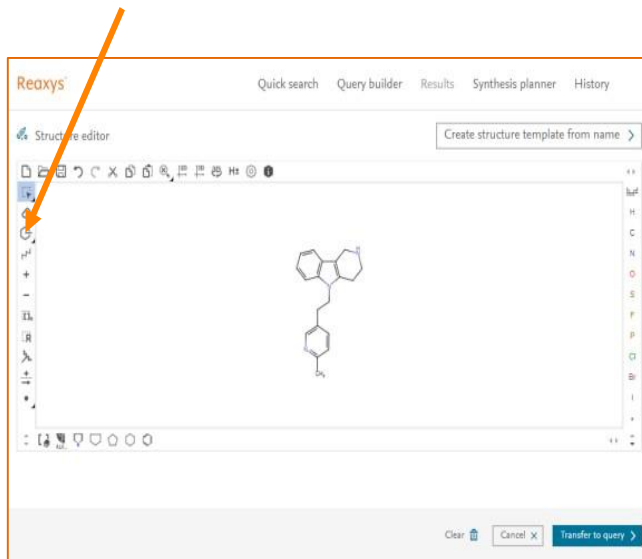
Удалите две метильные группы из верхних колец, нажав C и нажав Delete на клавиатуре.



Задать позиции плавающих связей

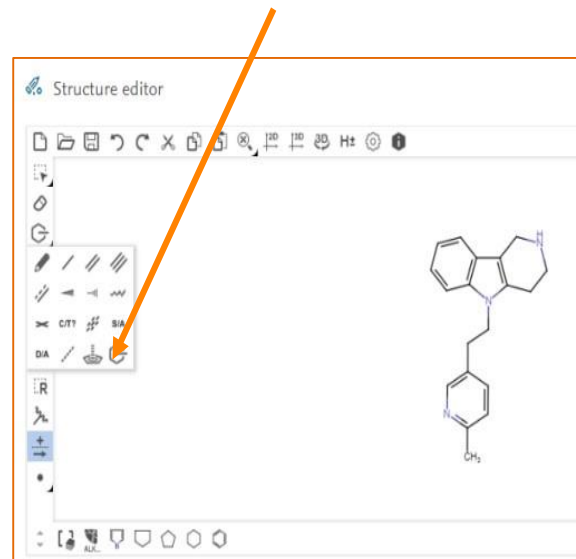
Открыть панель инструментов

a . Click here to open the tool panel.



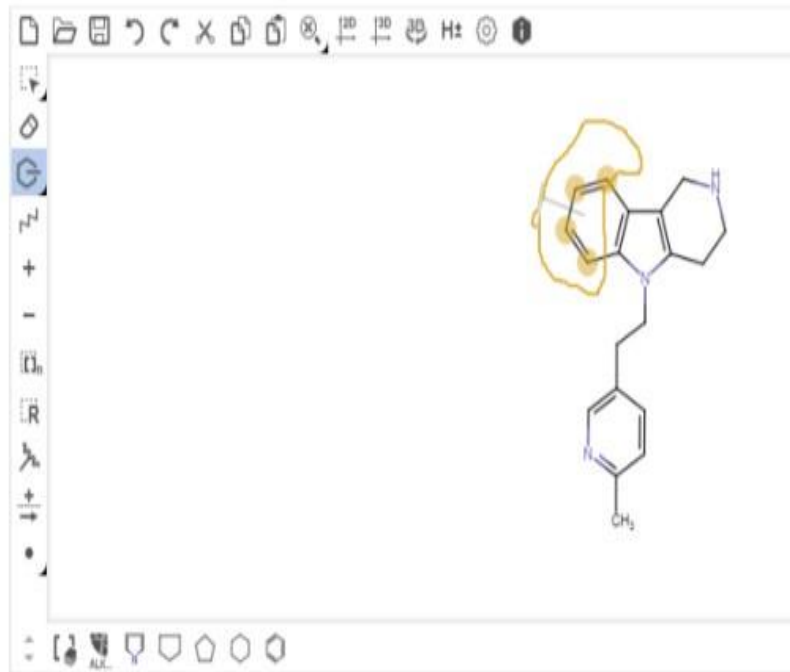
Открыть инструмент позиционирования плавающих связей

b . Select the position variation bond.

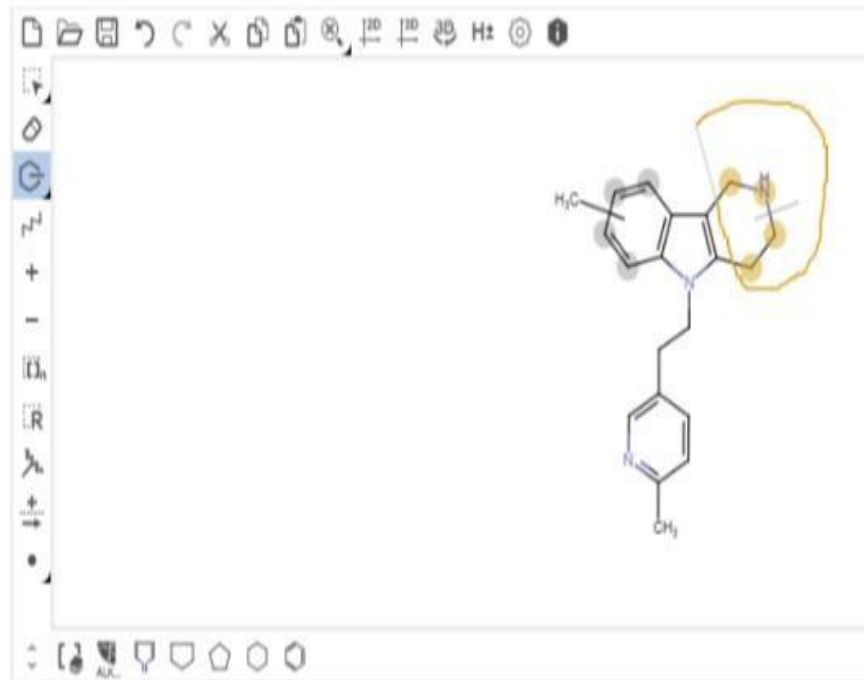


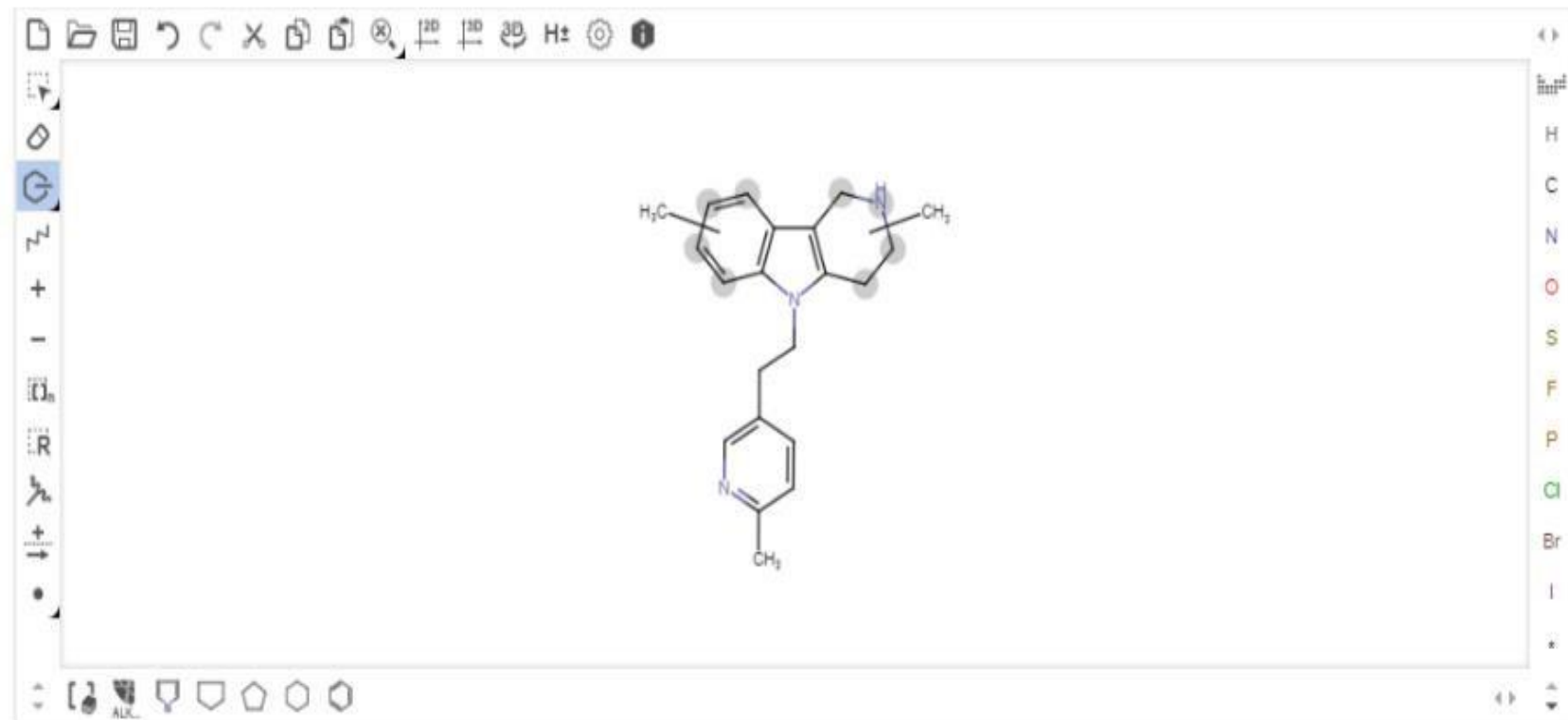
Выберите атомы для включения, нарисовав линию

Structure editor



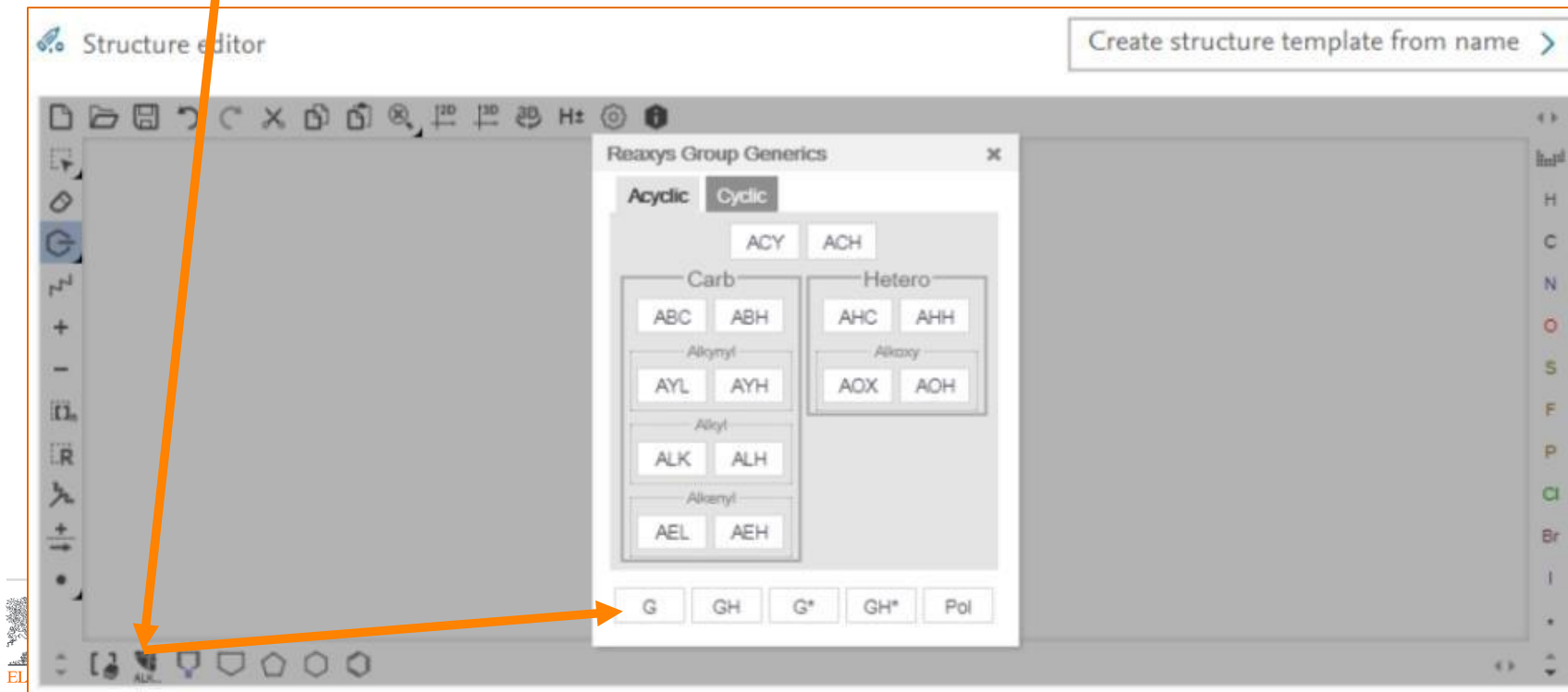
Structure editor





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

Structure editor

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

Chemical structure editor interface showing a complex molecule (a tricyclic system with a nitrogen atom and a side chain) and a search panel on the right. The search panel includes options for searching the structure as drawn, as substructure, or similar, and checkboxes for various search criteria like Tautomers, Stereo, Additional ring closures, Related Markush, Salts, Mixtures, Isotopes, Charges, and Radicals. A "Transfer to query" button is visible at the bottom right.

Clear Cancel X Transfer to query >

Нажмите find

Click **Transfer to query**

and then **Find** .

Reaxys

Quick search Query builder Results Synthesis planner History

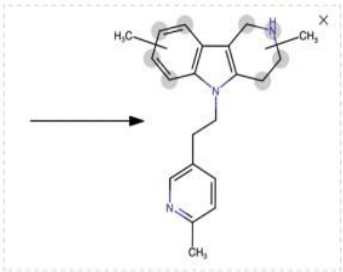
Import

Search for

Find

Documents, e.g. publications about quasicrystals

AND

A chemical structure of a quasicrystal building block, specifically a substituted indole derivative. The structure features a central indole ring system. The nitrogen atom of the indole is substituted with a 4-methylpyridin-2-ylmethyl group. The indole ring has a methyl group (H₃C) at the 2-position and a substituent (CH₂X) at the 3-position. The structure is enclosed in a dashed box, and an arrow points to it from the left.

As drawn



Исследуйте реакции вокруг определенных связей

Reaxys®

Quick search Query builder Results Synthesis planner History

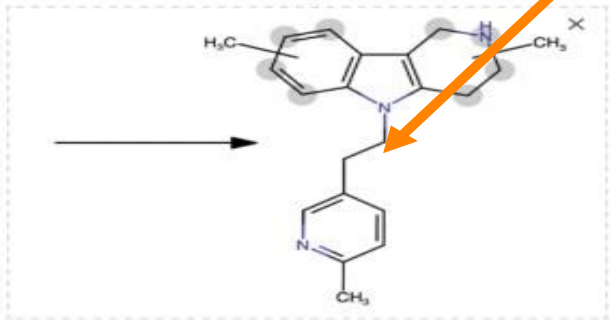
Import 

Search for 

Find >

Q Documents, e.g. publications about quasicrystals

AND



As drawn

Щелкните правой кнопкой мыши на связь 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»

Structure editor

Create structure template from name

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Mixed molecules
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

Bond properties

Absolute stereo (chiral)

(e.g. Peptide (2S+V))

Bond properties dialog box:

Type: single

Topology: undefined

Reacting center: undefined

Stereo search: Off

OK

Salts

Mixtures

Isotopes

Charges

Radicals

More options

Bond properties dialog box:

Type: single

Topology: undefined

Reacting center: make or break - ||

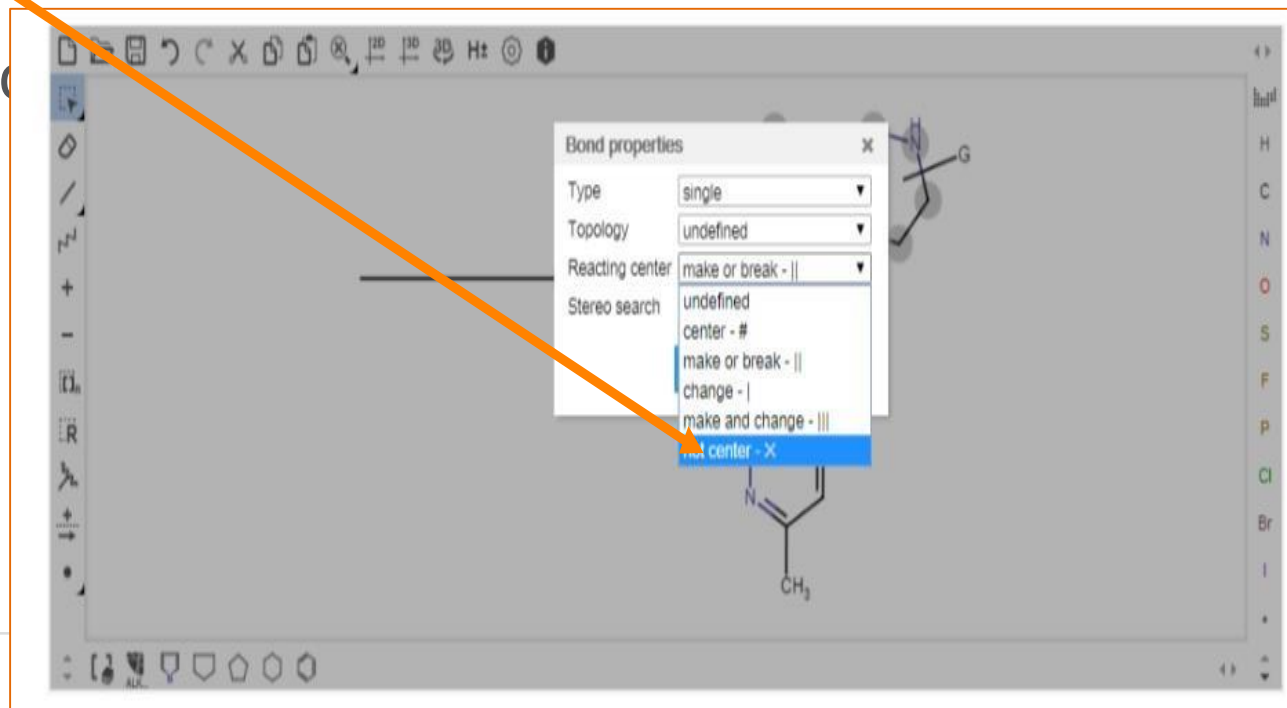
Stereo search: change - |

make and change - |||

not center - X

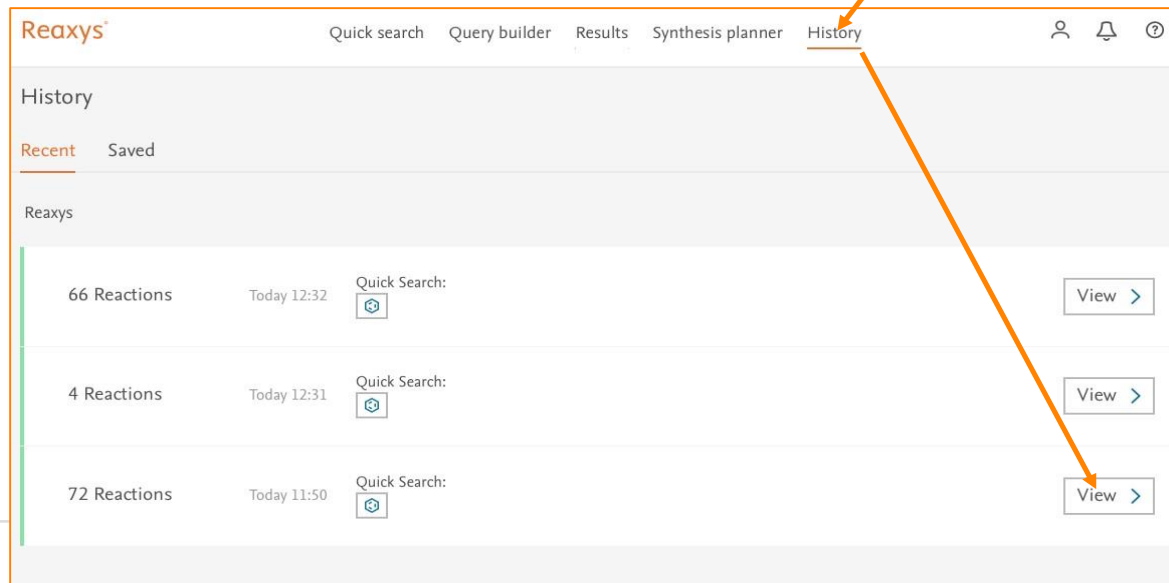
OK

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



Фильтрация результатов для конкретных промежуточных продуктов или реагентов.

View for the first set of results.



The screenshot shows the Reaxys web interface. At the top, there is a navigation bar with the Reaxys logo and several tabs: Quick search, Query builder, Results, Synthesis planner, and History. The History tab is selected and highlighted with an orange arrow. Below the navigation bar, the page is titled 'History' and has two sub-tabs: 'Recent' (selected) and 'Saved'. The main content area displays a list of search results under the heading 'Reaxys'. Each result entry includes the number of reactions, the time of the search, a 'Quick Search:' label with a magnifying glass icon, and a 'View >' button. The first result shows '66 Reactions' from 'Today 12:32'. The second result shows '4 Reactions' from 'Today 12:31'. The third result shows '72 Reactions' from 'Today 11:50'. An orange arrow points from the 'History' tab to the 'View >' button of the first result.

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

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

The screenshot displays a chemical reaction interface. At the top left, the reaction ID is 29081541. Below it, a chemical structure of a reactant is shown. To the right, the product structure is displayed. A table below the structures lists reaction conditions and yields. The 'Options' menu is open, showing several actions: Find Similar, View details, Copy structure to query, Copy reaction to query, Use as filter (highlighted with a red circle), and Open in database. The table below the menu lists reaction conditions and yields.

Yield	Conditions	References
80%	For 24h; Inert	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.; Kysil, Volodymyr M.; Khvat, Alexander V.; Okun, Ilya M.; Tkachenko, Sergey E. - Medicinal Chemistry Letters, 2009, vol. 19, # 12, p. 3183 - Show Less >

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 shows the Reaxys web interface. In the left sidebar, under 'Filters and Analysis', the 'Limit to' and 'Exclude' buttons are highlighted with an orange circle. The 'By Structure' filter is active, showing a chemical structure of 4-methyl-2-vinylpyridine. The main area displays a chemical reaction (Reaction ID: 29081341) and a table of results.

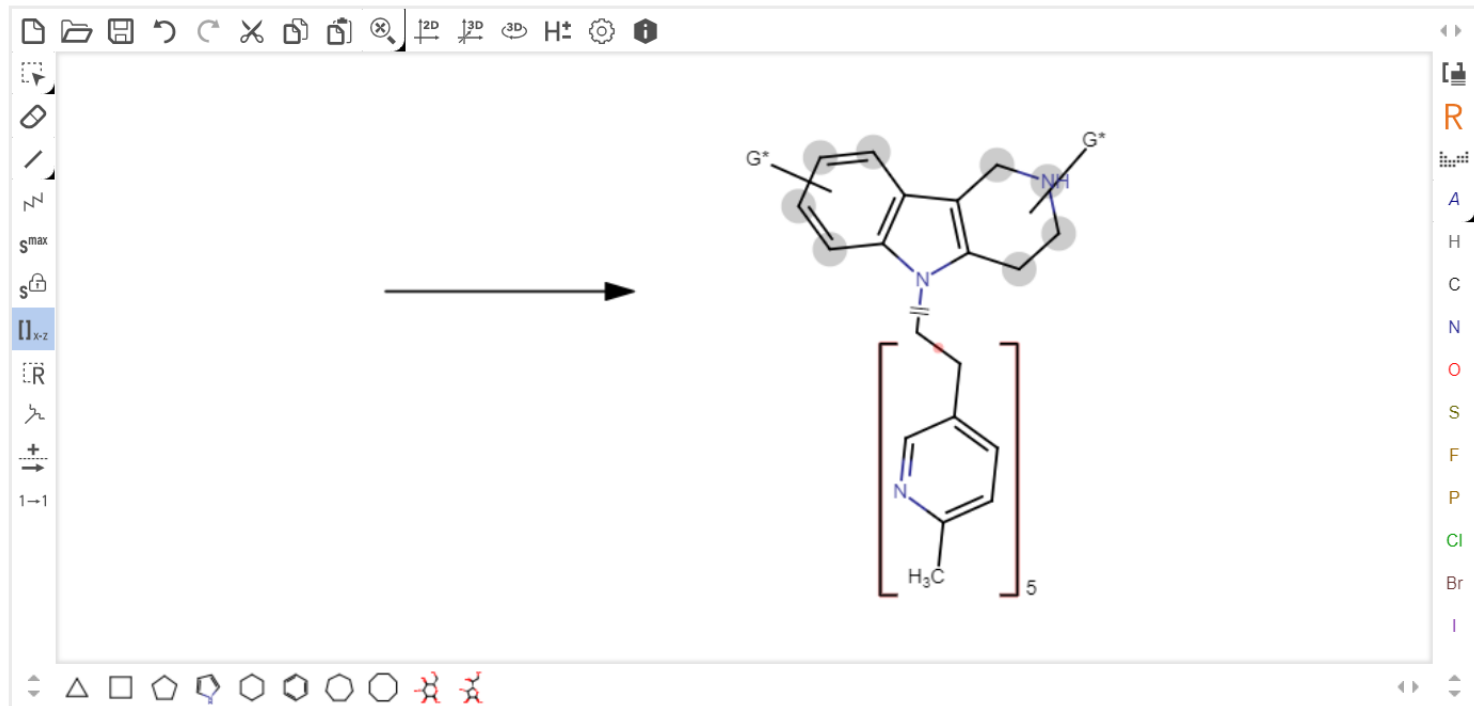
Reaction ID: 29081341

Chemical reaction scheme showing the reaction of 4-methyl-2-vinylpyridine with a substituted indole derivative to form a complex product.

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, Vladimir M.; Khusat, Alexander V.; Okun, Ilya M.; Tkachenko, Sergey E. - Medicinal Chemistry Letters, 2009, vol. 19, # 12, p. 3183 -

At the bottom of the table, there is a 'Show Less' button.

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

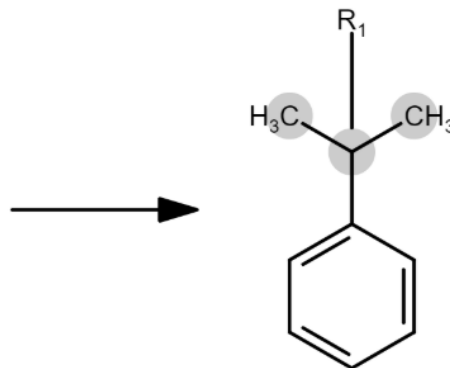


trigonal



AND

Structure



As drawn

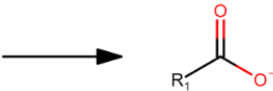
crystal system, crystal phase, crystal properties...

◇ 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 ⓘ

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

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

[QO](#) [Q](#) Sort by No of References ↓ [Grid](#) [Heatmap](#)

☐ 1 **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 >](#)

[Cart](#) [Close](#) [Search](#) [Menu](#) [Info](#)

[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.; Radhavarhari, Krishnan; Schlegel, H. Bernhard; Pople, John A. [Journal of the American Chemical Society, 1982, vol. 104, # 21, p. 5576 - 5580] Full Text Details Abstract Boche, Gernot; Bosold, Ferdinand; Lohrenz, John C. W. [Angewandte Chemie, 1994, vol. 106, # 11, p. 1228 - 1230] Full Text Details Abstract Musin; Lin [Journal of Physical Chemistry A, 1998, vol. 102, # 10, p. 1808 - 1814] Full Text Cited 26 times Details Abstract Knak Jensen; Csizmadia [Journal of Molecular Structure: THEOCHEM, 1999, vol. 459, # 1-3, p. 287 - 294] Full Text Cited 3 times Details Abstract Del Bene, Janet E.; Elguero, Jose [Journal of Physical Chemistry A, 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 [Journal of Physical Chemistry A, 2011, vol. 115, # 1, p. 122 - 123]

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. Al: 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*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*s*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*s*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*s*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*s*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*s*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*s*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*s*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*s*K); 25 Deg C	Smith, David S.; Fayette, Sylvain; Grandjean, Sylvie; Martin, Christian; Telle, Rainier; Tonnessen, 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



Reaxys предлагает своим клиентам лучший в своем классе AI. Нужно синтезировать молекулу? Спросите у Reaxys 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.



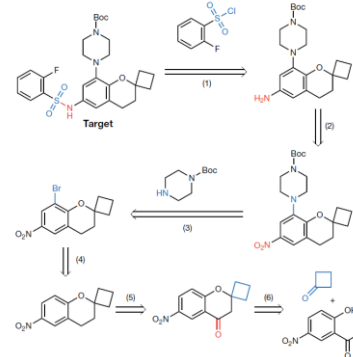
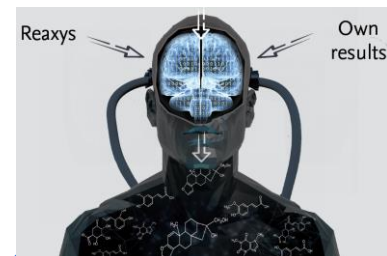
Инструмент ретросинтеза, разработанный в сотрудничестве с профессором Марком Уоллером, расширит синтез малых органических молекул прогностическим моделированием ранее неопубликованных синтетических путей.



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



В тридцать раз быстрее, чем традиционные компьютерные методы



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

Прогнозирующий ретросинтез: переосмысление химии и изменение синтетических маршрутов

Harvard
Business
Review

DATA

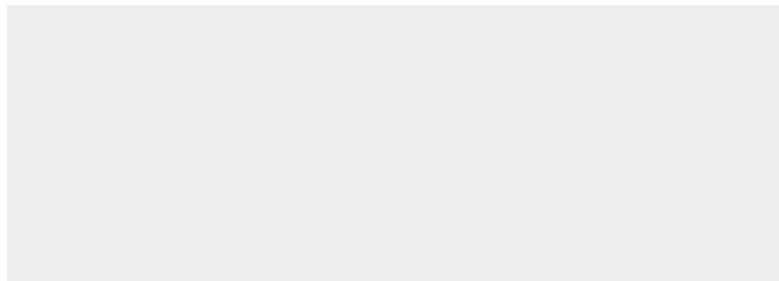
If Your Data Is Bad, Your Machine Learning Tools Are Useless

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.





ELSEVIER

Вопросы?

Моисеев Алексей Александрович
a.moiseev@elsevier.com +79251131255





ELSEVIER

Спасибо за внимание!

Моисеев Алексей Александрович
a.moiseev@elsevier.com +79251131255

