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

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Директор по развитию и обслуживанию клиентов
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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

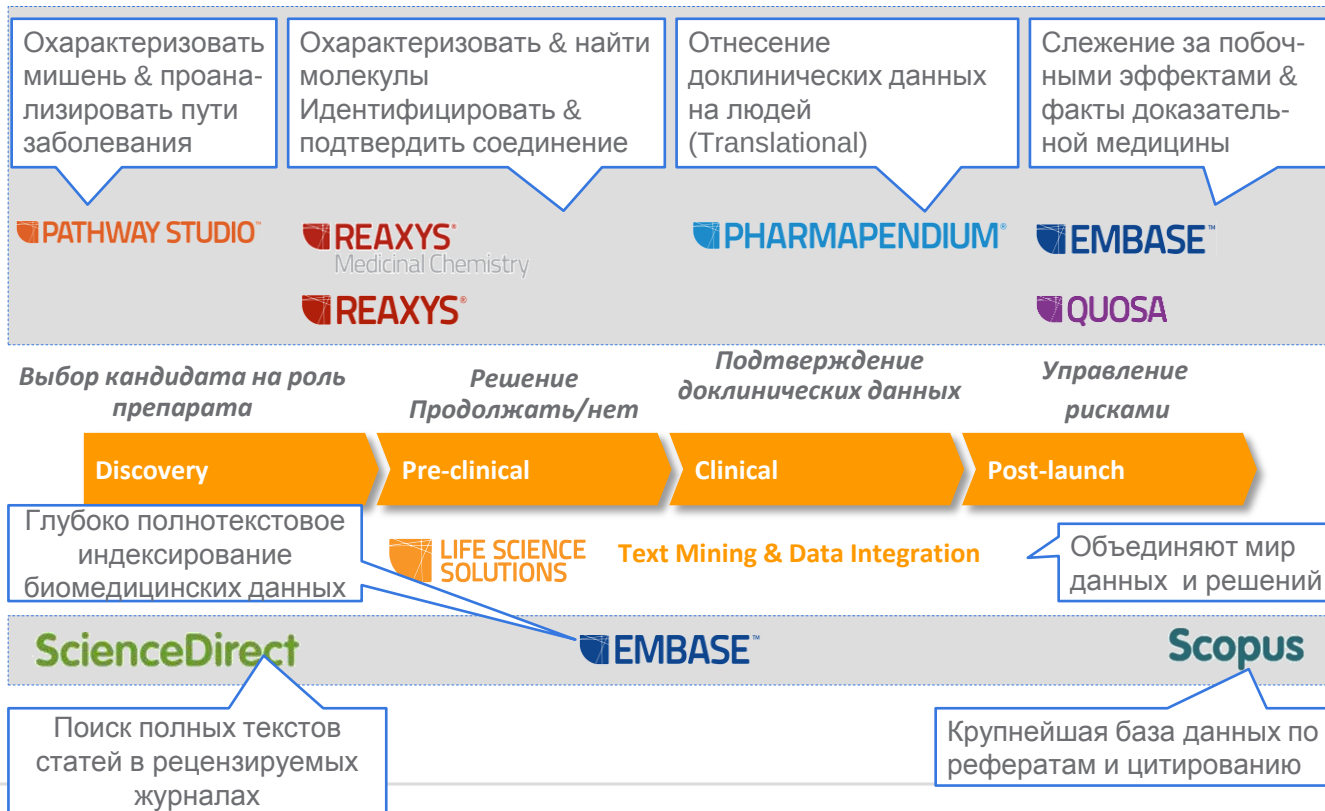
Моисеев Алексей Александрович

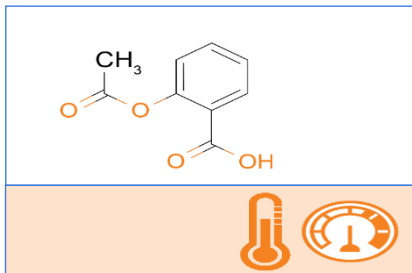
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Решения в области life sciences

НАПРАВЛЕННЫ 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



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 >]

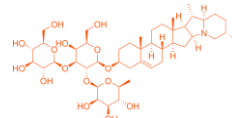
PO: JP, KR, CN, TW [2015 >]

380+k book chapters

Beilstein, Gmelin,



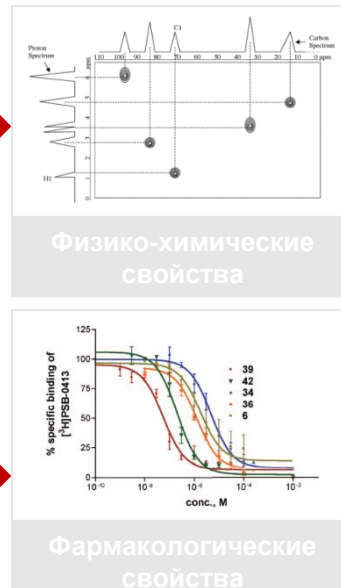
≈ 450 journals + PO
[manually excerpted]



Из экспериментальных данных статей из рецензируемых журналов и патентов



**Reaxys извлекает
все необходимые
данные даже из
примечаний и
текста**



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

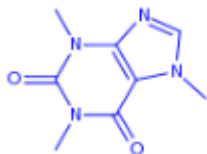
Solubility

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 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

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Поиск литературы. Поиск по ключевым словам

Reaxys®

Quick search

Query builder

Results

Synthesis planner

History ^{new}

Register >

Sign in ⓘ

Search in:

Reactions >

Targets >

Substances >

Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

◇ Keywords

is	▼	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 K

Filters and Analysis

Index Terms (List) ▾

Index Terms (ReaxysTree) ▾

Publication Year ▾

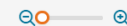
Document Type ▾

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 Moiseev

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

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Sort by Publication Year ↓ Heatmap

Filters and Analysis

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

1 Common roasting defects in coffee: Aroma composition, sensory characterization and consumer perception
Giacalone, Davide; Degen, Tina Kreuzfeldt; Yang, Ni; Liu, Chujiao; Fiek, Iara; Münchow, Morten - [Food Quality and Preference, 2019, vol. 71, p. 463 - 474]
Abstract Index Terms Substances (32) Full Text
Hit Substances (1)

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

3 Kohn-Sham energy decomposition for molecules in a magnetic field
Reimann, Sarah; Borgoo, Alex; 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)

4 Synthesis of new TiO₂/porphyrin-based composites and photocatalytic studies on methylene blue degradation
Min, Kyeong Su; Kumar, Rangaraju Satish; Lee, Jeong Hoon; Kim, Kang Seok; Lee, Seung Geol; Son, Young-A - [Dyes and Pigments, 2019, vol. 160, p. 37 - 47]
Abstract Index Terms Substances (17) Reactions (33) Full Text
Hit Substances (1)

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



Limit To



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Export



The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents

1

[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](#) ➤



Design, synthesis, and evaluation of new series of Imperatorin analogs with potential vas

2

[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](#) ➤



Synthesis and bioactivities of diamide derivatives containing a phenazine-1-carboxamide

3

[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)

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Query builder ^{New}

Results

Synthesis planner

History

Register >

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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 v

Identification v

Physical Properties ^

Melting Point

Boiling Point

Sublimation

Refractive Index

Density

Feedback

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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.



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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

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
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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
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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?

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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

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

EQ

is

▼

Original string

EQ

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

Q Search

×

☐ '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

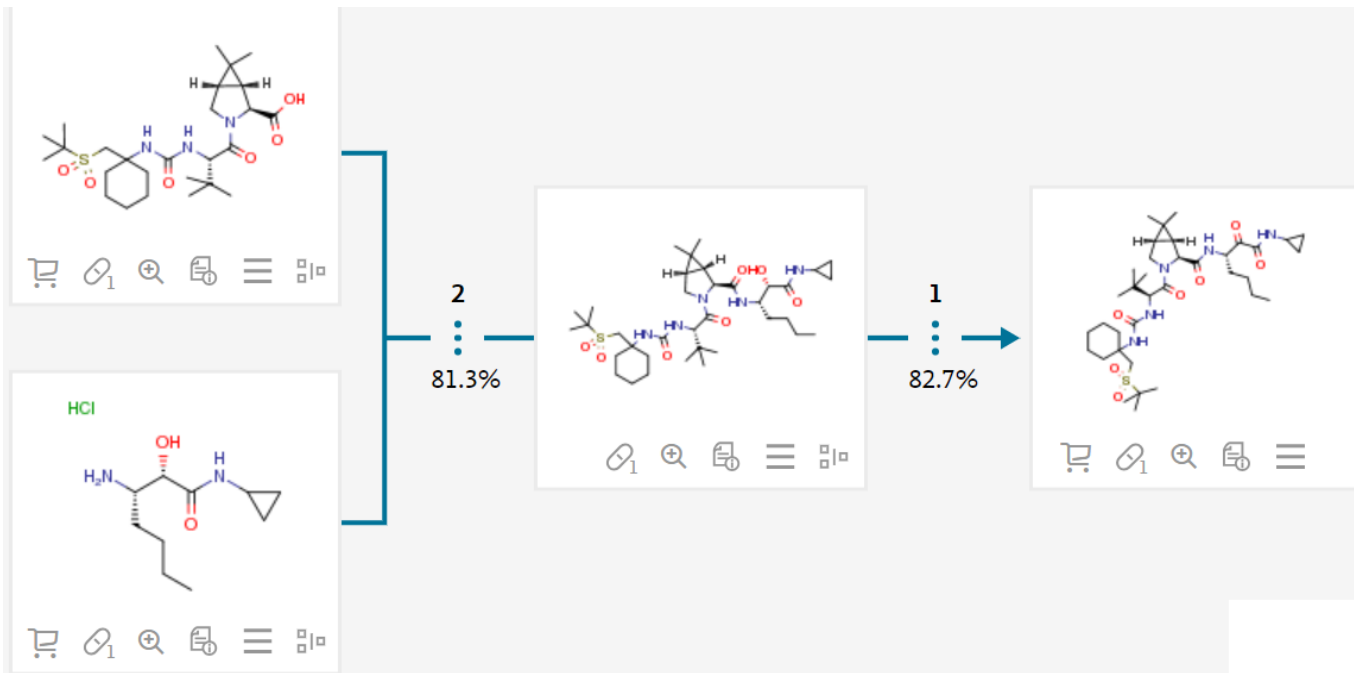
Химические реакции в Reaxys

-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?

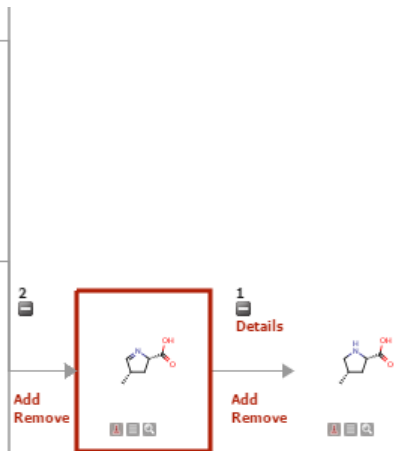
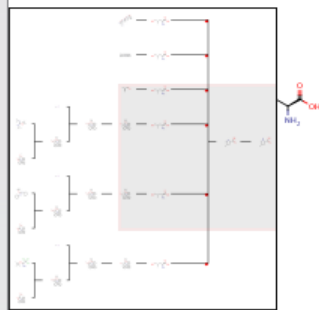
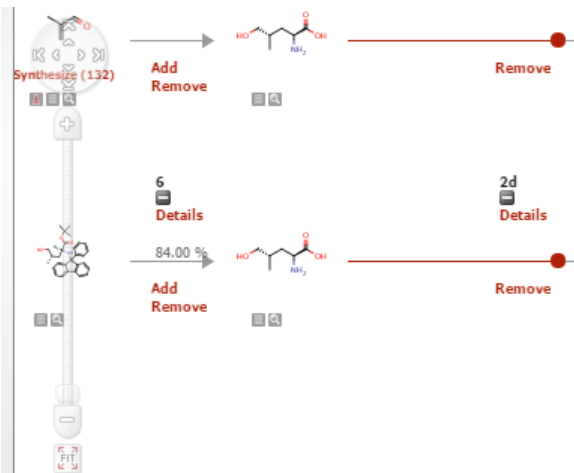
Как проверить доступность соединения



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



Разработка методики синтеза химических веществ (субстанций)



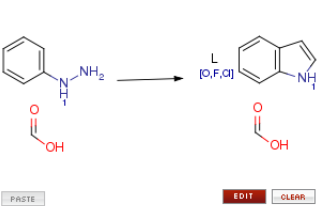
Также за секунды Reaxys может **построить многостадийный план синтеза** из базовых соединений, что сэкономит время сотрудников и **позволит выбрать метод, в котором не образуются опасные побочные продукты.**

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 × Formula Builder

Identification

Chemical Name is Lookup ×

Show AND Buttons

Please select role

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

Reaction Data

Yield (numerical)

= Lookup ×

Solvent (Reaction Details)

is Lookup ×

Reagent/Catalyst

is Lookup ×

Time (Reaction Details) (h)

= Lookup ×

Temperature (Reaction ... (°C)

= Lookup ×

Pressure (Reaction D... (Torr)

= Lookup ×

Reaction Type

is Lookup ×

Reaction Basic Index

is Lookup ×

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!!!

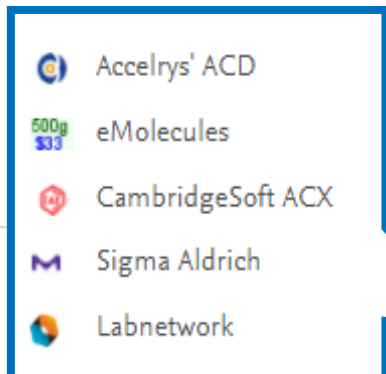
При планировании синтетической стратегии химии должны учитывать, как приобретать исходные материалы.

Три больших вопроса:

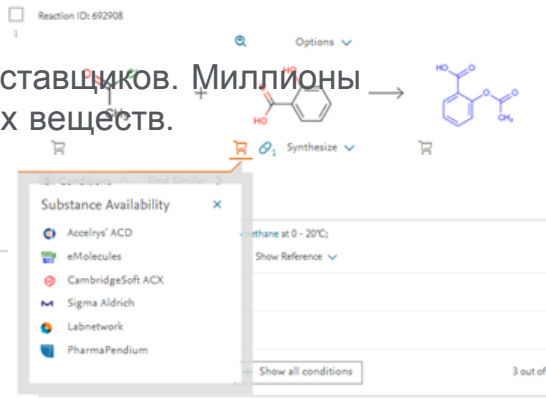
Есть ли этот материал на моей местном складе?

Есть ли материал присутствует на складе у любого поставщика?

Есть ли этот поставщик в моей системе покупки?



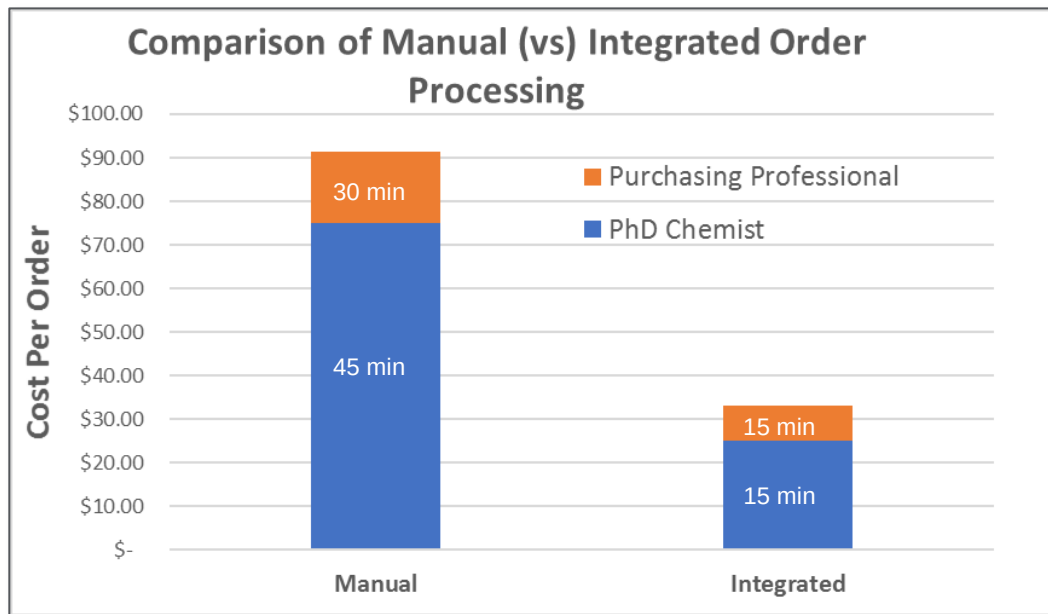
Тысячи поставщиков. Миллионы химических веществ.



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

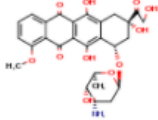
Export

☐ ☐

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 >



Import



Save



Reset form



Delete all



Structure



Molecular Formula



CAS RN



Doc. Index

Find search fields and forms

Q biological species



Reaxys ^

◇ Biological Species

is



chlamydiae



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

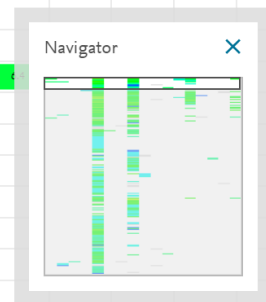
Value of Cells: Maximum of pX

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 ^ ×

is ☐ Isolation from Natural Product
camomile ☐

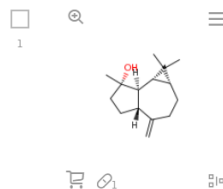
☐

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

☐ 0 selected Limit To Exclude Export

☐ Sort by No of References ↓

Grid ☐ Heatmap ☐



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 ☐



Single protein

1 **Acetylcholinesterase (Wild)**

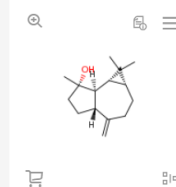
Synonyms: acetylcholinesterase

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 Natural Product

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

ELSEVIER

Reaxys®

LIFE SCIENCE SOLUTIONS

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

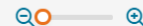
542 Substances out of 94,335 Documents, containing 28,875 Reactions, 1,688 Targets

☐ 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

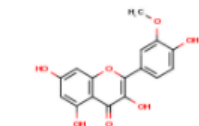
Какие соединения были найдены в тысячелистнике Yarrow?



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

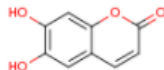
contains ▼ Isolation from Natural Product

Yarrow 



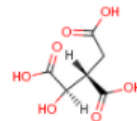
isorhamnetin
 $C_{16}H_{12}O_7$ 316.267

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



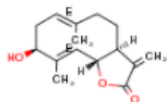
aesculetin
 $C_9H_6O_4$ 178.144 152788

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



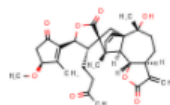
threo-D-isocitric acid
 $C_8H_8O_7$ 192.125 1727947

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



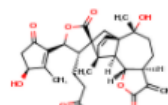
hanphyllin
 $C_{15}H_{20}O_3$ 248.322 1623169

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



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

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



C30H36O8

Synthesize ▼

Options ▼ **achillinin C**
 $C_{30}H_{36}O_8$ 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



☐	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 x

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

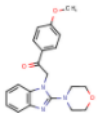
◇ Use Find any Hide fields ×

is ▼ Laboratory Use and Handling 🔍

is ▼ Use Pattern 🔍

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

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

Reaxys

Basic Indexes

Identification

Physical Properties

Spectra

MedChem

Other

Reactions

Bibliography

PubChem

eMolecules

LabNetwork

SigmaAldrich

Structure

Optical Rotatory Power

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

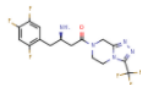
Molecular Formula

is Molecular Formula
F6N5C16*

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 ▾

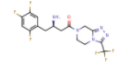
Type (Optical Rotatory Power)	Concentration (Optical Rotatory Power)	Length of Path, cm	Solvent (Optical Rotatory Power)	Optical Rotatory Power, deg	Wavelength (Optical Rotatory Power), nm	Temperature (Optical Rotatory Power), °C	Location	Reference
alpha	0.92 g/100ml		chloroform	-22.4	589	25	Page/Page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



ELSEVIER

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
C14H15F7N5O 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

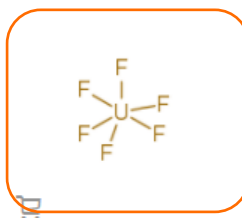


Substance Basic Index

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

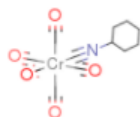
63.94

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:

Import Save Reset form Delete all

Structure Molecular Formula CAS RN Doc. Index

Search Substances

◇ 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

Search Reaxys interface showing results for "andalusite".

Search term: "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

Filters:

- 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

Results:

1 **andalusite**
SiAl₂O₅ 162.046 16453029
Identification Physical Data - 54 Other Data - 9 Preparations - 4
Druglikeness Spectra - 11 Reactions - 7
Documents - 93

2 **kyanite**
SiAl₂O₅ 162.046 16452963
Identification Physical Data - 26 Other Data - 6 Preparations - 3
Druglikeness Spectra - 14 Reactions - 11
Documents - 82

3 **sillimanite**
SiAl₂O₅ 162.046 16453049
Identification Physical Data - 34 Other Data - 8 Preparations - 5
Druglikeness Spectra - 10 Reactions - 15
Documents - 93



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. <i>Journal of Physical Chemistry A</i> , 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

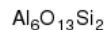
Transition Point(s) of Crystalline Modification(s)

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



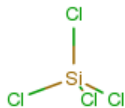
3 Conditions Find Similar Reaction ID: 26413460

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



$\text{Al}_2\text{O}_5\text{Si}$

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

2 out of 2

Поиск информации о минералах

ПОИСК ЛИТЕРАТУРЫ ПО АНДАЛУЗИТУ

◇ Document Basic Index

is

▼ andalusite

EQ X

1.60 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 ↓

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

[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...}

[Cited 1 times](#)

☐ 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

[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/m-3) 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 Substances out of 1,535 Documents, containing 403 Reactions, 0 Targets

Reaxys - 160

0 selected Limit To Exclude Export

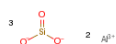
Sort by No of References ↓ Grid Heatmap

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 >

1



aluminum silicate
 $2Al^{3+} \cdot 3O_3Si^{2-}$ 282.214 14479534

Identification
Druglikeness
Other Data - 3

Documents - 688 >

2

$Al_6O_{13}Si_2$

mullite
 $3Al_2O_3 \cdot 2SiO_2 = Al_6Si_2O_{13}$ 426.052 16513662

Identification Physical Data - 313 Other Data - 8
Druglikeness Spectra - 44

Preparations - 140 >
Reactions - 169 >
Documents - 317 >

3

$Al_2O_7Si_2$

metakaolin
 $(Al_2O_3)(SiO_2)_2$ 222.13 11341013

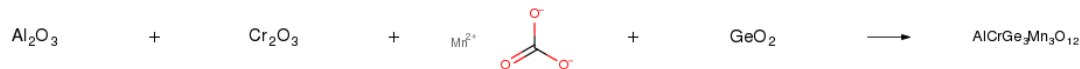
Identification Physical Data - 9 Other Data - 1
Druglikeness Spectra - 2

Preparations - 8 >
Reactions - 52 >
Documents - 162 >

andalusite

Feedback

Получение вещества



1 Conditions Find Similar Reaction ID: 26074679

Conditions

Yield

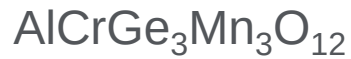
Reference

In neat (no solvent) triturating MnCO₃, Cr₂O₃, Al₂O₃ and GeO₂, 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

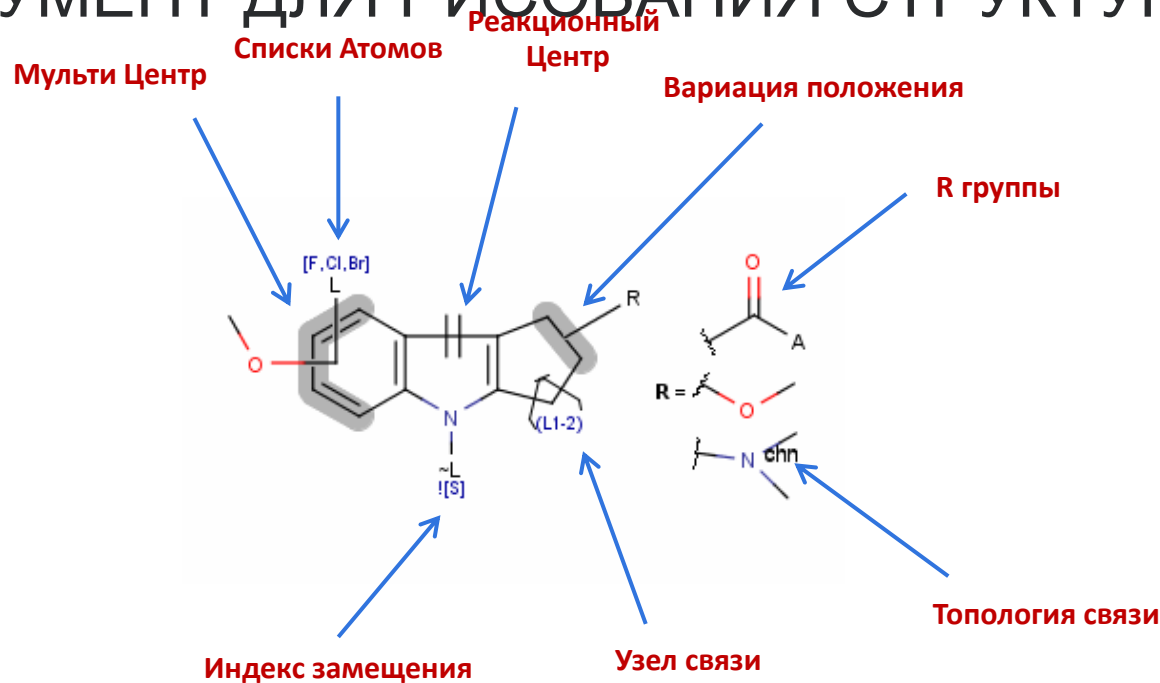
- Особенности и покрытие базы данных Reaxys.
- Оптимальная стратегия поиска литературы.
- Свойства веществ в Reaxys
- Химические реакции в Reaxys
- Биологическая активность и медицинская химия в Reaxys
- Вопросы



РИСОВАНИЕ СТРУКТУРЫ С ИСПОЛЬЗОВАНИЕМ MARVIN JS



MARVIN SKETCH – НАДЕЖНЫЙ ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ



MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ

Structure editor ChemAxon's MarvinJS

Create structure template from name

The screenshot shows the MarvinJS sketching interface. The central workspace displays the 'Marvin JS by ChemAxon' logo. The interface is surrounded by toolbars and panels. Red text annotations with blue arrows point to specific features: 'Выбор' (Selection) points to the selection tool in the left toolbar; 'Тип связей' (Bond type) points to the bond type tools; 'Повторяющиеся единицы' (Repeating units) points to the repeat button; 'Селектор R-групп' (R-group selector) points to the R-group selector; 'Прикрепление R-Group' (R-group attachment) points to the R-group attachment tool; 'Стрелка реакции/Мэппинг атомов' (Reaction arrow/Atom mapping) points to the reaction arrow; 'Общие шаблоны' (General templates) and 'Reaxys Generics' point to the template buttons at the bottom left; 'показать/ убрать водороды' (Show/hide hydrogens) points to the 'H+' button in the top toolbar; 'Список атомов (таблица Менделеева)' (List of atoms (Mendeleev table)) points to the periodic table on the right; and 'Основные атомы' (Basic atoms) points to the basic atoms list at the bottom right.

Выбор

Тип связей

Повторяющиеся единицы

Селектор R-групп

Прикрепление R-Group

Стрелка реакции/Мэппинг атомов

Общие шаблоны

Reaxys Generics

показать/ убрать водороды

Список атомов (таблица Менделеева)

Основные атомы

ИНСТРУМЕНТ ДЛЯ РИСОВАНИЯ СТРУКТУРЫ



MARVIN SKETCH – НАДЕЖНЫЙ

ИНСТРУМЕНТ ДЛЯ СОЗДАНИЯ СТРУКТУРЫ

The screenshot displays the Marvin.js web application in a Google Chrome browser. The main workspace shows a chemical structure of a bicyclic amine with two green circles highlighting specific atoms. Red text annotations with blue arrows provide instructions: "Нажмите на атом или связь, он будет выделен в зеленый, затем щелкните правой кнопкой мыши" (Click on an atom or bond, it will be highlighted in green, then right-click) and "Нажмите на атом или связь свойств чтобы найти дополнительные варианты" (Click on an atom or bond property to find additional options). Three context menus are shown: 1) A top menu with "Duplicate", "Atom properties", "Bond properties", and "Absolute stereo (chiral)". 2) A "Bond properties" menu with options for Type (single, double), Topology (undefined), and Reacting center (undefined, in ring, in chain). 3) An "Atom properties" menu with tabs for "Basic" and "Advanced", containing fields for Total H, Implicit H, Bond orders, Connections, Ring count, Smallest ring size, Ring bond, Substitutions, Unsaturated, and Aromaticity, each with a dropdown or input field and a lock icon. The interface includes a toolbar at the top with drawing tools and a sidebar on the right with a periodic table of elements.

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

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

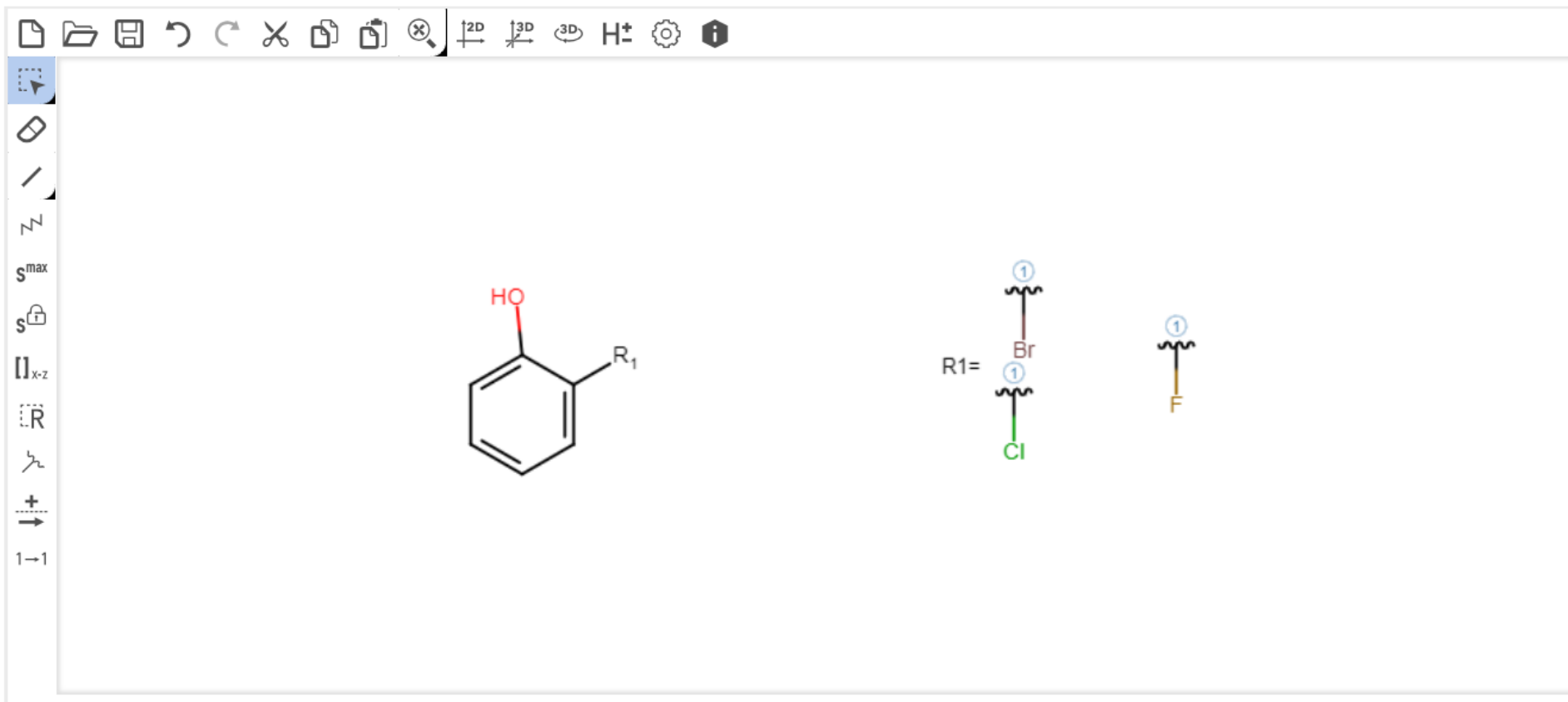
☒ Radicals

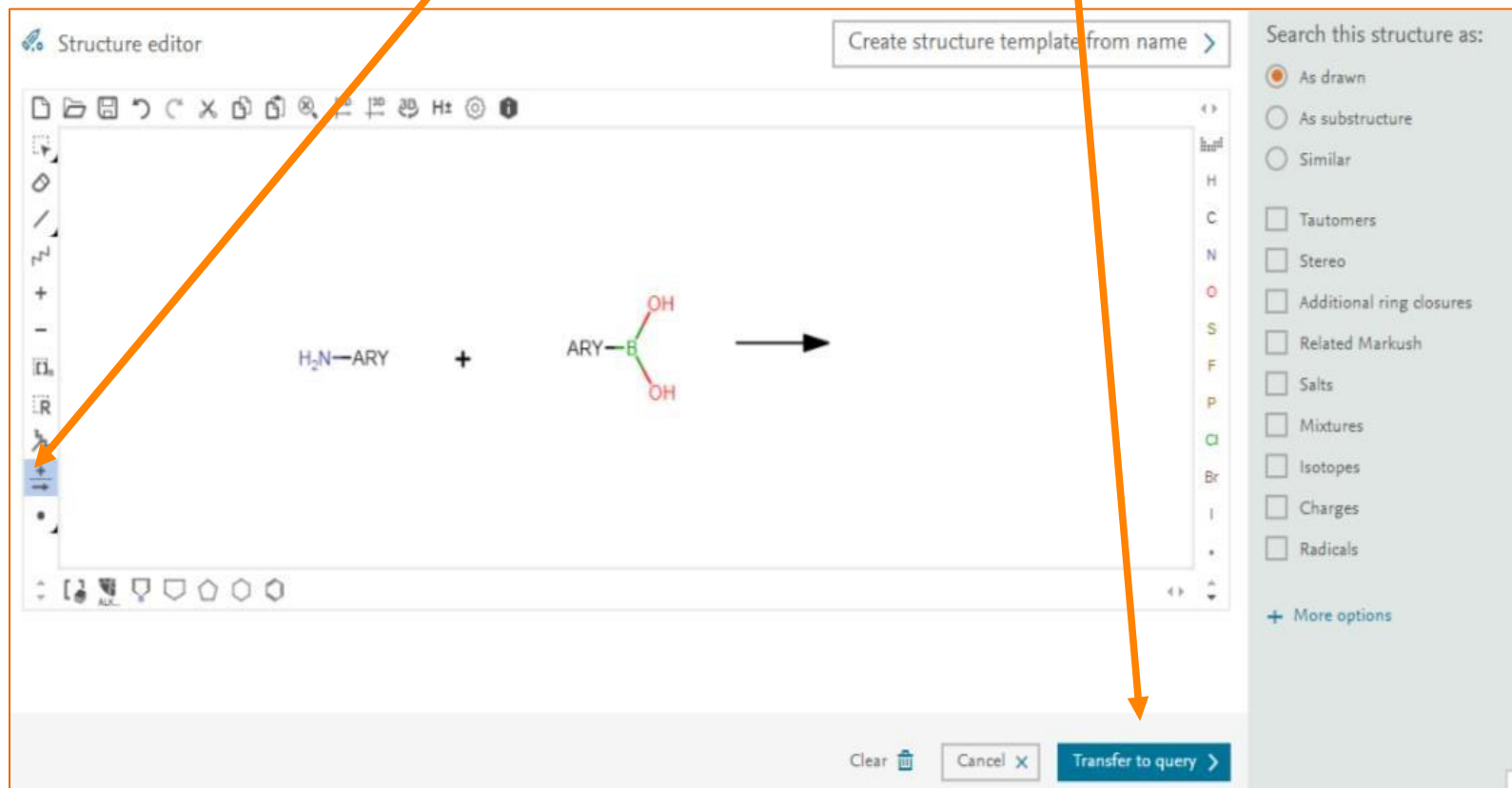
+ More options

В большинстве случаев можно создать структуру из названия

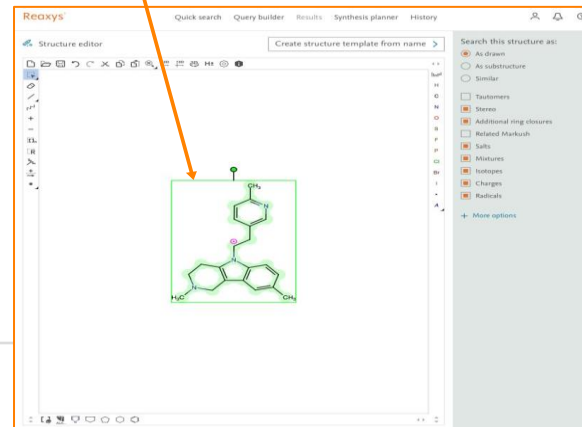
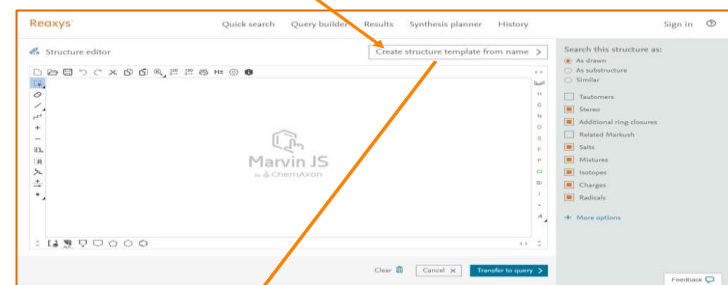
Marvin JS
by ChemAxon

Пример использования smart R-group

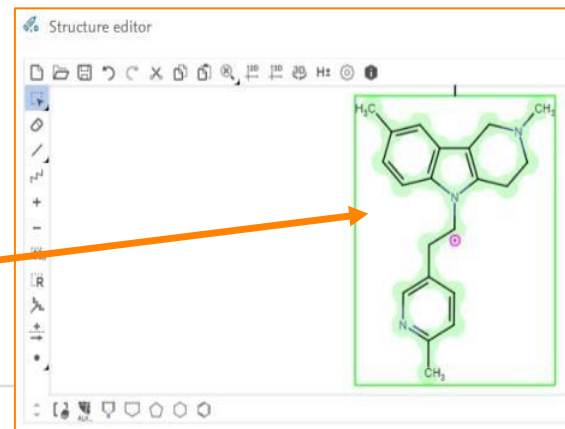
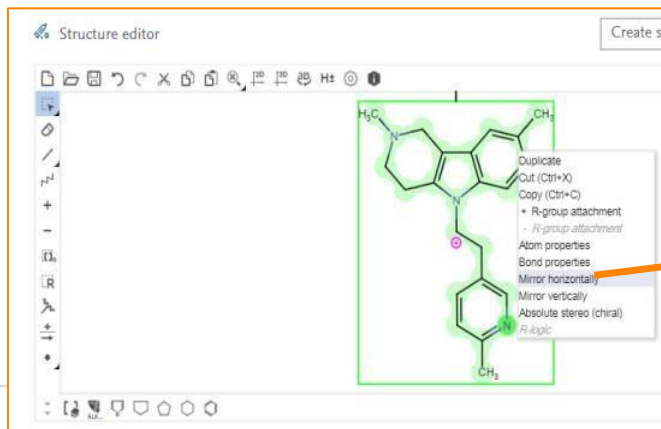
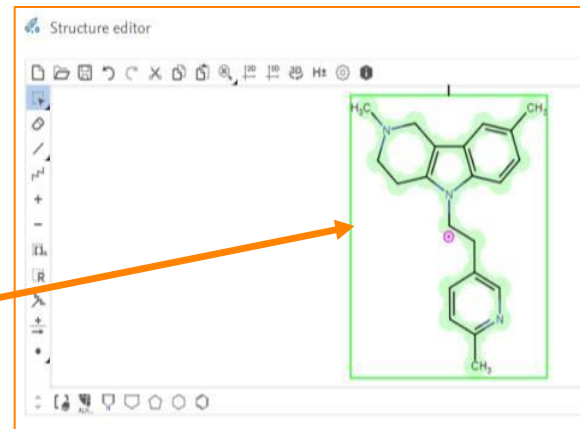
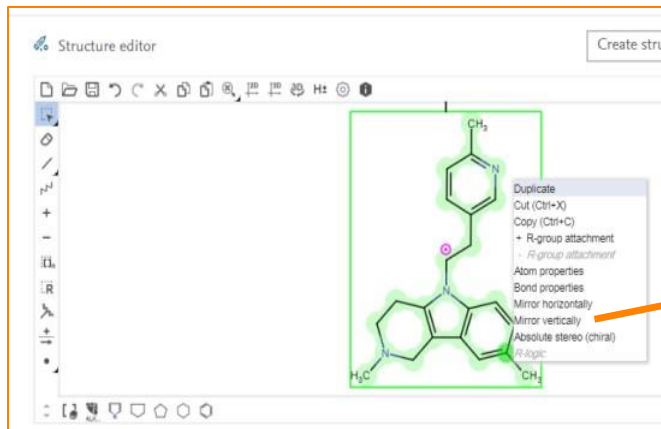




стратегия синтеза аналогов димебона Dimebon

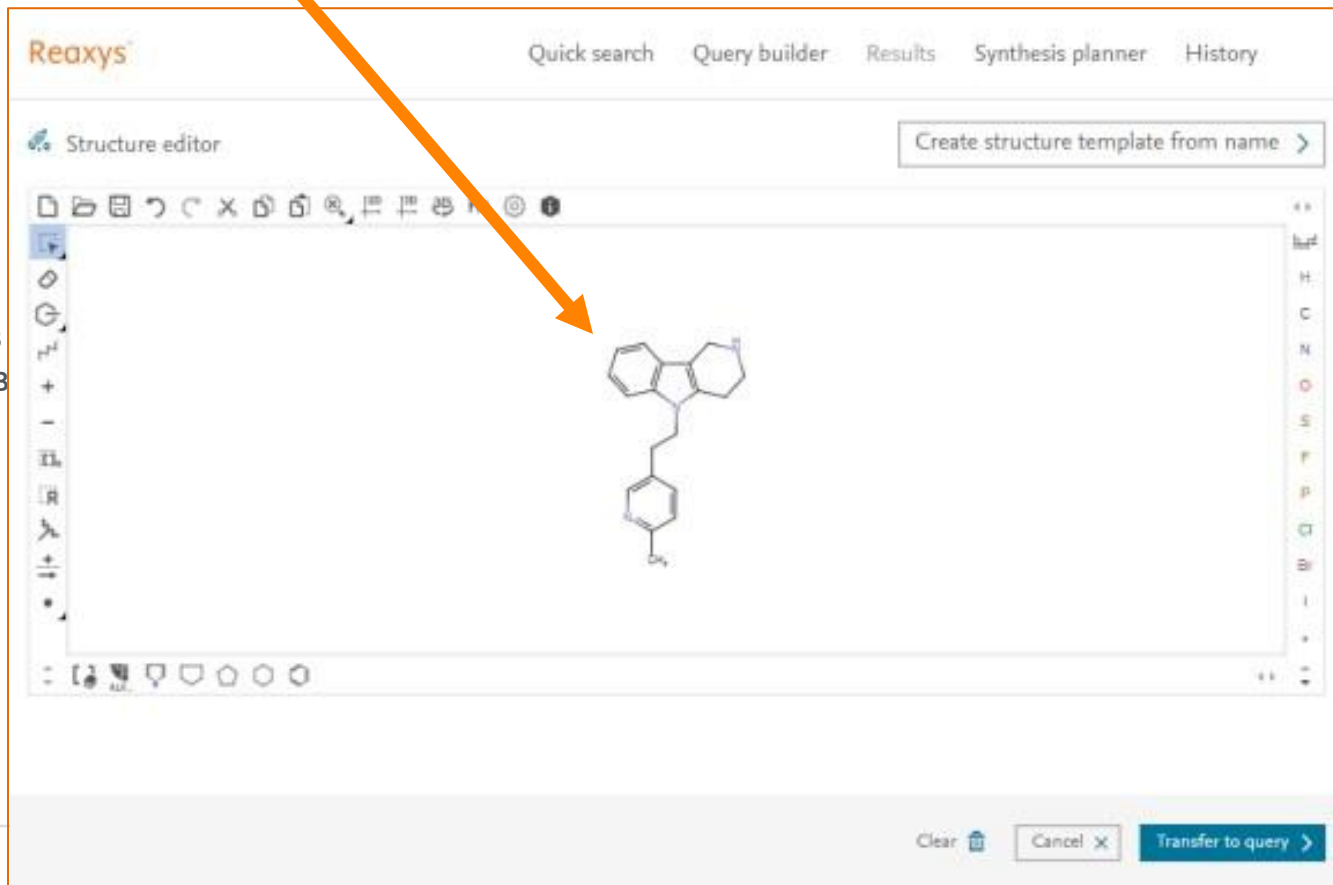


Чтобы изменить ориентацию структуры, щелкните правой кнопкой мыши на любом атоме и выберите «Отразить по вертикали» или «Отразить по горизонтали». Нужный участок структуры или вся структура должны быть выделены



Вы можете отрегулировать размер структуры, прокручивая вверх или вниз.

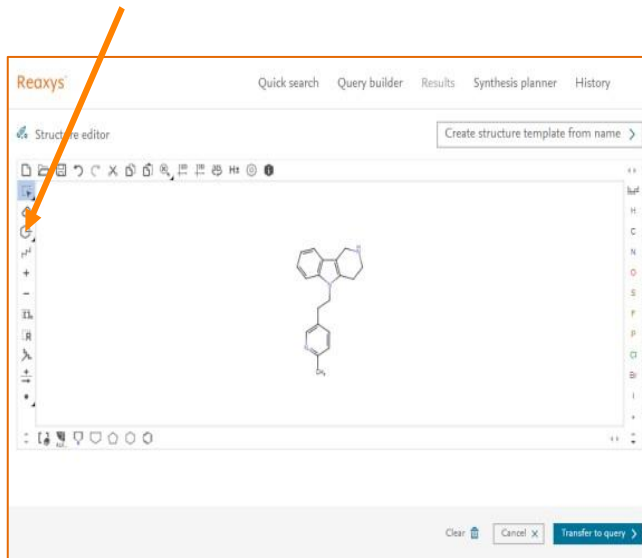
Удалите две метильные группы из верхних колец, нажав C и нажав Delete на клавиатуре.



Задать позиции плавающих связей

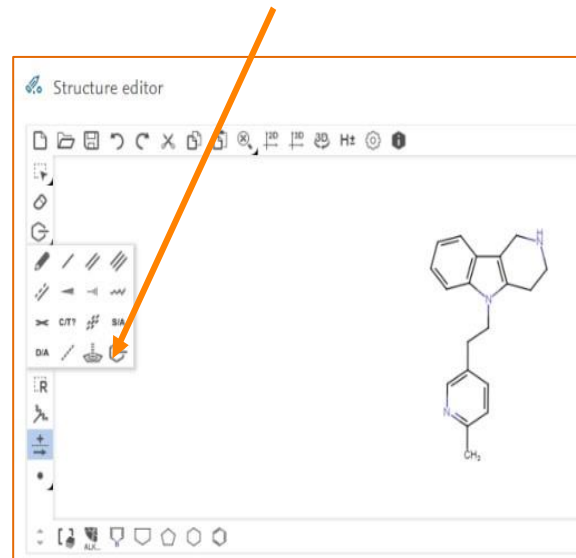
Открыть панель инструментов

a . Click here to open the tool panel.



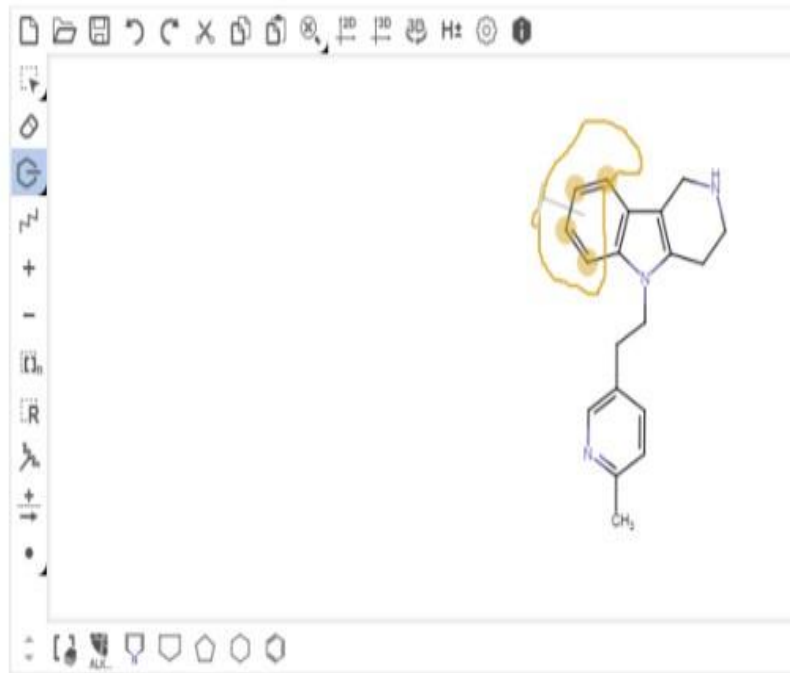
Открыть инструмент позиционирования плавающих связей

b . Select the position variation bond.

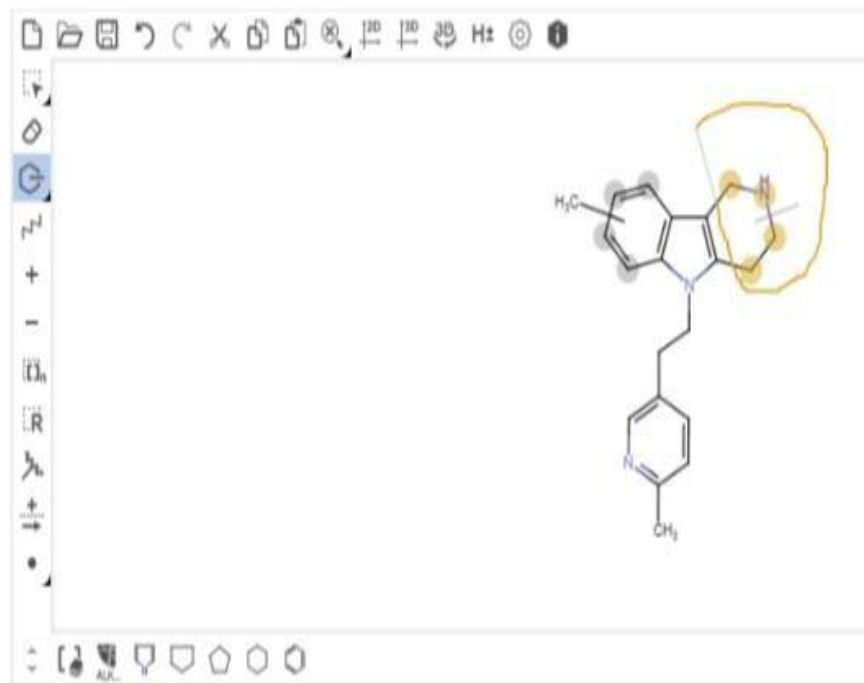


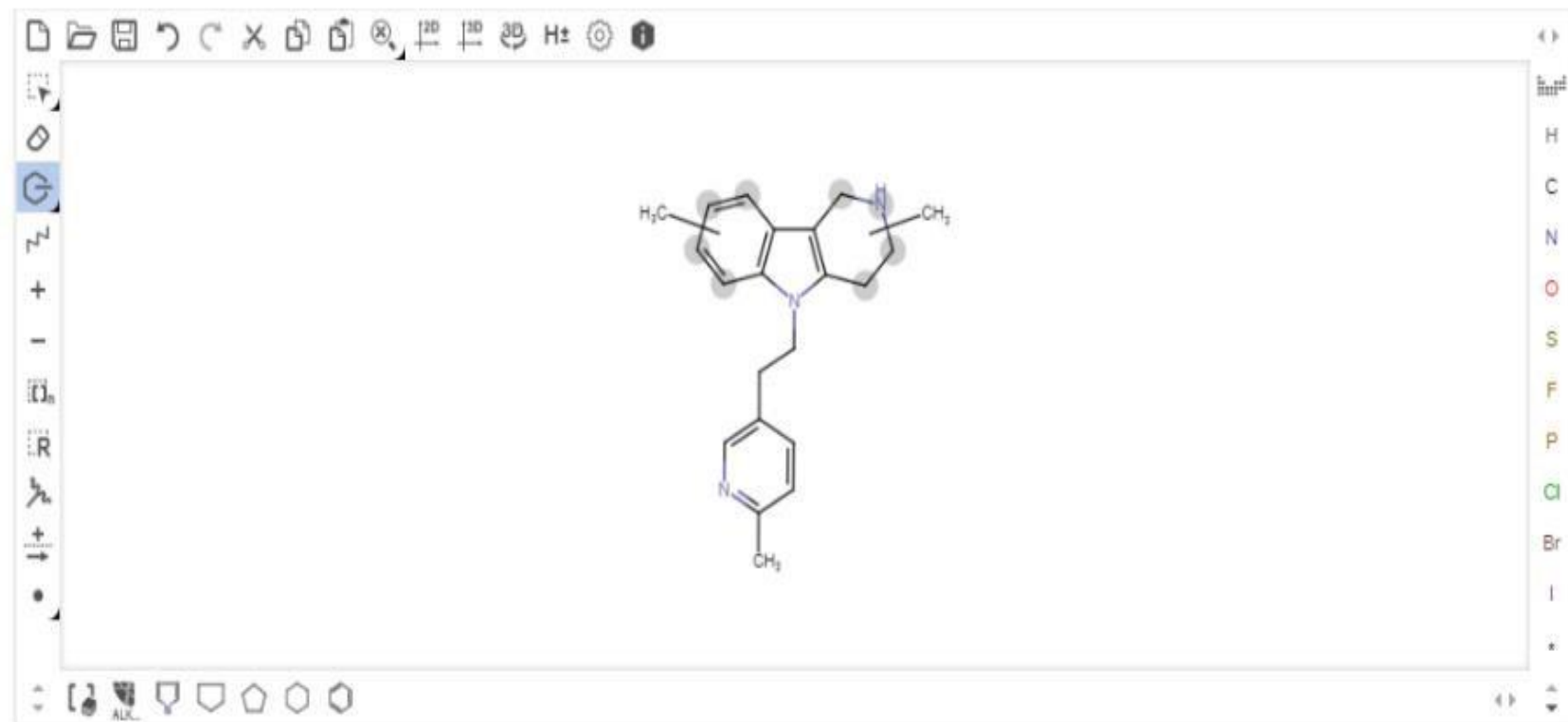
Выберите атомы для включения, нарисовав линию

Structure editor



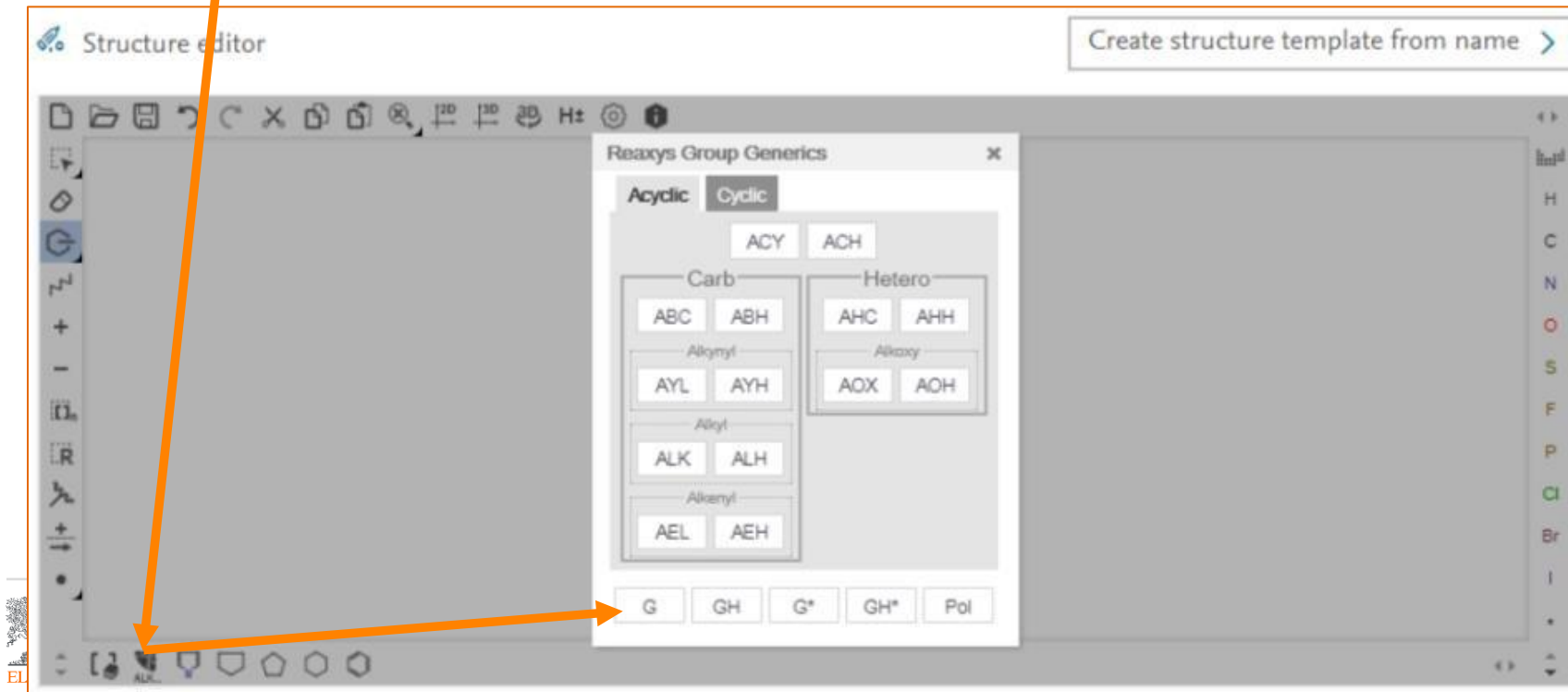
Structure editor





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

The screenshot displays a chemical structure editor window. At the top left, the text "Structure editor" is visible. Below it is a toolbar with various icons for editing chemical structures. In the center of the editor, a chemical structure is shown, consisting of a complex polycyclic aromatic system (a benzene ring fused to a five-membered ring, which is further fused to another benzene ring) connected via a two-carbon chain to a pyridine ring substituted with a methyl group (CH₃). An arrow points from the left towards this structure. To the right of the editor, there is a panel titled "Search this structure as:". It contains several radio buttons and checkboxes for different search criteria: "As drawn" (selected), "As substructure", "Similar", "Tautomers", "Stereo", "Additional ring closures", "Related Markush", "Salts", "Mixtures", "Isotopes", "Charges", and "Radicals". At the bottom of this panel is a link that says "+ More options". 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 arrow icon.

Нажмите find

Click **Transfer to query**

and then **Find** .

The screenshot shows the Reaxys web interface. At the top, there is a navigation bar with links: Quick search, Query builder, Results, Synthesis planner, and History. On the right side of the navigation bar, there are icons for user profile, notifications, and a settings gear. Below the navigation bar, there is a search bar with the text "Search for" and a search icon. To the left of the search bar is an "Import" button with a download icon. To the right of the search bar is a blue "Find" button with a right arrow. An orange arrow points from the text "Нажмите find" to this "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 diagram. The diagram shows a complex molecule with a central nitrogen atom (N) bonded to a benzene ring (with a methyl group, H₃C) and a pyridine ring (with a methyl group, CH₃). The nitrogen atom is also bonded to a chain that ends in a pyridine ring (with a methyl group, CH₃). The diagram is labeled "AND" at the top. Below the diagram, there is a small text label "As drawn".

Исследуйте реакции вокруг определенных связей

Reaxys®

Quick search Query builder Results Synthesis planner History

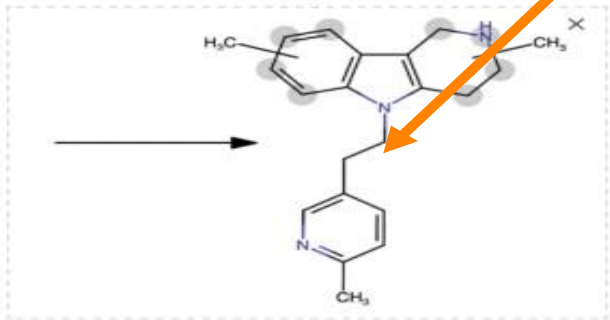
Import 

Search for 

Find >

Q Documents, e.g. publications about quasicrystals

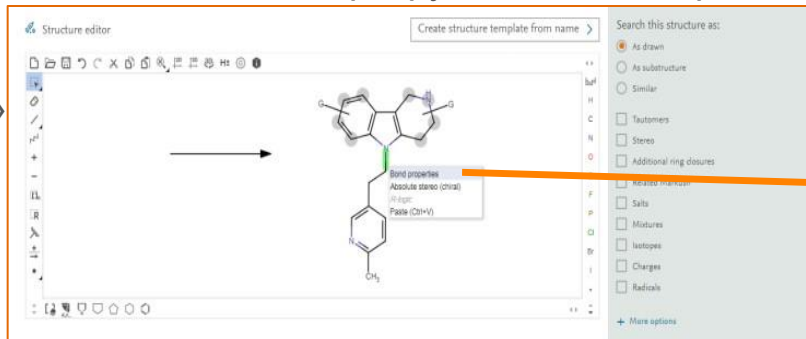
AND



As drawn

щелкните правой кнопкой мыши на связь и выберите связь 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)

As type: Pairs (C2H4)

Bond properties dialog:

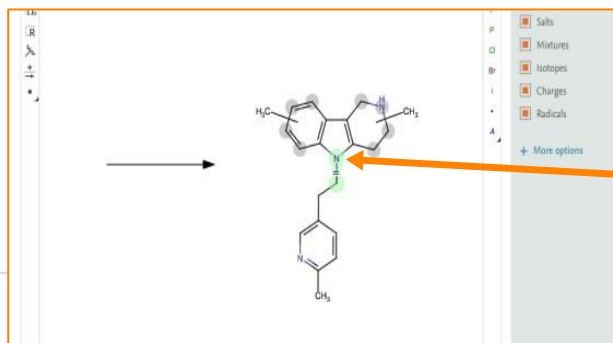
Type: single

Topology: undefined

Reacting center: undefined

Stereo search: Off

OK



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)

As type: Pairs (C2H4)

Bond properties dialog:

Type: single

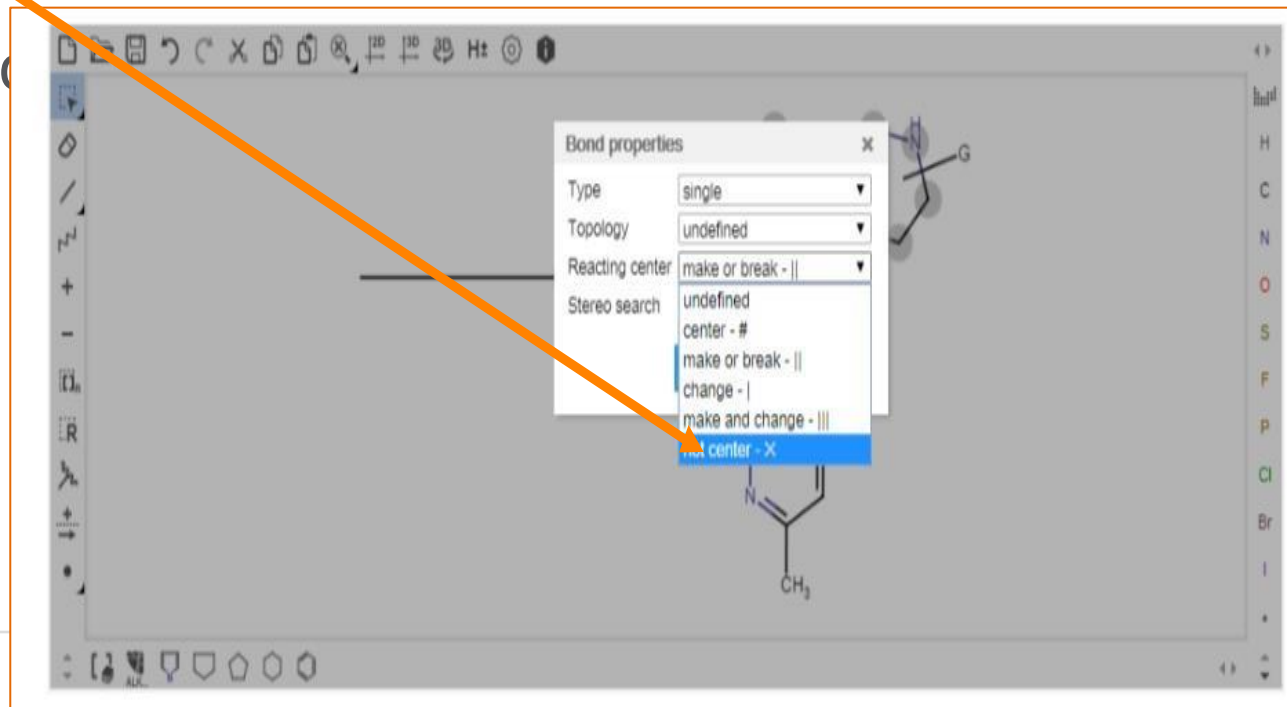
Topology: undefined

Reacting center: **make or break - ||**

Stereo search: Off

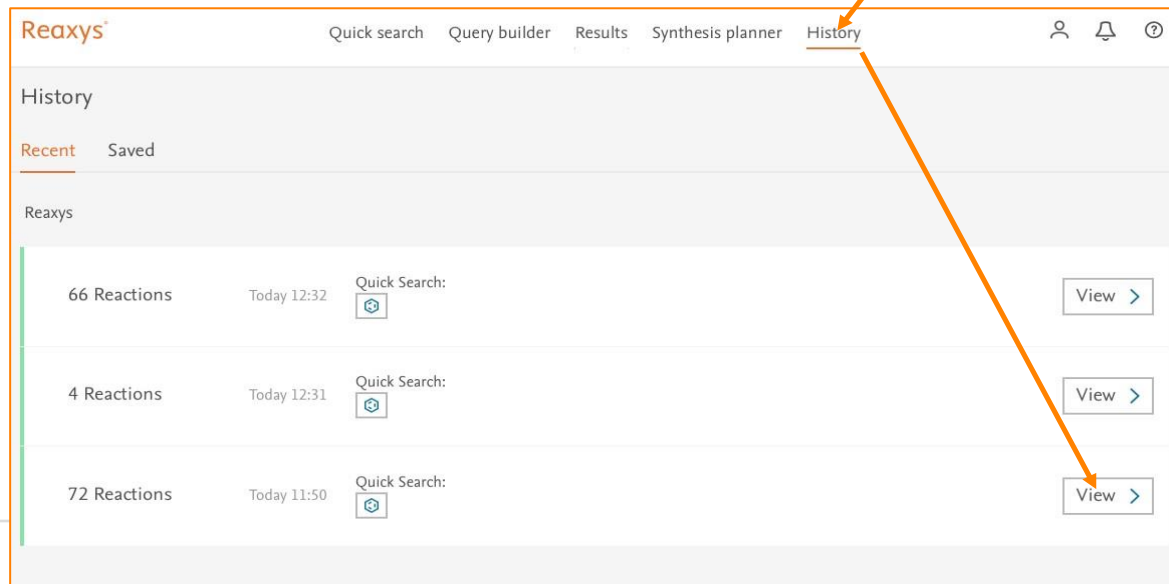
OK

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 displays the Reaxys web interface. At the top, a navigation bar includes the Reaxys logo and links for Quick search, Query builder, Results, Synthesis planner, and History. The History tab is selected. Below the navigation bar, there are tabs for Recent and Saved. The main content area shows 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 search icon, and a 'View >' button. Three orange arrows point to the 'View >' buttons for the first three results.

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. An 'Options' menu is open over the table, with the 'Use as filter' option highlighted. The table contains the following data:

Yield	Conditions	References
80%	With potassium hydroxide in 1-methyl-pyrrolidin-2-one at 100°C; 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 v	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 v	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 full text

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

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

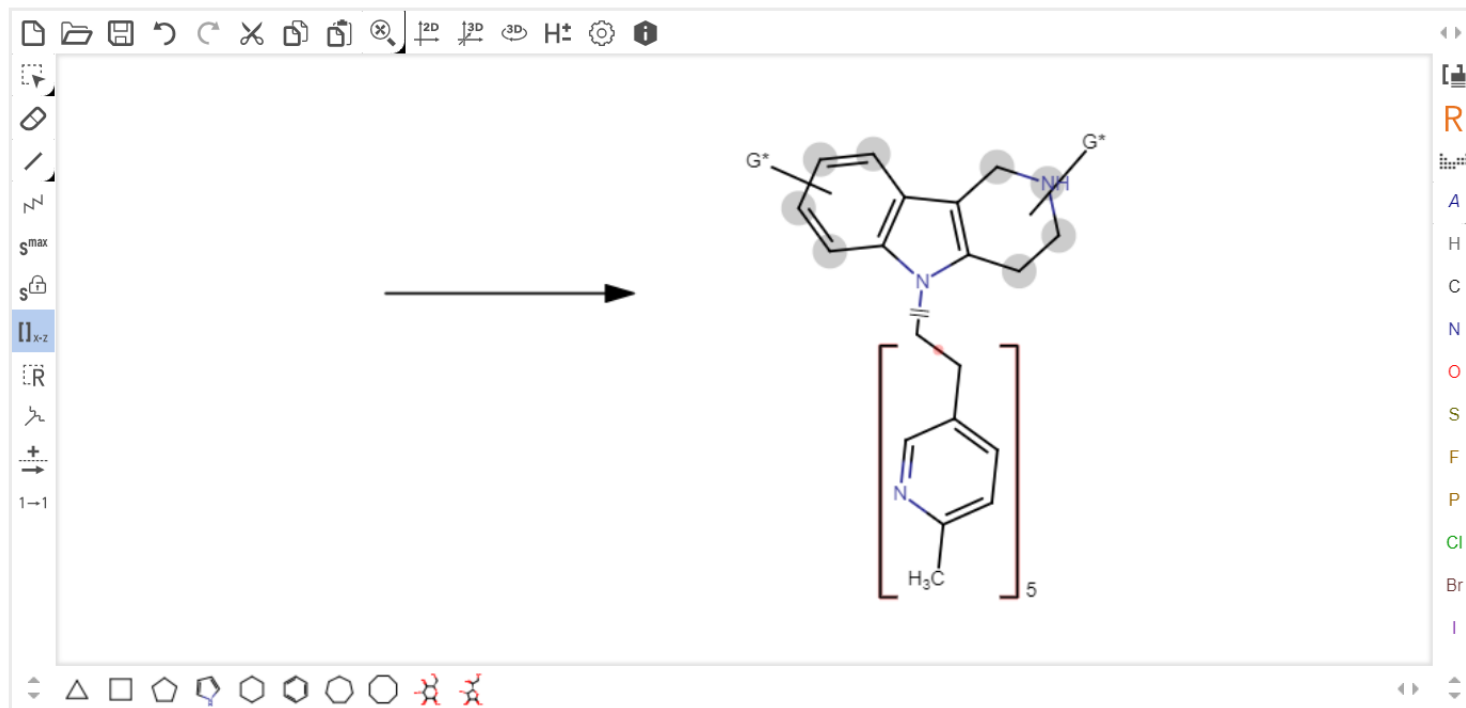
The screenshot shows the Reaxys web interface. On the left, the 'Filters and Analysis' sidebar is visible, with the 'Limit to' and 'Exclude' buttons highlighted by an orange circle. The 'By Structure' section shows a chemical structure of 4-methyl-3-vinylpyridine. The main area displays a chemical reaction (Reaction ID: 29081341) and a table of results.

Reaction ID: 29081341

Chemical reaction scheme showing the reaction of 4-methyl-3-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, Voldemur M.; Khvat, 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

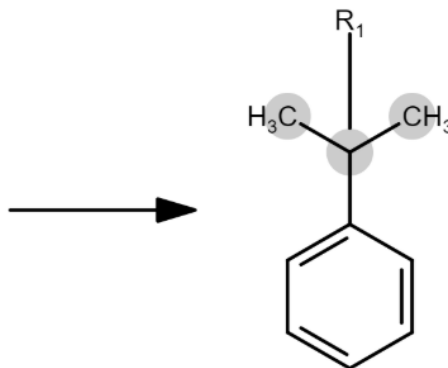


trigonal



AND

◇ Structure



As drawn

crystal system, crystal phase, crystal properties...

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

AND

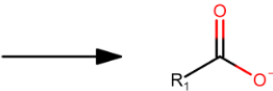
◇ Crystal Phase ☐ Find any Show fields ▾ (Description, Temperature, °C) ✕

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 ⓘ

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

☐ 0 selected



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 >

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

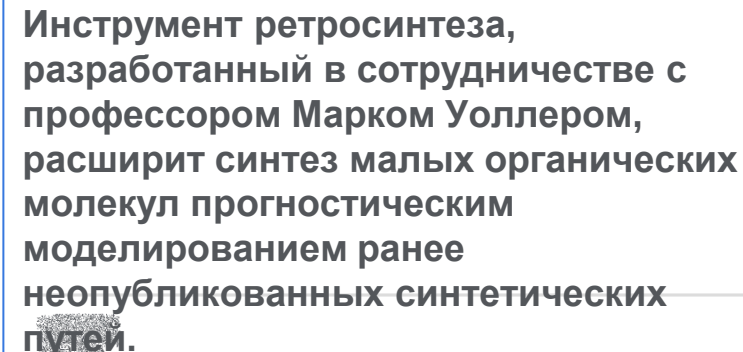
1500 - 1800	from α -Al ₂ O ₃ to β -Al ₂ O ₃			Goldschmidt, V. M.; Barth, T.; Lunde, G. ; Skr. Nor. Vidensk. - Akad., Kl. 1: Mat. - Naturvidensk. Kl.; nb. 7; (1925); p. 39, View in Reaxys ; vol. Al: MVol.B1; 2.9.1, page 78 - 80 ; (from Gmelin), View in Reaxys
Transport Data (92)				
Description (Transport 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

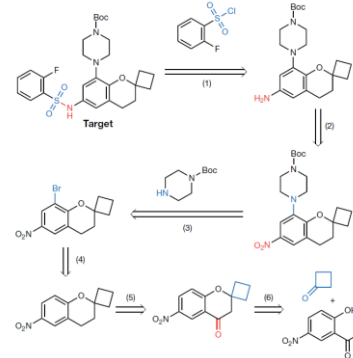
- Мы использовали наши данные для сотрудничества с некоторыми ведущими мировыми учеными в области хеминформатики, такими как профессор Марк Уоллер, для разработки возможности прогнозного ретросинтеза и доведения ее до наших клиентов. Очень скоро исследователи и химики смогут спросить ReaxysAI о том,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



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.



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



Прогнозирующий ретросинтез: переосмысление химии и изменение синтетических маршрутов

Harvard
Business
Review

DATA

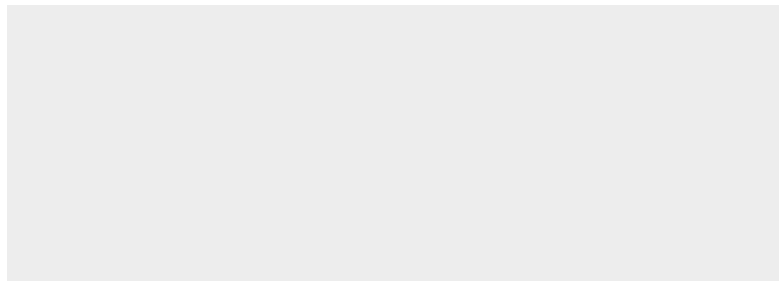
If Your Data Is Bad, Your Machine Learning Tools Are Useless

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?

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Спасибо за внимание!

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