

Reaxys



Самый короткий путь к эффективным
исследованиям и образованию в химии

The world's most prestigious award recognizing young chemists' work

The PhD Prize **recognises the research of extraordinary young chemists and celebrates the very best of chemistry research.**

No other award impacts the career of a young chemist like the Reaxys PhD Prize

It represents a great opportunity for **applicants, their research Group and academic institution to get further visibility** in Chemistry community.

2016 will mark the 7th edition of the prize. 2500 submissions have been received from over 400 universities in its 6-years history.

Each year, **45 finalists are selected by a panel of judges** out of hundreds of applicants. **3 winners** will then be awarded.

The **Chair of Reaxys PhD Prize Review Board** is a selection of **renowned chemistry experts** from around the world

All 45 entrants are given an opportunity to present their research **at the PhD Prize Symposium**

The **3 winners will be selected and announced at the banquet** closing the Symposium



Symposium is held in a different but equally **prestigious location**. In 2015, it was hosted in **Hong Kong**

All 45 finalists will be rewarded wide range of benefits including lifetime membership to **PhD Prize Club**, access to the **powerful network of 270 talented chemists** and **free access to Reaxys and Reaxys Medicinal Chemistry**

Each of the 3 winners receives an additional cheque for \$2000

Want to have a taste of PhD Symposium?



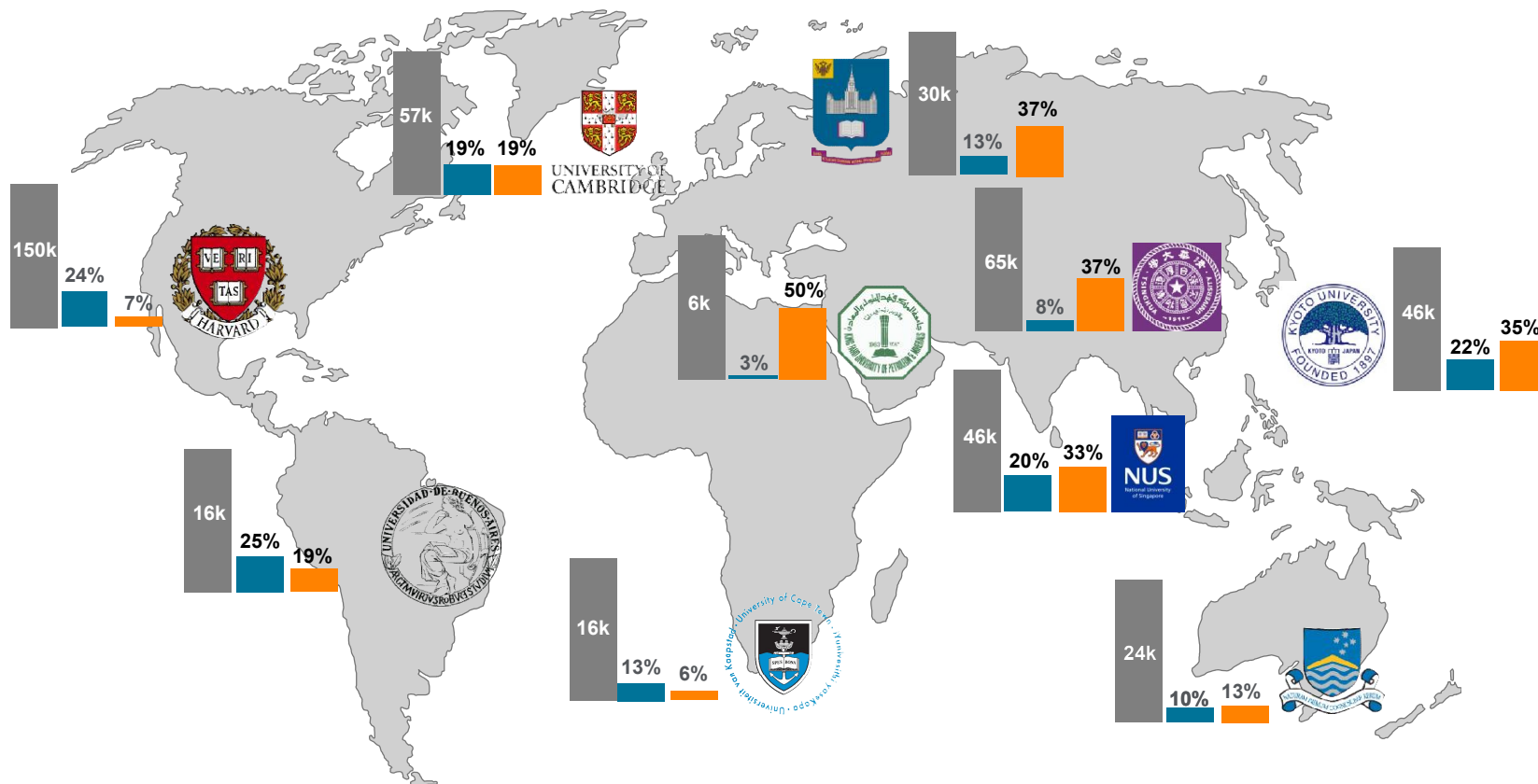
(click to play the video)

**Submissions for
2017 PhD Prize will
open soon**

Discover more on our website:
<http://inspiringchemistry.reaxys.com/phdprize>

Any question about the Reaxys PhD Prize?
Please email info@reaxys.ch

Химия является основным сегментом академической науки. Вклад химиков в публикационную активность составляет в среднем 30% по всему миру

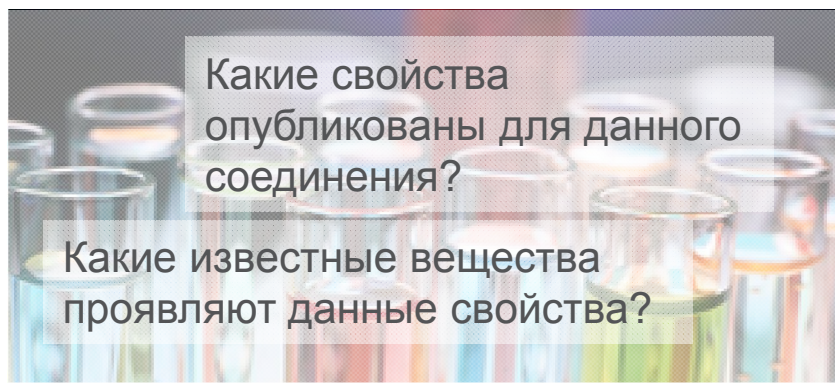


Всего публикаций 2010-2015

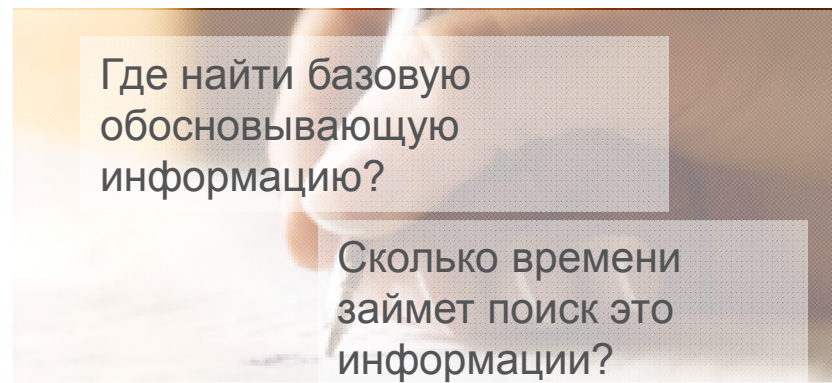
Науки о жизни

Химия

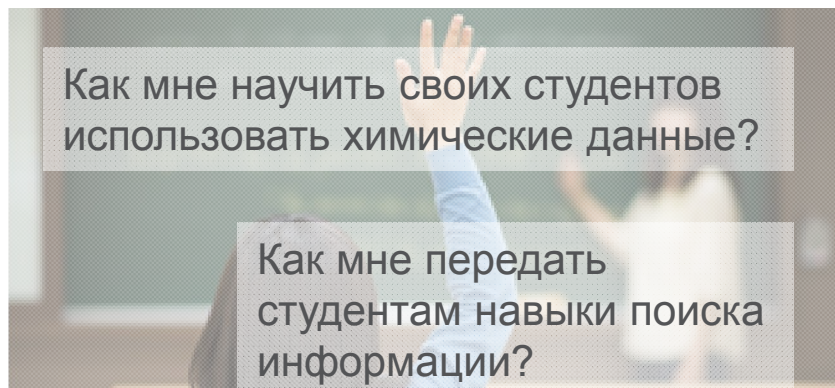
Химики в повседневной работе сталкиваются с рядом проблем, на решение которых затрачивается время, что снижает производительность труда



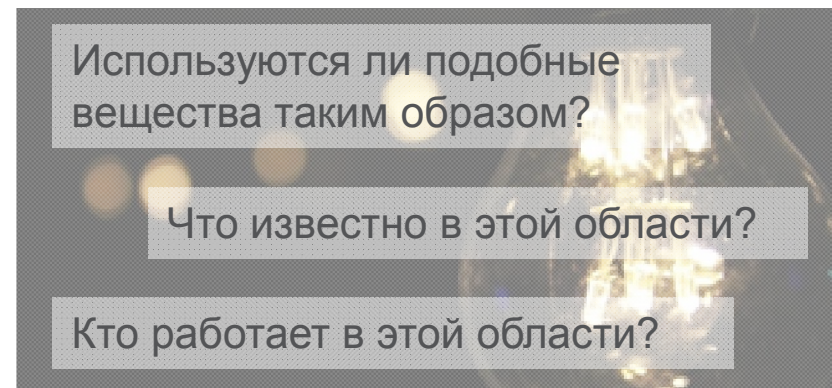
Руководство и планирование научной работой



Написание грантов



Обучение и наставничество



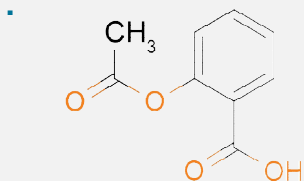
Новые идеи и сотрудничество

Поддержка работы студентов и сотрудников химиков:

- Повышает репутацию на международной арене
- Повышает эффективность научной работы
- Увеличивает финансовый отдачи от грантов, услуг, ИС
- Развивает инновационные технологии в рамках реализации стратегии импортозамещения
- Развивает российские фармацевтические НИОКР в рамках программы Фарма-2020

Вклад такой поддержки выходит далеко за пределы химического факультета

Знания о
соединениях..



...их
свойствах...



...и как это
поменять...



**Основные
принципы
химии**

... актуальны для широкого спектра других дисциплин

Наука о материалах
Природопользование
Геологические Науки
Археология
Палеонтология
Нанотехнологии

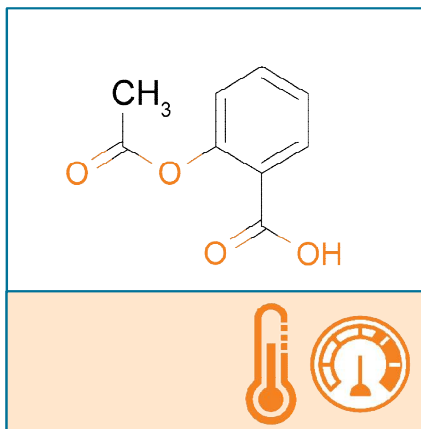
С-Х наук
Пищевых наук
Гидрологии
Лимнология
Токсикология
Исследование поверхности
Клинические исследований

Молекулярная
Биология
Клеточная Биология
Фармакология
Биохимия
Биомедицина
Биотехнологии
И многие другие...

**Используются
в различных
дисциплинах**

Reaxys

Информационная система, построенная для отражения реального использования химических знаний



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



40.7 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 материаловедения, биомедицины, наук о Земле, технических и экологических наук, фармакологии...

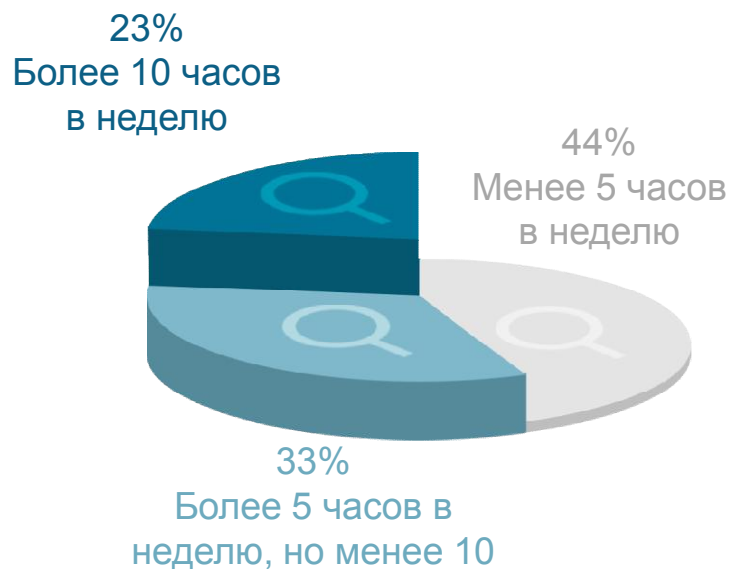
Применение в различных дисциплинах

Основные принципы химии

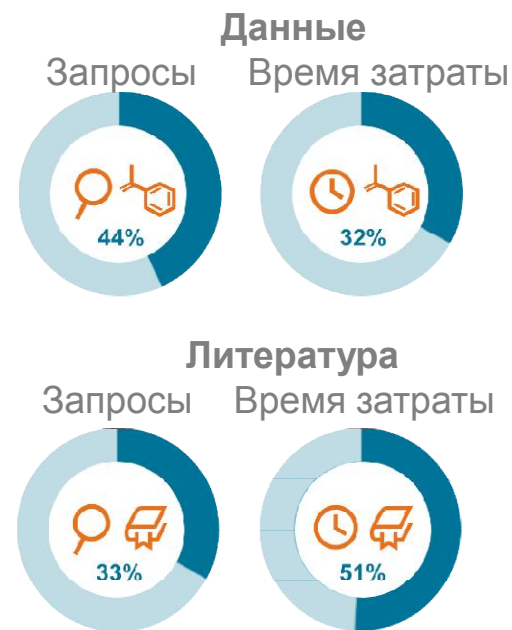
Reaxys

Снижает перегрузку информацией за счет курированных, качественно извлеченных данных

Более 50% химиков тратят не менее 5 часов в неделю в поиске информации.



Химики тратят непропорционально много времени на поиски литературы.



Retrieving extracted data is faster than finding answers in full-text literature.



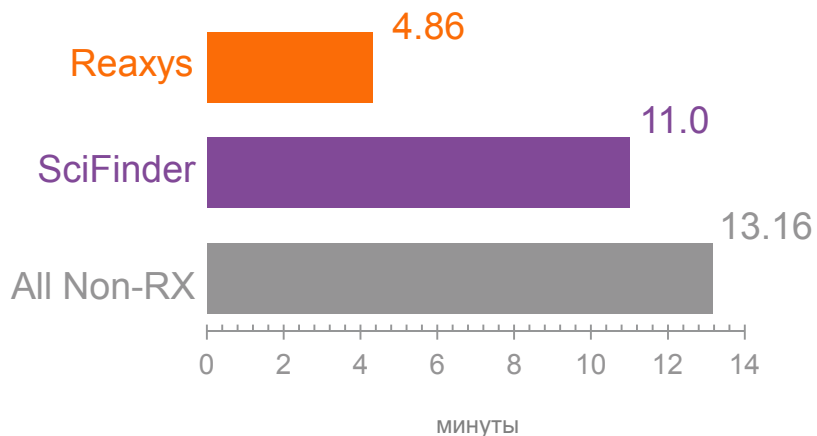
Поиск **извлеченных данных** выполняется **быстрее**, чем поиск **полнотекстовой литературы**

Reaxys

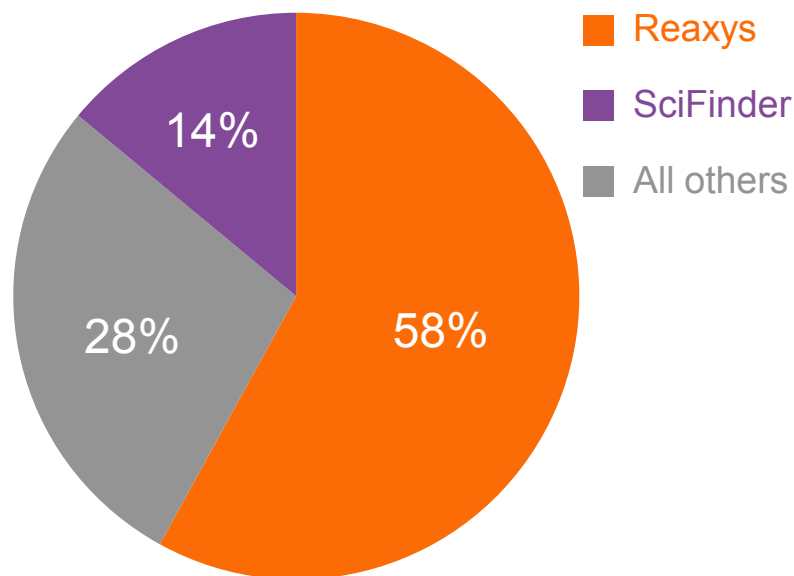
Информационная система, предназначенная для
ответа на исследовательские вопросы на лету

Опрос The ChemSearch Challenge

Пользователи Reaxys находят
ответы более чем вдвое быстрее,
чем другие пользователи



Лучшие конкурсанты,
58% использовали Reaxys



Reaxys

Responds to what really matters in chemistry (Re)search

Это мощный комплексный исследовательский инструмент для поиска фактов и литературы

Большинство пользователей используют содержащиеся записи **Соединений** и **Реакций**, но мало только некоторые воспользовались всеми преимуществами обширной, качественной базой **литературы**.



Synthesize
Find similar

Rx-ID: 24815350
Find similar reactions

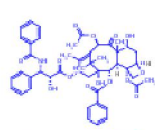
88.1%

Stage #1: With boron tribromide in chloroform
T=23 - 26°C; 0.283333 h;
Stage #2: With ammonia; water in chloroform
T=-5 - 0°C; 0.5 h;
[Show Experimental Procedure](#)

DR PHARMA NOVA, LLC
Patent: WO2006/91885 A2, 2006;
Location in patent: Page/Page column 51;
[Title/Abstract](#) [Full Text](#) [Show Details](#)

Title of the Document	Author's	Year	Source
Fused heterocyclic compounds Learning bridgehead nitrogen as patent HIV-1 NNRTIs. Part 1: Design, synthesis and biological evaluation of novel 5,7 disubstituted pyrazolo[1,5-a]pyrimidine derivatives	Tian, Ye; Dai, Daping; Rai, Divakar; Wang, Liu; Liu, Huigang; Zhan, Peng; De Clercq, Erik; Pannecouque, Christophe; Liu, Xinyong	2014	Bioorganic and Medicinal Chemistry, 2014, vol. 22, # 7 p. 2052-2059 Full Text View citing articles





Synthesize | [Show Details](#)
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Chemical Name:
PACLITAXEL

Reaxys Registry Number: 4290260
CAS Registry Number: 33069-62-4
Type of Substance: heterocyclic
Molecular Formula: C₄₇H₅₁NO₁₄
Linear Structure Formula: C₄₇H₅₁O₁₄N
Molecular Weight: 853.92
InChI Key: R.CINICONZJXQF-MZXODVADSA-N
Highest Clinical Phase: Marketed

Эти >51 Млн
Записей
документов
содержат ценную
информацию,
которую нельзя
найти в других
системах

Обеспечивает информационный „взгляд“ на содержание документа

European Journal of Medicinal Chemistry 92 (2015) 754–765

Contents lists available at ScienceDirect

European Journal of Medicinal Chemistry

journal homepage: <http://www.elsevier.com/locate/ejmech>

Original article

Fused heterocycles bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 3: Optimization of [1,2,4]triazolo[1,5-a]pyrimidine core via structure-based and physicochemical property-driven approaches

Boshi Huang^a, Cuicui Li^a, Wenmin Chen^a, Tao Liu^a, Mingyan Yu^b, Lu Fu^a, Yueyue Sun^a, Huiqing Liu^c, Erik De Clercq^d, Christophe Pannecouque^d, Jan Balzarini^d, Peng Zhan^{a,*}, Xinyong Liu^{a,*}

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^b Shandong Institute for Food and Drug Control, 2749 Xindao Street, 250101 Jinan, Shandong, PR China

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ARTICLE INFO

Article history:

Received 20 September 2014

Received in revised form 21 January 2015

Accepted 21 January 2015

Available online 22 January 2015

Keywords:

Triazolopyrimidines

Structure-based drug design

Biological activity

HIV-1 RT

Physicochemical properties

Molecular simulations

ABSTRACT

In our arduous efforts to develop new potent HIV-1 non-nucleoside reverse transcriptase (RT) inhibitors (NNRTIs), novel piperidine-linked [1,2,4]triazolo[1,5-a]pyrimidine derivatives were designed, synthesized and evaluated for their antiviral activities in MT-4 cell cultures. Biological results showed that all of the title compounds displayed moderate to excellent activities against wild-type (wt) HIV-1 strain (II₉) with EC₅₀ values ranging from 8.1 nM to 2284 nM in a cell-based assay. Among them, the most promising analog 7d possessed an EC₅₀ value of 8.1 nM against wt HIV-1, which was much more potent than the reference drugs DDI, 3TC, NVP and DLV. Additionally, 7d demonstrated weak activity against the double mutant HIV-1 strain (K103N + Y181C), and was more efficient than NVP in a RT inhibition assay. Besides, some measured and calculated physicochemical properties of 7d, like log P and water solubility, as well as the structure–activity relationships (SARs) analysis have been discussed in detail. Furthermore, the binding mode of the active compound 7d was rationalized by molecular simulation studies.

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Table 1
Anti-HIV-1 activity and cytotoxicity of the novel [1,2,4]triazolo[1,5-a]pyrimidine compounds in MT-4 cells infected with HIV-1 strain II₉.

7a–7f

7a, 7b

7c, 7d

7e, 7f

7g, 7h

7i, 7j

7k, 7l

7m, 7n

7o, 7p

7q, 7r

7s, 7t

7u, 7v

7w, 7x

7y, 7z

7aa, 7ab

7ac, 7ad

7ae, 7af

7ag, 7ah

7ai, 7aj

7ak, 7al

7am, 7an

7ao, 7ap

7aq, 7ar

7as, 7at

7au, 7av

7aw, 7ax

7ay, 7az

7ba, 7bb

7bc, 7bd

7be, 7bf

7bg, 7bh

7bi, 7bj

7bk, 7bl

7bm, 7bn

7bo, 7bp

7bq, 7br

7bs, 7bt

7bu, 7bv

7bw, 7bx

7by, 7bz

7ca, 7cb

7cc, 7cd

7ce, 7cf

7cg, 7ch

7ci, 7cj

7ck, 7cl

7cm, 7cn

7co, 7cp

7cq, 7cr

7cs, 7ct

7cu, 7cv

7cw, 7cx

7cy, 7cz

7da, 7db

7dc, 7dd

7de, 7df

7dg, 7dh

7di, 7dj

7dk, 7dl

7dm, 7dn

7do, 7dp

7dq, 7dr

7ds, 7dt

7du, 7dv

7dw, 7dx

7dy, 7dz

7ea, 7eb

7ec, 7ed

7ee, 7ef

7eg, 7eh

7ei, 7ej

7ek, 7el

7em, 7en

7eo, 7ep

7eq, 7er

7es, 7et

7eu, 7ev

7ew, 7ex

7ey, 7ez

7fa, 7fb

7fc, 7fd

7fe, 7ff

7fg, 7fh

7fi, 7fj

7fk, 7fl

7fm, 7fn

7fo, 7fp

7fq, 7fr

7fs, 7ft

7fu, 7fv

7fw, 7fx

7fy, 7fz

7ga, 7gb

7gc, 7gd

7ge, 7gf

7gg, 7gh

7gi, 7gj

7gk, 7gl

7gm, 7gn

7go, 7gp

7gq, 7gr

7gs, 7gt

7gu, 7gv

7gw, 7gx

7gy, 7gz

7ha, 7hb

7hc, 7hd

7he, 7hf

7hg, 7hh

7hi, 7hj

7hk, 7hl

7hm, 7hn

7ho, 7hp

7hq, 7hr

7hs, 7ht

7hu, 7hv

7hw, 7hx

7hy, 7hz

7ia, 7ib

7ic, 7id

7ie, 7if

7ig, 7ih

7ii, 7ij

7ik, 7il

7im, 7in

7io, 7ip

7iq, 7ir

7is, 7it

7iu, 7iv

7iw, 7ix

7iy, 7iz

7ja, 7jb

7jc, 7jd

7je, 7jf

7jg, 7jh

7ji, 7jj

7jk, 7jl

7jm, 7jn

7jo, 7jp

7jq, 7jr

7js, 7jt

7ju, 7jv

7jw, 7jx

7jy, 7jz

7ka, 7kb

7kc, 7kd

7ke, 7kf

7kg, 7kh

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7kq, 7kr

7ks, 7kt

7ku, 7kv

7kw, 7kx

7ky, 7kz

7la, 7lb

7lc, 7ld

7le, 7lf

7lg, 7lh

7li, 7lj

7lk, 7ll

7lm, 7ln

7lo, 7lp

7lq, 7lr

7ls, 7lt

7lu, 7lv

7lw, 7lx

7ly, 7lz

7ma, 7mb

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7ng, 7nh

7ni, 7nj

7nk, 7nl

7nm, 7nn

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7nq, 7nr

7ns, 7nt

7nu, 7nv

7nw, 7nx

7ny, 7nz

7oa, 7ob

7oc, 7od

7oe, 7of

7og, 7oh

7oi, 7oj

7ok, 7ol

7om, 7on

7oo, 7op

7oq, 7or

7os, 7ot

7ou, 7ov

7ow, 7ox

7oy, 7oz

7pa, 7pb

7pc, 7pd

7pe, 7pf

7pg, 7ph

7pi, 7pj

7pk, 7pl

7pm, 7pn

7po, 7pp

7pq, 7pr

7ps, 7pt

7pu, 7pv

7pw, 7px

7py, 7pz

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7qc, 7qd

7qe, 7qf

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7qo, 7qp

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7qy, 7qz

7ra, 7rb

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7rg, 7rh

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7rk, 7rl

7rm, 7rn

7ro, 7rp

7rq, 7rr

7rs, 7rt

7ru, 7rv

7rw, 7rx

7ry, 7rz

7sa, 7sb

7sc, 7sd

7se, 7sf

7sg, 7sh

7si, 7sj

7sk, 7sl

7sm, 7sn

7so, 7sp

7sq, 7sr

7ss, 7st

7su, 7sv

7sw, 7sx

7sy, 7sz

7ta, 7tb

7tc, 7td

7te, 7tf

7tg, 7th

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7tm, 7tn

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7tq, 7tr

7ts, 7tt

7tu, 7tv

7tw, 7tx

7ty, 7tz

7ua, 7ub

7uc, 7ud

7ue, 7uf

7ug, 7uh

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7uk, 7ul

7um, 7un

7uo, 7up

7uq, 7ur

7us, 7ut

7uu, 7uv

7uw, 7ux

7uy, 7uz

7va, 7vb

7vc, 7vd

7ve, 7vf

7vg, 7vh

7vi, 7vj

7vk, 7vl

7vm, 7vn

7vo, 7vp

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7vw, 7vx

7vy, 7vz

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7wo, 7wp

7wq, 7wr

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7wu, 7wv

7ww, 7wx

7wy, 7wz

7xa, 7xb

7xc, 7xd

7xe, 7xf

7xg, 7xh

7xi, 7xj

7xk, 7xl

7xm, 7xn

7xo, 7xp

7xq, 7xr

7xs, 7xt

7xu, 7xv

7xw, 7xx

7xy, 7xz

7ya, 7yb

7yc, 7yd

7ye, 7yf

7yg, 7yh

7yi, 7yj

7yk, 7yl

7ym, 7yn

7yo, 7yp

7yq, 7yr

7ys, 7yt

7yu, 7yv

7yw, 7yx

7yy, 7yz

7za, 7zb

7zc, 7zd

7ze, 7zf

7zg, 7zh

7zi, 7zj

7zk, 7zl

7zm, 7zn

7zo, 7zp

7zq, 7zr

7zs, 7zt

7zu, 7zv

7zw, 7zx

7zy, 7yz

Запись документа включает библиографическую информацию...

Title of the Document	Authors	Year	Source
Fused heterocyclic compounds bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 1: Design, synthesis and biological evaluation of novel 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives	Tian, Ye; Du, Deping; Rai, Diwakar; Wang, Liu; Liu, Huiqing; Zhan, Peng; De Clercq, Erik; Pannecouque, Christophe; Li, Xinyong	2014	Bioorganic and Medicinal Chemistry, 2014, vol. 22, # 7 p. 2052 - 2059 Full Text View citing articles

Ссылка

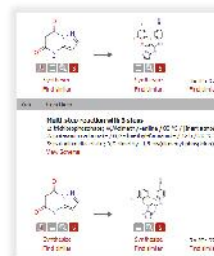
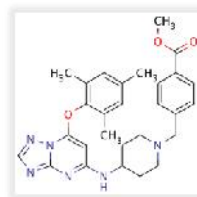
Название

Авторы

Резюме

Abstract
Fused heterocyclic compounds bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 1: Design, synthesis and biological evaluation of novel 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives
In our continuous efforts to identify novel potent HIV-1 NNRTIs, a novel class of 5,7-disubstituted pyrazolo[1,5-a]pyrimidine derivatives were rationally designed, synthesized and evaluated for their anti-HIV activities in MT-4 cell cultures. Biological results showed that all of the title compounds displayed moderate to excellent activity against wild-type HIV-1 with a wide range of EC₅₀ values from 5.98 to 0.07 μM. Among the active compounds, 5a was found to be the most potent compound with an EC₅₀ of 0.07 μM against wild-type HIV-1 and very high selectivity index (SI, 3999). Compound 5a was more effective than the reference drugs nevirapine (NVP) and delamanvir (DMV). In order to further confirm their binding target, an HIV-1 RT inhibitory assay was also performed. Furthermore, SAR analysis among the newly synthesized compounds was discussed and the binding mode of the active compound 5a was rationalized by molecular modeling studies.

...и связана с контентом, организованным в записи Соединений и Реакций, а также с полями свойств



Соединения

Реакции

Свойства

Отображает соответствие источника ряду дисциплин

В дополнение к ключевым словам автора записи Документов указывают индексацию с другими лидирующими на рынке базами данных



With geographic,
species and drug
tradename indexing

Keywords:

Author: [antiviral activity](#); Bignoniaceae; EMCV; HSV-1; in vitro assays; plant extracts; VACV

Compendex Free Language: [Antiviral activities](#); Bignoniaceae; EMCV; HSV-1; In-vitro assays

Compendex Descriptor: Assays; Bromine compounds; Ethanol

Compendex Mainhead: Viruses

EMTREE drug term: acidovir; alpha2a interferon; natural product; plant extract

GEObase Subject Index: [antimicrobial activity](#); dicotyledon; ethanol; ethnobotany; medic

EMTREE medical term: animal cell; [antiviral activity](#); article; Bignoniaceae; Brazil; controlled

Murine encephalomyelitis virus; nonhuman; plant leaf; plant stem; Vaccinia virus; Vero cell

Medline descriptor: Animals; [Antiviral Agents](#); Bignoniaceae; Brazil; Cercopithecus aethiop

Tests; Plant Extracts; Vaccinia virus; Vero Cells

Regional Index: Brazil; Minas Gerais

Species index: Bignoniaceae; Encephalomyocarditis virus; Human herpesvirus 1; Murinae; V

Reaxys Terms: 3-(4,5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide; [natural prod](#)

Tradename: bi 201335 (Boehringer Ingelheim)

Tradename: bms 650032 (Bristol Myers Squibb)

Tradename: bms 790052 (Bristol Myers Squibb)

Tradename: incivek (Novartis)

Tradename: nim 811 (Pharmasset)

Tradename: psi 7977 (Scynexis)

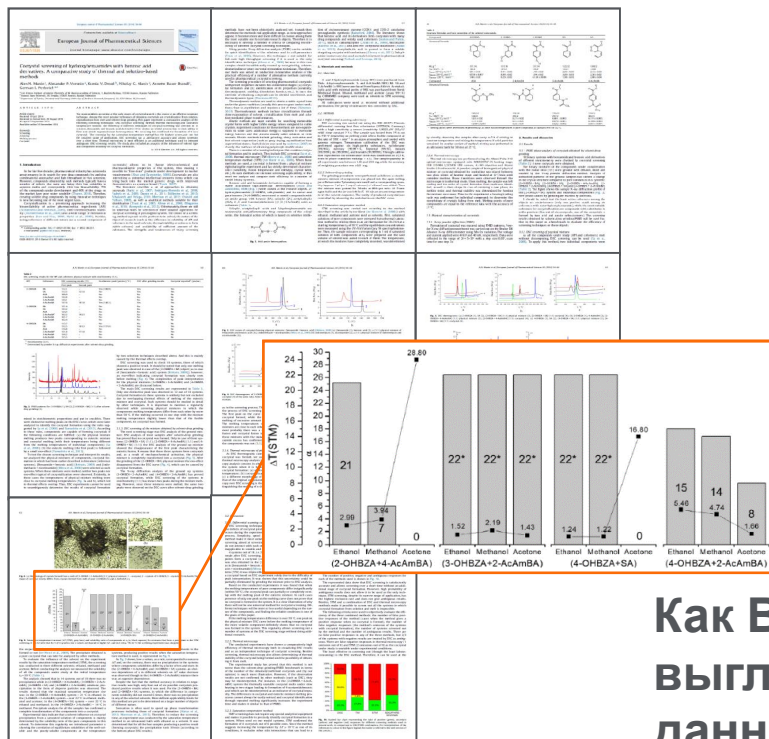
Tradename: scy 635 (Johnson and Johnson)

Tradename: tmc 435

Tradename: victrelis

Обеспечивает данными, которые можно использовать напрямую

Использование **растворимости соединения** требует знания **температуры** и **растворителя** использованных при измерении



Structure	Structure/Compound Data	N° of preparations All times, 1, all reactions	Available Data	Target	N° of ref.
	Chemical Name: acetylsalicylate Reaxys Registry Number: 779271 CAS Registry Number: 50-70-2 Type of Substance: isocyclic Molecular Formula: C ₉ H ₈ O ₄ Linear Structure Formula: C ₉ H ₈ O ₄ COOH Molecular Weight: 180.16 InChI Key: REHJWQWZBQCLUPFFACYSAN Highest Clinical Phase: Marketed	94 prep out of 958 reactions	HR Data (85) Druglikeness Bioactivity Identification Physical Data (323) Spectra (155) Ecological Data (5) Use/Application (222) Quantum Chemical Data (5)	Show Targets	3794
Chemical Names and Synonyms: acetylsalicylate, acetylsalicylic acid, acetylsalicylic Acid HR Data Solubility (mg/L) / (601818 out of 80 view all)					
181.781 g·l ⁻¹	20 °C	acetone			Masini, Alex N; Vercini, Alexander F; Drend, Ksenia V; Masin, Nikolay G; Bauer-Brandl, Annette; Penkovic, Gertman F; European Journal of Pharmaceutical Sciences, 2014, - vol. 65, p. 55 - 64 Title/Abstract Full Text View citing articles Show Details

181.781 g·l ⁻¹	20 °C	acetone
---------------------------	-------	---------

Как Вы
выглядят эти
данные в
литературе

Как Вы
выглядят эти
данные в
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 Constant
Ionization Potential
Isoelectric Point
Kinematic Viscosity
Liquid Phase
Magnetic Data
Mechanical Properties
Molecular Deformation
Optical Data
Thermomechanical Data
Solubility
Solution Behavior
Sound Properties
Static Dielectric Constant
Surface Tension
Transition Points
Transport Data

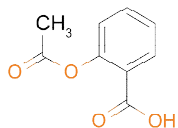
NMR Spectroscopy
IR Spectroscopy
Mass Spectroscopy
UV/VIS Spectroscopy
ESR Spectroscopy
NQR Spectroscopy
Raman Spectroscopy
Luminescence Spectroscopy
Fluorescence Spectroscopy
Exposure Assessment
Bioaccumulation
Biomagnification
Degradation
Stability in Soil
Oxygen Demand
Uses
Isolation from Natural 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...

Solubility

Делает информацию быстро и легко доступной



Записи Соединений
содержат все
извлеченные данные о
свойствах соединений.

Быстрый поиск
конкретных свойства
веществ

Легко найти все вещества,
которые имеют
определенное свойство



Записи документов
проиндексированы по
ключевым словам из
различных источников,
включая ведущие базы
данных EMBASE,
GeoBase и Compendex.

Используйте знакомые
термины, чтобы найти
релевантные результаты

Создание
высокоспецифичных
поисков



Записи реакций
содержат извлеченные
данные о реакциях
(выход, растворитель
температура и др.) из
множества исходных
источников.

Прямой поиск полезной
информацию для
планирования работы

Планировщик синтеза
упорядочивает реакции из
нескольких источников
для ретросинтетического
планирования



Новички



Промежуточные
пользователей



Эксперты

ПОВЫШЕНИЯ НАВЫКОВ В ПОИСКЕ ИНФОРМАЦИИ
ВСЕ БОЛЕЕ ИЗЯЩНЫЕ СПОСОБЫ ИСПОЛЬЗОВАНИЯ ИНФОРМАЦИИ

Простота использования

- Google-подобный поисковик
- Интуитивный Интерфейс
- Поддержка при поиске правильных поисковых терминов

Управление поиском

- Прозрачные функциональные возможности
- Объединение понятий в одном поиске
- Усечение, близость и логические операторы

Комплексное использование данных

- Инструменты расширенного поиска
- Интеллектуальный анализ данных и моделирование

и Reaxys становится только лучше

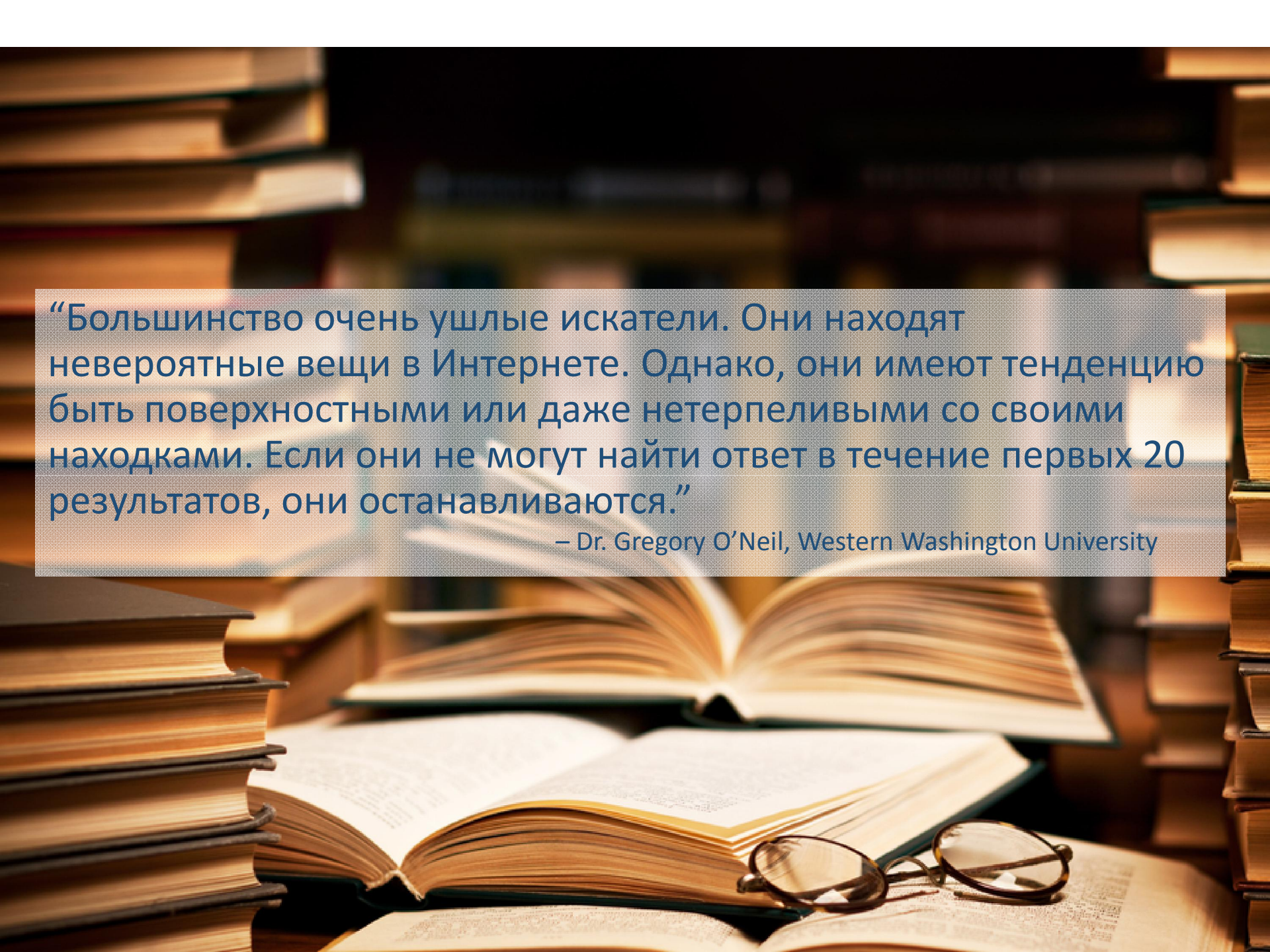
Выводы от 'педагогов'

Elsevier обзвонил преподавателей и библиотекарей в ВУЗах в США

Поговорили **138 людьми**

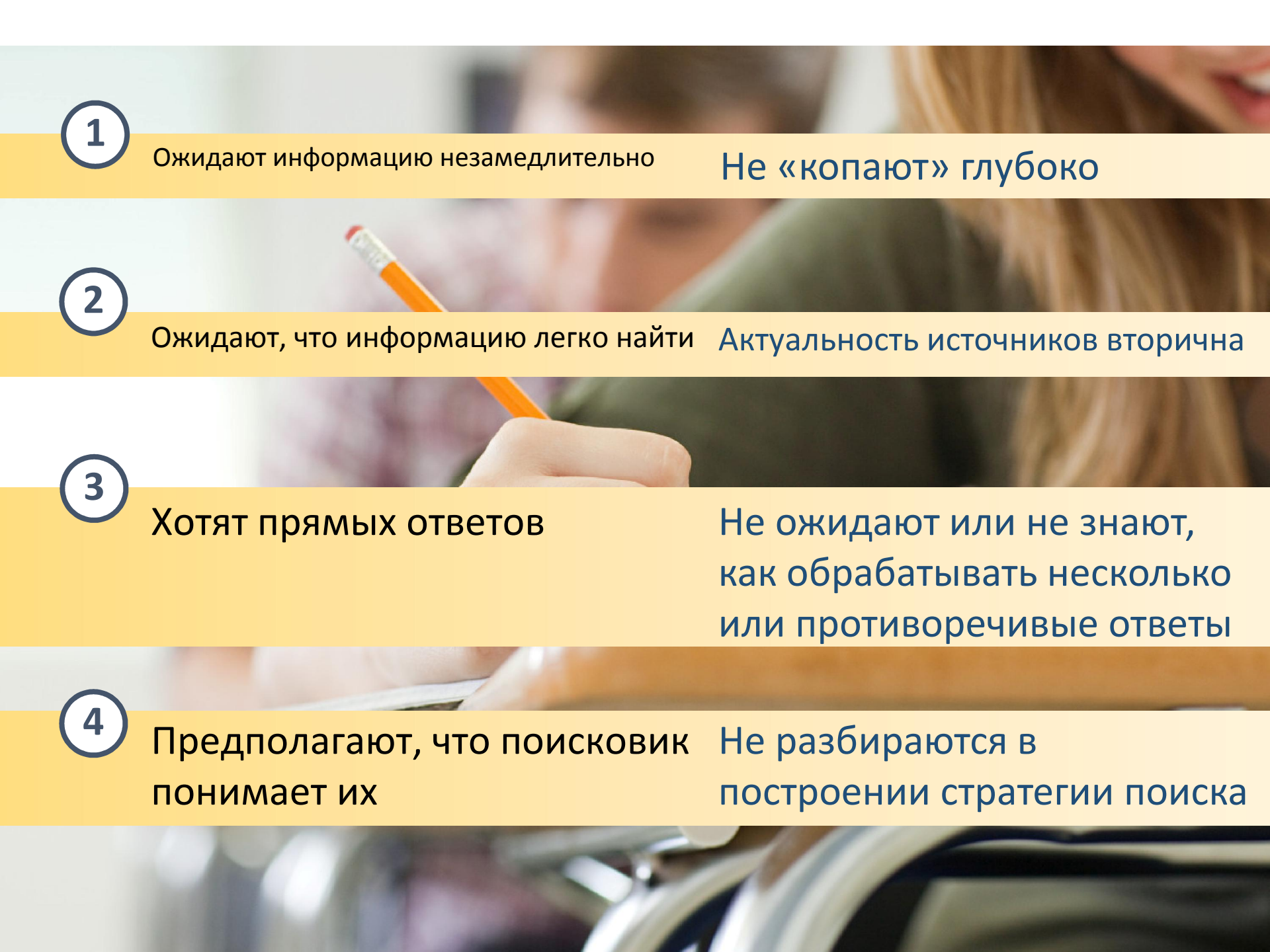
- 19 библиотекарей
- 119 сотрудники, лекторы, руководители лабораторных работ на химических факультетах

Открытая дискуссия о потребностях при преподавании



“Большинство очень ушлые искатели. Они находят невероятные вещи в Интернете. Однако, они имеют тенденцию быть поверхностными или даже нетерпеливыми со своими находками. Если они не могут найти ответ в течение первых 20 результатов, они останавливаются.”

– Dr. Gregory O’Neil, Western Washington University

A background image showing a blurred classroom scene with students. In the foreground, a hand holds an orange pencil, ready to write on a piece of paper. The image is divided into four horizontal yellow bands, each containing a numbered point.

1

Ожидают информацию незамедлительно

Не «копают» глубоко

2

Ожидают, что информацию легко найти

Актуальность источников вторична

3

Хотят прямых ответов

Не ожидают или не знают,
как обрабатывать несколько
или противоречивые ответы

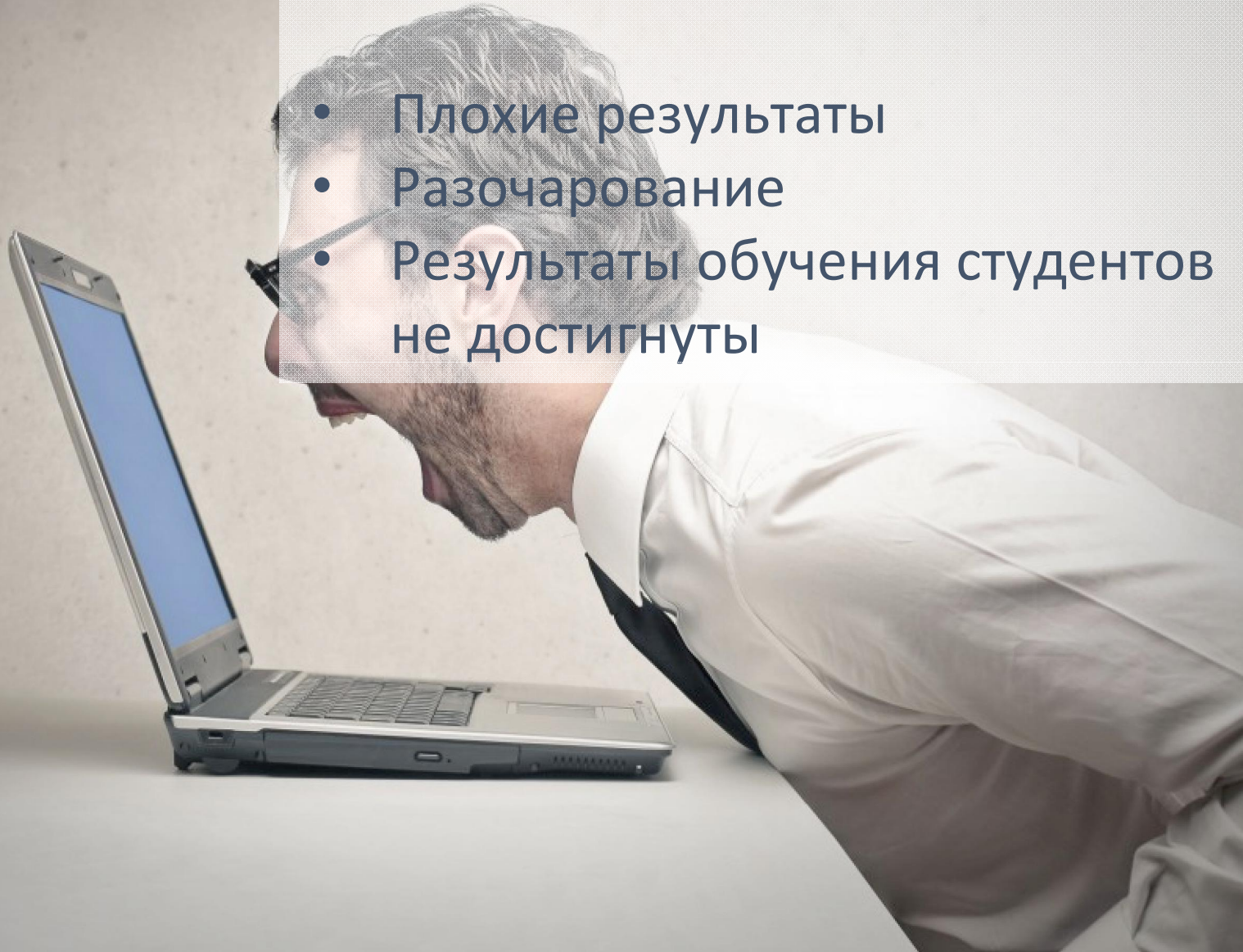
4

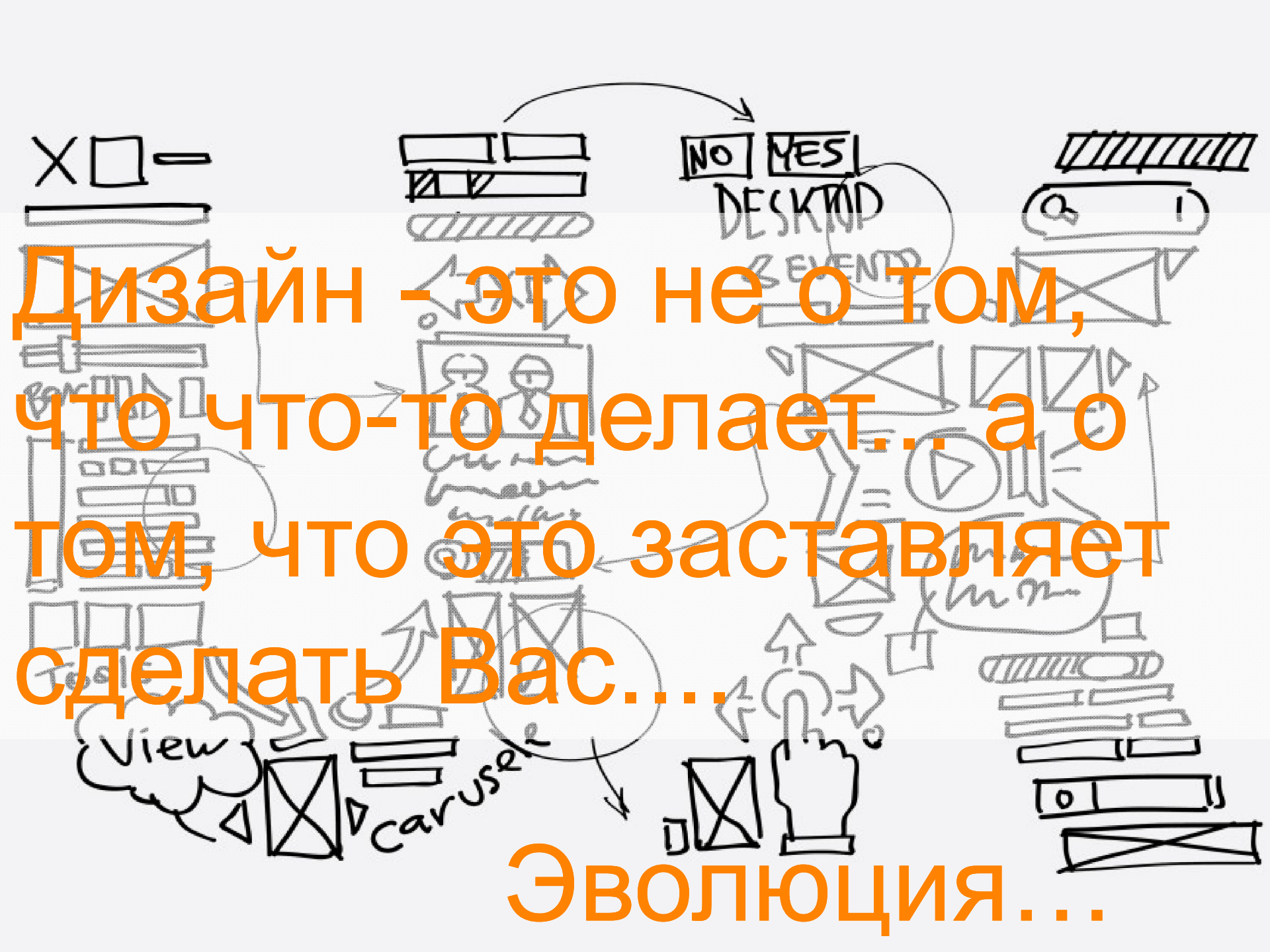
Предполагают, что поисковик
понимает их

Не разбираются в
построении стратегии поиска

Несоответствие структуры научной информации

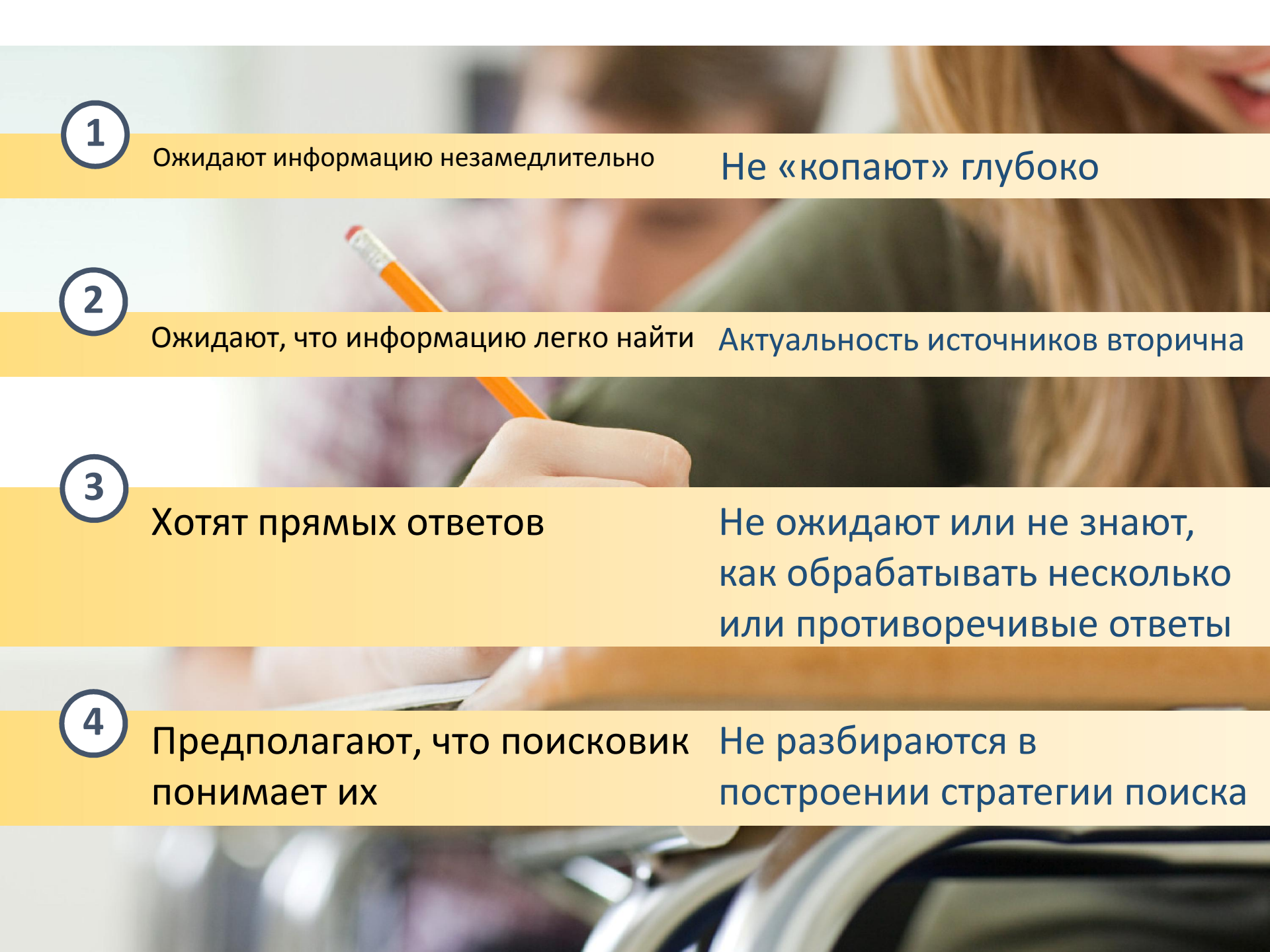
- Плохие результаты
- Разочарование
- Результаты обучения студентов не достигнуты



A hand-drawn sketch of a user interface design process. It features various UI elements like buttons, checkboxes, and text boxes, along with flow arrows indicating a sequence of actions. Labels include 'X', 'NO', 'YES', 'DESKTOP', 'EVENTS', 'View', and 'carousel'. There are also some scribbled-out elements and a hand icon pointing at a button.

Дизайн - это не о том,
что что-то делает... а о
том, что это заставляет
сделать Вас....

Эволюция...



1

Ожидают информацию незамедлительно

Не «копают» глубоко

2

Ожидают, что информацию легко найти

Актуальность источников вторична

3

Хотят прямых ответов

Не ожидают или не знают,
как обрабатывать несколько
или противоречивые ответы

4

Предполагают, что поисковик
понимает их

Не разбираются в
построении стратегии поиска

Устранение несогласованностей

4

Предполагают, что поисковик
понимает их

Не разбираются в
построении стратегии поиска

Дать студентам поисковик, который понимает их

или

Научить студентов строить стратегии поиска

или

И то и другое

Ask Reaxys

Search substances, reactions, citations and bioactivity data

 Substance Name, e.g. [Atenolol](#)



AND



Create Structure or Reaction Drawing

- Интерпретирует естественный язык
- Автоматически распознает замысел поиска (реакцию)
- Дает результаты незамедлительно

Позволяет быстрый поиск и беспрепятственное использование для НОВИЧКОВ

Search Reaxys

Q preparation of carbamazepine



Reaxys

Quick search

Query builder

Results

Synthesis planner

History

Logout

[← Back to Quick Search](#)

Choose a result for preparation of carbamazepine

Reactions

Product: carbamazepine (exact search)

[Preview Results](#)

[View Results](#)

4055

Documents

Titles, Abstracts and Keywords : Document Basic Index : formation; formations; make; making; manufacture; prep; preparation; preparation; preparations; prepare; prepared; preparing; preps; synthesis; synthesise AND Document Basic Index : carbamazepine

53876

Documents

Titles, Abstracts and Keywords : Document Basic Index : carbamazepine

[Preview Results](#)

[View Results](#)

7004798

Documents

Titles, Abstracts and Keywords : Document Basic Index : formation; formations; make; making; manufacture; prep; preparation; preparation; preparations; prepare; prepared; preparing; preps; synthesis; synthesise

[Preview Results](#)

[View Results](#)

Как Ask Reaxys
интерпретировал
поисковый запрос?

Как и в каком
контексте Ask
Reaxys получил
результаты?

Search Reaxys

Q alcohol oxidation ZrO2



Quick search

Query builder

Results

Synthesis planner

History

Logout



51

Documents

Document Basic Index : alcohol AND Document Basic Index : "oxidation"; "oxidation reaction"; "oxidation reactions"; "oxidations"; "oxydation"; "oxydations" AND Document Basic Index : ZrO2

Preview Results ▾

View Results >

4346

Documents

Document Basic Index : "oxidation"; "oxidation reaction"; "oxidation reactions"; "oxidations"; "oxydation"; "oxydations" AND Document Basic Index : ZrO2

564

Documents

Document Basic Index : alcohol AND Document Basic Index : ZrO2

Preview Results ▾

View Results >

19793

Documents

Document Basic Index : alcohol AND Document Basic Index : "oxidation"; "oxidation reaction"; "oxidation reactions"; "oxidations"; "oxydation"; "oxydations"

Preview Results ▾

View Results >

Как Ask Reaxys
интерпретировал
поисковый запрос?

Как и в каком
контексте Ask
Reaxys получил
результаты?

Documents

Document Basic Index : alcohol AND Document Basic Index : "oxidation"; "oxidation reaction"; "oxidation reactions"; "oxidations"; "oxydation"; "oxydations" AND Document Basic Index : ZrO2

[Preview Results](#) ^

[View Results](#) >

Top 3 results

Investigating the catalytic activity of monoclinic zirconia; **oxidation** of benzyl **alcohol** in aqueous medium at mild conditions

Sadiq; Ilyas; Alam - Tenside, Surfactants, Detergents, 2012, vol. 49, # 1, p. 37 - 42

[Abstract](#) v

[Index Terms](#) ^

[Full Text](#) ↗

Cited 2 times

Index terms

×

Author keyword: Benzoic acid, Benzyl alcohol, Monoclinic zirconia, **Oxidation**, Wastewater

Compendex Terms: Aqueous medium, Benzoic acid, Benzyl alcohol, Catalyst loadings, Contaminated water, Double-walled, Monoclinic phase, Monoclinic zirconia, Optimal conditions, Partial pressure of oxygen, Reaction parameters, Substrate solution

Compendex Terms: Atmospheric pressure, Batch reactors, Carboxylic acids, Catalyst activity, **Oxidation**, Sewage, Wastewater, Zirconia, Zirconium alloys

Reaxys Index Terms: catalyst, catalyst activity, catalytic reaction, industrial waste, monoclinic crystal system, **oxidation reaction**

Устранение несогласованностей

3

Хотят прямых ответов

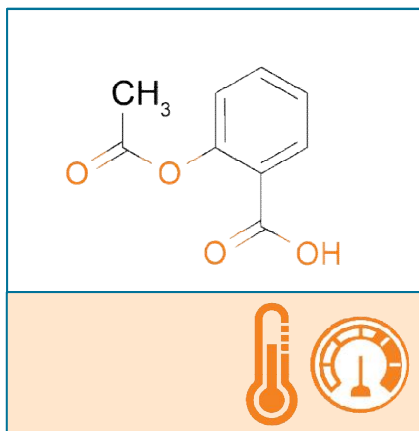
Не ожидают или не знают,
как обрабатывать несколько
или противоречивые ответы

Дать студентам реальные данные

Дать студентам возможность осмыслить
вариабельность данных

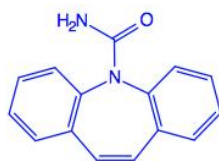
Извлеченные данные

Соединения могут иметь информацию во многих полях свойств, например, соединение carbamazepine содержит данные в ~3,000 полях и подполях.



>90 М записей соединений с >500 М извлеченных фактов о их **свойствах:** физических, химических, спектральных, экологических, биоактивность и др.

carbamazepin



Identification

Spectra - 120

Physical Data - 306

Bioactivity - 1203

Other Data - 1430

Preparations - 54 >

Reactions - 157 >

Documents - 1338 >

^ Spectra - 120

- ✓ Raman Spectroscopy - 9
- ✓ UV/VIS Spectroscopy - 40
- ✓ Mass Spectrometry - 30
- ✓ IR Spectroscopy - 24
- ✓ Fluorescence Spectroscopy - 3
- ✓ NMR Spectroscopy - 14

^ Physical Data - 306

- ✓ Liquid/Solid Systems (MCS) - 6
- ✓ Interatomic Distances and Angles - 4
- ✓ Further Information - 1
- ✓ Solubility (MCS) - 107
- ✓ Transport Phenomena (MCS) - 2
- ✓ Association (MCS) - 14
- ✓ Optics - 4
- ✓ Crystal Phase - 20
- ✓ Crystal System - 8
- ✓ Melting Point - 29

^ Bioactivity - 1203

- ✓ Pharmacological Data - 1154
- ✓ Ecotoxicology - 49

^ Other Data - 1430

- ✓ Abiotic Degradation, Hydrolysis - 3
- ✓ Abiotic Degradation, Photolysis - 14
- ✓ Transport and Distribution - 13
- ✓ Biodegradation - 5
- ✓ Exposure Assessment - 3
- ✓ Concentration in the Environment - 94
- ✓ Use - 1293
- ✓ Bioaccumulation, Biomagnification and Biomonitoring - 2
- ✓ Quantum Chemical Calculations - 3

Табулированные данные, позволяет студентам изучить эмпирические измерения и понять влияние экспериментальных условий

107 измерений
растворимости с
экспериментальными
данными и ссылками

^ Solubility (MCS) - 107

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Ratio of Solvents	Reference
0.164919	in pure solvent		water		Maswal, Masrat; Chat, Oyais Ahmad; Jabeen, Suraya; +4 others - RSC Advances, 2015, vol. 5, # 10, p. 7696 - 7712 Full Text ↗ Show details >
0.18 - 0.183	in pure solvent	37	water		Inoue, Yutaka; Sato, Sayuri; Yamamoto, Chisa; +2 others - Chemical and Pharmaceutical Bulletin, 2014, vol. 62, # 11, p. 1125 - 1130 Full Text ↗ Show details >
0.262		37	water		Shayanfar, Ali; Asadpour-Zeynali, Karim; Jouyban, Abolghasem - Journal of Molecular Liquids, 2013, vol. 187, p. 171 - 176 Full Text ↗ Cited 9 times ↗ Show details >

Устранение несогласованностей

2

Ожидают, что информацию
легко найти

Релевантность источников
вторична

Покажите студентам, как определить
релевантность документа-источника

Предоставить им "взгляд" в содержание
источника

Записи документов

Оценить релевантность в контексте ландшафта литературы

^ Solubility (MCS) - 107

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Ratio of Solvents	Reference
0.164919	in pure solvent		water		Maswal, Masrat; Chat, Oyais Ahmad; Jabeen, Suraya; +4 others - RSC Advances, 2015, vol. 5, # 10, p. 7696 - 7712
					Full Text ↗ Show details >

Solubilization and co-solubilization of carbamazepine and nifedipine in mixed micellar systems: Insights from surface tension, electronic absorption, fluorescence and HPLC measurements

Maswal, Masrat; Chat, Oyais Ahmad; Jabeen, Suraya; +4 others - RSC Advances, 2015, vol. 5, # 10, p. 7696 - 7712

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

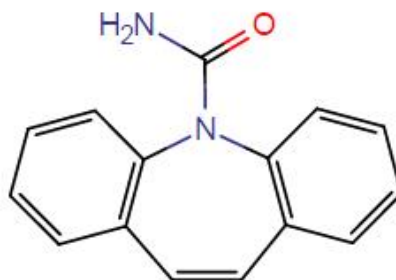
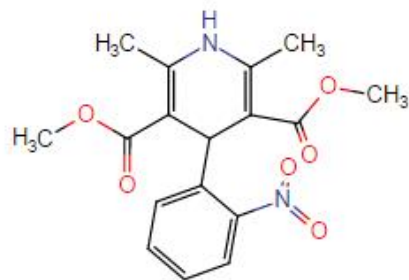


Abstract

UV absorption spectral and HPLC study on the solubilization and co-solubilization behavior of antiepileptic drug Carbamazepine (CBZ) and calcium channel blocker Nifedipine (NFD), which are reported to have a synergistic potentiation, was carried out in sodium cholate based binary and ternary mixed micellar systems with non-ionic polysorbate (Tween20, Tween40) and polyoxyethylene (Brij30, Brij35, Brij56 and Brij58) surfactants. The surfactant-surfactant interactions and their effect on the aggregation number, solubility of drugs, solubilization site, surfactant-drug interactions and drug-drug interactions were evaluated and explained. Synergism in mixed micellization increases the aggregation number and decreases the polarity of palisade layer resulting in enhancement of core solubilization of drugs with concomitant decrease in palisade layer solubilization. In the C_{12} series, CBZ shows a decrease in solubility upon surfactant mixing, indicating an appreciable solubilization in the palisade layer, whereas in the C_{16} series an increase in its solubility was observed. For NFD, a decrease in solubility follows the trend of synergism in mixed micellization, which is more for strongly interacting surfactant systems. During co-solubilization, because CBZ occupies preferentially the palisade layer, its solubility is decreased and the solubilization of NFD, which mainly occurs within the micellar core, is favored. The magnitude of drug-drug interactions increases in mixed micelles and is more for the surfactant systems, showing more synergism in the mixed micelle formation. The mixed micellar media used in the present study, being biocompatible, are expected to be employed as solubilization and drug delivery vehicles for co-administration of these two drugs in vivo. This journal is



Substances



Устранение несогласованностей

1

Ожидают информацию
незамедлительно

Не «копают» глубоко

Показать студентам, как сделать новейшие
взаимосвязи

Глубокое индексирование

Увидеть химию через междисциплинарные границы

Compendex

Embase

GeoBase

PubMed

Keywords:

Author: [antiviral activity](#); Bignoniaceae; EMCV; HSV-1; in vitro assays; plant extracts; VACV

Compendex Free Language: [Antiviral activities](#); Bignoniaceae; EMCV; HSV-1; In-vitro assays; Plant extract; VACV

Compendex Descriptor: Assays; Bromine compounds; Ethanol

Compendex Mainhead: Viruses

EMTREE drug term: acidovir; alpha2a interferon; natural product; plant extract

GEObase Subject Index: [antimicrobial activity](#); dicotyledon; ethanol; ethnobotany; medicinal plant; plant extract; taxonomy; virus

EMTREE medical term: animal cell; [antiviral activity](#); article; Bignoniaceae; Brazil; controlled study; cytopathogenic effect; cytotoxicity; ethnopharmacology; Murine encephalomyelitis virus; nonhuman; plant leaf; plant stem; Vaccinia virus; Vero cell

Medline descriptor: Animals; [Antiviral Agents](#); Bignoniaceae; Brazil; Cercopithecus aethiops; Encephalomyocarditis virus; Herpesvirus 1, Human; Humans; L Tests; Plant Extracts; Vaccinia virus; Vero Cells

Regional Index: Brazil; Minas Gerais

Species index: Bignoniaceae; Encephalomyocarditis virus; Human herpesvirus 1; Murinae; Vaccinia virus

Reaxys Terms: 3-(4,5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolium bromide; [natural products](#) - [antiviral agent](#)

Tradename: bi 201335 (Boehringer Ingelheim)

Tradename: bms 650032 (Bristol Myers Squibb)

Tradename: bms 790052 (Bristol Myers Squibb)

Tradename: incivek (Novartis)

Tradename: nim 811 (Pharmasset)

Tradename: psi 7977 (Scynexis)

Tradename: scy 635 (Johnson and Johnson)

Tradename: tmc 435

Tradename: victrelis

1

Технология И Инжиниринг

2

Биомедицины И Фармакологии

3

Геонауки и окружающая среда

4

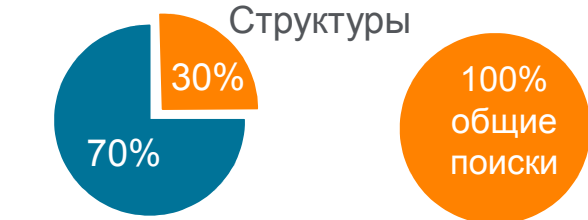
Науки о жизни и медицина

5

Химия

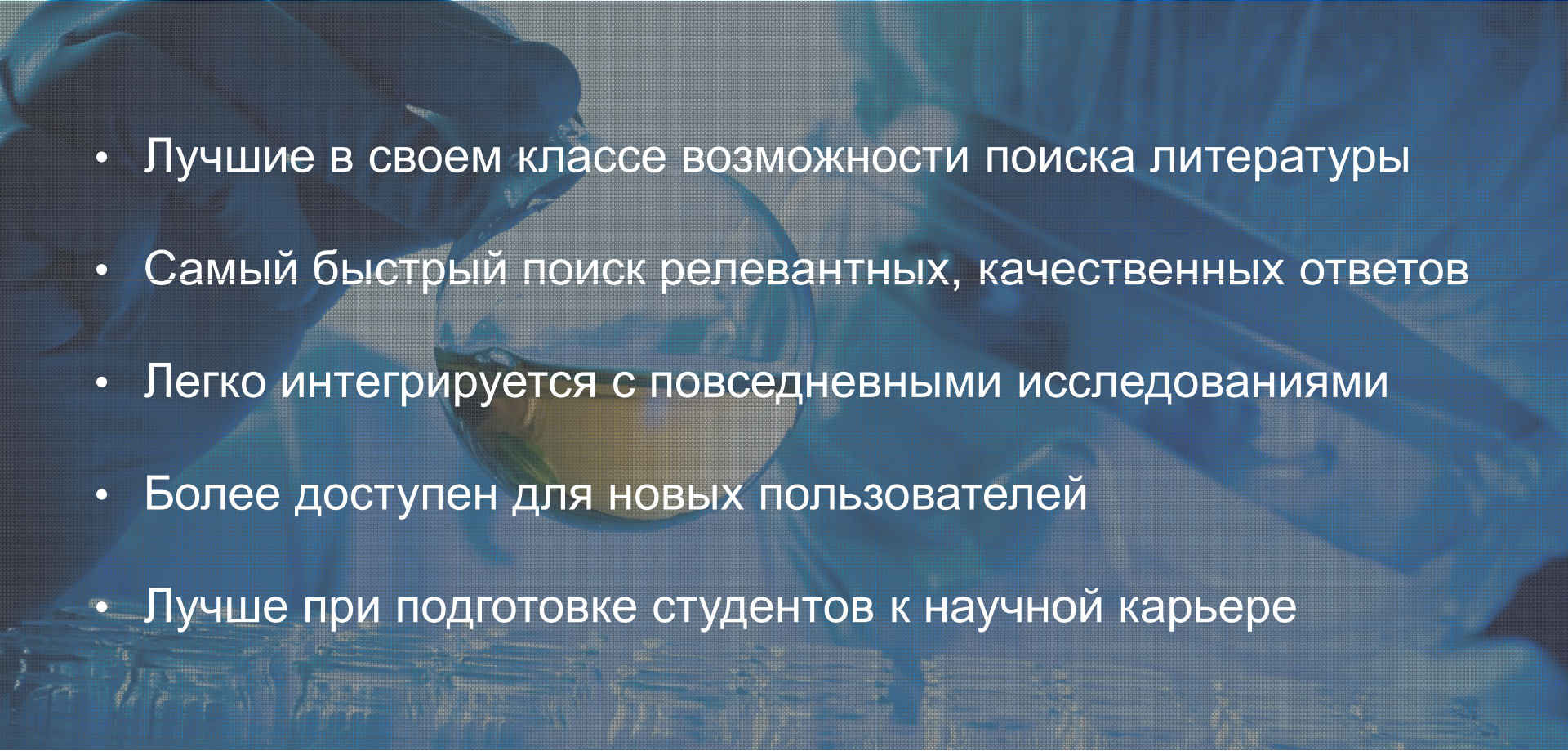
Препараты

Виды и география

	Изменение	Значение для вас
Дополнительное содержание	 Больше индексируемой периодики Больше охват патентов	• Больше соединений, свойств, реакций и литературы • Быстрое и глубокое понимание литературы из широкого спектра дисциплин • Актуальные и напрямую используемые данные, размещенные в мировой патентной литературе
Новый опыт пользователей	 Повышена производительность в 100% из наиболее распространенных видов поиска	• Легкий доступ к запросам, которые вы используете чаще всего • Помощь в поиске и предпросмотр результатов • Интуитивная навигация и анализ результатов
Улучшенная интеграция	 Улучшенный API Оптимизированное управление данными	• Мгновенный доступ к контенту Reaxys • Беспрепятственная интеграция с платформами и инструментами обработки данных • Быстрый и простой мэшап данных

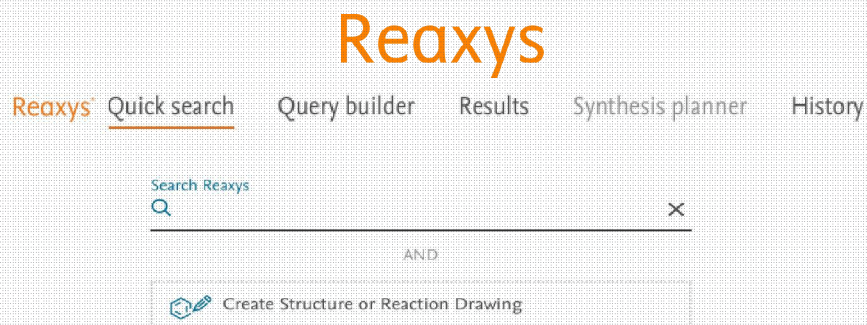
Reaxys – устраняет препятствия в академической науке

Помогает укрепить научные исследования, инновации и образование в вашем учреждении

- Лучшие в своем классе возможности поиска литературы
 - Самый быстрый поиск релевантных, качественных ответов
 - Легко интегрируется с повседневными исследованиями
 - Более доступен для новых пользователей
 - Лучше при подготовке студентов к научной карьере
- 

Возможности поиска литературы

Резюме по основным параметрам текстового поиска



- **Содержит автозаполнения**
- **Осмысляет естественный язык**
- Автоматически распознает формы единственного/множественного числа, английский/американский варианты написания, синонимы
- **Автоматически распознает намерение поиска (темы, вещества, реакции, свойства, авторов, источник публикации) – не делает ни одна другая поисковая система**
- Дает возможности для комбинации введенных понятий
- Интерпретирует усечения и логическое/близость
- **Позволяет одновременно производить текстовой/числовой поиск совместно с структурным поиском**
- **Также позволяет пользователям управлять усечения и близость**

Результаты поиска ранжируются по релевантности.

Конкурирующая база данных

Возможность текстового поиска является Explore by Research Topic (ERT):

ERT работает, если пользователи знают, что надо поставить связи между понятиями: A с b с C.

Затем пользователи выбирают из списка кандидатов:

A, B, B – 'тесно связана'

A, B, B – 'В любом месте в записи'

Комбинации A, B; A, C; B, C, то a; B; B – 'тесно связаны и в любом месте в записи'

Для одного понятия автоматически включено: форм единственного/множественного числа (в основном), английский/американский варианты написания, синонимы из 'словарь синонимов'; записи соединений, если они обнаружены, также осуществляется автоматически.

Нет автозаполнения или подсказок.

Не показывает, как происходил поиск.

Ответы всегда ранжируются в обратном хронологическом порядке.

Возможности поиска литературы

Резюме по охвату литературы

Reaxys

Часть Elsevier

(ScienceDirect, Scopus, Embase, Ei Village and more)

Конкурирующая база данных

Покрытие более 16000 периодических изданий.

>53 М оригинальных реферативных статей
~1М патентных документов

Замечание: Индексируемые ключевые слова из Compendex, EMTREE, GeoBase, MEDLINE, Reaxys находятся в единой Литературной записи.

Если их считать “независимо“, Reaxys будет покрывать **>82 млн документов**

“Итого”
>82 М

>>

“Итого”
>67 М

Покрытие более 10000 периодических изданий

Общий
индекс

>35 млн оригинальных записей

(включая абстракты конференций /заметки ред коллегии)

MEDLINE: ~24млн оригинальных записей

Общий
индекс

>8М патентных документов

Общий
индекс

и MEDLINE размещены раздельно. Всего записей **>67 млн.**

Возможны повторяющиеся записи!!!

Reaxys содержит на много больше реферируемых статей из журналов. В Reaxys отсутствуют дублирующиеся записи, которые необходимо разделять в ручную.

Поиска Reaxys обеспечивает результат напрямую

1. Введите термины на естественном языке без усечения/близости...

Search Reaxys

solubility of duloxetine



2. Обзор вариантов. Поиск дает одно вещество с информацией в области растворимости.

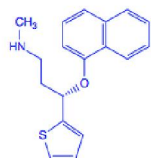
Reaxys

Quick search Query builder Results Synthesis planner History

Back to Quick Search

Choose a result for solubility of duloxetine

1	Substances	Solubility MCS exists AND Compound: duloxetine (exact search)	Preview Results	View Results
14	Documents	"Titles, Abstracts and Keywords : Document Basic Index : 'solubilities'; 'solubilities'; 'solubility'; 'solubility mcs' AND Document Basic Index : duloxetine"	Preview Results	View Results
6775	Documents	"Titles, Abstracts and Keywords : Document Basic Index : duloxetine"	Preview Results	View Results
213406	Documents	"Titles, Abstracts and Keywords : Document Basic Index : 'solubilities'; 'solubilities'; 'solubility'; 'solubility mcs'"	Preview Results	View Results



Duloxetine

Hit Data - 1

Identification

Spectra - 31

Physical Data - 17

Bioactivity - 269

Preparations - 63

Reactions - 94

Documents - 307

Hit Data - 1

Solubility (MCS) - 1 hits out of 1

Solubility, g·l ⁻¹	Saturation	Temperature (Solubility (MCS)), °C	Solvent (Solubility (MCS))	Ratio of Solvents	Reference
0.14871	in solution	25	phosphate buffer		Alayunas, Yun W.; Empfield, James R.; McCarthy, Dennis; +4 others - Bioorganic and Medicinal Chemistry Letters, 2010, vol. 20, # 24, p. 7312 - 7316 Full Text ↗ Cited 17 times ↗ Show details ↗

3. Нажмите View Results ... и Reaxys показывает конкретные данные в записи соединения

Поиска Reaxys обеспечивает результат напрямую

Как Reaxys трактует запрос.

Search Reaxys

esterification of benzoic acid



Create Structure or Reaction Drawing

82 Reactions

Reactions: 'benzoic acid'(structured) as starting, exact AND (Reaction Type = 'esterification'; 'esterifications' OR Other Conditions = 'esterification'; 'esterifications')

[View Results >](#)

[Preview Results](#) ▾

392 Documents

Documents: Search in Titles, Abstracts and Keywords = Document Basic Index = "esterification"; "esterification"; "esterifications" AND Document Basic Index = 'benzoic acid'

[View Results >](#)

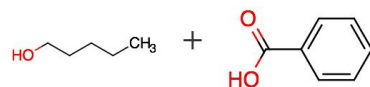
[Preview Results](#) ▾



[Find Similar Reactions >](#)

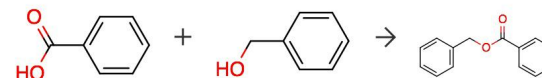
Yield	Conditions
95%	With carbon ;toluene-4-sulfonic acid D=0.00972222 h;

[Show All Details](#) ▾



[Find Similar Reactions >](#)

Yield	Conditions
94%	With carbon ;toluene-4-sulfonic acid D=0.00972222 h;



[Find Similar Reactions >](#)

Yield	Conditions	Reference
100%	With (tributylphosphoranylidene)acetonitrile In benzene T=100 °C; D=24 h;	Tsunoda, Tetsuto; Ozaki, Fumie; Ito, Sho - Tetrahedron Letters, 1994, vol. 35, # 28, p. 5081 - 5082

[Full Text](#) [Show details](#) >

[Show All Details](#) ▾

Применение Reaxys Ингибирование коррозии?

Reaxys

Обеспечивает релевантные ответы по дисциплинам,
связанным с химией



Записи в Reaxys
глубоко
проиндексированных по
ключевым словам из
автора, таксономии
Reaxys, а также
ведущими на рынке
базами данных **EMBASE**,
MedLine, **GeoBase** и
Compendex.



**Детализированные
данные о свойствах**
с **>500 полей данных для
поиска**, Reaxys является
крупнейшим хранилищем
данных о свойствах
вещества в мире.

Получает литературу по большим
веществам — **полимерам биологическим
продуктам и материалам** — используя
общеизвестные имена

Находит сведения о свойствах малых
молекул — **органических, неорганических,
координационных соединений и
мономеров** — которые имеют отношение к
вашей дисциплине

Осуществлять целенаправленный поиск по
**процессам и продуктам, характерным
для вашей отрасли.**

Фармацевтика
Биотехнологии
Исследования в
области полимеров
Материаловедение
Биомедицина
Окружающая среда
Синтетическая химия

Токсикология
Нанотехнологии
Инженерия
Тонкая химия
Нефть И Газ
Новые материалы
и многое другое...

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 Constat
Surface Tension
Transition Points
Transport Data

NMR Spectroscopy
IR Spectroscopy
Mass Spectroscopy
UV/VIS Spectroscopy
ESR Spectroscopy
NQR Spectroscopy
Raman Spectroscopy
Luminescence Spectroscopy
Fluorescence Spectroscopy
Exposure Assessment
Bioaccumulation
Biomagnification
Biodegradation
Abiotic Degradation
Stability in Soil
Oxygen Demand
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
Data
Exponent
Viscosity
Electrolytic Conductivity
Enthalpy of Fusion
Enthalpy of Vaporization
Explosion Limits
Interatomic Distance/Angle
Kinematic Viscosity
Liquid/Solid Systems
Liquid/Vapor Systems
Metarotation

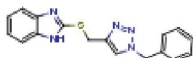
Информация о
применении

And many more...

Reaxys нашел 191 запись соединений, применяемых как “corrosion inhibitor”

Bioactivities (13818) Reactions (681845) **Substances (191)** Targets (835) Citations (393990) go to Page Page 21 of 22

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as:

Structure	Structure/Compound Data	Nº of preparations All Preps All Reactions	Available Data	Target	Nº of ref.
  Synthesize Hide Details Find similar	Chemical Name: 2-[(1-benzyl-1H-1,2,3-triazol-4-yl)methylthio]-1H-benzimidazole Reaxys Registry Number: 27469611 Molecular Formula: C ₁₇ H ₁₅ N ₅ S Linear Structure Formula: C ₁₇ H ₁₅ N ₅ S Molecular Weight: 321.406 InChI Key: WDDDYHVZDSGHDS-UHFFFAOYSA-N	2 prep out of 2 reactions.	Hit Data (1) Druglikeness Identification Physical Data (2) Spectra (4) Use/Application (2)	Show Targets	1

Chemical Names and Synonyms
 2-[(1-benzyl-1H-1,2,3-triazol-4-yl)methylthio]-1H-benzimidazole

Hit Data
 Use (1 Hits out of 2 view all)

Use Pattern	Reference
acidic corrosion inhibitor of steel	Cruz-Gonzalez, Deysi Y.; Gonzalez-Olvera, Rodrigo; Negron-Silva, Guillermo E.; Lomas-Romero, Leticia; Gutierrez-Carrillo, Atilano; Palomar-Pardave, Manuel E.; Romero-Romo, Mario A.; Santillan, Rosa; Uruchurtu, Jorge Synthesis (Germany), 2014 , vol. 46, # 9 art. no. 55-2013-M0842-OP, p. 1217 - 1233 Title/Abstract Full Text View citing articles Show Details

Druglikeness
 Identification
 Physical Data
 Spectra
 Use/Application

Reaxys нашел 21473 запись документов по теме ингибиторов коррозии

[← Back to Quick Search](#)

Choose a result for corrosion inhibitor

21473

Documents

Titles, Abstract, Keywords : corrosion, inhibitor

[Preview Results](#) ^

[View Results](#) >

Top 3 results

Streptomycin: A commercially available drug as corrosion inhibitor for mild steel in hydrochloric acid solution

Cited 91 times

Shukla, Sudhish Kumar; Singh, Ashish Kumar; Ahamad, Ishtiaque; +1 other - Materials Letters, 2009, vol. 63, # 9-10, p. 819 - 822

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

Inhibition effect of thioureidoimidazoline inhibitor for the flow accelerated corrosion of an elbow

Cited 4 times

Zeng; Zhang; Guo; +1 other - Corrosion Science, 2015, vol. 90, p. 202 - 215

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

Inhibition of microbiologically influenced corrosion of mild steel and stainless steel 316 by an organic inhibitor

Sheng, Xiaoxia; Ting, Yen-Peng; Pehkonen, Simo Olavi - Biohydrometallurgy: From the Single Cell to the Environment, IBS 2007, 2007, vol. 20-21, p. 379 - 382

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

21,473

Filters and Analysis

Index Terms (List) ^

☐ electrooxidation	17,475
☐ adsorption	5,102
☐ spectroscopy	3,720
☐ impedance	2,776
☐ impedance spectroscopy	2,770
☐ isotherm	2,070
☐ adsorption isotherm	2,070

+ More

Index Terms (ReaxysTree) v

Publication Year ^

☐ 2013	1,487
☐ 2012	1,414
☐ 2014	1,389
☐ 2015	1,386
☐ 2011	1,353
☐ 2010	1,089
☐ 2009	899

[Back to Results Preview](#)

21,473 Documents with 6,138 Substances, 9,866 Reactions

☐ 0 selected: [Limit To](#)  [Export](#) Relevance   

- ☐ **Streptomycin: A commercially available drug as corrosion inhibitor for mild steel in hydrochloric acid solution** Cited 91 times

1

Shukla, Sudhish Kumar; Singh, Ashish Kumar; Ahamad, Ishtiaque; +1 other - Materials Letters, 2009, vol. 63, # 9-10, p. 819 - 822

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

- ☐ **Inhibition effect of thioureidoimidazoline inhibitor for the flow accelerated corrosion of an elbow** Cited 6 times

2

Zeng; Zhang; Guo; +1 other - Corrosion Science, 2015, vol. 90, p. 202 - 215

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

- ☐ **Inhibition of microbiologically influenced corrosion of mild steel and stainless steel 316 by an organic inhibitor** Cited 6 times

3

Sheng, Xiaoxia; Ting, Yen-Peng; Pehkonen, Simo Olavi - Biohydrometallurgy: From the Single Cell to the Environment, IBS 2007, 2007, vol. 20-21, p. 379 - 382

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

- ☐ **Inhibition effect of 3-amino-5-mercapto-1,2,4-triazole on copper corrosion** Cited 6 times

4

Yu; Gan; Jiang - Corrosion, 2008, vol. 64, # 12, p. 900 - 904

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

Поля поиска помогают разобраться в исследовательском вопросе и найти конкретные ответы

Identify an unknown substance isolated from a **natural product**³. Experimental results indicate that the substance has **30 carbon atoms**¹ and an **optical rotation of 75-85°**². Has it been tested for **antimicrobial** activity⁴?

1

⋮ Molecular Formula

eg.C₆H₅COOH
C₃₀*

Look up

3

⋮ Isolation from Natural Product

Exist ✓

2

⋮ Optical Rotatory Power

is ✓ Type (Optical Rotatory Power)

is ✓ Concentration (Optical Rotatory Power)

= ✓ Length of Path, cm

is ✓ Solvent (Optical Rotatory Power)

= ✓ Optical Rotatory Power, deg
75-85

= ✓ Wavelength (Optical Rotatory Power), nm

= ✓ Temperature (Optical Rotatory Power), °C

4

⋮ Basic Indexes

is ✓ Substance Basic Index
antimicrobi*

This search illustrates how searches through querylets can be combined to give very precise answers. When this search is done, 6 substances are obtained and it is a simple task to look through data for all of them.



Пост-обработка литературного запроса

711

13,011

Filters and Analysis

Index Terms (List)

☐ cyclic voltammetry

711

☐ x-ray diffraction

349

☐ electrochemical property

321

☐ scanning electron microscopy

275

☐ impedance spectroscopy

258

☐ transmission electron microscopy

124

☐ sol gel process

82

+ More

Index Terms (ReaxysTree)

Publication Year

☐ 2014

127

☐ 2013

99

☐ 2015

86

☐ 2012

69

☐ 2011

55

☐ 2010

42

☐ 2008

41

+ More

Document Type

☐ article

632

☐ conference paper

77

☐ review

1

Tsutsumi, Hiromori; Oyari, Yoshiaki; Onimura, Kenjiro; +1 other - Journal of Power Sources, 2001, vol. 92, # 1-2, p. 228 - 233

Abstract Index Terms Full Text

Synthesis, characterization and application of $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ nanoparticles as cathode of lithium-ion rechargeable batteries

Cited 11 times

Karami, Hassan; Taala, Foroozandeh - Journal of Power Sources, 2011, vol. 196, # 15, p. 6400 - 6411

Abstract Index Terms Full Text

Abstract

This work introduces a new method to synthesize $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ electrochemical performance by cyclic voltammetry and combustion method based on polyvinyl alcohol (PVA). It includes 8 wtpercent PVA, 0.34 wtpercent lithium salt, 1 phosphate, ethanol-water 50:50 as solvent, 675 °C core. Characterization of the samples is performed by the scanning electron microscopy (SEM), EDX analysis, XRD patterns, BET surface area, and electrochemical performance. The optimized sample shows 12.5 $\text{m}^2 \text{g}^{-1}$ specific surface area. The synthesized compound has good reversibility and high tests. The obtained results show that the synthesized $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ shows 125.5 mAh g^{-1} approximately same with its theoretical

Index terms

Author keyword: Cathode material, Cyclic voltammetry, Compendex Terms: Ammonium dihydrogen phosphate, Gel combustion, Gel-combustion method, Iron cycles, Nano powders, Optimum conditions, SEM, TEM, Compendex Terms: Ammonium compounds, Bioelectrochemistry, Lithium alloys, Lithium compounds, Nanoparticles, Nanotechnology, Transmission electron microscopy

Reaxys Index Terms: combustion, cyclic voltammetry, Lithium ion batteries

Effects of MoS_2 doping on the electrochemical performance of lithium-ion batteries



Synthesis, characterization and application of $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ nanoparticles as cathode of lithium-ion rechargeable batteries

Hassan Karami*, Foroozandeh Taala

New Research Laboratory, Chemistry Department,

Article history:
Received 26 January 2011
Received in revised form 24 March 2011
Accepted 27 March 2011
Available online 1 April 2011

Keywords:
Lithium ion phosphate
Gel combustion
Nanoparticles
Cathode material
Cyclic voltammetry
Lithium-ion batteries

1. Introduction

Lithium ion secondary batteries have been used in many electronic devices, mobile phones, cellular phones, and digital cameras and electric vehicles [1–3]. $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ [26–37] have been used as cathodes.

Lithium ion phosphates are new cathode materials. Among the iron compounds, $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ [26–37] and $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ [28] can be used as positive poles vs. LiFePO_4 and $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ as positive poles. They have been used successfully as cathodes in lithium-ion batteries. Lithium ion phosphate LiFePO_4 and $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$. In LiFePO_4 , it is of 2+ and in $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$, it has 3+

* Corresponding author. Tel.: +98 91 2 390 8211.
E-mail address: karami.hassan@yahoo.com (H. Karami).
0378-7753/\$ – see front matter © 2011 Elsevier Ltd.
doi:10.1016/j.jpowsour.2011.03.029

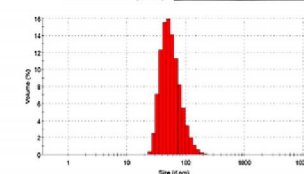
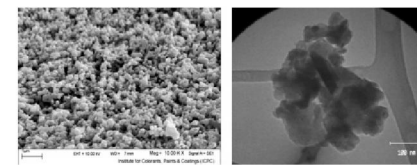


Fig. 11. SEM and TEM images and particle size distribution diagram for the optimized sample.

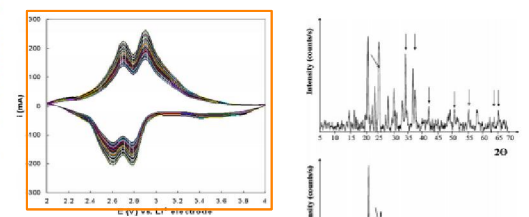


Fig. 12. Cyclic voltammograms of the synthesized $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ sample in the electrolyte including 1 M LiPF_6 solution in 1:1 EC and DMC as mixed solvent under nitrogen atmosphere in a two-electrode system and reference electrodes.

Fig. 13. XRD patterns for the dried paste of working electrode which was used in CV studies before (top image) and after 20 cycles CV experiments (bottom image).

Как искать информацию в области катализа?

Что ищет каталитик?



Synthesize
Find similar

Rx-ID: 24815350
Find similar reactions

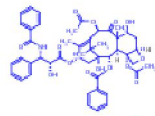
88.1%

Stage #1: **With** boron tribromide **in** chloroform
T=23 - 26°C; 0.283333 h;
Stage #2: **With** ammonia; water **in** chloroform
T=-5 - 0°C; 0.5 h;
[Show Experimental Procedure](#)

DR PHARMA NOVA, LLC
Patent: WO2006/91885 A2, **2006**;
Location in patent: Page/Page column 51;
[Title/Abstract](#) [Full Text](#) [Show Details](#)

Title of the Document	Author's	Year	Source
Fused heterocyclic compounds bearing bridgehead nitrogen as potent HIV-1 NNRTIs. Part 1: Design, synthesis and biological evaluation of novel 5,7 disubstituted pyrazolo[1,5-a]pyrimidine derivatives	Tian, Ye; Dai, Daping; Rai, Divakar; Wang, Liu; Liu, Huigang; Zhang, Peng; De Clercq, Erik; Pannecoque, Christophe; Liu, Xinyong	2014	Bioorganic and Medicinal Chemistry, 2014, vol. 22, # 7 p. 2052-2059 Full Text View citing articles





Synthesize | [Show Details](#)
[Find similar](#)

Chemical Name:
PACLITAXEL

Reaxys Registry Number: 4290260
CAS Registry Number: 33069-62-4
Type of Substance: heterocyclic
Molecular Formula: C₄₇H₅₁NO₁₄
Linear Structure Formula: C₄₇H₅₁O₁₄N
Molecular Weight: 853.92
InChI Key: R.CINICONZJXQF-MZXODVADSA-N
Highest Clinical Phase: Marketed

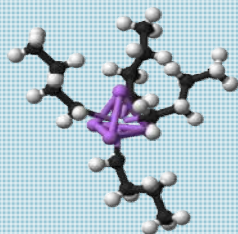
Поиск информации в области катализа

Находятся в записях Веществ REAXYS ...
и ...

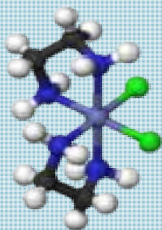
Находятся в КЛЮЧЕВЫХ СЛОВАХ в REAXYS
БИБЛИОГРАФИЧЕСКИХ Записях



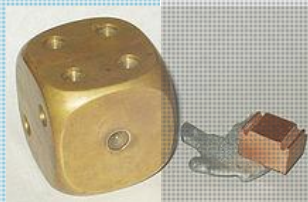
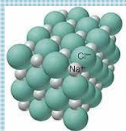
Органические
вещества



Металлоорганические
Координационные
соединения



Неорганические



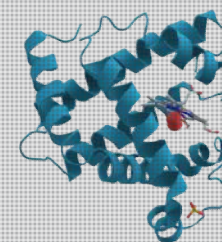
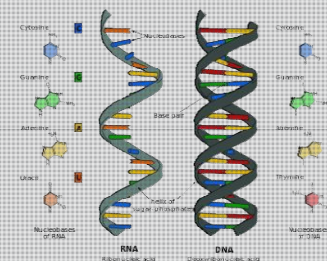
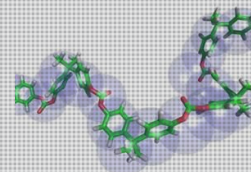
Сплавы & Металлы

Катализатор

Керамика



Полимеры



Нуклеиновые кислоты
и Белки

Поиск в записях Соединений

Поиск в записях Литературы

Search Reaxys: Bibliographic Records

The two main ways to search for text terms in bibliographic records are:

- Ask Reaxys

- » An intelligent natural language search interface
- » Used to find initial information quickly

- Citation Basic Index Querylet

- » Allows users to control the search
- » Allows truncation (left-, right- and left/right-)
- » Allows proximity/Boolean (NEAR, NEXT, AND, NOT, OR)
- » Suggests individual terms or phrases through auto-suggest as you type in the Entry Box or in the box through Lookup

Over 50 million bibliographic records are searched

The screenshot displays the Reaxys web application interface. At the top, a navigation bar includes links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this, a search bar is labeled 'Ask Reaxys' and contains the text 'e.g. Ask Reaxys for "publications about quasicrystals"'. A row of icons represents different search categories: Reactions, Substances, Literature (highlighted with a red box), ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Structure' section is open, showing a 'selected query editor' with the MarvinSketch logo. To the right of the editor are options for 'As drawn', 'Substructure', and 'Similarity'. A list of checkboxes on the right allows for refining the search, including 'Include tautomers', 'Ignore stereo', 'No salts', 'No mixtures', 'No isotopes', 'No charges', 'No radicals', 'No ring closures', and 'Align results with query' (which is checked). Below the 'Structure' section, the 'Bibliographic Data' section is visible, featuring a 'Citation Basic Index' querylet (highlighted with a red box) and a 'Lookup' button. At the bottom, a 'Search Literature' button is present.

Search Reaxys: Substance Records

- The main ways to search for substances in substance records are:
 - Full/part structure through the Structure Editor(s)
 - Full/part name through the Chemical Name or Chemical Name Segment Querylets
 - Full/part formula through the Formula Builder (=> Molecular Formula Querylet)
- Substances may be found through the > 500 Property Querylets
 - Specific querylets may be set up through Add/Remove fields...
- The Substance Basic Index Querylet is very useful to search for specific terms in substance records
- Notes
 - Information on all substances may also be found through bibliographic searches (previous slide)
 - For substances with “simple names” try Ask Reaxys

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

- Navigation Bar:** Includes icons for Reactions, Substances (highlighted), Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced.
- Structure Section:** Features a "selected query editor" with MarvinSketch by ChemAxon. It includes radio buttons for "As drawn" (selected), "Substructure" (with sub-options "on heteroatoms" and "on all atoms"), and "Similarity". On the right, there are checkboxes for "Include tautomers", "Ignore stereo", "No salts", "No mixtures", "No isotopes", "No charges", "No radicals", "No ring closures", and "Align results with query" (checked). A "More options" link is also present.
- Molecular Formula Section:** Contains a "Molecular Formula" input field, a "Lookup" button, and a "Formula Builder" button.
- Identification Section:** Includes fields for "Chemical Name", "Chemical Name Segment", "Catalyst Investigation", and "Investigated characteristi...". Each field has a dropdown menu (set to "is"), a text input, and a "Lookup" button. The "Catalyst Investigation" field also has an "exists" checkbox.
- Ecological Data Section:** Includes checkboxes for "Exposure Assessment" and "Bioaccumulation, Biomagnif...", each with an "exists" checkbox and a "Lookup" button.
- Basic Indexes Section:** Features a "Substance Basic Index" dropdown menu (set to "is"), a text input, and a "Lookup" button.
- Footer:** Includes a "Show AND Buttons" link, an "Add to Query:" section with buttons for "Structure", "Molecular Formula", and "Alloy", an "Add/Remove Fields..." link, and a prominent red "Search Substances" button.

Search Reaxys: Reaction Records

- The main ways to search in reaction records are through:
 - Full/part structure for reactants, catalysts, products through the Structure Editor(s)
 - Reaction-based Querylets
 - » For example through the Reaction Type Querylet that searches for Named Reactions and Types of Reactions
 - Reaction Basic Index Querylet is particularly useful to search for specific terms in reaction records (including in the Experimental Details)
- Remember that auto-suggest terms appear as you type in the Entry Box or in the box through Lookup in all Querylets

The screenshot displays the Reaxys search interface for Reaction Records. At the top, a navigation bar includes icons for Reactions, Substances, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Reactions' icon is highlighted. Below this, the 'Structure' search panel is active, showing a 'selected query editor' with the MarvinSketch logo by ChemAxon. To the right of the editor are radio buttons for 'As drawn' (selected), 'Substructure' (with sub-options 'on heteroatoms' and 'on all atoms'), and 'Similarity'. Further right are checkboxes for various search criteria: 'Include tautomers', 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No ring closures', 'Ignore atom mappings', 'Align results with query' (checked), and 'Keep fragments' (with sub-options 'separate' and 'together'). Below the structure panel, a 'Please select role' section has radio buttons for 'Product' (selected), 'Starting material', 'Reagent / Catalyst', and 'Any role'. The 'Reaction Data' section contains five rows of search criteria: 'Yield (numerical)', 'Solvent (Reaction Details)', 'Reagent/Catalyst', 'Reaction Type', and 'Reaction Basic Index'. Each row has a dropdown menu (currently showing '=' or 'is'), a text input field, and a 'Lookup' button with a close 'X' icon. At the bottom, a 'Show AND Buttons' link is present. The footer includes an 'Add to Query:' section with tabs for 'Structure', 'Molecular Formula', and 'Alloy', followed by an 'Add/Remove Fields...' link and a prominent red 'Search Reactions' button.

Гомогенные, металлоорганические, твердые растворы и др. в качестве катализаторов.

ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ СОЕДИНЕНИЙ. Zr⁴⁺ В КАЧЕСТВЕ КАТАЛИЗАТОРА ?


Reactions


Substances

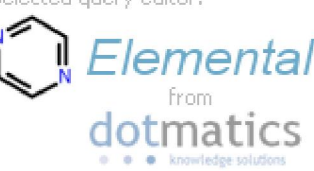

MedChemistry


Literature


ReaxysTree

Structure

selected query editor:



PASTE STRUCTURE EDITOR

https://www.reaxys.com/reaxys/js/sre_5_4_2_01/child_js.html

C

N

O

S

H

F

Cl

Br



[]_n





+

-



H																	He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uu	Uq	Up	Uh	Us	Uo				
			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					

A R1

Q R2

X R3

AH R4

QH R5

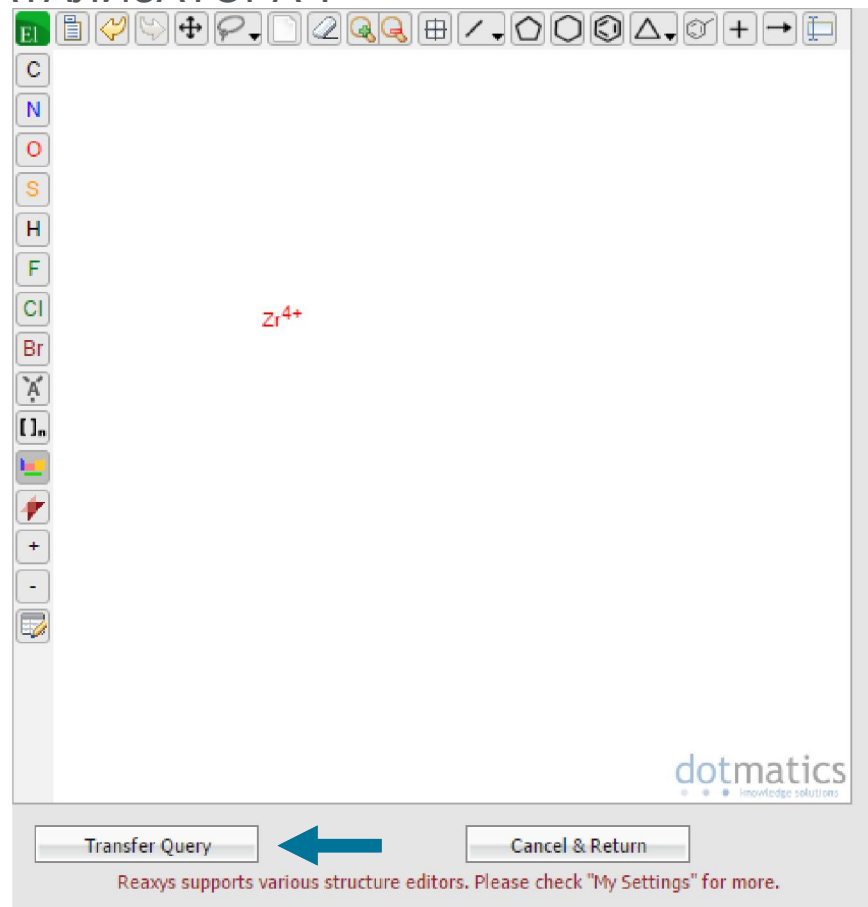
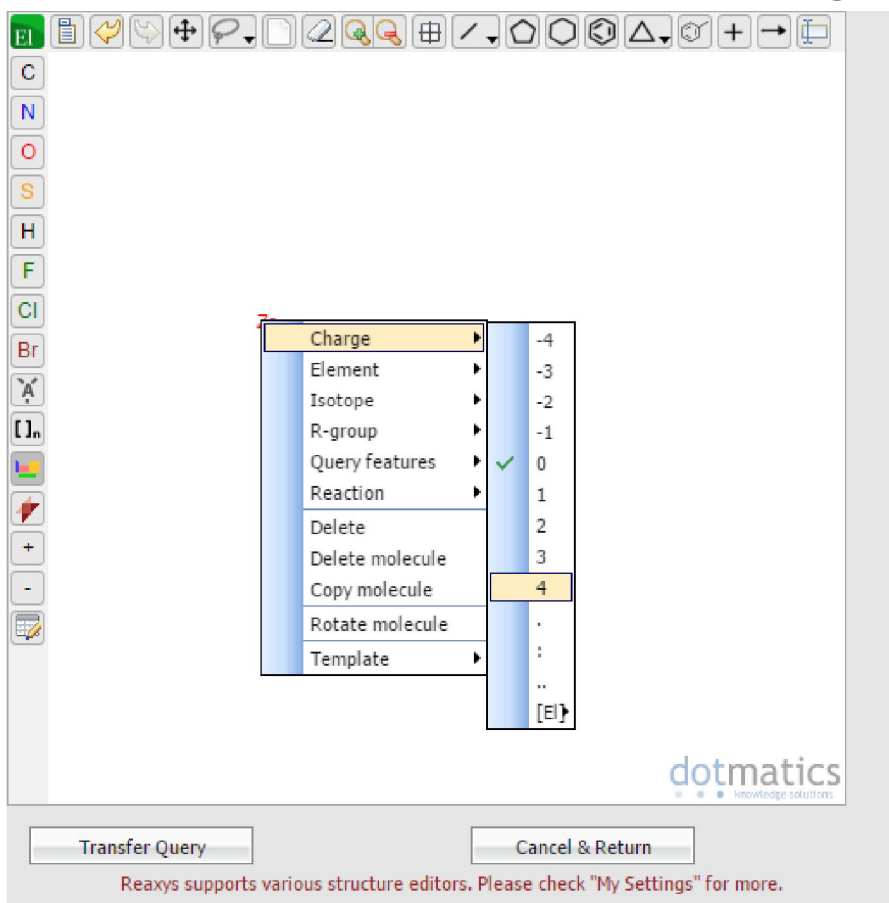
XH R6

* R7

Гомогенные, металлоорганические, твердые растворы и др. в качестве катализаторов.

ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ СОЕДИНЕНИЙ.

Zr^{4+} В КАЧЕСТВЕ КАТАЛИЗАТОРА ?



Гомогенные, металлоорганические, твердые растворы и др. в качестве катализаторов.

ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ СОЕДИНЕНИЙ.
 Zr^{4+} В КАЧЕСТВЕ КАТАЛИЗАТОРА ?

Structure

Zr^{4+}

PASTE EDIT CLEAR

Create Structure Template from Name

☐ As drawn

☒ Substructure 

☐ on heteroatoms

☒ on all atoms

☐ Similarity



Substance Basic Index

contains

Lookup X

Search Substances

Гомогенные, металлоорганические, твердые растворы и др. в качестве катализаторов.

ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ СОЕДИНЕНИЙ.
 Zr^{4+} В КАЧЕСТВЕ КАТАЛИЗАТОРА ?

Bioactivities (1) Reactions (2988) **Substances (1196)** [Targets \(0\)](#) Citations (1751) [go to Page](#)

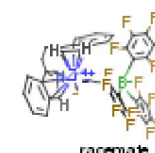
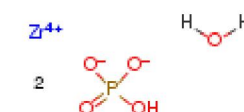
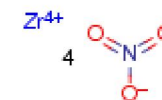
Limit to Exclude Export Print Zoom in Zoom out Hide Sort by **No of References** Display as:

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data
 1 Synthesize Hide Details Find similar	Chemical Name: zirconium(IV) sulfate Reaxys Registry Number: 14201579 Molecular Formula: $2O_4S \cdot Zr$ Linear Structure Formula: $Zr^{(4+)} \cdot 2SO_4^{(2-)} = Zr(SO_4)_2$ Molecular Weight: 283.351 InChI Key: QMBDLUWQOUXKMJ-UHFFFAOYSA-L	21 prep out of 144 reactions.	Hit Data (14) Druglikeness Identification Physical Data (31) Spectra (8) Use/Application (10)

Chemical Names and Synonyms
 zirconium(IV) sulfate, zirconium (IV) sulphate, zirconium bis-sulphate, zirconium disulfate, zirconium sulphate, zirconium sulfate, sulfated zirconia

Hit Data
 Further Information (11 Hits out of 11 [view all](#))
 Use (3 Hits out of 10 [view all](#))

Use Pattern	Reference
Acetalization catalyst	CLARIANT PRODUKTE (DEUTSCHLAND) GMBH Patent: WO2006/119940 A1, 2006 ; Title/Abstract Full Text Show Details
catalyst for deodorize the polyether-modified siloxane composition	Nishijima, Kazuhiro; Tamura, Seiki; Shoji, Hiroaki Patent: US2006/18935 A1, 2006 ; Title/Abstract Full Text Show Details
catalyst	Nishijima, Kazuhiro; Tamura, Seiki; Shoji, Hiroaki Patent: US2006/18935 A1, 2006 ; Title/Abstract Full Text Show Details

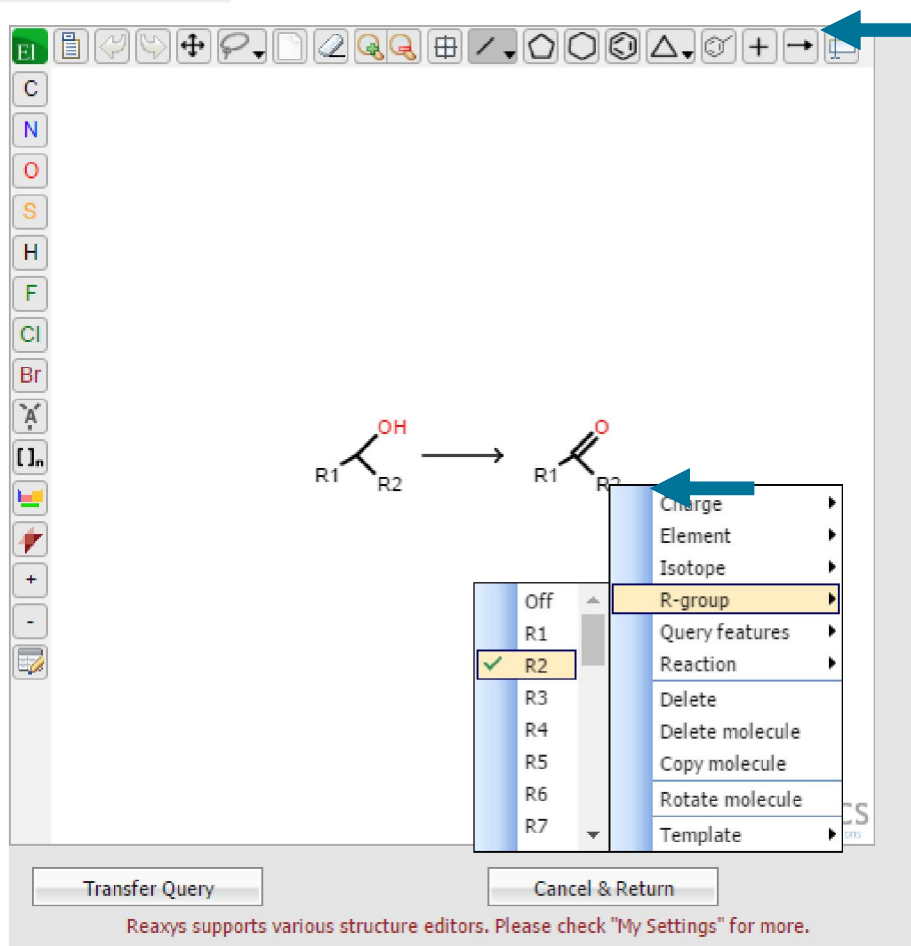


Molecular Formula: $5H^+O_{40}PW_{11}Zr$

Конкретная реакция, проходящая на Zr катализаторе.



ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ
СОЕДИНЕНИЙ.
Zr⁴⁺ В КАЧЕСТВЕ КАТАЛИЗАТОРА ?

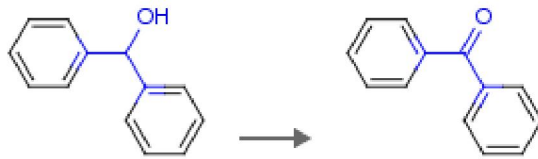


Конкретная реакция, проходящая на Zr катализаторе.

ПОИСК ИНФОРМАЦИИ В ЗАПИСЯХ СОЕДИНЕНИЙ.
Zr⁴⁺ В КАЧЕСТВЕ КАТАЛИЗАТОРА ?

Bioactivities (12893) **Reactions (38)** Substances (66) Targets (625) Citations (1774)

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
	    Rx-ID: 140976 Find similar reactions	
Hit Details (1)		
	in acetonitrile 0.0166667 h; Microwave irradiation Green chemistry; Catalytic behavior; Reagent/catalyst Solvent; Hide Experimental Procedure	Shojaei, Abdollah Fallah; Tabatabaei Zoha Journal of the Iranian Chemical Society, 2 Title/Abstract Full Text View citing
General procedure for the oxidation reaction General procedure: A mixture of benzyl alcohol (1 mmol), t-BHP 70 percent (0.3 ml) and RuO ₂ (at)ZrO ₂ 4 (20 mg) in acetonitrile (5 ml) was used. The progress of the reaction was followed using thin layer chromatography and after completion of the reaction, the products were filtered out from the mixture using a gas chromatograph with a GC capillary column HP 6890 and FID detector.		

Поиск литературы по окислению спирта на ZrO_2

Поиск Литературы

Контекст

Два основных пути:

- **Ask Reaxys**
 - Разумная “Google-like” функция обработки естественного языка
 - Нет автоматических форм единственного/множественного числа, английское/американское правописание
 - Часто дает отличные ответы, очень быстро
- Citation Basic Index поле для поиска
 - Позволяет искать по усеченным формам
 - Позволяет соседство и логические операции
 - Предлагает авто-продолжение терминов и фраз
 - Пользователь контролирует поиск

- 
- Ответы
 - Пост-обработка (Analysis View, Filter by:)

Усеченная форма

left-, right-, L-/R- *

Близость/Логическ ие

NEXT NEAR AND NOT OR
Parentheses Help!
(A NEAR B) AND (C OR D)

Синонимы

Auto-suggest Help!!

Где искать литературу в области катализа в Reaxys

1. Выберите Иконку Literature

2. Основное поле для поиска терминов и тем

Ask Reaxys
Быстрый поиск терминов или тем

The screenshot displays the Reaxys web application interface. At the top, there is a navigation bar with links: Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this is a search bar labeled "Ask Reaxys" with a "Start Over" button and a placeholder text "Enter a keyword, concept or author".

The main content area features a row of icons for different search categories: Reactions, Substances, Literature (highlighted with a red border), ReaxysTree, Physical, Spectra, Natural Product, and Advanced. Below these icons is a "Structure" section with a "selected query editor" (MarvinSketch by ChemAxon) and various search options like "As drawn", "Substructure", "Include tautomers", etc.

The "Bibliographic Data" section contains a list of search fields with dropdown menus and "Lookup" buttons:

Field	Operator	Value	Action
Document Type	is		Lookup X
Authors	is		Lookup X
Common Patent Number	is		Lookup X
Patent Country Code	is		Lookup X
Journal Title	is		Lookup X
Publication Year	=		Lookup X
DOI	is		Lookup X
Title	is		Lookup X
Abstract	is		Lookup X
Keywords	is		Lookup X
Citation Basic Index	is		Lookup X

At the bottom, there is a "Show AND Buttons" section and a "Search Literature" button.

Поисковые
поля

Поиск информации в области катализа в Reaxys

Поиск литературы по окислению спирта на ZrO_2

Citation Basic Index

contains ▼

(Alcohol NEAR oxidation) AND (ZrO2)

Lookup ✕

ИЛИ

Citation Basic Index

1)

contains ▼

Lookup ✕

Select index items and click 'Transfer'

Reaxys

Search for: alcohol oxidat 2)

alcohol oxidation (2123)
alcohol oxidation by gold (2)
alcohol oxidation catalysis (1)
alcohol oxidation catalysts (1)
alcohol oxidation in alkaline media (1)
alcohol oxidation reaction (3)
alcohol oxidation reactions (1)
alcohol oxidation reduction (2)
alcohol oxidation, mars-van krevelen mechanism (2)
alcohol oxidation, pd complexes (1)
alcohol oxidations (13)
alcohol oxidations in water (1)
alcohol oxidizing agent (1)
alcohol oxidizing enzymes (1)
alcohol oxidoreductase (2)
alcohol oxidoreductase inhibitor (1)
alcohol oxidoreductases (10449)
alcohol oxidoreductases/analysis (3)
alcohol oxidoreductases/analysis/antagonists &x0026;x0026 (1)
alcohol oxidoreductases/antagonists &x0026;x0026 (1)

Page 147716 of 1549140

Transfer Reset Cancel

Citation Basic Index

3)

contains ▼

zro2

Lookup ✕

Query

Reaxys 4)

Synthesis Plans

History

Report

My Alerts

My Settings

Help



42

Edit Create Alert

Literature: (Citation Basic Index = '*zro2*')

37757 citations

Literature: (Citation Basic Index = '*zro2*')



38

Edit Create Alert

Literature: (Citation Basic Index = '*alcohol oxidation';'alcohol oxidations*')

29342 citations

Literature: (Citation Basic Index = '*alcohol oxidation';'alcohol oxidations*')

Select how you want to combine the hitsets



Merge 42 with 38



Overlap 42 with 38



Exclude 42 from 38



Exclude 38 from 42

Cancel

Combine hitsets

6)

Поиск информации в области катализа в Reaxys

Поиск литературы по окислению спирта на ZrO₂

Bioactivities (0) Reactions (32) Substances (73) Targets (0) Citations (61) go to Page Page 1 of 7

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by Relevance

Title of the Document	Authors	Year	Source	Times cited
Selective oxidation of alcohols with molecular oxygen over Ru/CaO-ZrO ₂ catalyst	Yasu-eda, Takashi; Kitamura, Susumu; Ikenaga, Na-oki; Miyake, Takanori; Suzuki, Toshimitsu	2010	Journal of Molecular Catalysis A: Chemical, 2010 , vol. 323, # 1-2 p. 7 - 15 Full Text View citing articles	27

Title/Abstract
Selective **oxidation of alcohols with molecular oxygen over Ru/CaO-ZrO₂ catalyst**
 Selective **oxidation** of alcohols to carbonyl compounds with molecular oxygen was carried out over ruthenium supported on a CaO-ZrO₂ solid solution prepared by the co-precipitation method. In the **oxidation** of benzyl **alcohol**, the Ru/CaO-ZrO₂ catalyst gave benzaldehyde in a yield higher than 98percent at 90 °C, and the turnover frequency reached 224 h⁻¹. The Ru/CaO-ZrO₂ catalyst also exhibited high catalytic activities and selectivities to carbonyl compounds in the **oxidation** of aromatic ring-substituted benzylic, allylic, and aliphatic alcohols. Moreover, this catalyst exhibited high activities in the **oxidation** of alcohols at a low temperature (40 °C). The catalytic activity and **oxidation** state of ruthenium depended on the Ca/Zr molar ratio of the support, and the highest catalytic activity was obtained with Ca/Zr = 0.125. DRIFT and XPS analyses revealed that Ruⁿ⁺-OH (n = 3, 4) on the surface of CaO-ZrO₂ were likely the active species in the **oxidation** of alcohols.

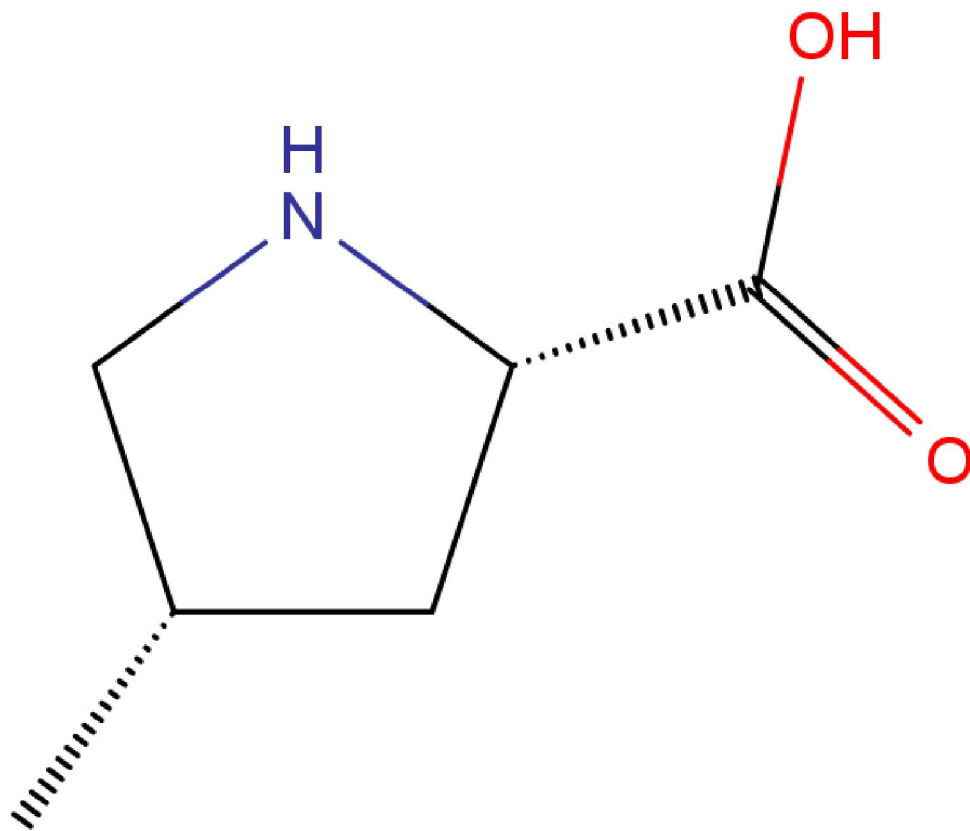
Keywords:
Author: Basic support; CaO-ZrO₂ solid solution; Heterogeneous catalyst; Oxidative dehydrogenation; Ruthenium
Compendex Free Language: Active species; **Aliphatic alcohol**; Aromatic rings; Basic support; **Benzyl alcohol**; Benzylic; Carbonyl compounds; Catalytic activity; Coprecipitation method; Heterogeneous catalyst; High activity; Low temperatures; Molar ratio; **Oxidation of alcohols**; **Oxidation state**; Oxidative dehydrogenation; Oxidative dehydrogenations; **Selective oxidation**; Turnover frequency; XPS analysis
Compendex Descriptor: Aldehydes; Carbonylation; Catalyst selectivity; **Catalytic oxidation**; Crystallization; Dehydrogenation; Electrochemical sensors; Molecular oxygen; Organic polymers; Precipitation (chemical); Ruthenium; Solid solutions; Solidification; Zirconium alloys
Compendex Mainhead: Catalyst activity
Reaxys Terms: catalyst; catalyst activity; **oxidation reaction**; turnover frequency

⚡ Show All Reactions (10)
 ⚡ Show All Substances (19)

Разработка методики синтеза химических веществ

С помощью Reaxys можно гораздо эффективнее решать задачу поиск оптимальных условий синтеза **неорганического или органического соединения**.

Допустим, Вас интересует методика синтеза данного соединения



Разработка методики синтеза химических веществ

Reactions

Substances

MedChemistry

Literature

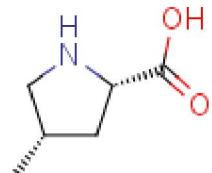
ReaxysTree

Physical

Spectra

Natural Product

Structure



PASTE

EDIT

CLEAR

☒ 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 from Name

Molecular Formula

Lookup

Formula Builder

Please select role

☒ Product

☐ Starting material

☐ Reagent / Catalyst

☐ Any role

Опции поиска соединений

Вызов
графического
редактора формул.

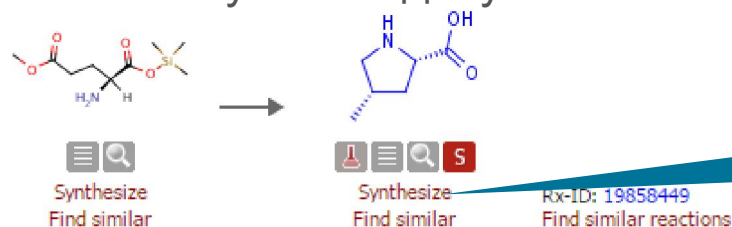
Вы рисуете его в графическом редакторе формул или пишете название.

Также можно выбрать поиск всех подструктур.

Нажимаете кнопку **Search Reaction**

Разработка методики синтеза химических веществ

Reaxys выдает Вам все реакции синтеза заданного соединения сразу с обзором экспериментальных условий, что позволит сэкономить деньги на реактивах, так как Вы сможете выбрать оптимальную методику.



Synthesize - Запускает автоматического построения ретросинтетического

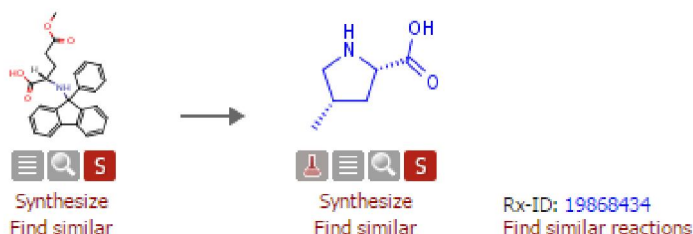
Multi-step reaction with 6 steps

- 1: lead nitrate, Et₃N / CHCl₃ / 87 h / Ambient temperature
- 2: 75 percent / CH₂Cl₂ / 16 h / Ambient temperature
- 3: 1.) potassium hexamethyldisilazide (KHMDs) / 1.) THF, toluene, -78 deg C, 1 h, 2.) THF, toluene, 3 h
- 4: 24 percent / LiAlH₄ / tetrahydrofuran / 4 h / -78 °C
- 5: 88 percent / PPh₃, CBr₄, iPr₂NEt / tetrahydrofuran / 1 h / Ambient temperature
- 6: 90 percent / CF₃CO₂H / CH₂Cl₂ / 16 h

[View Scheme](#)

Koskinen, Ari M. P.; Rapoport, Henry

Journal of Organic Chemistry, **1989**, vol. 54, # 8 p. 1859 - 1866
[Title/Abstract](#) [Full Text](#) [View citing articles](#) [Show Details](#)



Multi-step reaction with 5 steps

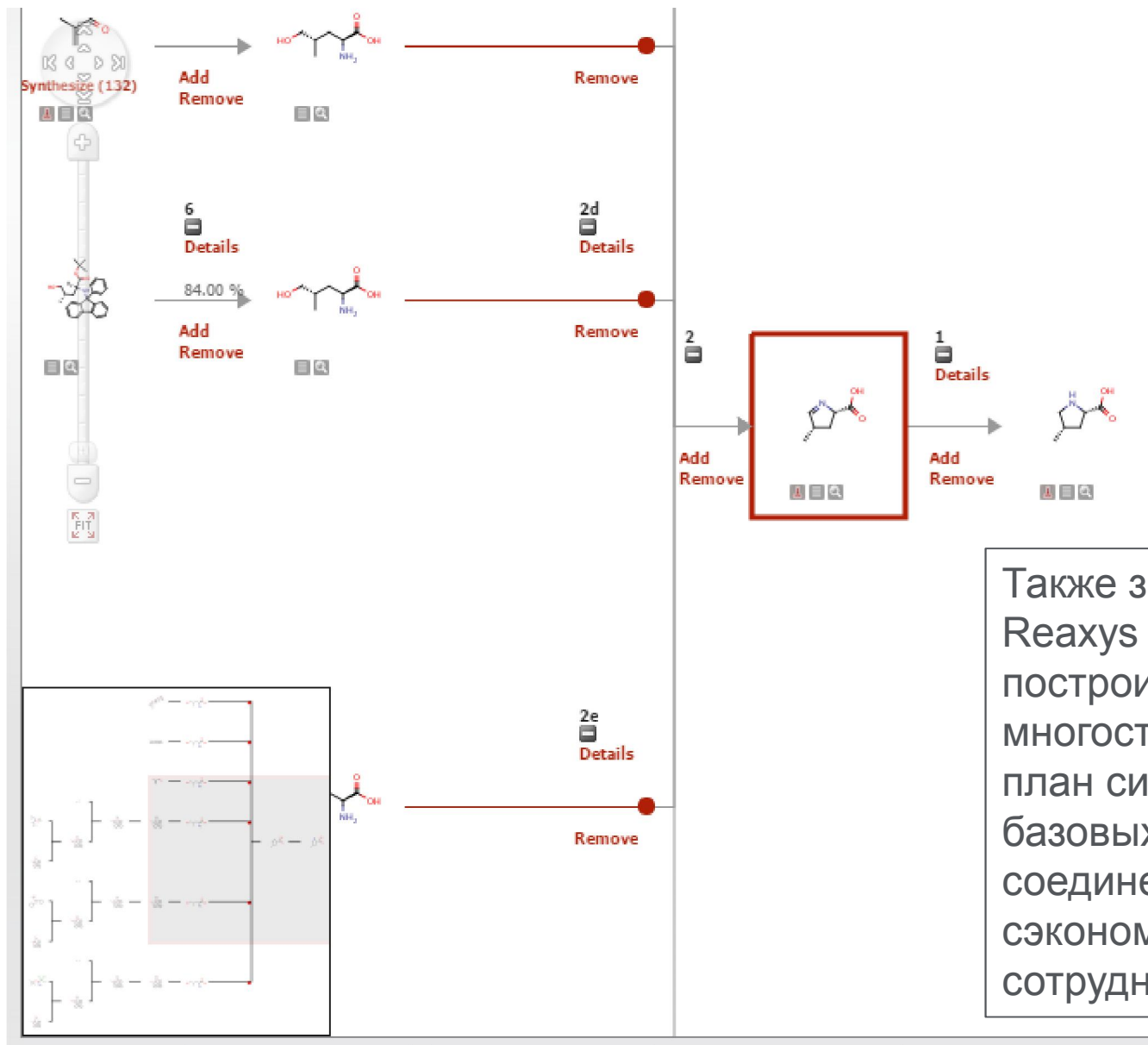
- 1: 75 percent / CH₂Cl₂ / 16 h / Ambient temperature
- 2: 1.) potassium hexamethyldisilazide (KHMDs) / 1.) THF, toluene, -78 deg C, 1 h, 2.) THF, toluene, 3 h
- 3: 24 percent / LiAlH₄ / tetrahydrofuran / 4 h / -78 °C
- 4: 88 percent / PPh₃, CBr₄, iPr₂NEt / tetrahydrofuran / 1 h / Ambient temperature
- 5: 90 percent / CF₃CO₂H / CH₂Cl₂ / 16 h

[View Scheme](#)

Koskinen, Ari M. P.; Rapoport, Henry

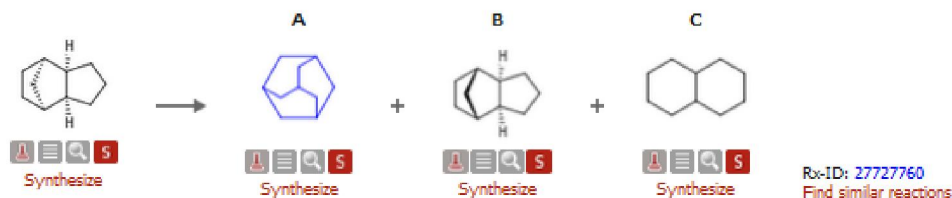
Journal of Organic Chemistry, **1989**, vol. 54, # 8 p. 1859 - 1866
[Title/Abstract](#) [Full Text](#) [View citing articles](#) [Show Details](#)

Разработка методики синтеза химических веществ



Также за секунды Reaxys может построить многостадийный план синтеза из базовых соединений, что сэкономит время сотрудников

Просмотр экспериментальных условий



With AlCl_3 , aluminium chloride in dichloromethane

T: -20°C ; 16 h;

Hide Experimental Procedure

Tsao, Ying-Yen; Liao, Chyuan-Neng; Chen, Chi-Yu; Lin, Chin-Ming; Wei, Kuo-Min

Patent: US2008/249341 A1, 2008 ;

Location in patent: Page/Page column 8 ;

[Title/Abstract](#)

[Full Text](#)

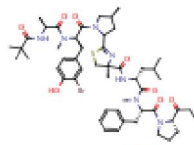
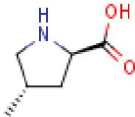
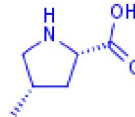
[Show Details](#)

5:

EXAMPLE 5 is the comparative example of EXAMPLE 4. 65 g of endo-THDCPD crystals from the same source of EXAMPLE 4 are placed in a 250 ml of glass bottle, followed by adding 40 g of dichloromethane thereto to dissolve these crystals, purging with dry nitrogen and stirring in the ice bath. Subsequently, 10 g of AlCl_3 is added to the dichloromethane solution of endo-THDCPD, followed by stirring for 2 hours in the ice bath, and continuously stirring for 16 hours at room temperature. The resulting mixture is washed with 100 ml of saturated KCl solution, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the upper layer in the separatory funnel. The above saturated KCl solution washing procedure is repeated for three times. Subsequently, the mixture washed with the saturated KCl solution is washed with 100 ml of deionized water, followed by adding it to a separatory funnel, shaking to allow to separate into two layers and leaving the lower layer in the separatory funnel. The above deionized water washing procedure is repeated for three times. Subsequently, the lower layer is distilled to remove dichloromethane and water. The bottoms is collected, and determined by chemical analysis. The chemical analysis shows that the bottoms is composed of 85.7 wt percent of exo-THDCPD, 0.5 wt percent of endo-THDCPD, 1.2 wt percent of Decalin, 5.8 wt percent of adamantane, 1.3 wt percent of exo-THMDCPD, and the other two-stage hydrotreated and saturated C_{11}^+ derivatives, namely CPD and/or MCPD dimers. The bottoms has a volumetric heating value of 39.17 MJ/L, a density of 0.9339 at 15°C , and a viscosity of 3.52 cSt at 20°C , and more than 26.7 cSt at -20°C . In this example, the isomerization reaction is violent because isomerization reaction time is too long so that portions of exo-THDCPD is further isomerized to adamantane which will increase the viscosity of the high energy fuel. Under such a violent reaction conditions, a small amount of THDCPD will be ring opened by hydrogen to give decalin (the side product) with relatively less volumetric heating value as well as density. Therefore, the isomerization reaction of this example is not suitable for preparing the high energy fuels because the freezing point of the isomerization product is too high.

В Reaxys приведены экспериментальные методики проведения реакция из более чем 280 химических журналов, что позволяет выбрать оптимальную процедуру химического синтеза. Тем самым экономя деньги на реактивы и время для выхода на стадию доклинических исследований

Проверка коммерческой доступности

Yield	Conditions	References
    Synthesize Find similar	A     Synthesize Find similar	B      Available through...  Accelrys' ACD  eMolecules  CambridgeSoft ACX
Stage #1: With ozone in methanol T=-78°C; 0.5 h; Stage #2: With dimethylsulfide in methanol T=-78 - 20°C; Inert atmosphere; Stage #3: With hydrogenchloride; water T=100°C; 48 h; Sealed vessel; optical yield given as percent de; Show Experimental Procedure		182625 Find similar reactions Sasaki, Hiroaki; Teruya, Toshiaki; Fukazawa, Hidesuke; Suenaga, Kiyotake Tetrahedron, 2011, vol. 67, # 5 p. 990 - 994 Title/Abstract Full Text View citing articles Show Details

Чтобы разработать наиболее экономически эффективную методику синтеза в Reaxys есть информация о стоимости молекул

Теплопроводность Алюминия при различных температурах

Ask Reaxys

Heat Capacity Cp of Aluminium

Search

Smart searching with Ask Reaxys. [See examples >](#)

Bioactivities (0) Reactions (8) **Substances (14)** Targets (0) Citations (8)

go to Page Page 1 of 2

Limit to Exclude Export Print Zoom In Zoom Out Hide Sort by No of References Display as Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.																																
	Chemical Name: copper Reaxys Registry Number: 4122947 CAS Registry Number: 12775-06-1, 15158-11-9, 15721-63-8, 16941-75-6, 17492-90-6, 19490-52-3, 20499-83-6, 20499-84-7, 20499-85-8, 20499-86-9, 20573-10-8, 20573-11-9, 21595-51-7, 21595-52-8, 22206-52-6, 26445-28-3, 28959-95-7, 37362-93-9, 39417-05-5, 54603-16-6, 54603-23-5, 54603-32-6, 54603-40-6, 54603-48-4, 54603-81-5, 54603-89-3, 58316-56-4, 95985-91-4, 122297-32-9, 7440-50-8 Type of Substance: Coordination compound/Isotope or isotope containing compound/Solid solution Molecular Formula: Cu Linear Structure Formula: Cu Molecular Weight: 63.546 InChI Key: RYGMFSIKBFXOCR-UHFFFAOYSA-N	1321 prep out of 18112 reactions.	Druglikeness Bioactivity Identification Physical Data (8551) Spectra (159) Use/Application (552) Quantum Chemical Data (310)	Show Targets	22248																																
	Chemical Name: aluminium Reaxys Registry Number: 7365459 CAS Registry Number: 7429-90-5 Type of Substance: Alloy Molecular Formula: Al Linear Structure Formula: Al Molecular Weight: 26.9815 InChI Key: AZDRQVAHNSJQ-UHFFFAOYSA-N	357 prep out of 14636 reactions.	Heat Capacity Cp (476) <table border="1"> <thead> <tr> <th>Heat Capacity Cp</th> <th>Temperature (Heat Capacity Cp)</th> <th>Comment (Heat Capacity Cp)</th> <th>Reference</th> </tr> </thead> <tbody> <tr> <td>0.011 Jmol⁻¹K⁻¹</td> <td>-267.876 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.035 Jmol⁻¹K⁻¹</td> <td>-263.49 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.085 Jmol⁻¹K⁻¹</td> <td>-259.08 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.181 Jmol⁻¹K⁻¹</td> <td>-254.71 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.341 Jmol⁻¹K⁻¹</td> <td>-250.34 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.602 Jmol⁻¹K⁻¹</td> <td>-246.04 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> <tr> <td>0.992 Jmol⁻¹K⁻¹</td> <td>-241.67 °C</td> <td>1 atm Solid</td> <td>Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011, vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details</td> </tr> </tbody> </table>	Heat Capacity Cp	Temperature (Heat Capacity Cp)	Comment (Heat Capacity Cp)	Reference	0.011 Jmol ⁻¹ K ⁻¹	-267.876 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.035 Jmol ⁻¹ K ⁻¹	-263.49 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.085 Jmol ⁻¹ K ⁻¹	-259.08 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.181 Jmol ⁻¹ K ⁻¹	-254.71 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.341 Jmol ⁻¹ K ⁻¹	-250.34 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.602 Jmol ⁻¹ K ⁻¹	-246.04 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details	0.992 Jmol ⁻¹ K ⁻¹	-241.67 °C	1 atm Solid	Morishita, Masao; Yamamoto, Hiroaki; Koder, Masahiro; Ikeda, Keiichi; Miura, Seiji; Yamada, Yoshihiro Thermochimica Acta, 2011 , vol. 526, # 1-2 p. 90 - 98 Title/Abstract Full Text View citing articles Show Details		
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Chemical Names and Synonyms
aluminium, anhydrous aluminium, aluminium Powder, aluminum powder, ALUMINIUM, ALUMINUM, alumina

Hit Data
Heat Capacity Cp (71 Hits out of 476 view all)
Druglikeness

Поиск сплавов титана с температурой плавления 1320 – 1370 °C, Содержащих не менее 10% Ti

Reactions Substances MedChemistry Literature ReaxysTree Physical Spectra Natural Product

Structure

selected query editor:

 Elemental
from
dotmatics
knowledge solutions

PASTE STRUCTURE EDITOR

Create Structure Template from Name

☒ As drawn
☐ Substructure
☐ on heteroatoms
☒ on all atoms
☐ Similarity

☐ Include tautomers
☐ Ignore stereo
☐ No salts
☐ No mixtures
☐ No isotopes
☐ No charges
☐ No radicals
☐ No ring closures
☒ Align results with query

More options

Molecular Formula

Molecular Formula Lookup

Alloy

Component Formula

Ti

Percentage

10-100

Percentage Type: Weight

Additional Components: ☒

Поиск информации в области Наук о материалах в Reaxys

Поиск сплавов титана с температурой плавления 1320 – 1370 °С, Содержащие не менее 10% Ti

Open Analysis View

Жмем сюда

Bioactivities (0) Reactions (882) **Substances (2540)** Targets (0) Citations (1362)

go to Page Page 1 of 283

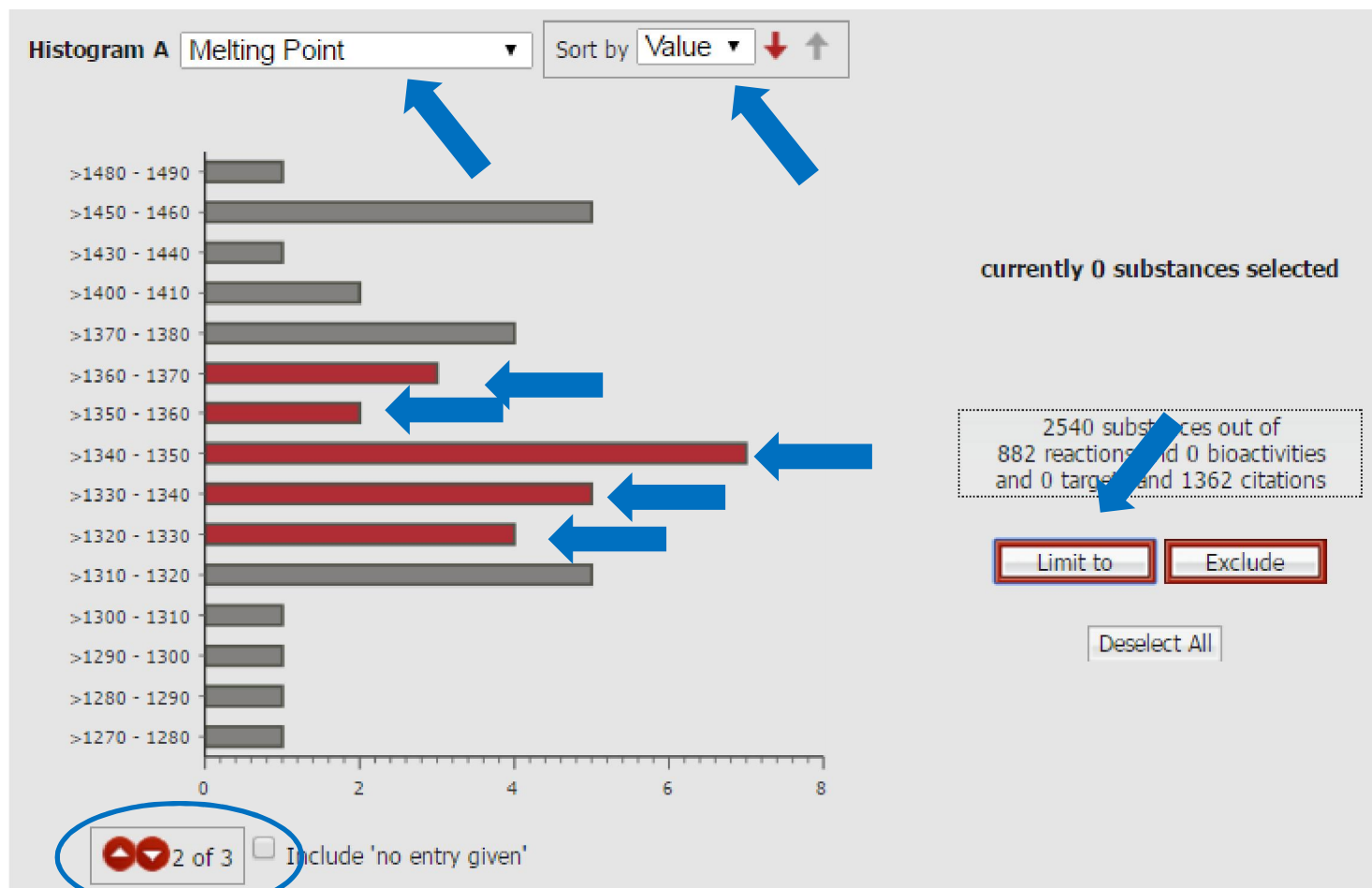
Limit to Exclude Export Print Zoom in Zoom out Hide

Sort by No of References Display as Exclude GOSTAR data

	Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
☐ 1	mixture (composition completely given) : titanium nickel Synthesize Show Details	Reaxys Registry Number: 16911764 Type of Substance: mixture (composition completely given) Alloy	2 prep out of 3 reactions.	Physical Data (15) Spectra (2)	Show Targets	23
☐ 2	mixture (composition completely given) : titanium aluminium vanadium Show Details	Chemical Name: TA6V Reaxys Registry Number: 16911805 Type of Substance: mixture (composition completely given) Alloy	0 prep out of 1 reactions.	Physical Data (15) Spectra (1)	Show Targets	19
☐ 3	mixture (composition completely given) : titanium vanadium Show Details	Reaxys Registry Number: 16911805 Type of Substance: mixture (composition completely given) Alloy	0 prep out of 1 reactions.	Physical Data (14)	Show Targets	18

Для каждого сплава приведены свои свойства и литературные записи.

Поиск сплавов титана с температурой плавления 1320 – 1370 °С, Содержащие не менее 10% Ti



Мы нашли 21 соединение титана с заданной температурой плавления

Bioactivities (0) Reactions (2) **Substances (21)** Targets (0) Citations (6) go to Page Page 1 of 3

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
1 mixture (composition completely given) : silicon titanium vanadium Hide Details	Reaxys Registry Number: 16566456 Type of Substance: mixture (composition completely given) Alloy	no reactions.	Hit Data (1) Physical Data (1)	Show Targets	2

Composition

silicon (10 weight percent)

Si

Synthesize
Find similar

titanium (30 weight percent)

Ti

Synthesize
Find similar

vanadium (60 weight percent)

V

Synthesize
Find similar

Hit Data

Melting Point (1 Hits out of 1 view all)

Melting Point	Reference
1350 - 1380 °C	Komjathy, S. Journal of the Less-Common Metals, 1961 , vol. 3, p. 468 - 488 Full Text View citing articles Show Details Gmelin Handbook: V: MVol.B2, 137, page 659 - 662 Full Text Show Details

Поиск сплавов любых железа с магнитными свойствами



1.

Add to Query: Structure Molecular Formula **Alloy** Add/Remove Fields... **Search Substances**

2.

Alloy

Component Formula	Percentage
Fe	5-100

Percentage Type: Unspecified Additional Components: ☒

3.

Add/Remove Fields...

4.

Insert/Remove Properties
Define the "Substances" query layout

Find any property: **magne** **RESET**

Reaxys

Physical Data

Magnetic Data exists

Description (Magnetic Data) (MAG.KW)

Temperature (Magnetic Data), °C (MAG.T)

Moment (Magnetic Data), Acm² (MAG.MMOM)

Magnetic Susceptibility exists

Magnetic Susceptibility, 10⁻⁶cm³mol⁻¹ (MSUS.MSUS)

Temperature (Magnetic Susceptibility), °C (MSUS.T)

Add >>

Remove

Remove all

Add Defaults

Electrochemical Behaviour (in Reaxys)

Electrochemical Characteristics (in Reaxys)

Electrochemistry Data (in Reaxys)

Electrolytic Conductivity (in Reaxys)

Electron Binding (in Reaxys)

Optical Data (MCS) (in Reaxys)

Optical Rotatory Dispersion (in Reaxys)

Optical Rotatory Power (in Reaxys)

Optics (in Reaxys)

Solubility (MCS) (in Reaxys)

Solubility Product (MCS) (in Reaxys)

Use Pattern (in Reaxys)

Substance Basic Index (in multiple)

Available to add Already selected Searches in multiple databases

Save

Поиск сплавов железа с магнитными свойствами

5.

Physical Data

Magnetic Data	☒ exists	×
Magnetic Susceptibility	☐ exists	×

Show AND Buttons

6.

Search Substances

Поиск информации в области Наук о материалах в Reaxys

Сплавы железа с магнитными свойствами

Bioactivities (1) Reactions (887) **Substances (4646)** Targets (0) Citations (3465)

go to Page Page 1 of 517

Limit to Exclude Export Print Zoom In Zoom out Hide Sort by No of References Display as Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of ref.
1 mixture (composition completely given) : iron nickel Synthesize Hide Details	Reaxys Registry Number: 16555145 Type of Substance: mixture (composition completely given) Alloy	1 prep out of 1 reactions.	Hit Data (7) Physical Data (21) Spectra (3)	Show Targets	95

★ Magnetic Data (7 Hits out of 7 view all)

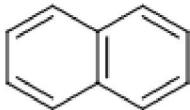
Description (Magnetic Data)	Temperature (Magnetic Data)	Moment (Magnetic Data)	Reference
Ferromagnetic			Ali; Mahmoud; Farid; Atef Physica Status Solidi (A) Applied Research, 1998 , vol. 165, # 2 p. 377 - 387 Title/Abstract Full Text View citing articles Show Details
Magnetostriction			Auwers, O. v. Wiss. Veroeffentl. Siemens-Werke, 1936 , vol. 15, # 2 p. 117 - 117 Full Text Show Details
Magnetization diagram			Dahl, O.; Pfaffenberger, J. Metallwirtsch., Metallwiss., Metalltech., 1934 , vol. 13, p. 528 - 528 Full Text Show Details Dahl, O.; Pfaffenberger, J. Z. Tech. Phys., 1934 , vol. 15, p. 103 - 103 Full Text Show Details

Curie temperature	562 °C	
Magnetic moment		1.5469E-19 Acm ²

Найдем в Reaxys органометаллические соединения кобальта с нафталиновым фрагментом.

Какие соединения известны?

Structure



PASTE

EDIT

CLEAR

Create Structure Template from Name

☐ As drawn

☒ Substructure

☐ on heteroatoms

☒ on all atoms

☐ Similarity

☐ Include tautomers

☐ Ignore stereo

☐ No salts

☐ No mixtures

☐ No isotopes

☐ No charges

☐ No radicals

☐ No ring closures

☒ Align results with query

More options

Molecular Formula

Molecular Formula

Co[1-5]*

Lookup

Formula Builder

За один запрос в Reaxys найдено 2646 соединений кобальта с нафталиновым фрагментом

Что известно о электрохимических свойствах этих соединений?

Все найденные соединения в Reaxys можно отфильтровать. И оставить только те, по которым известны электрохимические свойства

Filter by:

- Substructure
- Molecular Weight
- Number of Fragments
- Physical Data
 - ☐ Crystal Property Description 1254
 - ☐ Magnetic Data 614
 - ☐ Conformation 466
 - ☐ Solubility (MCS) 453
 - ☐ Crystal Phase 444
 - ☐ Space Group 394
 - ☐ Crystal System 367
- More
 - Limit to
 - Exclude
- Spectroscopic Data
- Ecological Data
- Natural Product
- Availability
- Availability in other DBs
- LogP
- H Bond Donor (HBD)
- H Bond Acceptor (HBA)
- Polar surface Area (PSA)
- Highest clinical phase

Bioactivities (429) Reactions (2289) **Substances (2646)** Targets (9) Citations (1167)

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as

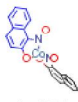
Structure Structure/Compound Data

1


Synthesize | Show Details
Find similar

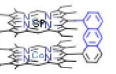
Chemical Name: {Co(2-C10H7NC)5}I
Reaxys Registry Number: 16724032
Type of Substance: Coordination compound
Molecular Formula: C₅₅H₃₅CoN₅I
Linear Structure Formula: {Co(C₁₀H₇NC)5}⁽¹⁺⁾*I⁽¹⁻⁾={Co(C₁₀H₇NC)5}I
Molecular Weight: 951.814
InChI Key: AGAFRGUCUCJHBM-UHFFFAOYSA-M

2


Synthesize | Show Details
Find similar

Chemical Name: {Co(αβ-C10H6NO2)2}
Reaxys Registry Number: 16947113
CAS Registry Number: 32248-55-8, 24412-90-6
Type of Substance: Coordination compound
Molecular Formula: C₂₀H₁₂CoN₂O₄
Linear Structure Formula: {Co(C₁₀H₆NO₂)2}
Molecular Weight: 403.319
InChI Key: JOGYIIBGYSRWMB-UHFFFAOYSA-L

3


Synthesize | Show Details
Find similar

Chemical Name: Co-Co-1,8-anthryldiporphyrin
Reaxys Registry Number: 16470482
CAS Registry Number: 94250-18-7
Type of Substance: Coordination compound
Molecular Formula: C₇₈H₇₈Co₂N₈
Linear Structure Formula: {Co(CcN(CH₂CH₂)CH₂)4H₂)2C₁₄H₆

Electrical Data available (24)

Description is
Electric Conductivity =
Temperature of Electric Conductivity =
Critical Superconductivity Temperature =

Electrical Moment available (4)

Description is
Moment =
Temperature =
Method is
Solvent is

Electrochemical Behaviour available (6)

Description is

Electrochemical Characteristics available (259)

Description is
Solvent is
pH-Value =
Temperature =

Electrochemistry Data available (4)

Electrochemical Cell is
Cell Potential =
Description is

Electrolytic Conductivity available (212)

Description is
Electrolytic Conductivity =

Electron Binding available (11)

Description is

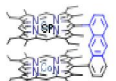
За один запрос в Reaxys найдено 2646 соединений кобальта с нафталиновым фрагментом

Что известно о электрохимических характеристиках этих соединений?

Activities (16) Reactions (156) **Substances (259)** Targets (0) Citations (108)

go to Page Page 1 of 29

Limit to Exclude Export Print Zoom in Zoom out Hide Sort by No of References Display as Exclude GOSTAR data

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	Target	N° of re
	Chemical Name: Co-Co-1,8-anthryldiporphyrin Reaxys Registry Number: 16470482 CAS Registry Number: 94250-18-7 Type of Substance: Coordination compound Molecular Formula: C ₇₈ H ₇₈ Co ₂ N ₈ Linear Structure Formula: (Co(C ₅ N(CH ₂ CH ₃)CH ₃) ₂ C ₁₄ H ₈) Molecular Weight: 1245.52 InChI Key: QFSWQSYTBKLGAM-NEIXCZRWSA-N	1 prep out of 5 reactions.	Hit Data (4) Druglikeness Identification Physical Data (7) Spectra (2)	Show Targets	7

Synthesize | Hide Details
Find similar

Chemical Names and Synonyms

Co-Co-1,8-anthryldiporphyrin

Hit Data

Electrochemical Characteristics (4 Hits out of 4 view all)

Description (Electrochemical Characteristics)	Solvent (Electrochemical Characteristics)	Product XRN (Electrochemical Characteristics)	Product	Comment (Electrochemical Characteristics)	Reference
Electrochemical characteristics given					Chen, Ping; Lau, Hoyi; Habermeyer, Benoît; Gros, Claude P.; Barbe, Jean-Michel; Kadish, Karl M. Journal of Porphyrins and Phthalocyanines, 2011 , vol. 15, # 5-6 p. 467 - 479 Title/Abstract Full Text View citing articles Show Details
cyclovoltammetry	benzonitrile	16706155	[Co(C32H35N4)]2C14H8O2(1+)	transmitted electrons: 1; ferrocene/ferrocenium; 0.2 M Bu4NPF6; -0.04 V	Mest, Yves Le; Inisan, Claude; Laouenan, Andre; L'Her, Maurice; Talarmin, Jean; Khalifa, Moulay El; Saillard, Jean-Yves Journal of the American Chemical Society, 1997 , vol. 119, # 26 p. 6095 - 6106 Title/Abstract Full Text View citing articles Show Details
cyclovoltammetry	benzonitrile	16706157	[Co(C20H3N4(CH3)4(C2H5)4)]2(C14H8) (2+)	transmitted electrons: 2; ferrocene/ferrocenium; 0.2 M Bu4NPF6; 0.05 V	Le Mest, L'Her; Saillard Inorganica Chimica Acta, 1996 , vol. 248, # 2 p. 181 - 191 Title/Abstract Full Text View citing articles Show Details
cyclovoltammetry	methylene chloride=methylene dichloride			saturated calomel electrode (SCE); potential diagram; 0.1 M (C4H9)4NClO4	Liu, Hsue-Yang; Abdulmuhdi, I.; Chang, C. K.; Anson, Fred C. Journal of Physical Chemistry, 1985 , vol. 89, # 4 p. 665 - 670 Title/Abstract Full Text View citing articles Show Details