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Ростов-на-Дону, 23.05.2017



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Chemical Abstracts Service



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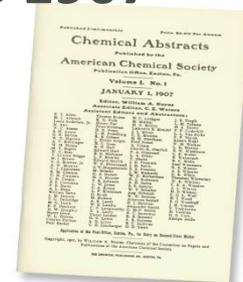
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The CAS REGISTRY represents the world's largest collection of small molecules.

Cc1ccc(cc1)C(=O)N2CCNCC2

- **CAS - мировой лидер в области химической информации, первый выпуск Chemical Abstracts опубликован в 1907**
- **1,400 сотрудников, из них 1,000 научные редакторы “индексаторы” в Колумбусе, США**
- **является подразделением Американского химического общества, *American Chemical Society, ACS***
- **производит и поставляет такие ресурсы, как *SciFinder[®]*, *STN[®]***



Специалисты “индексаторы” CAS анализируют полные тексты статей и патентов


 US 20070078189A1

(19) **United States**
 (12) **Patent Application Publication** (10) **Pub. No.: US 2007/0078189 A1**
 Sarshar (43) **Pub. Date: Apr. 5, 2007**

(54) **NOVEL THERAPEUTIC AGENTS FOR THE TREATMENT OF CANCER, METABOLIC DISEASES AND SKIN DISORDERS** (52) **U.S. CL.** 514/090; 568/314; 568/326; 568/328

(75) **Inventor:** Sephr Sarshar, Cardiff by the Sea, CA (US) (57) **ABSTRACT**

Correspondence Address:
 DL A PIPER US LLP
 436 EXECUTIVE DRIVE
 SUITE 1100
 SAN DIEGO, CA 92121-2133 (US)

(73) **Assignee:** Auspex Pharmaceuticals, Vista, CA
 (21) **Appl. No.:** 11/592,009
 (22) **Filed:** Nov. 1, 2006

Related U.S. Application Data

(63) **Continuation-in-part of application No. PCT/US05/15366, filed on May 2, 2005.**
 (60) **Provisional application No. 60/567,965, filed on May 3, 2004.**

The present invention is directed to novel compounds according to formulae




wherein R₁, R₂, R₃, and R₄ are as defined herein. The invention also discloses methods of preparation, pharmaceutical compositions, and methods of disease treatment utilizing pharmaceutical compositions comprising these compounds. The compounds of this invention are novel therapeutic agents for the treatment of cancer, diabetes, metabolic diseases and skin disorders in mammalian subjects. These compounds are also useful modulators of gene

CRYSTAL GROWTH AND DESIGN
 XXXX
 VOL. XXX, NO. XX

A Dynamic Microporous Metal–Organic Framework with BCT Zeolite Topology: Construction, Structure, and Adsorption Behavior

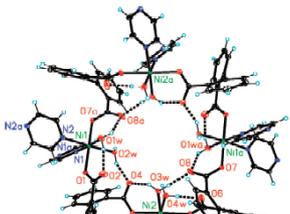
Sheng Hu,¹ Jie-Peng Zhang,² Hao-Xiang Li,¹ Ming-Liang Tong,^{3,4} Xiao-Ming Chen,^{3,4} and Susumu Kitagawa¹

MOE Laboratory of Bioinorganic and Synthetic Chemistry/State Key Laboratory of Optoelectronic Materials and Technologies, School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and Department of Synthetical Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Katata, Nishikyo-ku, Kyoto 615-8510, Japan

Received June 30, 2007; Revised Manuscript Received August 14, 2007

ABSTRACT: A new microporous metal–organic framework (MOF) material [Ni₄(dpa)(pyz)(H₂O)]·11H₂O (1) with BCT zeolite topology has been hydrothermally synthesized. The framework components undergo dynamic structural transformation in response to removal and rebinding of the suitable guest molecules.

Microporous metal–organic framework (MOF) materials have received increasing attention mainly because of their potential application in adsorption, ion exchange, and catalysis, as well as intriguing architectures and topologies.^{1–2} In particular, dynamic porous MOF materials retain crystallinity after some structural transformations, including stretching, rotational, “breathing”, and scissoring mechanisms, responding to external stimuli, which is essentially distinct from that of the rigid classical porous materials.³ Those reversibly dynamic structural changes, being induced by removal/readsorption of guest molecules and/or caused by the removal/addition of ligands from/to the host framework itself, may be used for the accommodation and separation of specific molecules. However, it is still a challenge to control the pore size and chemical characteristics of the internal surface as well as to decorate the topology of dynamic porous MOF materials.⁴ A promising route to such materials is the rational choice of suitable inorganic compositions as secondary building units (SBUs) and flexible organic ligands as the spacers. 1,1'-Biphenyl-2,2'-dicarboxylic acid




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И добавляют индексные термины – ключевые слова и регистрационные номера веществ, описанных в первоисточнике

Crystallography and Liquid Crystals (Section75-11)

Concepts

Liquid crystals

chiral; study on chiral liq. crystals based on optical active isoamyl alc.

Esterification
Phase transition
Thermal stability

Heating
Temperature

study on chiral liq. crystals based on optical active isoamyl alc.

Substances

1403559-75-0P 
1403559-78-3P 
1403559-79-4P 
1403559-80-7P 
1403559-81-8P 

study on chiral liq. crystals based on optical active isoamyl alc.

Properties; Synthetic preparation; Preparation

137-32-6 2-Methyl-butan-1-ol 
149-91-7 3,4,5-Trihydroxy-benzoic acid, reactions 
38289-28-0 

study on chiral liq. crystals based on optical active isoamyl alc.

Reactant; Reactant or reagent



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 - PCTFULL
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Term Explorer ?

Term:

CAplus Controlled Terms (Lexicon)

[Select All](#) | [Deselect All](#) | [Expand All](#) | [Collapse All](#)

Liquid crystals (115544)

- liquid crystals
- liquid crystals, polymeric

- Chiral liquid crystals (414)
 - Chiral smectic liquid crystals (437)
 - Cholesteric liquid crystals (3059)
 - Liquid crystal optical filters (79)
 - Liquid crystal transition (4092)
 - Liquid crystals, polymeric (27598)
- Nematic liquid crystals (8605)
 - Cholesteric liquid crystals (3059)
 - Polymer-dispersed liquid crystals (1761)
- Smectic liquid crystals (3117)
 - Chiral smectic liquid crystals (437)

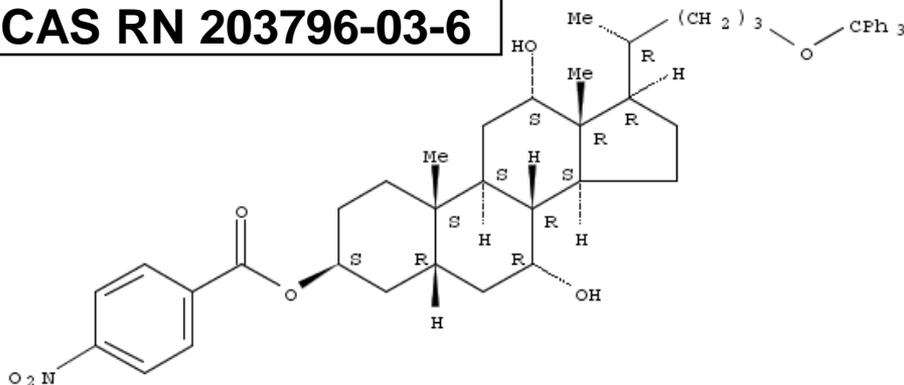
Term	Current
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Ученые CAS обнаруживают существенные данные, такие как неявно описанные структуры, которые отсутствуют в других базах данных

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO₃ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na₂SO₄. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO₂ chromatography (Et₂O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H) 5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 2 H), 0.70 (s, 3 H). ¹³C NMR (CDCl₃, 75 MHz) δ 164.21, 150.56,

CAS RN 203796-03-6



Absolute stereochemistry.

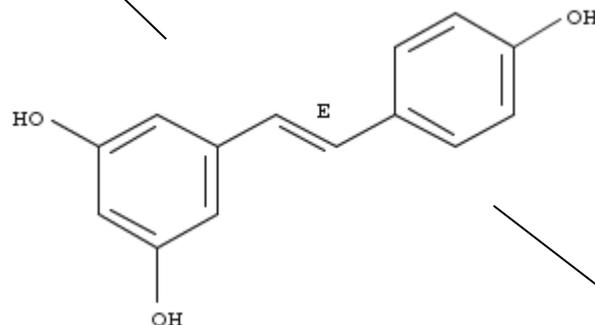


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Что нам известно об этом соединении?

- ~6,730 References
- Reactions
- Commercial Sources
- Regulatory Information



CAS Registry Number: 501-36-0

C₁₄ H₁₂ O₃

1,3-Benzenediol, 5-[(1E)-2-(4-hydroxyphenyl)ethenyl]-
 1,3-Benzenediol, 5-[2-(4-hydroxyphenyl)ethenyl]-, (E)-; 3,4',5-Stilbenetriol (7CI,8CI); Resveratrol (6CI); (E)-2-(3,5-Dihydroxyphenyl)-1-(4-hydroxyphenyl)ethene; (E)-3,4',5-Trihydroxystilbene; (E)-5-(p-Hydroxystyryl)resorcinol; (E)-Resveratrol; 3,4',5-Trihydroxy-trans-stilbene; 5-[(1E)-2-(4-Hydroxyphenyl)ethenyl]-1,3-benzenediol; CA 1201; Resveratrol P 5; Resvida; Vineatrol 20M; trans-3,5,4'-Trihydroxystilbene; trans-Resveratrol

Biological Properties	Value	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	(2) CAS
Half-Life (Biological)	See full text	(9) CAS
LC50	See full text	(13) CAS
Minimum Inhibitory Concentration	See full text	(43) CAS

Lipinski and Related Properties	Value
Freely Rotatable Bonds	5
H Acceptors	3
H Donors	3
H Donor/Acceptor Sum	6
logP	3.024±0.267
Molecular Weight	228.24

Spectra Properties	Value
Carbon-13 NMR Spectrum	See spectrum
Proton NMR Spectrum	See spectrum

Если это важно, это есть в SciFinder!

Базы данных входящие в SciFinder

CAplus® – библиография 10,000+ журналов (185 стран) патенты из 63 ведомств	44+ млн. ссылок (5,000 ежедневно), Рефераты и индексирование с 1802 г., цитаты с 1997–
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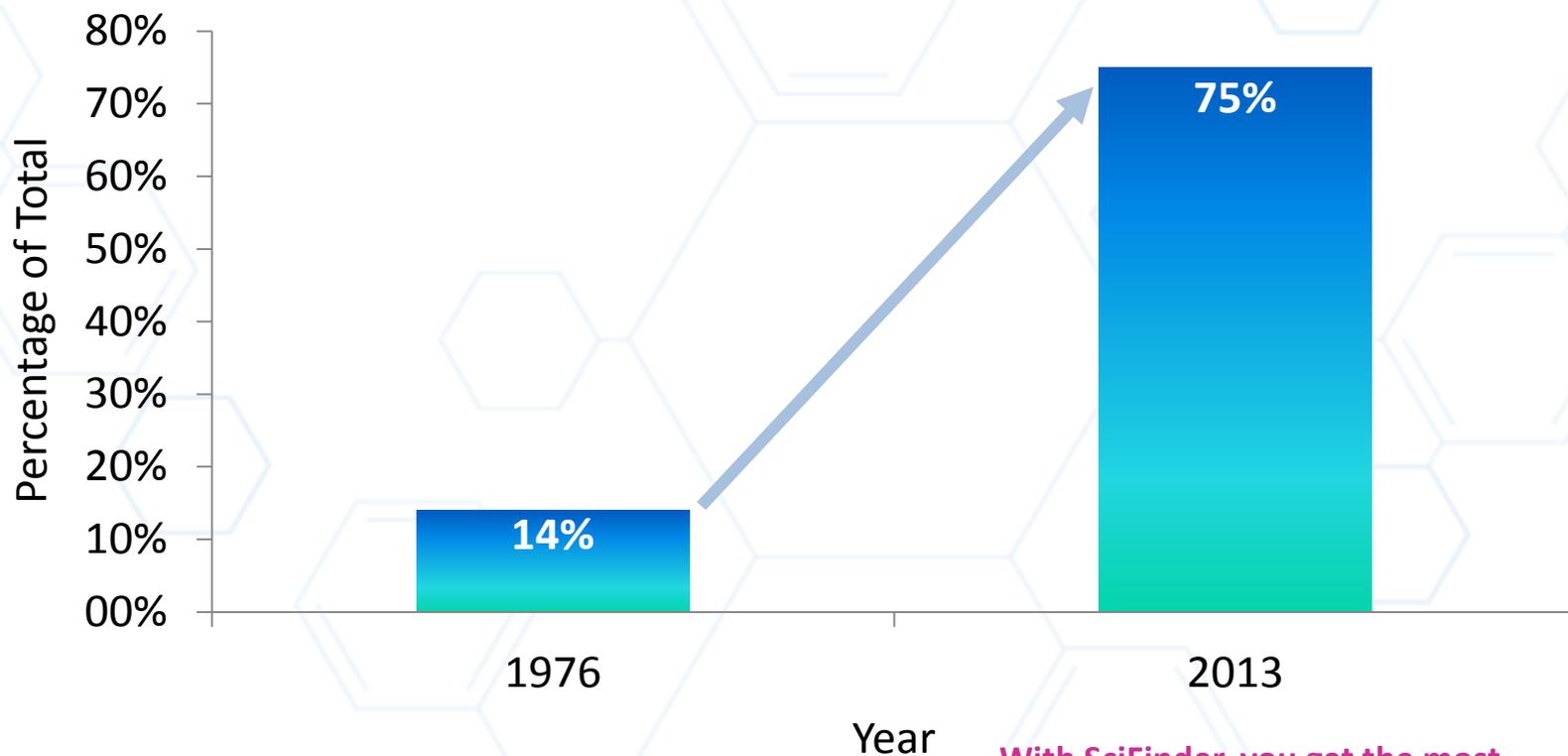
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Базы данных CAS обеспечивают широкий охват публикаций в области **биологии и медицины**

Молекулярная биология и генетика

- *Annual Review of Genetics*
- *Cell*
- *Developmental Cell*
- *Genome Research*
- *Journal of Cell Biology*
- *Molecular Genetics and Genomics*
- *Nature*
- *New England Journal of Medicine*
- *Proceedings of the National Academy of Sciences*
- *Science*

Биохимия

- *ACS Chemical Biology*
- *ACS Synthetic Biology*
- *Annual Review of Biochemistry*
- *Biochemistry and Cell Biology*
- *Cellular Physiology and Biochemistry*
- *Journal of Biological Chemistry*
- *Journal of Cellular Biochemistry*
- *Molecular and Cellular Biochemistry*
- *Preparative Biochemistry and Biotechnology*

Фармацевтика и медицинская химия

- *Advanced Drug Delivery Reviews*
- *Annual Review of Pathology: Mechanisms of Disease*
- *Anti-Inflammatory Anti-Allergy Agents in Medicinal Chemistry*
- *Circulation Research*
- *Immunity*
- *Journal of the American Medical Association*
- *Journal of Experimental Medicine*
- *Nature Reviews Drug Discovery*
- *Trends in Immunology*

Дополнительные возможности SciFinder

6.8 млн+

Экспериментальных методик реакций – более 1 млн было добавлено только в этом году!

Методики из журналов **Springer and Thieme Verlag**

1.4 млн

Экспериментальных спектров >22,000 гетероатомных ЯМР спектров

> 4.5 млн экспериментальных свойств

100,000+

Реакций из наиболее авторитетных источников

Science of Synthesis из Thieme и Wiley's *Encyclopedia of Reagents for Organic Synthesis and Organic Reactions (EROS)* в качестве примера

1,800+

Наименований белков и синонимов

Охват диссертаций был увеличен за счет работ из Китая

SciFinder Smart Search – продвинутая система поиска для помощи пользователям



- **Интеллектуальная расшифровка поисковых терминов**
 - синонимы: cancer → e.g. tumor
 - различные словоформы : freeze → frozen
 - единственное и множественное число : mouse → mice
 - аббревиатура : HPLC
 - сокращенное написание : solvable → solv
- **Альтернативные варианты написания**
- **Структурные таутомеры и комплексы**

Эффективные инструменты интерфейса SciFinder

Stay current in
your field and
keep track of
competition

Quickly find and
analyze information
(research topic,
structure, reaction)

Share ideas with
colleagues and
collaborators

The screenshot displays the SciFinder web interface. At the top, there is a navigation bar with 'SciFinder' logo, 'Preferences', 'SciFinder Help', and 'Sign Out'. Below this is a secondary bar with 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', and 'Export'. The main search area shows a query: 'Keep Me Posted "carbon nanotubes"[May 17, 2014] (234)'. A toolbar contains options like 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner'. The 'Analyze' tab is active, showing a dropdown menu for 'Analyze by:' with 'Company-Organization' selected. Below this is a table of results:

Company-Organization	Count
East China Normal University, Peop Rep China	3
University of Toronto, Can	3
...	2

The main content area shows a list of references, with the first one selected: '1. In vivo biodistribution of platinum-based drugs encapsulated into multi-walled carbon nanotubes'. The abstract text is visible below the title.

Применение фильтров Categorize и Analyze облегчает поиск релевантной информации

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.

Category Heading	Category	Index Terms	Selected Terms
All	Substances in biology (221)	Select All Deselect All	
General chemistry	Animal pathology (69)	<input type="checkbox"/> Interferons 7 ▲	
Biotechnology	Immunology (72)	<input type="checkbox"/> Antibodies and Immunoglobulins 5	
Synthetic chemistry	Processes & systems (44)	<input type="checkbox"/> Interferons, α 5	
Genetics & protein chemistry	Endocrinology (48)	<input type="checkbox"/> Vaccines 5	
Physical chemistry	Anatomy (27)	<input type="checkbox"/> Interleukin 2 3	
Polymer chemistry	Substances in adverse effects (16)	<input type="checkbox"/> Interleukin 4 3	
Biology		<input type="checkbox"/> Leukotriene B4 3	
Technology		<input type="checkbox"/> RANTES (chemokine) 3	
Analytical chemistry		<input type="checkbox"/> Spleen 3	
Environmental chemistry		<input type="checkbox"/> Tumor necrosis factor α 3	
		<input type="checkbox"/> Anti-HIV agents, vaccines 2	
		<input type="checkbox"/> CD4 antigens 2	
		<input type="checkbox"/> CXC chemokines 2	
		<input type="checkbox"/> Etanercept 2	
		<input type="checkbox"/> High throughput screening 2 ▼	

Biology > Immunology

SUBSTANCES ⓘ

Get References Get Reactions Get Commercial Sources

Sort by: CAS Registry Number ▼

0 of 1 Substance Selected

1. **28911-01-5** 🔍

~2061 📄 ~34 🧪

C₁₇ H₁₂ Cl₂ N₄
4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-

Regulatory Information
Spectra
Experimental Properties

Analyze by: ⓘ

- Target Indicators
- Bioactivity Indicators**
- Commercial Availability
- Elements
- Reaction Availability
- Substance Role
- Target Indicators**
- Receptors (any)

Transport proteins (all) 1

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Российская наука в Chemical Abstracts (как пример, с 2009-)

- Более **207,800** публикаций российских авторов включены в **Chemical Abstracts** с 2009 года
 - **136,900** статей из журналов и **70,900** патентов
- Включены статьи из **400** наименований журналов, опубликованных на русском языке, или имеющих указание на то, что журнал российских в их названиях (**Russian Chemical Reviews, Russian Journal of Organic Chemistry** и т.д.)

Специалисты CAS переводят на английский рефераты

В. В. Быкова, Г. А. Ананьева, Н. В. Усольцева

ХИРАЛЬНЫЕ ЖИДКИЕ КРИСТАЛЛЫ НА ОСНОВЕ ОПТИЧЕСКИ АКТИВНОГО ИЗОАМИЛОВОГО СПИРТА

Ивановский государственный университет, НИИ Наноматериалов
153025 Иваново, ул. Ермака, 39. E-mail: nv_usoltseva@mail.ru

С целью изучения влияния строения каламитных соединений на их мезоморфные свойства осуществлен синтез и изучены текстурные характеристики пяти производных изоамилового спирта. Установлено, что из пяти соединений только два (алкилзамещенные) проявляют хиральную нематическую фазу. Алкоксизамещенные и производные со сложноэфирной связью формируют нематическую фазу без признаков хиральности.

Ключевые слова: синтез, хиральные жидкие кристаллы, мезоморфизм, оптически активный изоамиловый спирт. (С. 43 – 47)

□ 1. **Chiral liquid crystals based on optical active isoamyl alcohol** 🔍 📖 Full Text

By Bykova, V. V.; Anan'eva, G. A.; Usoltseva, N. V.

From Zhidkie Kristally i Ikh Prakticheskoe Ispol'zovanie (2011), (1), 43-47. | Language: Russian, Database: CAPLUS

To study the influence of the calamitic compds. structure on their mesomorphic properties, the synthesis and study of the texture characteristics of S isoamil alc. derivs. were carried out. Only two (alkyl substituted) from 5 compds. possess chiral nematic phase. The alkoxy substituted and the ester derivs. from nematic phase without chirality features.

Список российских журналов (top list) в Chemical Abstracts

Journal	Refs 2009-
RUSS CHEM BULL	1478
IZV VYSSH UCHEBN ZAVED KHIM KHIM TEKHNOL	1429
RUSS J GEN CHEM	1380
RUSS J PHYS CHEM A	1170
RUSS J APPL CHEM	1143
RUSS J ORG CHEM	1064
BULL RUSS ACAD SCI PHYS	996
RUSS J INORG CHEM	930
BASHK KHIM ZH	645
RUSS J GENET	610
PLAST MASSY	595
ESTESTV TEKH NAUKI	547
RUSS PHYS J	526
KHIM FIZ	497
TSVETN MET MOSCOW RUSS FED	483
RUSS J ELECTROCHEM	474
KHIM RASTIT SYR YA	470
FIZ MET METALLOVED	445
KHIM PROM ST SEGODNYA	434

Основные дисциплины в российских публикациях

Section	Title	Refs
56	Non Ferrous Metals	2636
51	Fossil Fuels (oil)	2579
55	Ferrous metals	2088
53	Mineralogy	1881
22	Physical Organic Chem	1589
76	Electric Phenomena	1513
57	Ceramics	1339
59	Air Pollution	1229
54	Extractive Metallurgy	1213
73	Mass Spectroscopy	1071
14	Mammalian Biochem	1046
78	Inorganic reactions	1010
1	Pharmacology	1004
61	Water	988
48	Chemical Engineering	928
37	Plastics	884
60	Waste treatment	878
71	Nuclear Technology	857
68	Thermodynamics	835

Организации по всему миру доверяют SciFinder



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Источники:

- *The Academic Ranking of World Universities*
- *Chemical & Engineering News*
- *Genetic Engineering & Biotechnology News*
- *PharmaExec.com*

Спасибо за внимание ! 😊

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