

CAS

The World's Chemical Information Authority

Veli-Pekka Hyttinen

Regional Marketing Manager Central and Eastern Europe

Denis Erokhin

ACS International Russia

BEH PAH Moscow 11.-12.4.2017



A division of the American Chemical Society

www.cas.org

Chemical Abstracts Service



CAS is the
WORLD'S AUTHORITY
for **CHEMICAL INFORMATION**

CAS is the only organization in the world whose objective is to find, collect and organize all publicly disclosed substance information.

We build and maintain the world's largest collection of molecular substances, reactions, and related content that is vital to the work of researchers.

70 Million: No one else has

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

Cc1ccc(cc1)C(=O)N2CCNCC2

- **CAS - мировой лидер в области научно-технической 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®***

CAS специалисты “индексаторы” изучают и 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: **Sepehr Sarshar**, Cardiff by the Sea, CA (US)

(57) **ABSTRACT**
 The present invention is directed to novel compounds according to formulae

Correspondence Address:
DLA PIPER US LLP
 4365 EXECUTIVE DRIVE
 SUITE 1100
 SAN DIEGO, CA 92121-2133 (US)

(73) Assignee: **Auspex Pharmaceuticals**, Vista, CA

(21) Appl. No.: **11/892,009**

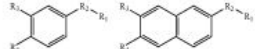
(22) Filed: **Nov. 1, 2006**

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.

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

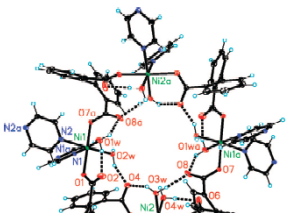
Sheng Hu,¹ Jie-Peng Zhang,² Hao-Xiang Li,¹ Ming-Liang Tong,^{3,†} Xiao-Ming Chen,^{3,†} and Susumu Kitagawa¹

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 Synthesis Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Katata, Nishikyō-ku, Kyoto 615-8510, Japan

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

ABSTRACT: A new microporous metal–organic framework (MOF) material [Ni₂(dpa)₂(pyz)₂(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/adsorption 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 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



STN®
 THE CHOICE OF PATENT EXPERTS™

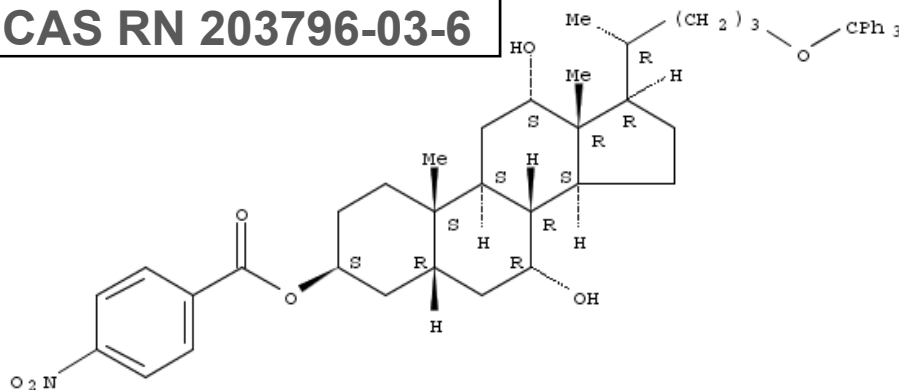
SciFinder®

Сотрудники CAS находят химическую информацию и экономят Ваше время!

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, 3 H), 0.70 (s, 3 H). ¹³C NMR (CDCl₃, 75 MHz) δ 164.21, 150.56

CAS RN 203796-03-6

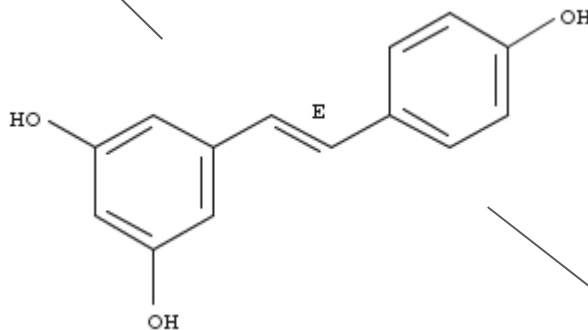


Absolute stereochemistry.



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

Lipinski and Related Properties

Property	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

Property	Value
Carbon-13 NMR Spectrum	See spectrum
Proton NMR Spectrum	See spectrum

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

Если это важно, это есть в SciFinder!

CAS covers all chemistry and key areas of life science, biology, pharmacology, physics and many others

- Biochemical methods
- Biochemistry
- Bioinformatics
- Biophysics
- Cellular biology
- Clinical
- Drug metabolism
- Enzymology
- Genetics
- Microbiology
- Molecular biology
- Pharmacogenetics
- Pharmacokinetics
- Pharmacology
- Proteomics
- Toxicology

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

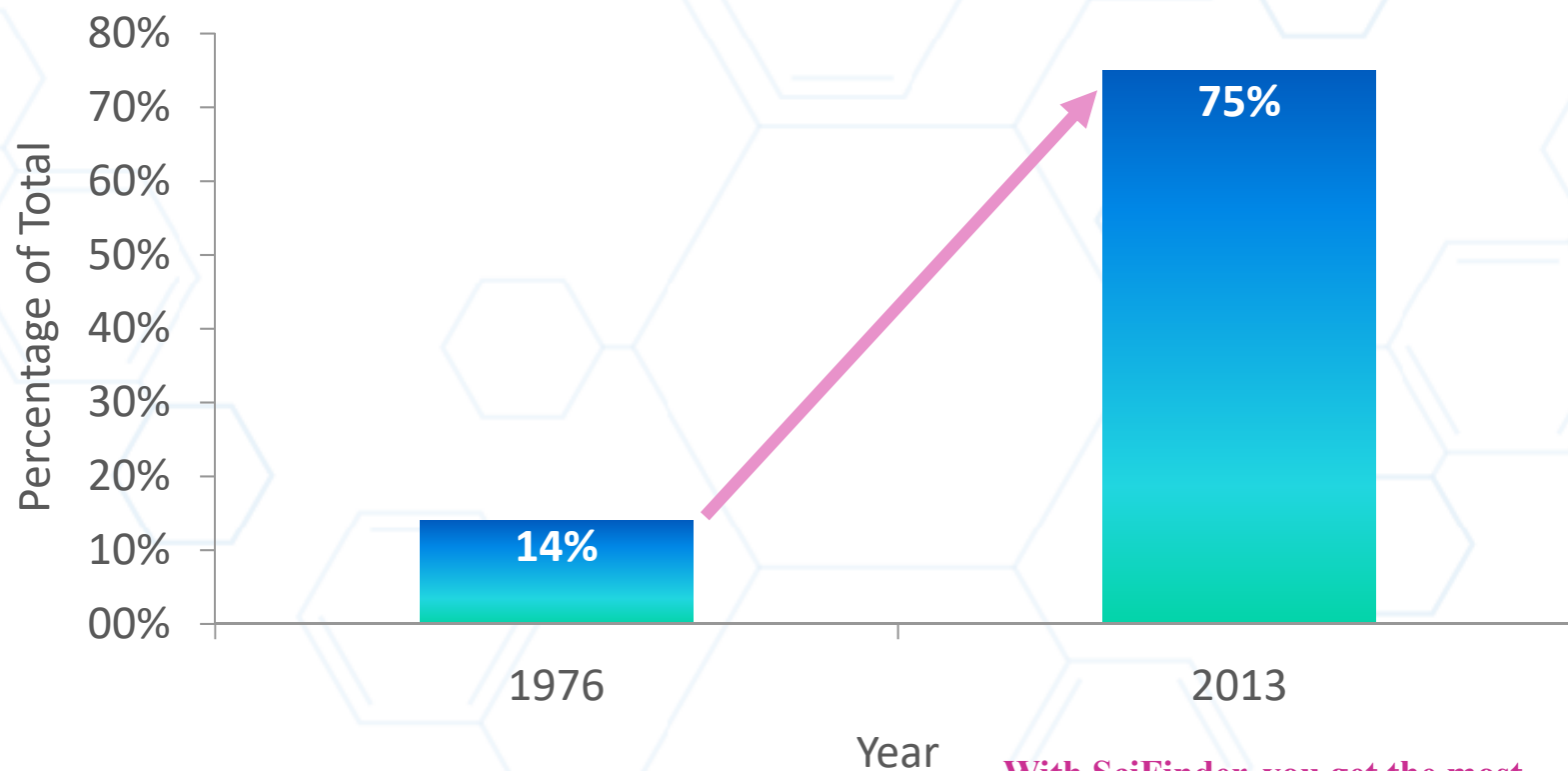
- *ACS Chemical Biology*
- *ACS Synthetic Biology*
- *Annual Review of Biochemistry*
- *Biochemistry and Cell Biology*
- *Cellular Physiology and Biochemistry*
- *Journal of Biological Chemistry*
- *Journal of Cellular Biochemistry*
- *Molecular and Cellular Biochemistry*
- *Preparative Biochemistry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

Новые химические соединения все чаще впервые описываются в патентах

Процент новых соединений из патентов



**With SciFinder, you get the most
comprehensive, timely patent data.**

Максимальный охват азиатских патентов



CAS is a division of the American Chemical Society.
Copyright 2014 American Chemical Society. All rights reserved.



CAS[®]
A DIVISION OF THE
AMERICAN CHEMICAL SOCIETY

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, a secondary bar contains 'Explore', 'Saved Searches', 'SciPlanner', 'Save', 'Print', and 'Export'. The main search bar contains the query 'Keep Me Posted "carbon nanotubes"[May 17, 2014] (234)'. Below the search bar, there are several tool icons: 'Get Substances', 'Get Reactions', 'Get Related Citations', 'Get Full Text', 'Tools', 'Create Keep Me Posted Alert', and 'Send to SciPlanner'. The 'Send to SciPlanner' button is highlighted with a red box. Below the tools, there are tabs for 'Analyze', 'Refine', and 'Categorize'. The 'Analyze' tab is active, showing a dropdown menu for 'Analyze by:' with 'Company-Organization' selected. Below this, a table lists organizations and their counts: East China Normal University, Peop Rep China (3), University of Toronto, Can (3), and another entry (2). The main content area shows a list of references, with the first one highlighted: '1. In vivo biodistribution of platinum-based drugs encapsulated into multi-walled carbon nanotubes'. The abstract of this reference 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"/> CXCL 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



Substance Detail is now more customer-friendly

SUBSTANCE DETAIL ?

Get References Get Reactions Get Commercial Sources

[Return](#)

CAS Registry Number 13292-46-1

~17,438 ~124

$C_{13}H_{28}N_4O_{12}$

Rifamycin, 3-[[[(4-methyl-1-piperazinyl)imino]methyl]-

Molecular Weight
822.94

pKa (Predicted)
Value: 4.81±0.70 | Condition: Most Acidic Temp: 25 °C

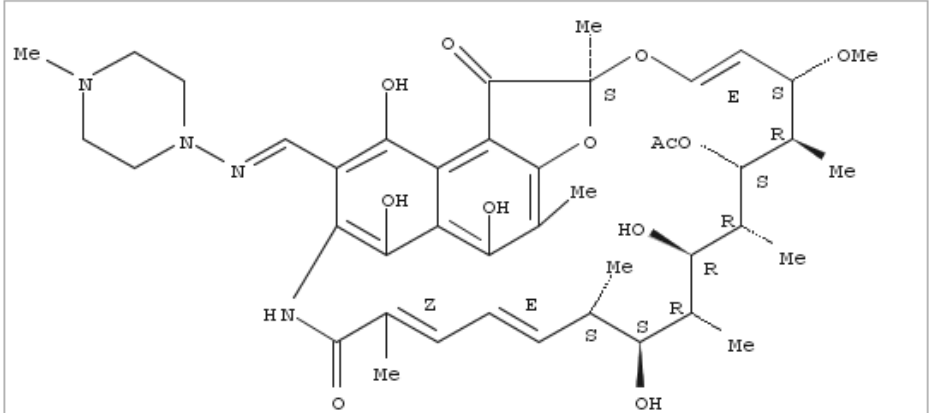
Melting Point (Experimental)
Value: See full text | Condition: 1 of 2

Boiling Point (Predicted)
Value: 937.4±65.0 °C | Condition: Press: 760 Torr

Density (Predicted)
Value: 1.34±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr

Other Names
2,7-(Epoxy-pentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan-1,11(2*H*)-dione, 5,6,9,17,19,21-hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-, 21-acetate (8CI)
2,7-(Epoxy-pentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan-1,11(2*H*)-dione, 5,6,9,17,19,21-hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-, 21-acetate (7CI)
2,7-(Epoxy-pentadeca[1,11,13]trienimino)naphtho[2,1-*b*]furan, rifamycin deriv.
3-[(4-Methyl-1-piperazinyl)iminomethyl]rifamycin SV
5,6,9,17,19,21-Hexahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-8-[*N*-(4-methyl-1-piperazinyl)formimidoyl]-2,7-(epoxy-pentadeca[1,11,13]trienimino)-naphtho[2,1-*b*]furan-1,11(2*H*)-dione 21-acetate

[View more...](#)



Absolute stereochemistry. Double bond geometry as described by E or Z.

Property and Spectra Data Collated tabs organize information scientifically

EXPERIMENTAL PROPERTIES

Biological Chemical Lipinski Optical and Scattering Structure Related Thermal

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 16	(2) CAS
Half-Life (Biological)	See full text	1 of 6	(5) CAS
LD50	See full text	1 of 2	(9) CAS
Median Lethal Dose(LD50)	1073.9 mg/kg	Organism: mouse Route: oral	(13)
Median Lethal Dose(LD50)	885 mg/		
Median Lethal Dose(LD50)	840 mg/		
Median Lethal Dose(LD50)	800 mg/		
Median Lethal Dose(LD50)	610 mg/		
Median Lethal Dose(LD50)	260 mg/		
Minimum Inhibitory Concentration	See full t		

Notes

(2) Quenelle, Debra; Drug Delivery 2004, V11(1), 1-10
 (5) Gurumurthy, Prema; Antimicrobial Agents and Chemotherapy 2006, V50(12), P4011-4017
 (9) Solov'ev, V. N.; Antibiotiki (Moscow) 1974, V19(5), P427-32
 (13) Bykova, M. A.; Antibiotiki (Moscow) 1977, V22(1), P1-6
 (14) "Drugs - Synonyms and Properties" data v
 (15) Balabanova, E. L.; Gigiena Truda i Professionalnye Zabolevaniya 1981, (11), P52-4
 (16) Gol'dberg, L. E.; Antibiotiki (Moscow) 1974, V19(5), P427-32
 (20) Murillo, O.; Antimicrobial Agents and Chemotherapy 2006, V50(12), P4011-4017

EXPERIMENTAL SPECTRA

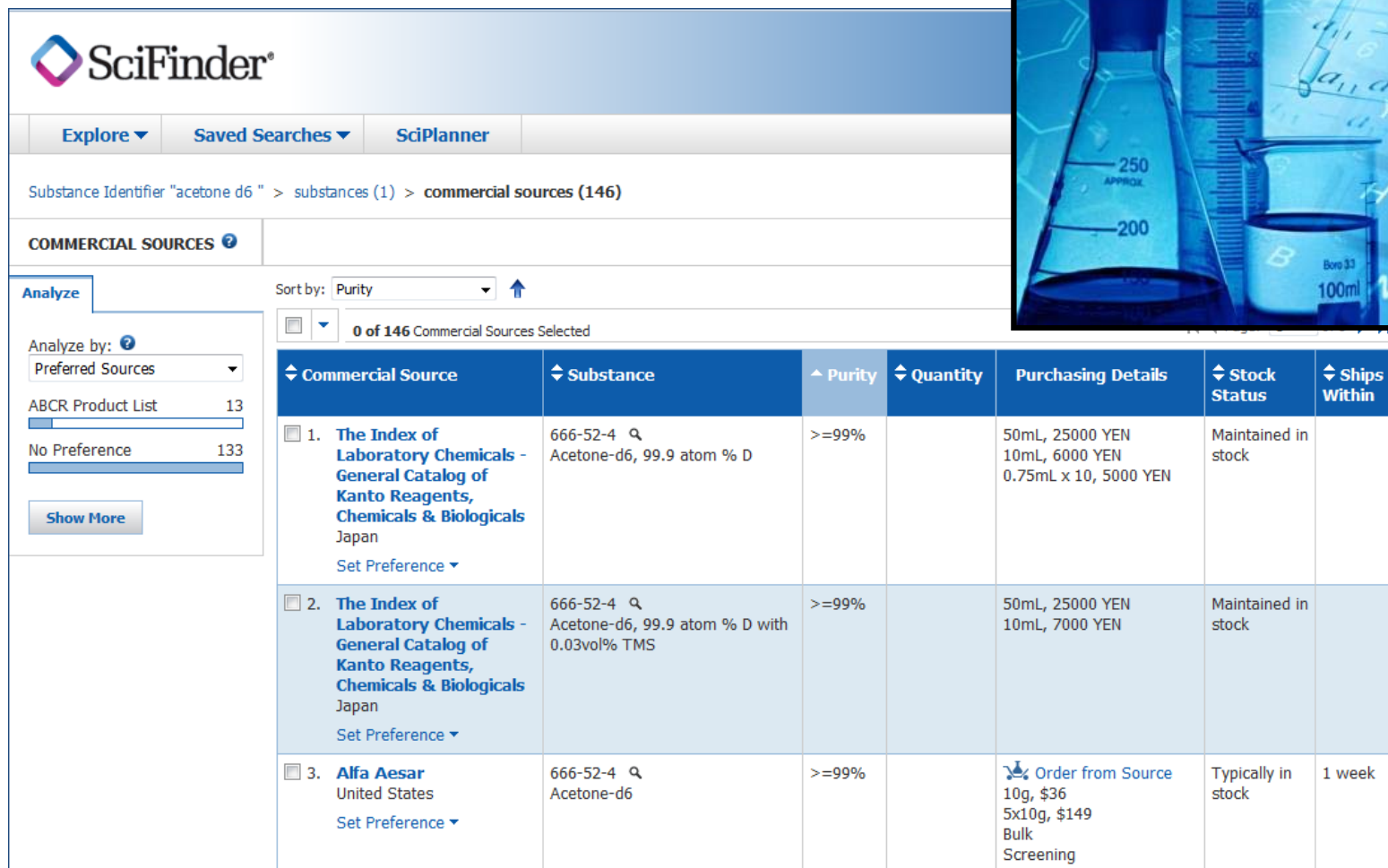
¹H NMR ¹³C NMR IR Mass Raman UV and Visible

IR Properties	Value	Condition	Note
IR Absorption Spectrum	See spectrum		(6) BIORAD
IR Absorption Spectrum	See spectrum		(6) BIORAD
IR Absorption Spectrum	See full text	1 of 5	(7)CAS
IR Spectrum	See full text	1 of 2	(8)CAS

Notes

(6) BIORAD: Infrared spectral data from the Bio-Rad/Sadtler IR Data Collection was obtained from Bio-Rad Laboratories, Philadelphia, PA (US). Copyright © Bio-Rad Laboratories. All Rights Reserved.
 (7) Gupta, K. C.; Journal of Applied Polymer Science 2007, V104(3), P1942-1956
 (8) Sabri, Nagwa A.; Egyptian Journal of Pharmaceutical Sciences 2003, V44(1), P19-38

CHEMCATS[®] is the definitive collection of commercially available chemicals and suppliers



SciFinder[®]

Explore ▾ Saved Searches ▾ SciPlanner

Substance Identifier "acetone d6" > substances (1) > commercial sources (146)

COMMERCIAL SOURCES ⓘ

Analyze

Sort by: Purity ▾ ↑

0 of 146 Commercial Sources Selected

Analyze by: ⓘ
 Preferred Sources ▾
 ABCR Product List 13
 No Preference 133
 Show More

Commercial Source	Substance	Purity	Quantity	Purchasing Details	Stock Status	Ships Within
1. The Index of Laboratory Chemicals - General Catalog of Kanto Reagents, Chemicals & Biologicals Japan Set Preference ▾	666-52-4 Q Acetone-d6, 99.9 atom % D	>=99%		50mL, 25000 YEN 10mL, 6000 YEN 0.75mL x 10, 5000 YEN	Maintained in stock	
2. The Index of Laboratory Chemicals - General Catalog of Kanto Reagents, Chemicals & Biologicals Japan Set Preference ▾	666-52-4 Q Acetone-d6, 99.9 atom % D with 0.03vol% TMS	>=99%		50mL, 25000 YEN 10mL, 7000 YEN	Maintained in stock	
3. Alfa Aesar United States Set Preference ▾	666-52-4 Q Acetone-d6	>=99%		Order from Source 10g, \$36 5x10g, \$149 Bulk Screening	Typically in stock	1 week

CHEMLIST[®] is the comprehensive source for information on regulated chemicals

SciFinder[®]

Explore ▾ Saved Searches ▾ SciPlanner

REGULATORY INFORMATION

[Return](#)

CAS Registry Number: 1920-90-7

Plumbane, tetrabutyl- (TSCA, NDSL)
 Tetrabutylplumbate (French) (NDSL, EINECS)
 tetrabutylplumbane (REACH, EINECS)
 Tetrabutylplumbat (German) (EINECS)
 tetrabutylplumbato (Spanish) (EINECS)
 Lead, tetrabutyl-
 NSC 179770
 Tetrabutyllead

$$\begin{array}{c}
 n\text{-Bu} \\
 | \\
 n\text{-Bu} - \text{Pb} - \text{Bu-n} \\
 | \\
 n\text{-Bu}
 \end{array}$$

File Segment

CANADA: NDSL
 EEC: EINECS
 EU: REACH
 Restricted Chemical Lists: RSTR
 USA: TSCA

Regulatory List Number

EC No.: 217-649-2
 EINECS No.: 217-649-2
 SINGAPORE PCDTBL111

Inventory Status

On TSCA Inventory
 June 2013 TSCA Inventory
 On NDSL
 Canada Gazette, Part I, January 31, 1998
 On REACH



SCIFINDER включает 7 баз данных	
CAplus® – библиограф. данные 10,000+ научных журналов (185 стран) патенты из 63 патентных ведомств	44+ млн ссылок с рефератами и индексными терминами с 1802, цитирование с 1997
REGISTRY® – химические вещества органические и неорганические соединения, последовательности	129+ миллионов органических и неорганических веществ, 65+ млн биопоследовательностей, 5,0+ блн записей о свойствах
CASREACT® – химический синтез структурные диаграммы продуктов и реактантов/реагентов	96+ миллионов реакций (синтетическое получение) с 1840
CHEMLIST® – правовая информация REACH, EINECS, U.S. Gov. Register	345,000 промышленно важных химических соединений с 1979
CHEMCATS® – коммерческие источники 1,200 поставщиков	химических веществ с ценами (28+млн уникальный)
MARPAT® – структуры Маркуша из 440к патентов (INPI 1961)	1,1 миллионов структуры Маркуша из патентов
MEDLINE – рефераты из 5,200 медико-биологических журналов	25+ млн ссылок NML с рефератами и индексными терминами с 1947

ch.™

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.


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**

Новый дизайн SciFinder – познакомьтесь!

Ваша работа становится более удобной. Максимальное количество научной, релевантной и исчерпывающей информации по химии и смежным дисциплинам.

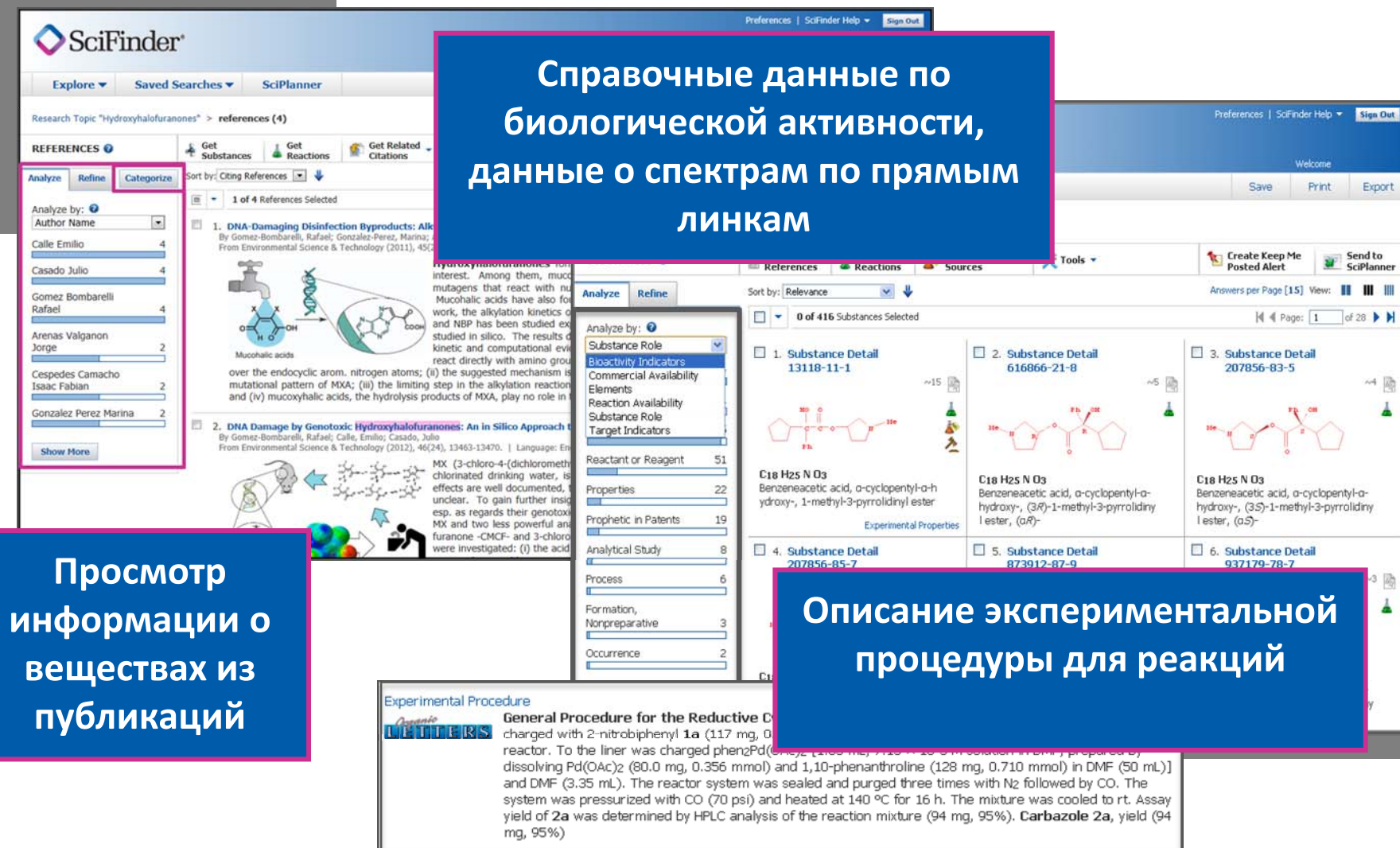


The collage displays various features of the SciFinder interface:

- Top Left:** Navigation tabs for Explore, Saved Searches, and SciPlanner. A sidebar menu lists categories like REFERENCES, SUBSTANCES, and REACTIONS.
- Top Center:** A search results page for "SUBSTANCES: CHEMICAL STRUCTURE" showing a chemical structure of a complex organic molecule and search options (Exact Structure, Substructure, Similarity).
- Bottom Left:** A detailed view of a reaction search for "Duloxetine", showing a list of 126 reactions and a table of results filtered by "Company-Organization".
- Bottom Center:** A chemical reaction scheme showing the synthesis of Carbazole (2a) from 2-nitrobiphenyl (1a) and 1,10-phenanthroline.
- Bottom Right:** A snippet of an experimental procedure for the reductive cyclization of Carbazole (2a), detailing reagents, conditions, and yield.
- Right Side:** A text snippet discussing "DNA-Damaging Disinfection Byproducts: Alkylation Mechanism of Mutagenic Mucohalic Acids" and "Hydroxyhalofuranones".

Результаты точно соответствуют запросам, охватывают “свежие” публикации

Справочные данные по
биологической активности,
данные о спектрах по прямым
линкам



The screenshot displays the SciFinder search results page. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. The search topic is 'Hydroxyhalofuranones' with 4 references found. A sidebar on the left allows filtering by author name, listing authors like Calle Emilio, Casado Julio, Gomez Bombarelli Rafael, Arenas Valganon Jorge, Cespedes Camacho Isaac Fabian, and Gonzalez Perez Marina. The main content area shows two references, each with a chemical structure diagram and a brief abstract. A central blue box highlights the availability of biological activity and spectral data. A bottom-left blue box points to the 'Analyze' tab, which provides detailed experimental and analytical data for selected substances. A bottom-right blue box points to the 'Substance Detail' view, which includes chemical structures and experimental procedures.

Просмотр
информации о
веществах из
публикаций

Описание экспериментальной
процедуры для реакций

Оптимизация путей синтеза с помощью специальных инструментов в базе данных по реакциям в SciFinder

Группирование результатов по типам превращения

Substance Identifier "vanillin " > substances (1) > get reactions (490)

REACTIONS

Get References

Tools

Send to SciPlanner

Analyze

Refine

Group by: Transformation Sort by: Frequency

Answers per Page [50]

0 of 436 Reactions Selected

Page: 1 of 2

Analyze by:

Reagent (New)

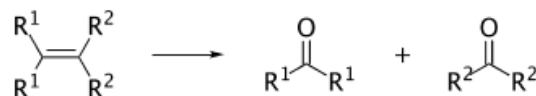
O₂ 89

NaOH 59

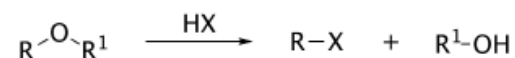
H₂O 37

H₂O₂ 35

1. Ozonolysis
99 Reactions

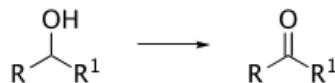


2. Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ether
60 Reactions



R¹ = CR₃, SiR₃

3. Oxidation or Dehydrogenation of Alcohols to Aldehydes and
46 Reactions



Экспериментальная процедура доступна из публикаций издательств ACS, Springer, Thieme, T&F, патентов и Chinese Inst Org Synth.

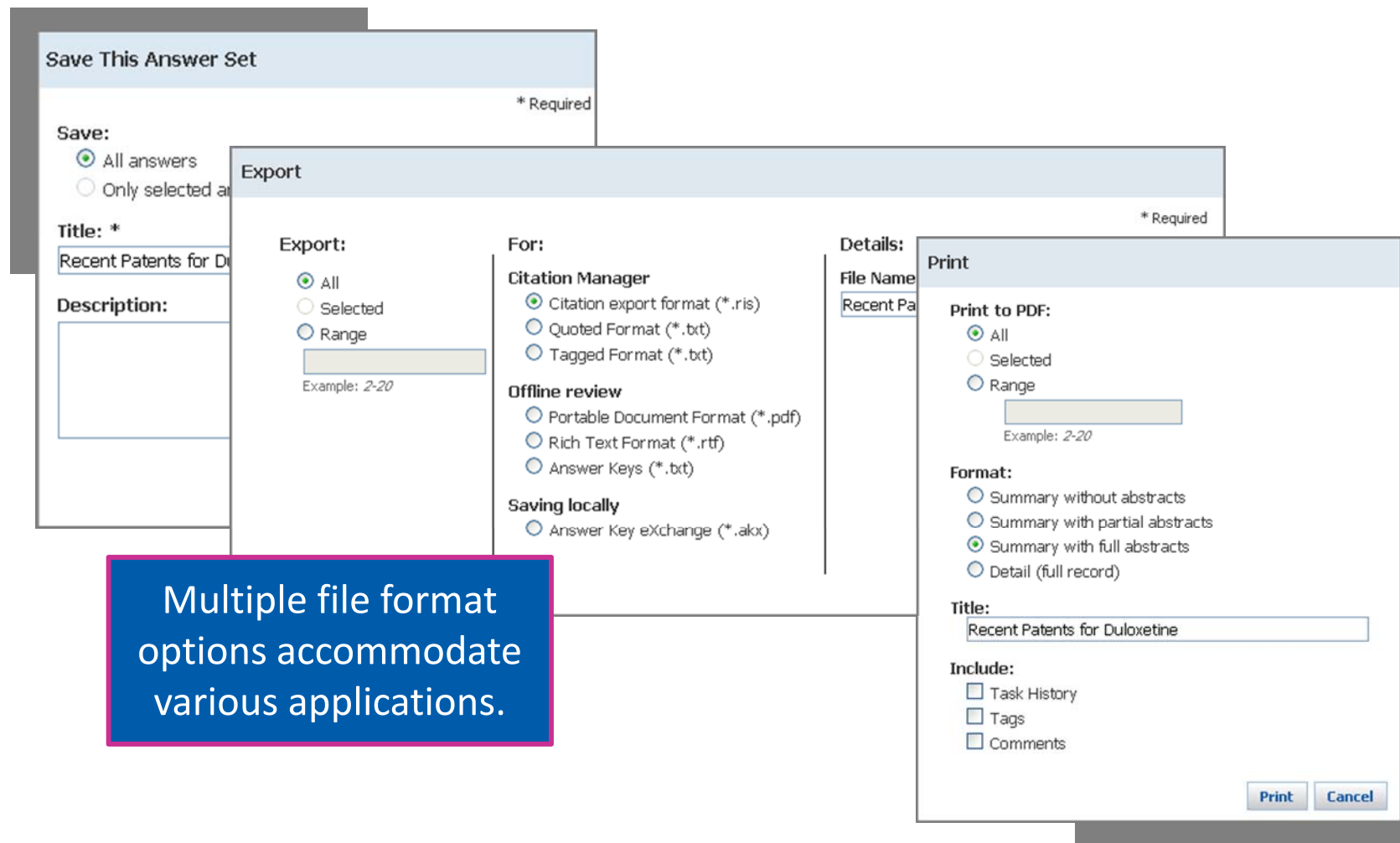
Анализ по реагентам (добавлен на прошлой неделе)

Experimental Procedure

 Springer

Growing Cells Biotransformation For the preparation of *C. galli*/PGO6 growing cells, a twostep biotransformation process was used. Cells were first incubated in 250-ml Erlenmeyer flasks (30 °C, 200 rpm) containing 50-ml YPD (2% glucose, 2% peptone, 1% yeast extract) medium. When the strain grew to the late-exponential of growth phase (28 h growth), the biotransformation was started by adding directly isoeugenol at the concentration of 0.1% (v/v). Time-course samples were withdrawn at different times to assess the isoeugenol and the main products of its biotransformation by HPLC. vanillin, yield 48%; vanillic acid, yield 19%.

Сохранить, печати или экспорта ответы на? Последующего анализа и сотрудничества



Save This Answer Set * Required

Save:

- All answers
- Only selected answers

Title: *

Recent Patents for Duloxetine

Description:

Export * Required

Export:

- All
- Selected
- Range

Example: 2-20

For:

Citation Manager

- Citation export format (*.ris)
- Quoted Format (*.txt)
- Tagged Format (*.txt)

Offline review

- Portable Document Format (*.pdf)
- Rich Text Format (*.rtf)
- Answer Keys (*.txt)

Saving locally

- Answer Key eXchange (*.akx)

Details: * Required

File Name:

Recent Patents for Duloxetine

Print

Print to PDF:

- All
- Selected
- Range

Example: 2-20

Format:

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

Title:

Recent Patents for Duloxetine

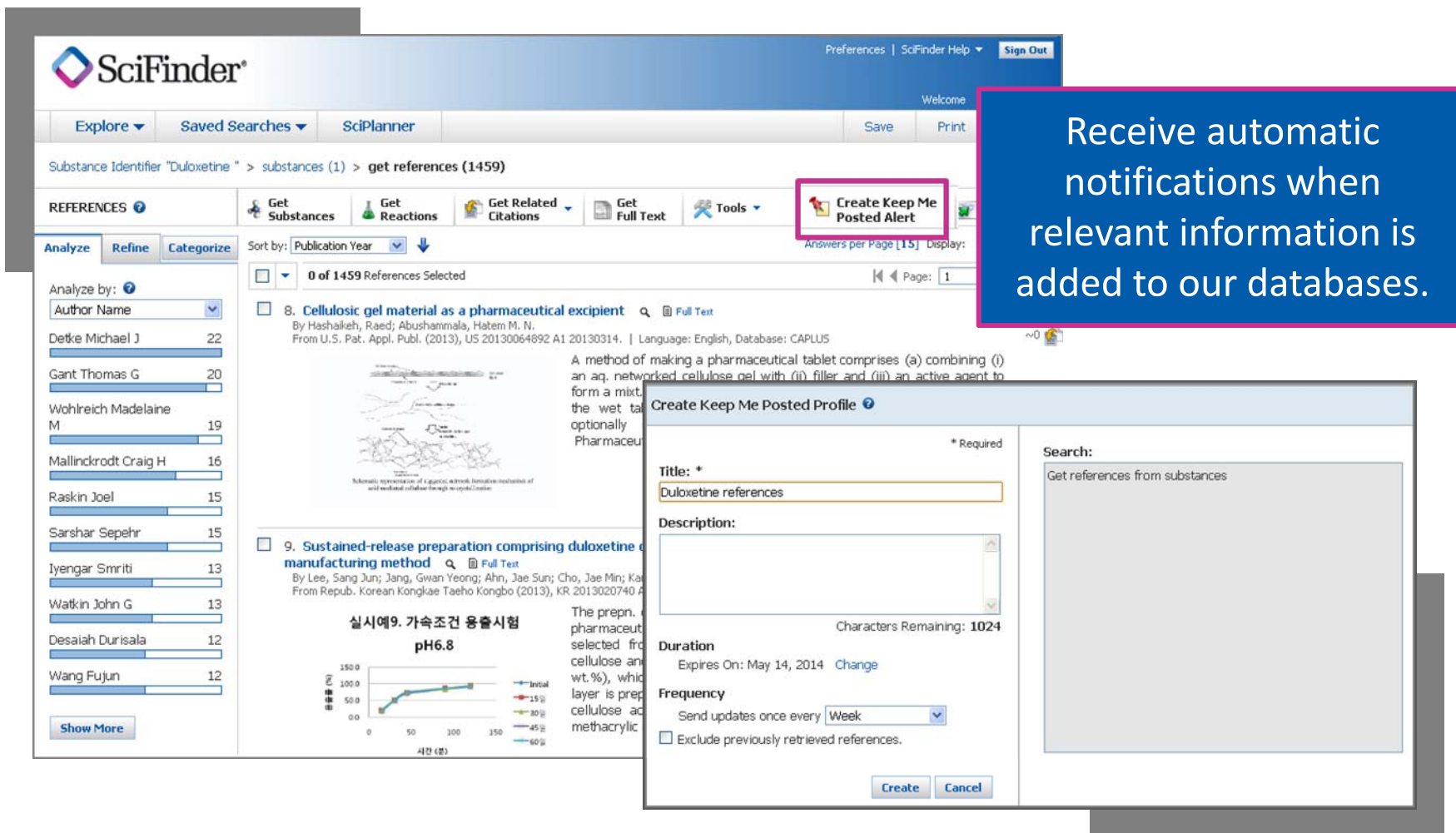
Include:

- Task History
- Tags
- Comments

Print **Cancel**

Multiple file format options accommodate various applications.

мониторинга с «Keep Me Posted alerts»



The screenshot displays the SciFinder web interface. At the top, there are navigation tabs for 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows search results for 'Duloxetine' with 1459 references. A 'Create Keep Me Posted Alert' button is highlighted with a red box. A blue callout box on the right contains the text: 'Receive automatic notifications when relevant information is added to our databases.'

The 'Create Keep Me Posted Profile' dialog box is open, showing the following fields:

- Title:** * Duloxetine references
- Description:** (Empty text area)
- Duration:** Expires On: May 14, 2014 (Change)
- Frequency:** Send updates once every: Week (dropdown menu)
- Exclude previously retrieved references.

Buttons for 'Create' and 'Cancel' are at the bottom of the dialog.

Спасибо – Kiitos – Thank you



Access SciFinder at:

scifinder.cas.org