# SciFinder®
## Searching for Science

## *Знакомство с SciFinder ⁿ*

ННГУ
Н. Новгород, 22.11.2019

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AMERICAN CHEMICAL SOCIETY

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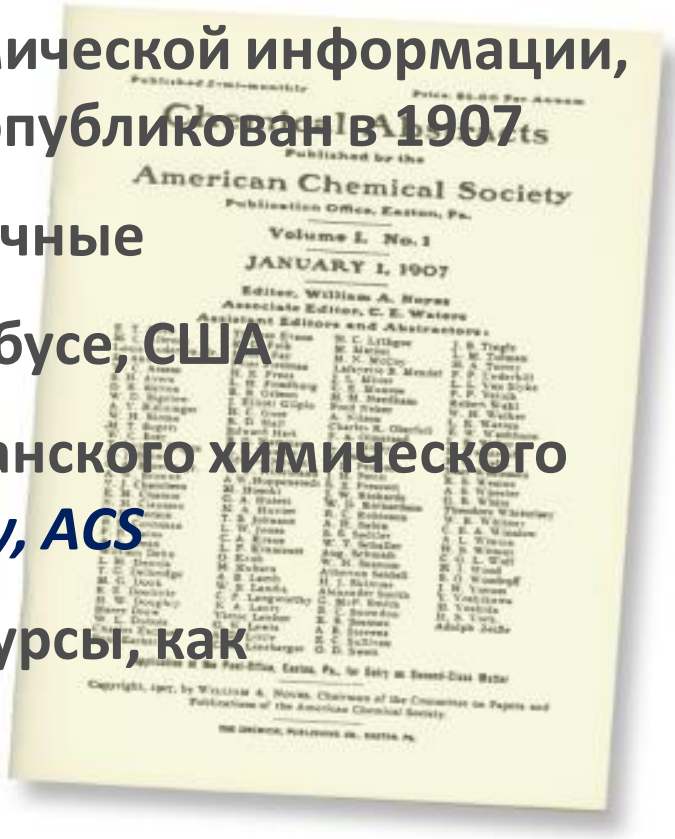
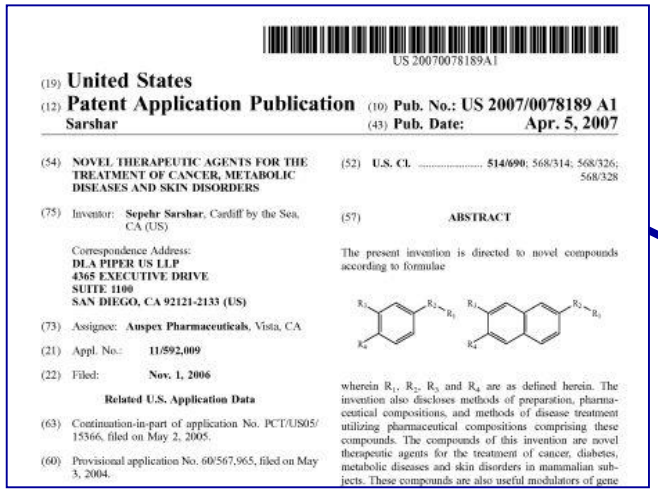
# Chemical Abstracts Service (CAS)


- **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 публикаций, в которых фигурирует **вещество**



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**

(75) Inventor: **Sepehr Sarshar**, Cardiff by the Sea, CA (US)

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.: **11/592,009**

(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.

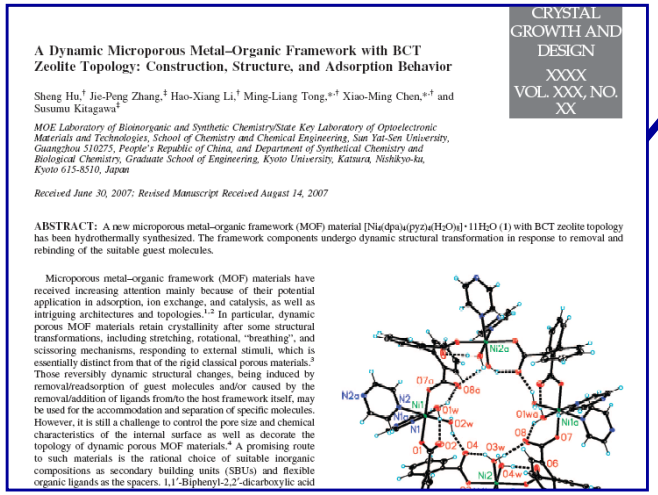
(52) **U.S. Cl.** ..... **514/690**; 568/314; 568/326; 568/328

(57) **ABSTRACT**

The present invention is directed to novel compounds according to formulae



wherein $R_1$, $R_2$, $R_3$ and $R_4$ 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**

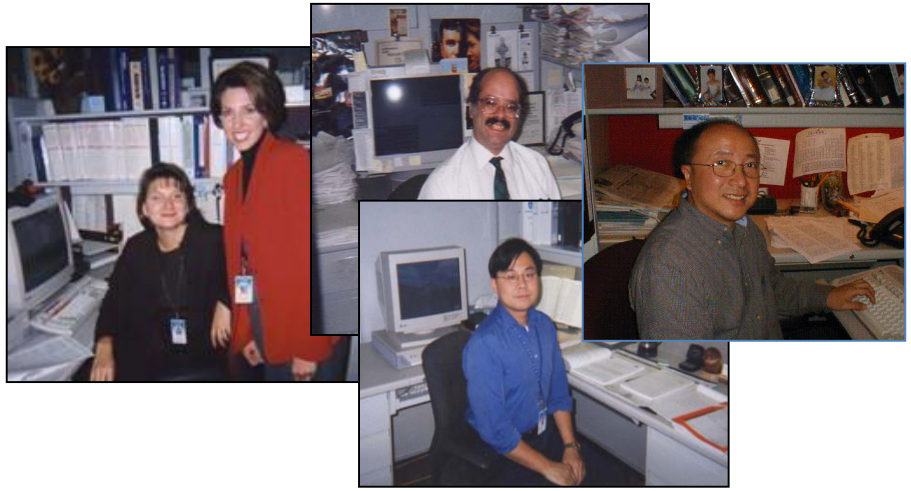
Sheng Hu,[†] Jie-Peng Zhang,[‡] Hao-Xiang Li,[†] Ming-Liang Tong,*[,†] Xiao-Ming Chen,*[,†] and Susumu Kitagawa[‡]

*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, Katsura, 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 $[Ni_4(dpa)_4(pyz)_4(H_2O)_4]\cdot 11H_2O$ (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 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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STN®
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# И добавляют **индексные термины** – ключевые слова и регистрационные номера веществ (**CAS RN**) согласно критериям **новизны и/или значимости**

Crystallography and Liquid Crystals (Section75-11)

**Concepts**

Liquid crystals

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

Esterification
Heating
Phase transition
Temperature
Thermal stability

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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## Особенности контента CAS:

- Независимый выбор экспертом-индексатором стандартизированных ключевых слов (концепций), веществ, биологических обьектов, процессов , материалов, реакций из первоисточников

- Информация анализируется экспертами в каждой конкретной области и владеющими языком оригинала публикации

- Полнота охвата и взаимосвязанность контента



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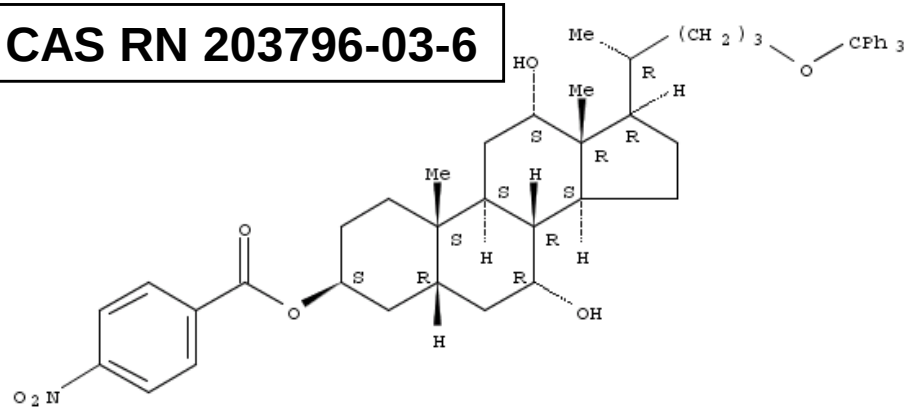
# Ученые CAS обнаруживают **существенные данные**, такие как неявно описанные структуры, которые **отсутствуют в других базах данных**

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 $NaHCO_3$ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous $Na_2SO_4$. The desired product (2.72 g, 85% yield) was obtained as white powder after $SiO_2$ chromatography ($Et_2O$/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 $cm^{-1}$ ; $^1H$ NMR ($CDCl_3$, 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); $^{13}C$ NMR ($CDCl_3$, 75 MHz) δ 164.21, 150.56

**CAS RN 203796-03-6**




Absolute stereochemistry.

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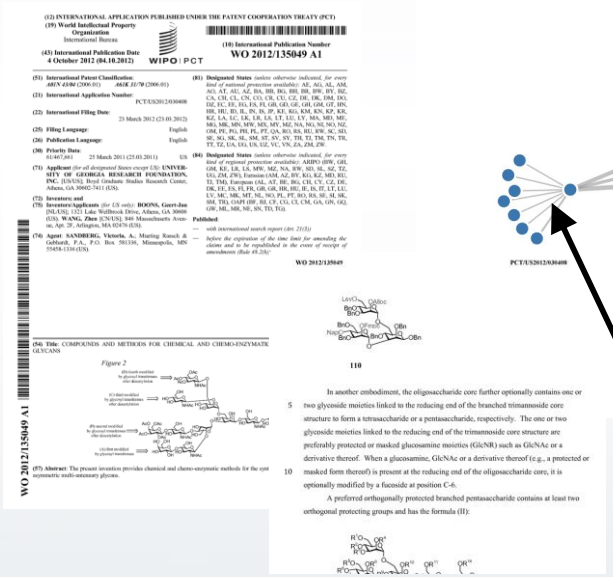
# ПРИМЕР ПАТЕНТА

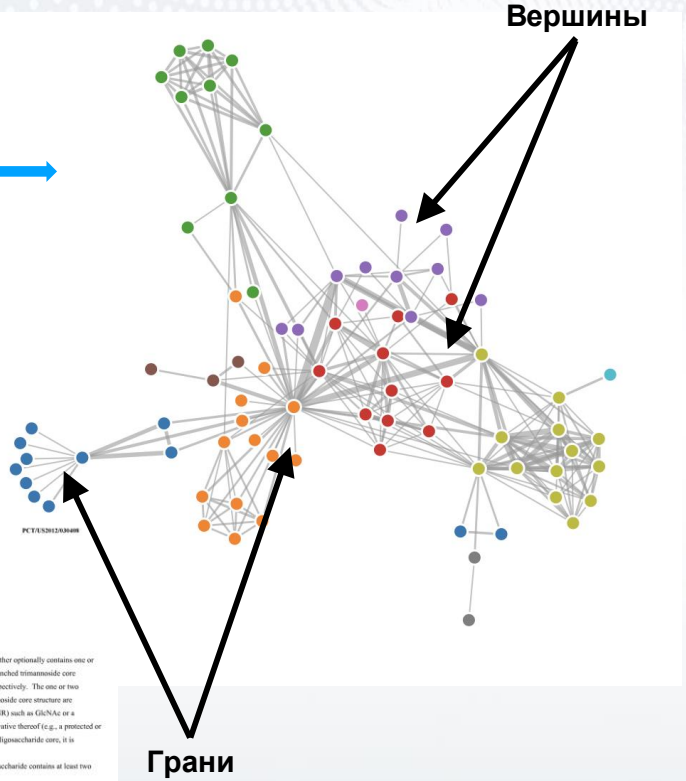
## CAS EXTRACTS MORE KNOWLEDGE THAN ANYONE ELSE

WO 2012135049

**Compounds and methods for chemical and chemo-enzymatic synthesis of complex glycans**

7 концепций
138 соединений
4614 реакций
4 членов патентных семейств
3 цитируемых документа

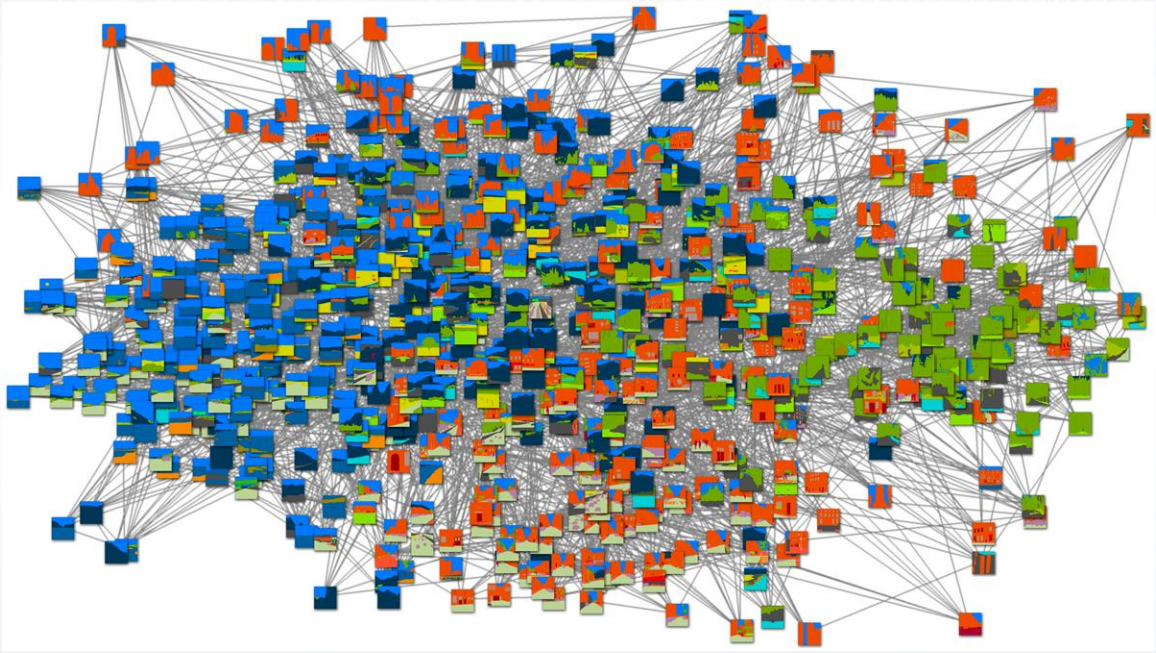

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
(19) World Intellectual Property Organization
International Bureau
(43) International Publication Date
4 October 2012 (04.10.2012)
WIPO | PCT
(10) International Publication Number
WO 2012/135049 A1
(54) Title: COMPOUNDS AND METHODS FOR CHEMICAL AND CHEMO-ENZYMATIC GLYCANS
Figure 2
(57) Abstract: The present invention provides chemical and chemo-enzymatic methods for the synthesis of complex, multi-antennary glycans.
WO 2012/135049 A1
In another embodiment, the oligosaccharide core further optionally contains one or two glycoside moieties linked to the reducing end of the branched trimannoside core structure to form a tetrasaccharide or a pentasaccharide, respectively. The one or two glycoside moieties linked to the reducing end of the trimannoside core structure are preferably protected or masked glucosamine moieties (GlcNR) such as GlcNAc or a derivative thereof. When a glucosamine, GlcNAc or a derivative thereof (e.g., a protected or masked form thereof) is present at the reducing end of the oligosaccharide core, it is optionally modified by a fucoside at position C-6.
A preferred orthogonally protected branched pentasaccharide contains at least two orthogonal protecting groups and has the formula (II):



# CAS ПОНИМАЕТ КАК ВЗАИМОСВЯЗАНЫ РАЗЛИЧНЫЕ ОБЛАСТИ ЗНАНИЯ

*1.4 млрд вершин*

*14 млрд граней*



**See Blog:** [Innovation Drives Transformation]

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TRANSCENDING
BOUNDARIES
SCIENCE, SYNTHESIS & SERVICE

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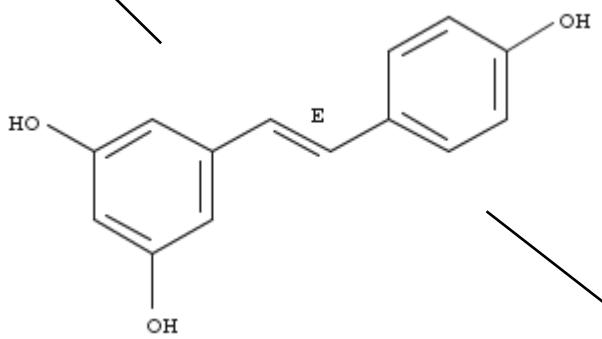
Стандартный инструмент

для более *500000* химиков по всему миру

# Что нам известно об этом соединении?

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




**CAS Registry Number:** 501-36-0

$C_{14}H_{12}O_3$

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**<br>10,000+ журналов (185 стран)<br>патенты из 63 ведомств | **45+ млн. ссылок (5,000 ежедневно), Рефераты и индексирование с 1802 г., цитаты с 1997–** |
| **REGISTRY® – соединения**<br>Органические и неорганич. структуры, последовательности | **155+ млн. малых молекул (15,000 ежедневно), 67+ млн. последовательностей, 5,0+ млрд. свойств** |
| **CASREACT® – реакции**<br>Структурные диаграммы, детали | **98+ млн. реакций и синтезов с 1840г.** |
| **CHEMLIST® – регулируемая химия**<br>REACH, EINECS, US. Gov/Fed. Register | **348 k регулируемых соединений с 1979 г.** |
| **CHEMCATS® – поставщики реактивов**<br>Химические каталоги | **Миллионы соединений от поставщиков, в том числе с уникальными CAS RNs** |
| **MARPAT® – структуры Маркуша**<br>440k патентов, INPI с1961 г. | **1,1+ млн.структур Маркуша (75 новых патентов ежедневно)** |
| **MEDLINE – библиография**<br>5,200 биомедицинских журналов | **24+ млн.библиографических NLM-ссылок с 1947 г.** |

# Преимущества SciFinder для пользователей в РФ:

- При производстве контента для SciFinder, CAS равномерно охватывает *все* области химии и смежных дисциплин
- Для пользователей в РФ важно знать, что публикуется и *патентуется* в *России*, а также быстро развивающихся *Китае, Корее и Индии*



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***Новый продукт в семье SciFinder…***



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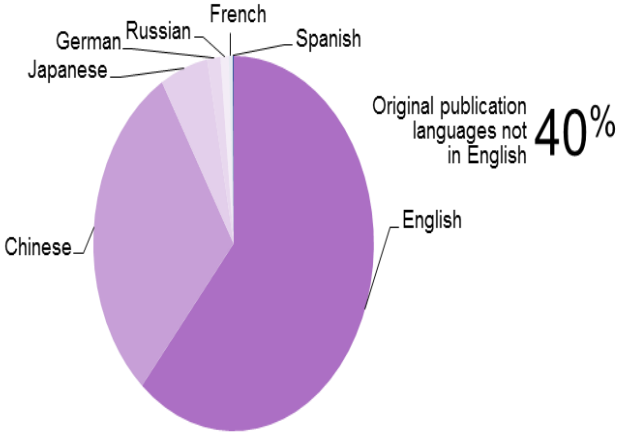
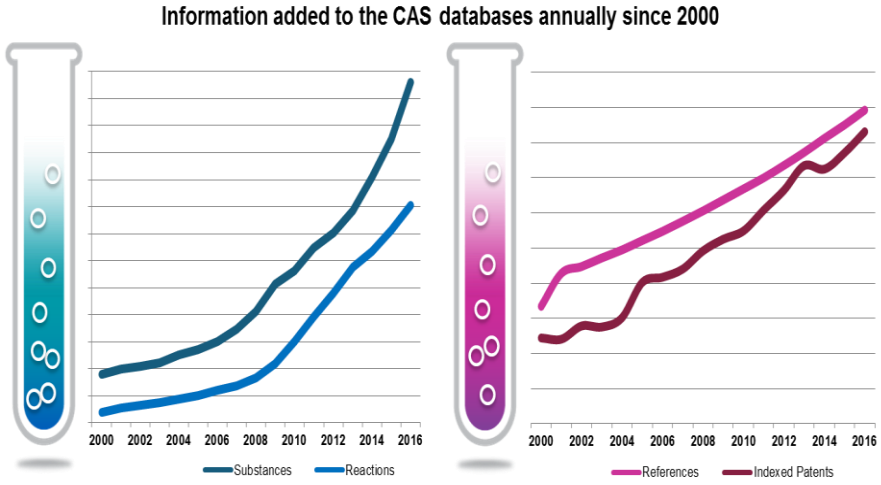
# Обьем доступной химической информации неуклонно растет!

- В некоторых случаях это рост по экспоненте
- Возрастает сложность, особенно в патентах
- Рост глобален




**Original publication languages in CAS databases**

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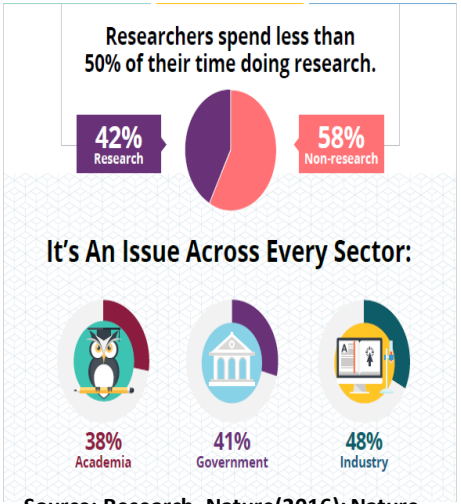
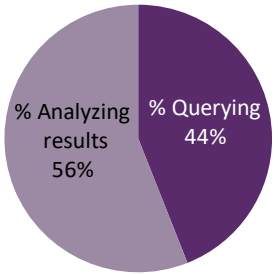
## К сожалению исследователи вынуждены тратить больше половины своего рабочего времени на поиск информации




**Source: Research, Nature(2016): Nature Salary and job satisfaction survey**

## И больше 50% времени поиска уходит на обработку первичных ответов от поисковых систем




**Source: CAS Global Customer Satisfaction Survey**

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## Почему понадобился новый продукт?

- Некоторым пользователям нужен не просто портал химических данных, а платформа, которая:
  - Дает что-то большее чем просто набор ответов;
  - Понимает логику исследователей и их способ постановки вопросов;
  - Быстро работает, тем самым высвобождает время для собственно исследований.

- Мнение клиентов за каждым решением. *Свыше 1,000 непосредственных интервью с учеными и дополнительно свыше тысячи опросов.*

- Ожидания от нового продукта:
  - Мощный, но легкий в использовании – *интуитивно понятный интерфейс*
  - Умный – *правильная интерпретация запросов пользователей*
  - Быстрый – *существенный рост скорости, экономия времени ученого*
  - Легкий переход пользователей обычного SciFinder на новую платформу

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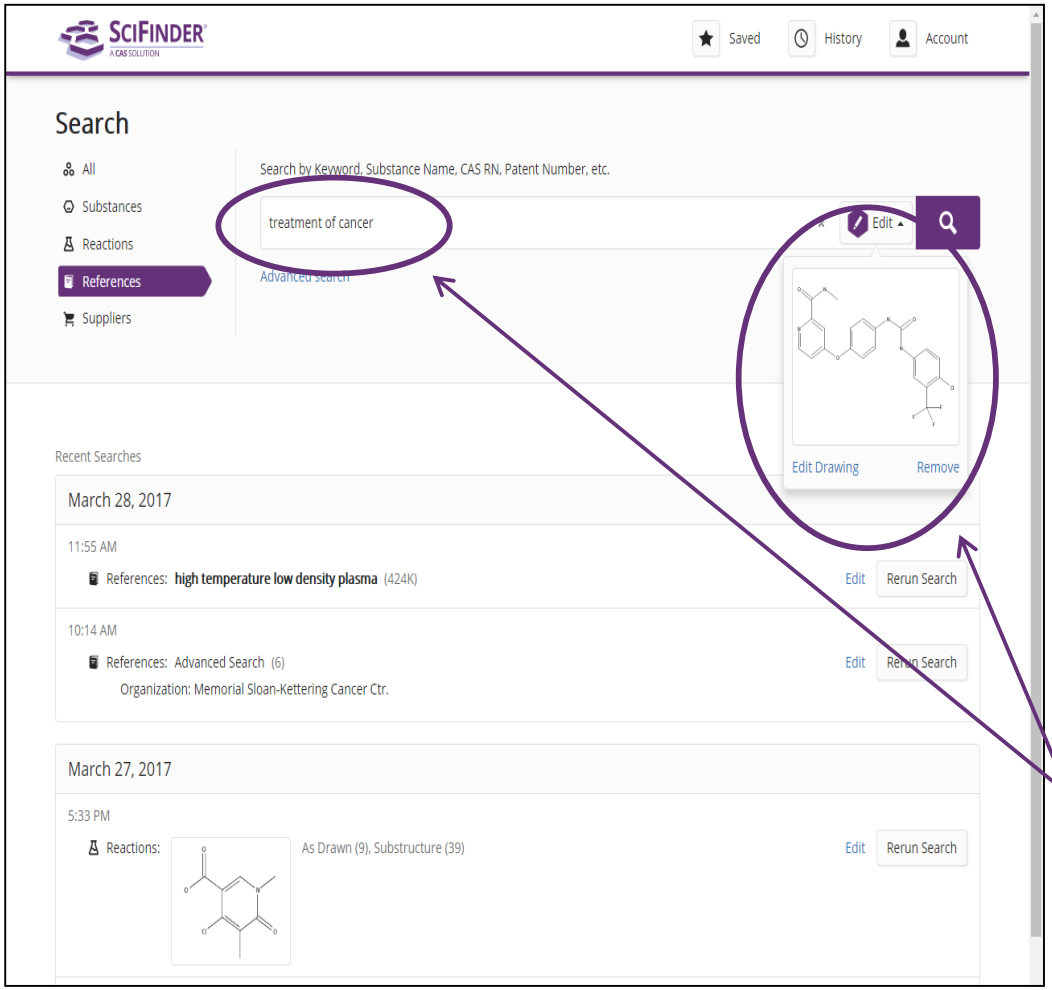
# Новый интерфейс, новые возможности поиска и многое другое!

Выбор поисковых опций

Удобная история




Одновременный поиск по тексту и структуре

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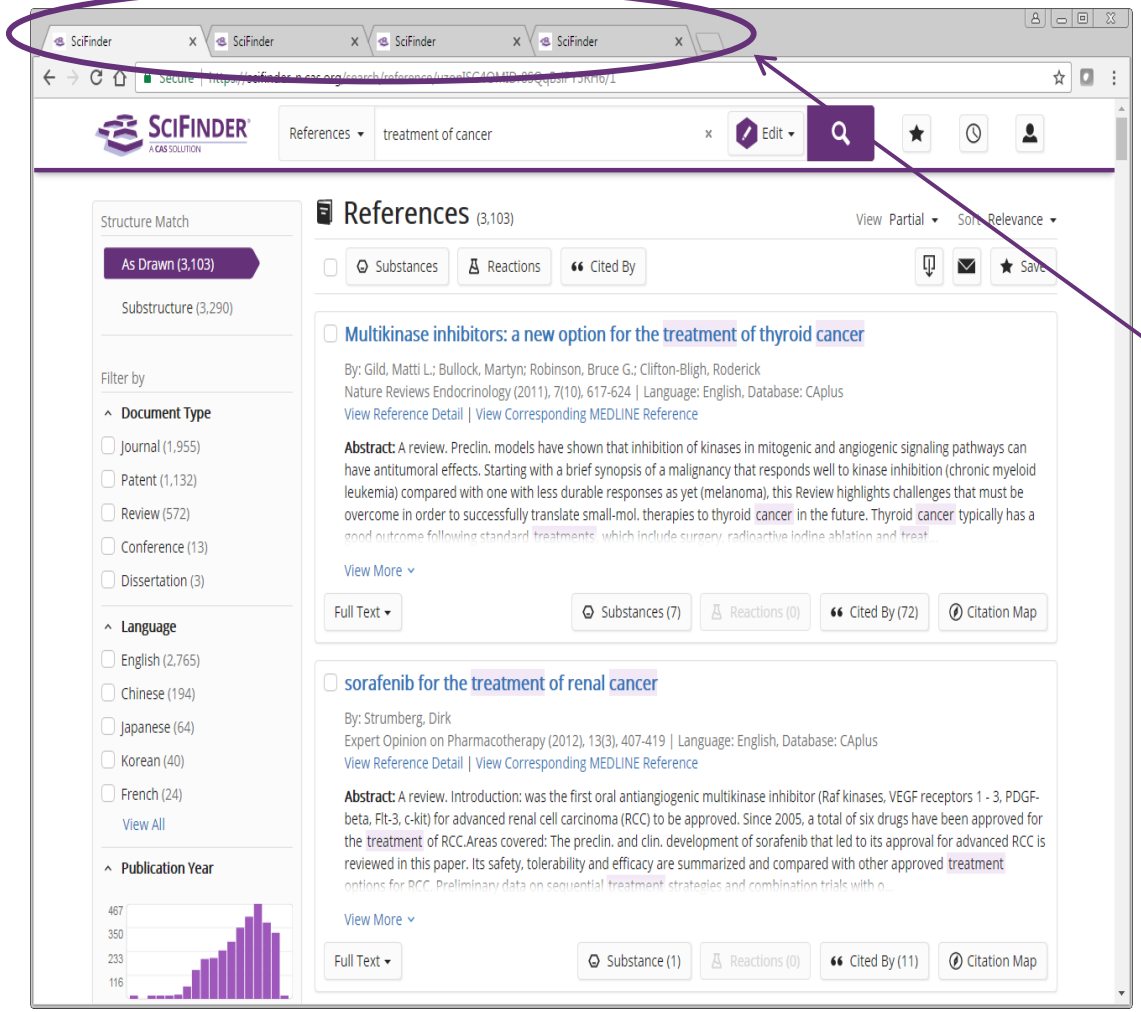
# SciFinder$^n$ поддерживает touch screen и многостраничность!




Одновременный поиск в нескольких вкладках/окнах

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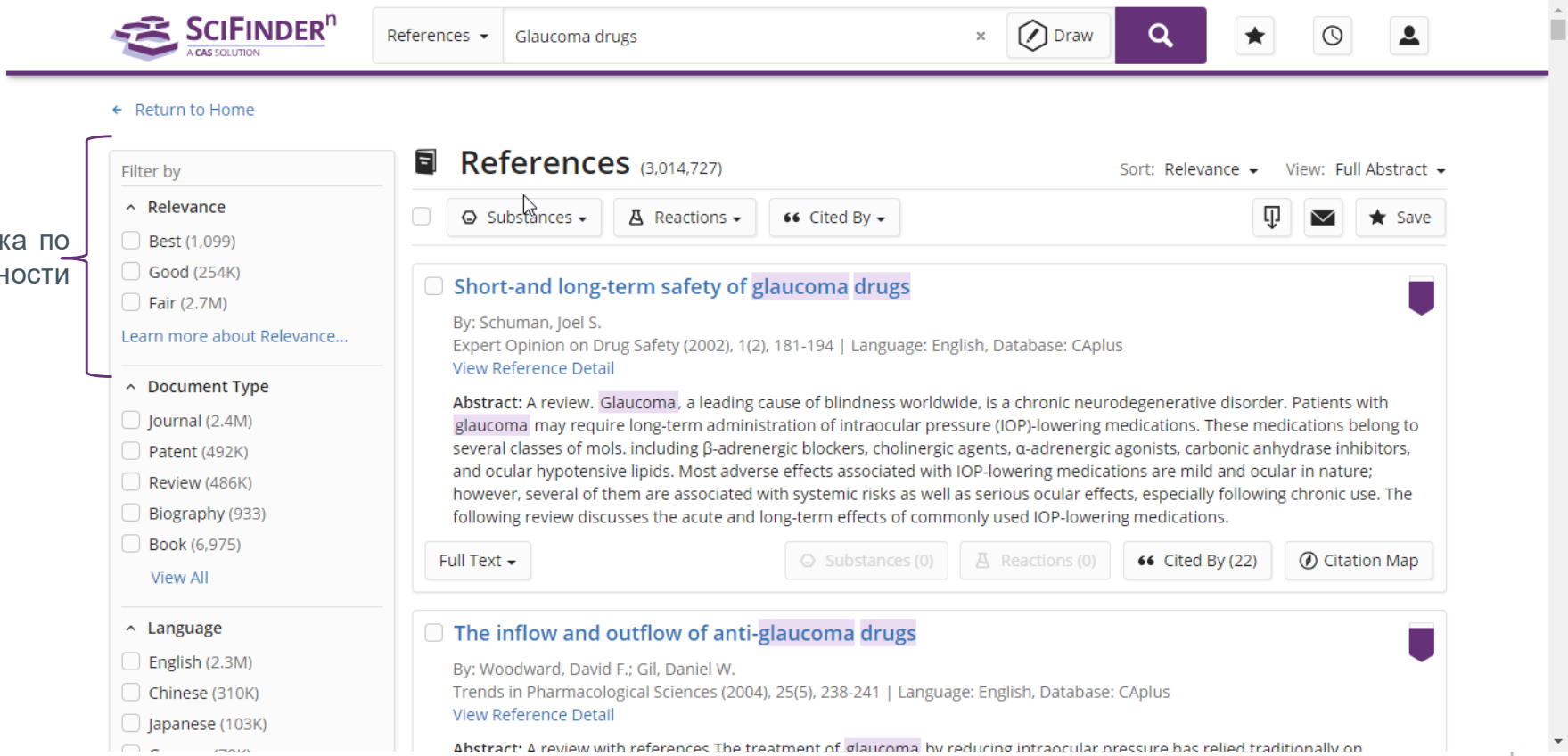
# Отбор наиболее релевантных вариантов ответов

Сортировка по релевантности




SciFinder n
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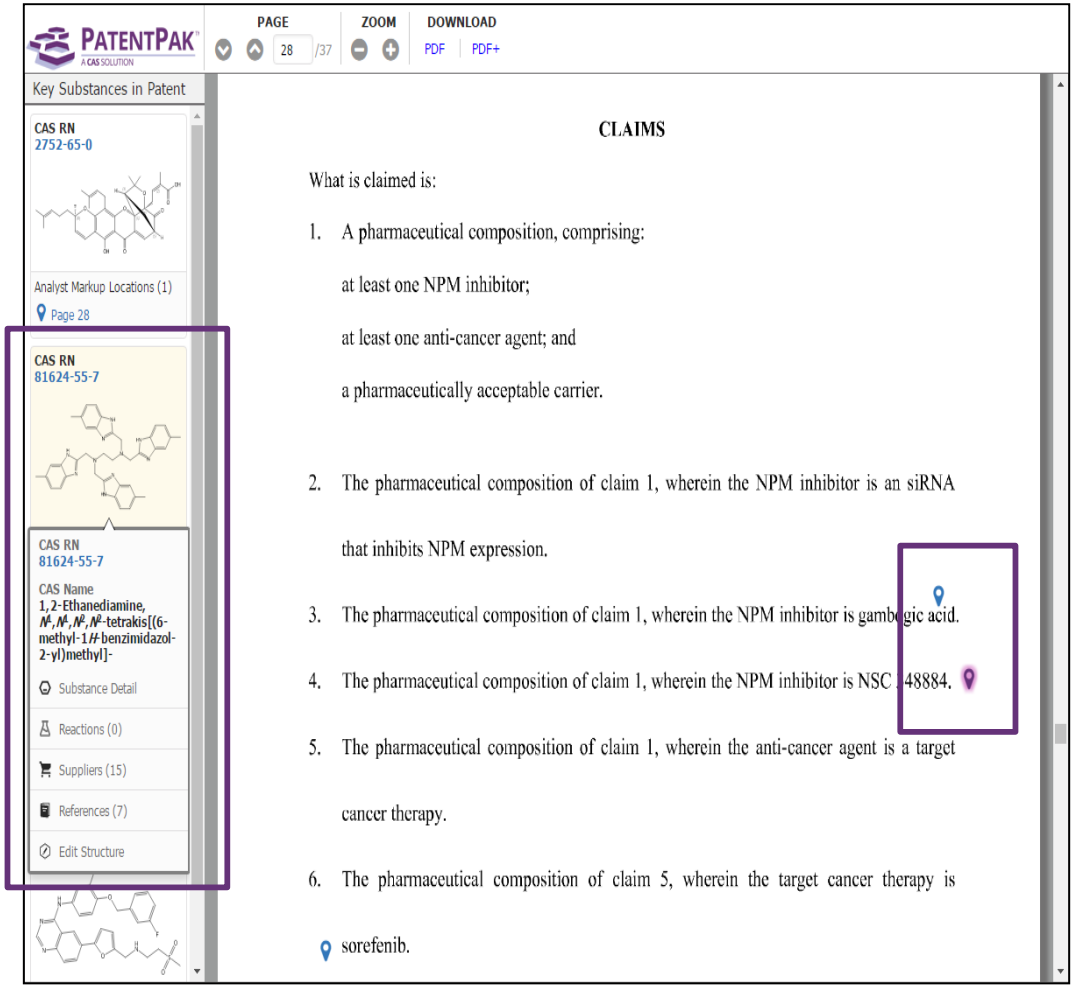
# Встроенный модуль для работы с патентами

Поиск химических структур в патенте




Метки химических структур в тексте патента

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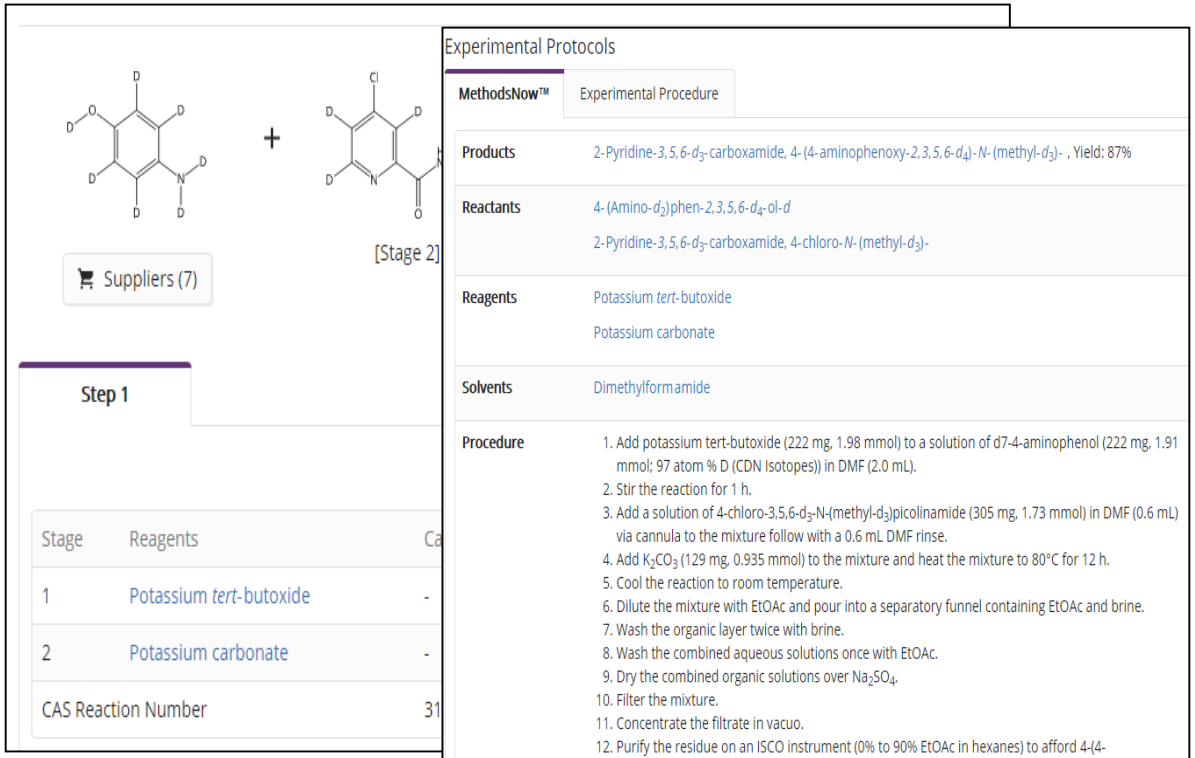
# Встроенный модуль синтетических протоколов




Experimental Protocols

MethodsNow™ | Experimental Procedure

| | |
|---|---|
| **Products** | 2-Pyridine-3,5,6-$d_3$-carboxamide, 4-(4-aminophenoxy-2,3,5,6-$d_4$)-N-(methyl-$d_3$)- , Yield: 87% |
| **Reactants** | 4-(Amino-$d_2$)phen-2,3,5,6-$d_4$-ol-$d$<br>2-Pyridine-3,5,6-$d_3$-carboxamide, 4-chloro-N-(methyl-$d_3$)- |
| **Reagents** | Potassium *tert*-butoxide<br>Potassium carbonate |
| **Solvents** | Dimethylformamide |

**Procedure**

1. Add potassium tert-butoxide (222 mg, 1.98 mmol) to a solution of d7-4-aminophenol (222 mg, 1.91 mmol; 97 atom % D (CDN Isotopes)) in DMF (2.0 mL).
2. Stir the reaction for 1 h.
3. Add a solution of 4-chloro-3,5,6-$d_3$-N-(methyl-$d_3$)picolinamide (305 mg, 1.73 mmol) in DMF (0.6 mL) via cannula to the mixture follow with a 0.6 mL DMF rinse.
4. Add $K_2CO_3$ (129 mg, 0.935 mmol) to the mixture and heat the mixture to 80°C for 12 h.
5. Cool the reaction to room temperature.
6. Dilute the mixture with EtOAc and pour into a separatory funnel containing EtOAc and brine.
7. Wash the organic layer twice with brine.
8. Wash the combined aqueous solutions once with EtOAc.
9. Dry the combined organic solutions over $Na_2SO_4$.
10. Filter the mixture.
11. Concentrate the filtrate in vacuo.
12. Purify the residue on an ISCO instrument (0% to 90% EtOAc in hexanes) to afford 4-(4-amino(phenoxy-$d_4$))-3,5,6-$d_3$-N-(methyl-$d_3$)picolinamide.

| | |
|---|---|
| **Transformation** | Aromatic Substitution by Oxygen Nucleophiles |
| **Scale** | milligram |

**Characterization Data**

2-Pyridine-3,5,6-$d_3$-carboxamide, 4-(4-aminophenoxy-2,3,5,6-$d_4$)-N-(methyl-$d_3$)-

| | |
|---|---|
| **Mass Spectrum** | MS (M + H): 254.0 |

Ключевые компоненты реакции

Пошаговая инструкция

Дополнительная информация

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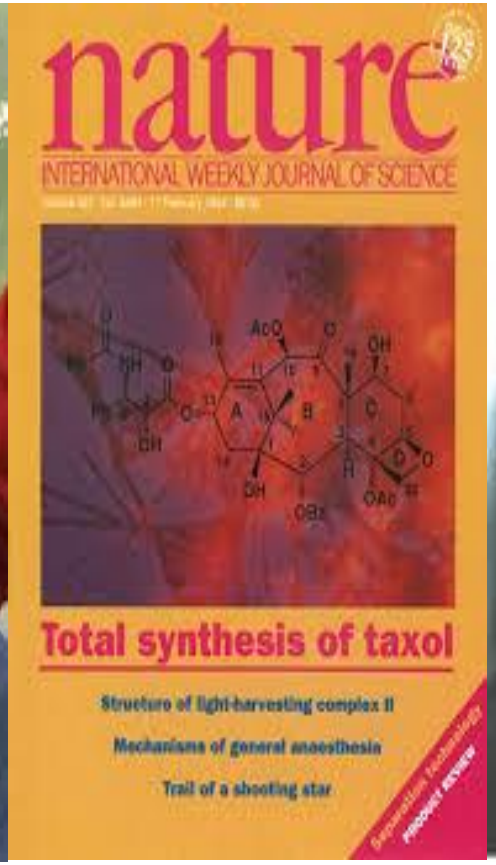
# Пример: полный синтез таксола







Кирьякос Николау – номинация на Нобелевскую премию по химии 2015

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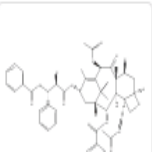
References: **synthesis**



As Drawn (2,746), Substructure (2,782)

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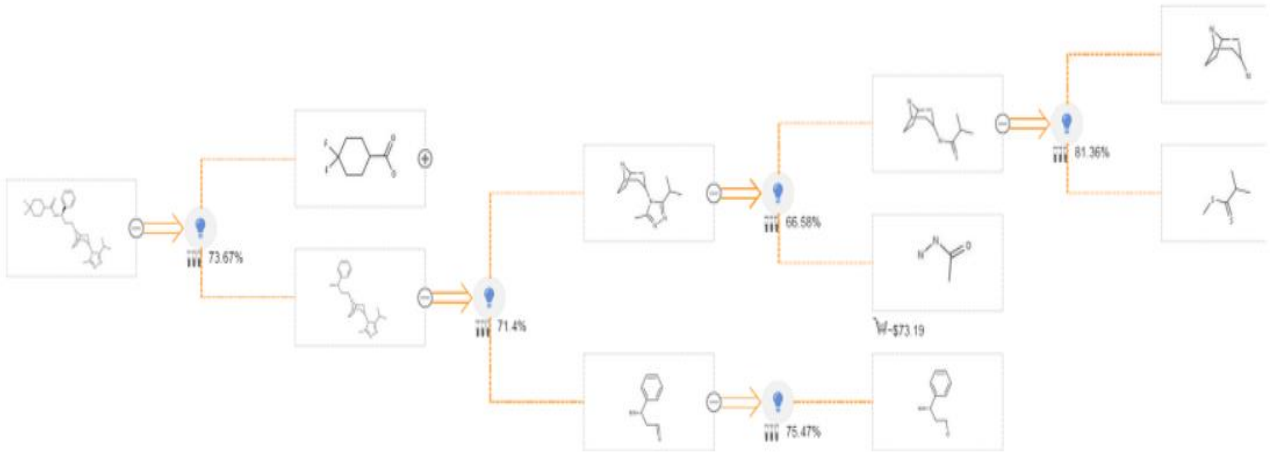
# В SciFinder$^n$ появился ретросинтез!

- Экспериментальный и теоретический ретросинтез
  - Альтернативные стратегии синтеза известных соединений
  - Предсказание стадий синтеза новых целевых молекул

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# Спасибо за внимание !

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