化学及相关学科信息资源概述

林佳　　清华大学图书馆

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主要内容

- 化学及相关学科文献信息源的特点
- 常用专业信息源概览
- 信息资源的合理选择
- 获取全文
- 了解本学科领域高影响力期刊

1. 化学及相关学科文献信息源的特点

①记录内容包含大量化学特有信息

- **题录信息（基本同其他学科信息资源）**

  标题、责任者、来源、文摘……

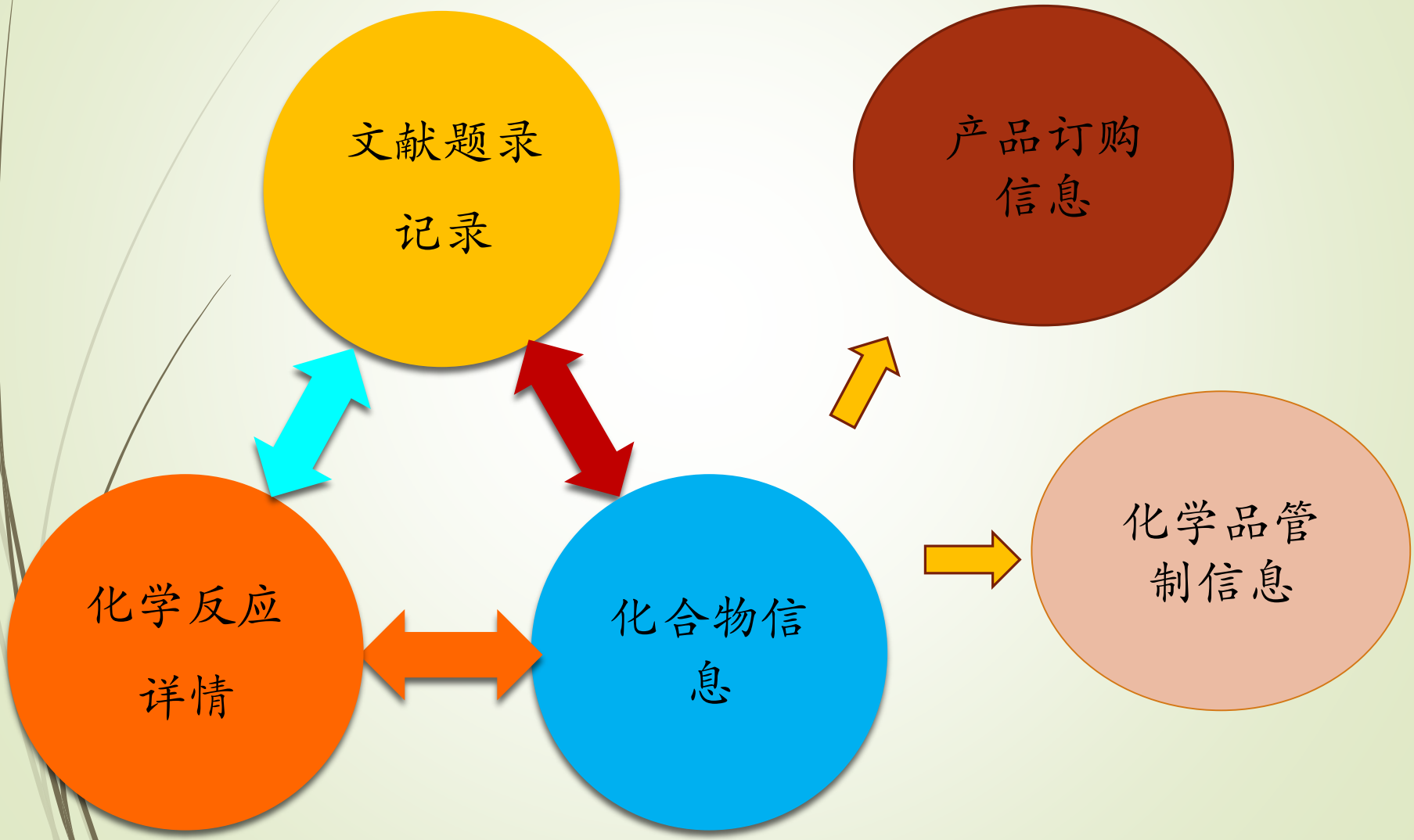
- **反应信息**

  反应式（步骤、条件、中间体、产率……）、反应条件……

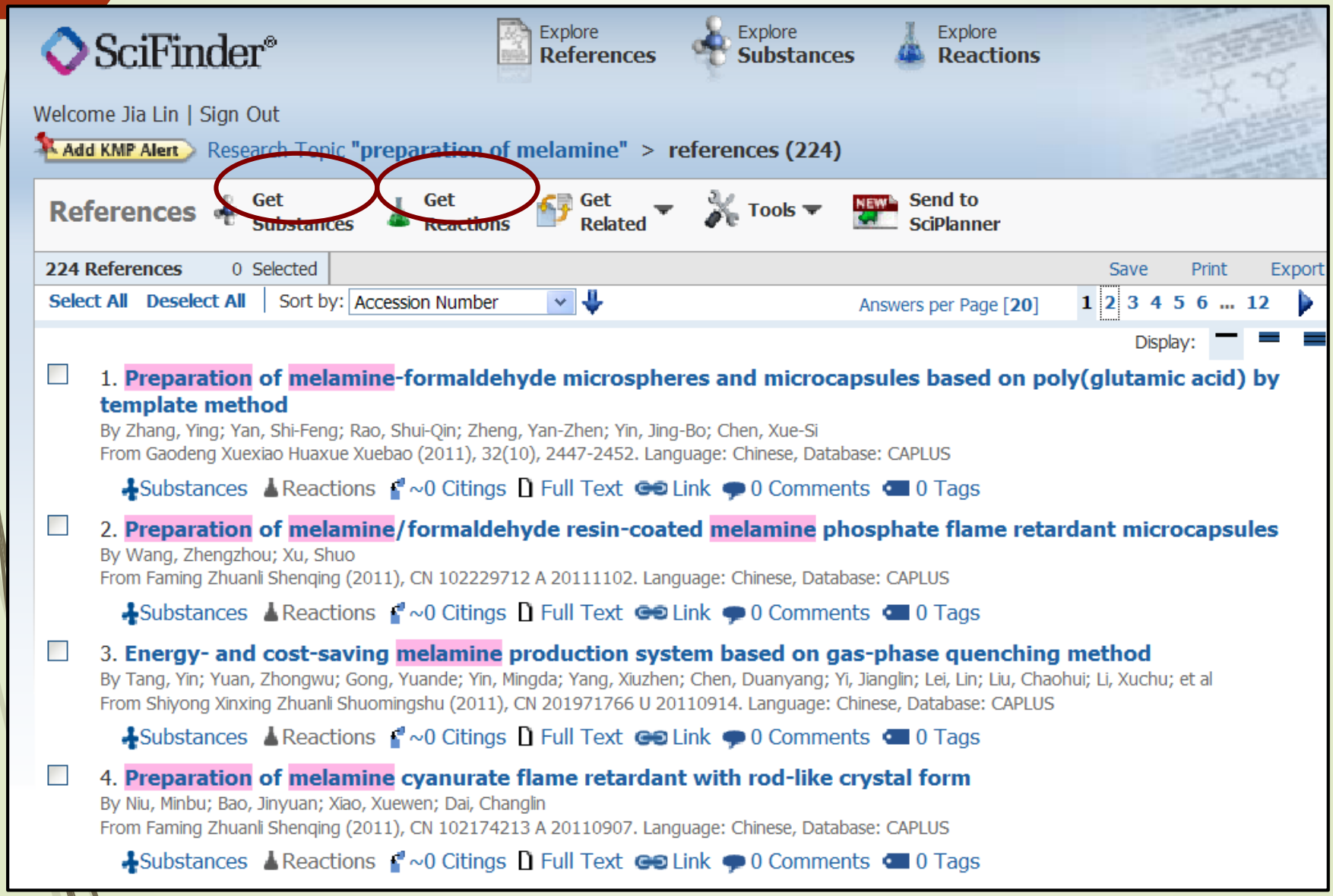
- **化合物信息**

  结构式、名称（系统命名、商品名、俗名、药品名……）、代码（CASRN……）、物理、化学、药理学、生物性质、商业信息及化学品管制信息

②文献信息、化合物、反应之间无缝链接



②文献信息、化合物、反应之间无缝链接（SciFinder应用实例）



②文献信息、化合物、反应之间无缝链接（SciFinder应用实例）

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31 Substances | 0 Selected | Save | Print | Export

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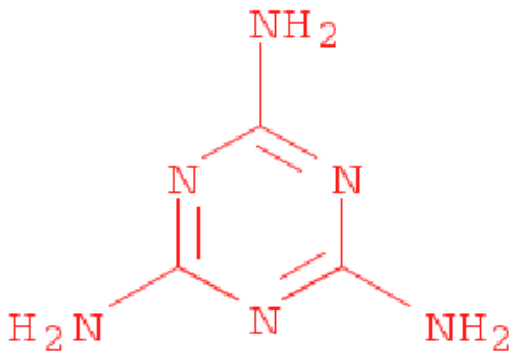
View:

1. **Substance Detail**
   1260170-50-0



$C_3H_6N_6$

~1 References

Reactions

2. **Substance Detail**
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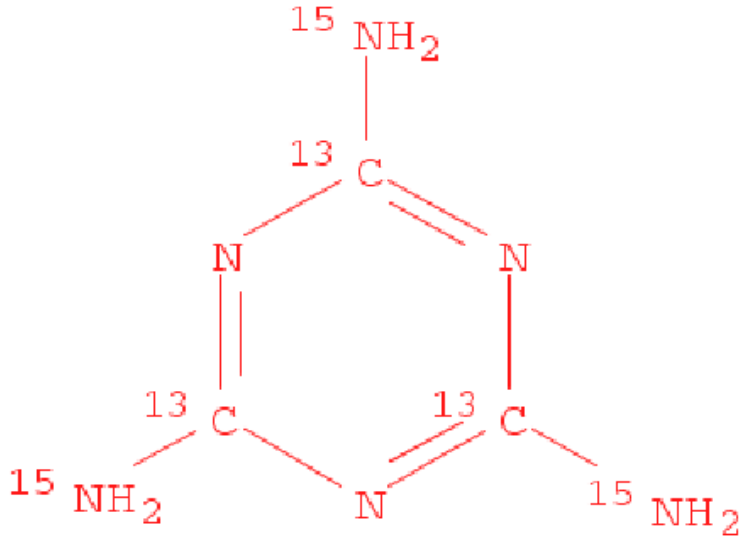

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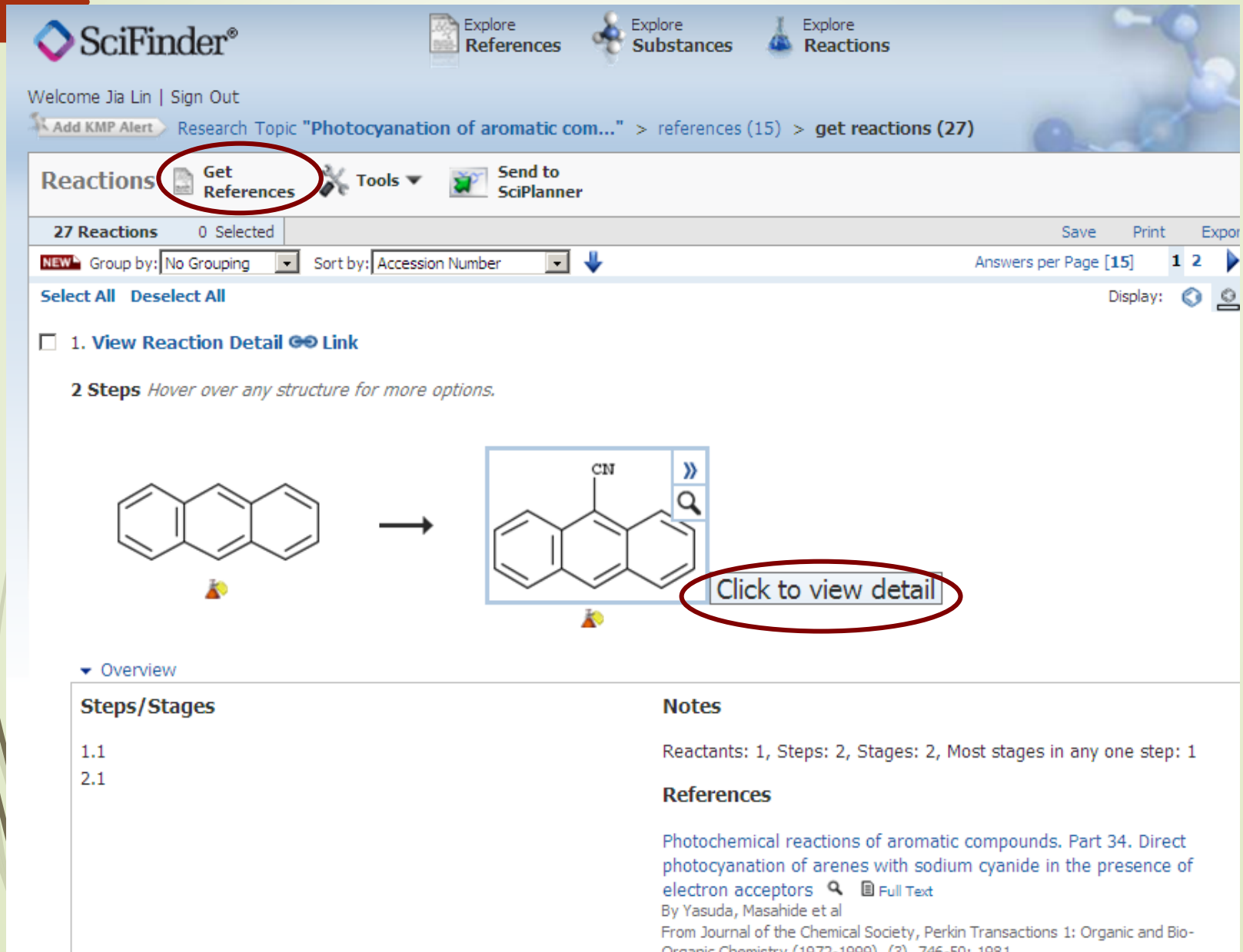
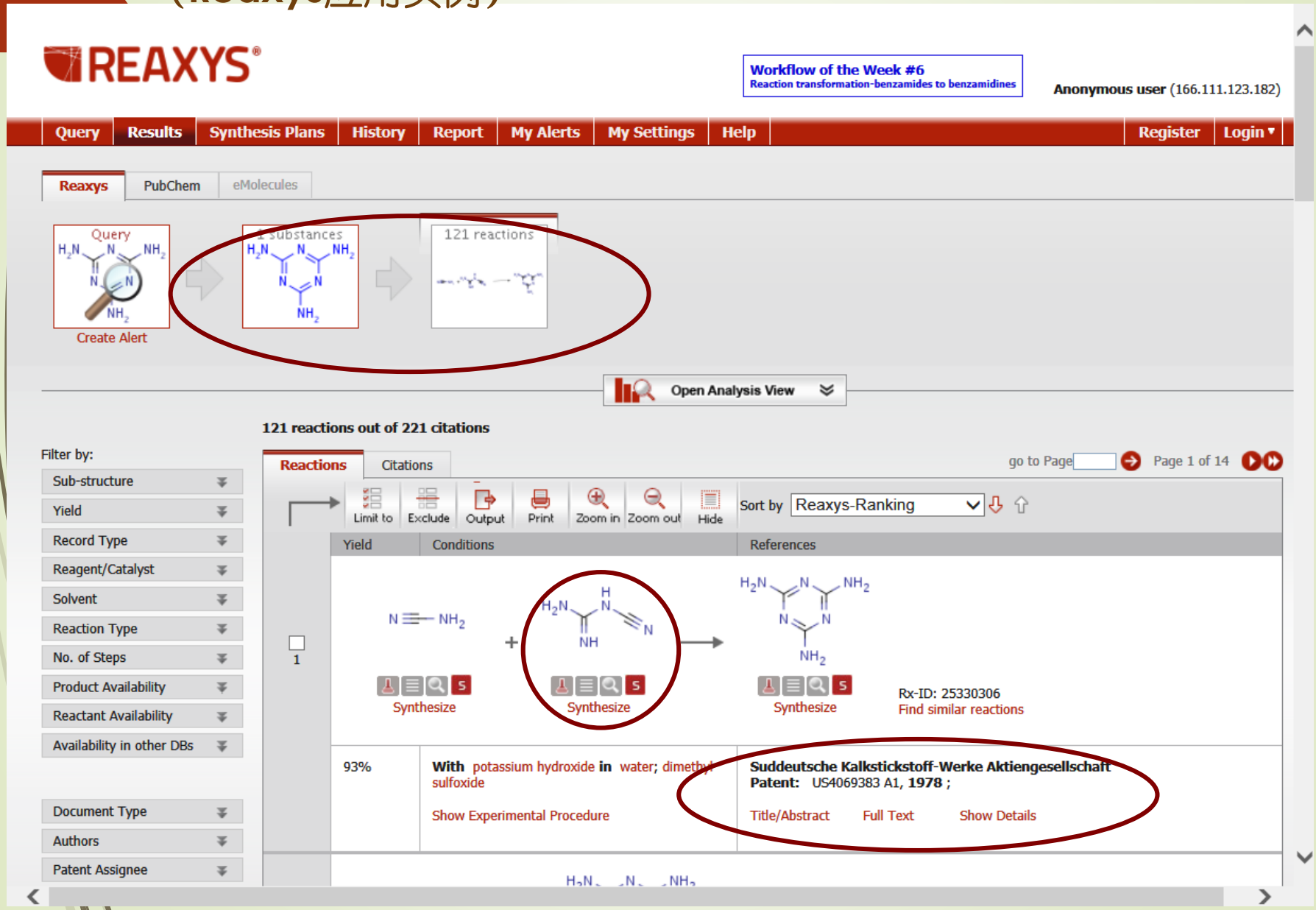
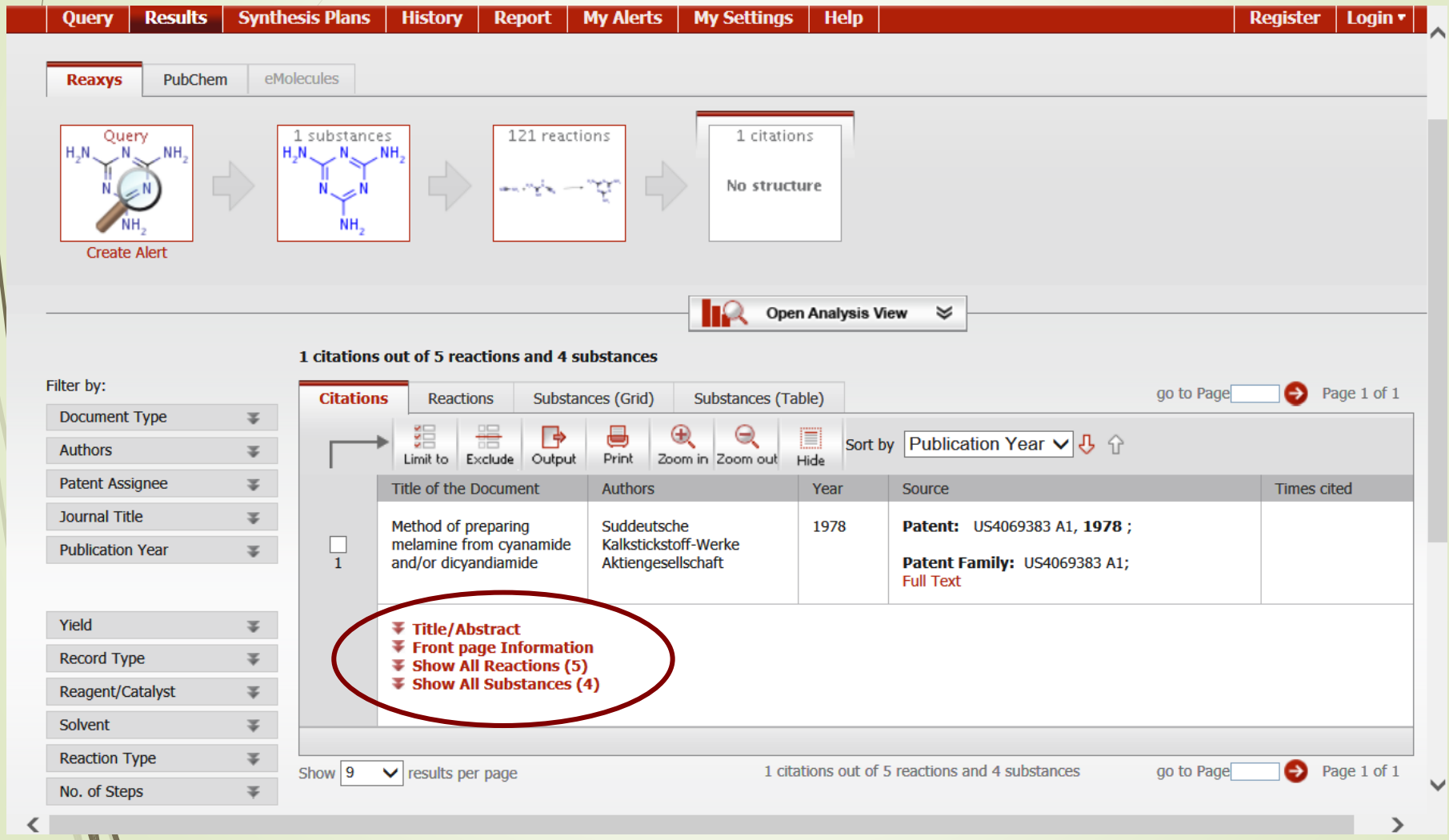


②文献信息、化合物、反应之间无缝链接（Reaxys应用实例）



②文献信息、化合物、反应之间无缝链接（Reaxys应用实例）



③丰富实用的检索途径、检索字段和检索限定

- 书目信息（基本同其他学科信息资源）

  主题、人名、来源……

- 反应信息

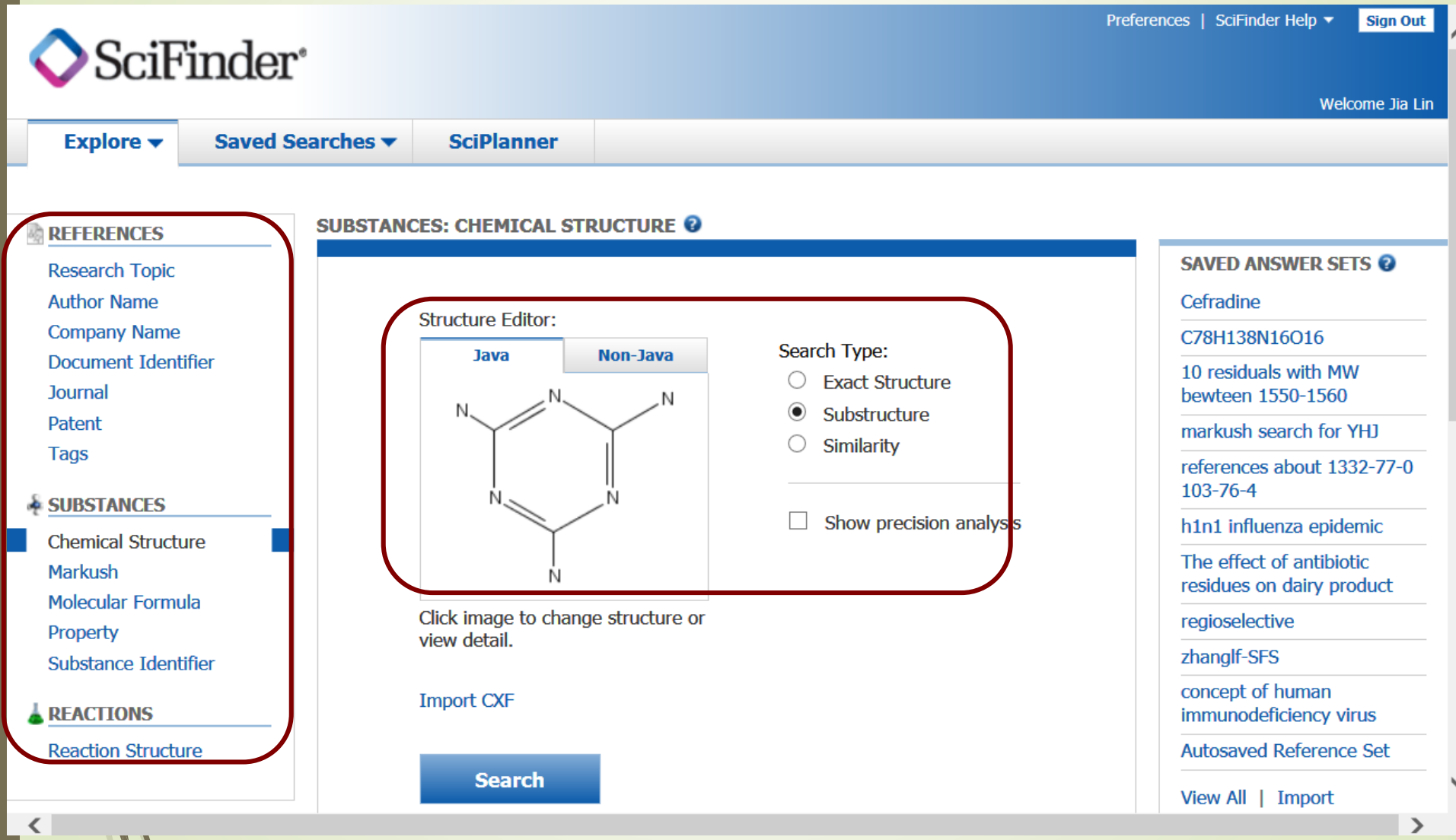
  反应式（完整/部分）、反应条件、产率、反应步骤……

- 化合物信息

  结构式、名称、代码、物理化学性质

不同数据库有各自不同的检索字段，检索时可辅以多种限定条件

③丰富实用的检索途径、检索字段和检索限定



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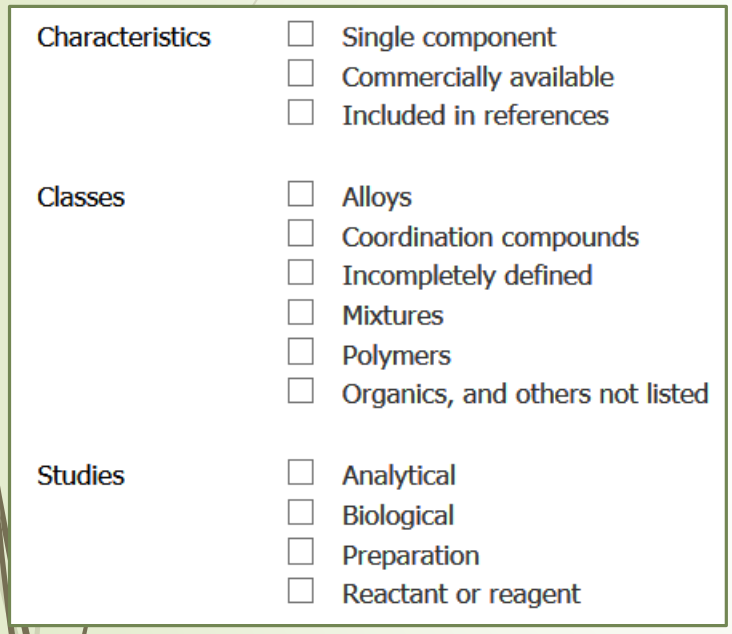
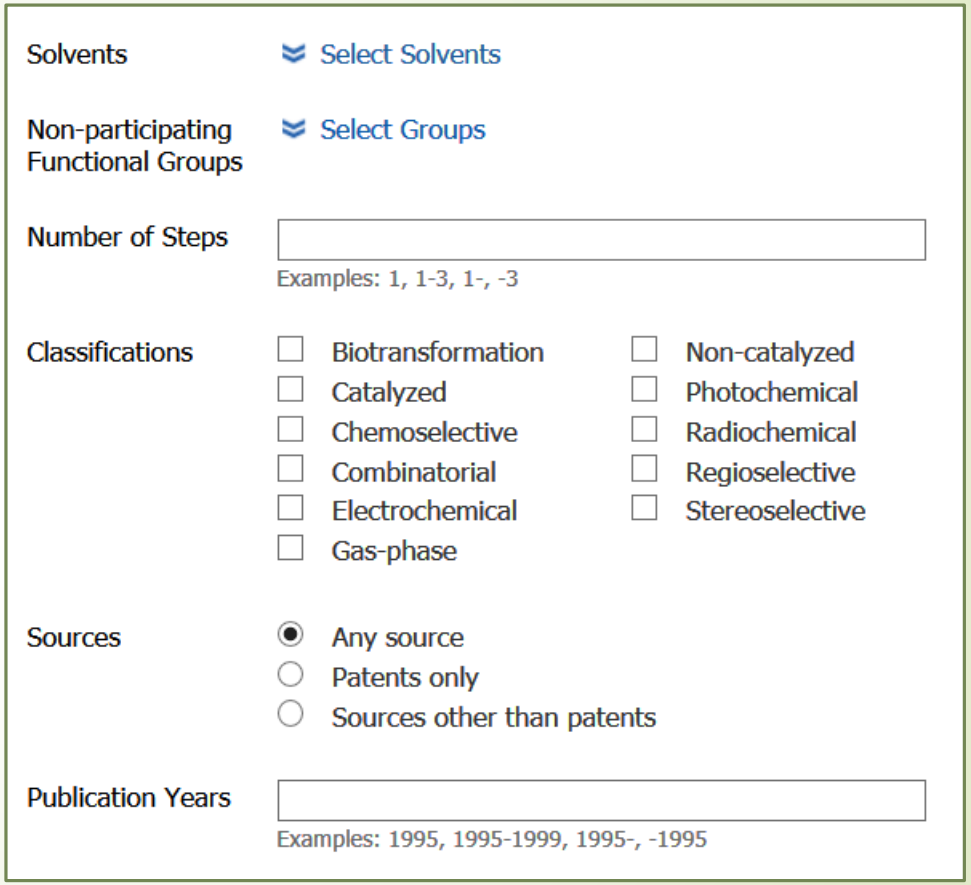


化合物限定



化学反应限定

2. 常用专业信息源概览

常用专业信息源

- **SciFinder——可检索研究进展及化学反应和化合物信息**
- **Reaxys——包含**丰富的数值、事实等化学信息
- **DII之Chemicals——专利信息数据库**
- **ACS Publications/RSC Publishing——两大化学学会的电子出版物**
- **Knovel-**Chemistry & Chemical Engineering**——交互式参考工具**
- **更多？**

  推荐使用“清华大学学术信息资源门户”、“电子去期刊导航系统”
- **网络免费资源**
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- ACS-Chemical Abstracts Service出版发行的基于网络的信息检索系统
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- 需要注册个人账号（须用……tsinghua.edu.cn邮箱，且在校园网内，参见 http://www.lib.tsinghua.edu.cn/database/scifinder.htm）
- 访问入口：https://scifinder.cas.org

统一平台上的多个数据库

- **CAPLUS** (reference)
- **MEDLINE** (reference)
- **REGISTRY** (substance)
- **CASREACT** (reaction)
- **CHEMLIST**（regulated chemicals）
- **MARPAT**（patents by Markush structure）

检索模式和检索途径

根据已有线索和检索目的选择模式和途径

检索模式	检索途径	对象数据库	记录内容
References（查找文献）	Research Topic	CAplus MEDLINE	●文献标题 ●著者、编者、发明人 ●机构名称、专利受让人 ●出版年 ●来源、出版物名称、出版时间、出版者、卷、期、页码、CODEN 码和 ISSN ●专利标识，包括专利授权、申请、优先权、以及专利族信息 ●文摘 ●索引标题及补充术语 ●引文 ●原文中涉及的化合物、序列和反应
	Author Name		
	Company Name		
	Document Identifier		
	Journal		
	Patent		
	Tags		

检索模式	检索途径	对象数据库	记录内容
Substances（查化合物）	Chemical Structure Molecular Formula Markush Property Identifier	REGISTRY	● 化学名称 ● CAS 登记号 ● 分子式 ● 结构图示 ● 序列信息，包括 GenBank® 和专利文献中的注解 ● 数据性质，包括光谱谱图 ● 商业来源信息 ● 化学品管制信息 ● 编者注解 ● 涉及对象化合物的文献信息 ● 对象化合物参与的化学反应信息
Reactions（查反应）	Reaction Structure	CASREACT	● 反应图示，包括反应物、产物、试剂 、催化剂、溶剂、以及反应步骤 ● 涉及对象反应的文献信息 ● 参与反应的所有化合物信息，包括化学品管制信息、商业来源信息等

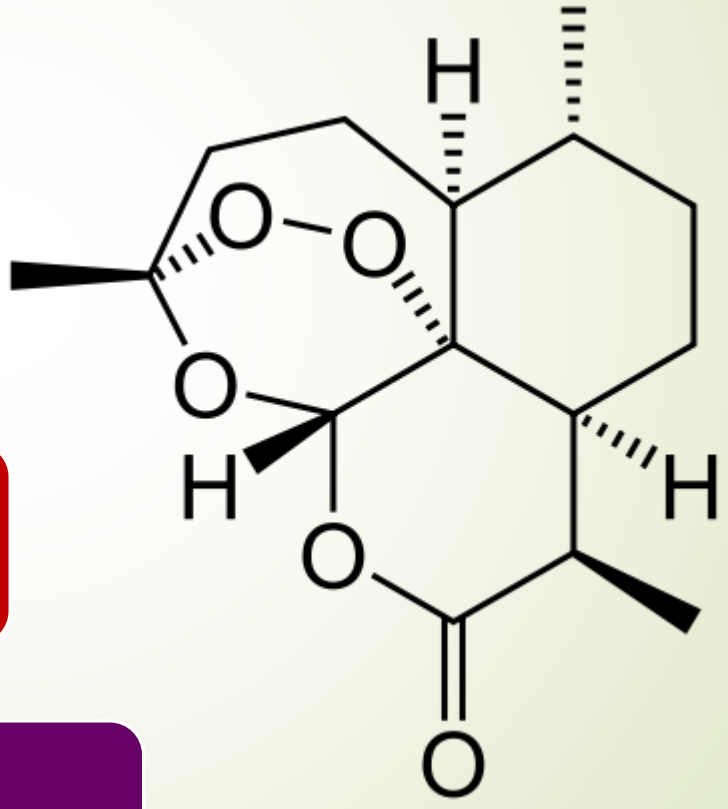
检索实例

2015生理或医学诺奖

屠呦呦

青蒿素

疟疾



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Analyze by: Substance Role

- Analytical Study 1
- Biological Study 1
- Formation, Nonpreparative 1
- Miscellaneous 1
- Occurrence 1
- Preparation 1
- Process 1
- Properties 1
- Prophetic in Patents 1
- Reactant or Reagent 1

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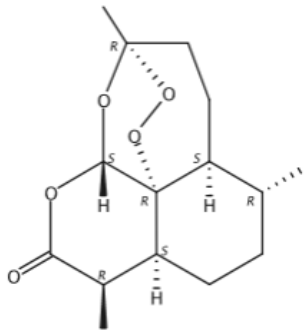
1. 63968-64-9

~4094 ~165



Quick View

Absolute stereochemistry.

$C_{15}H_{22}O_5$

3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, (3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-

Key Physical Properties

Regulatory Information

Spectra

Experimental Properties

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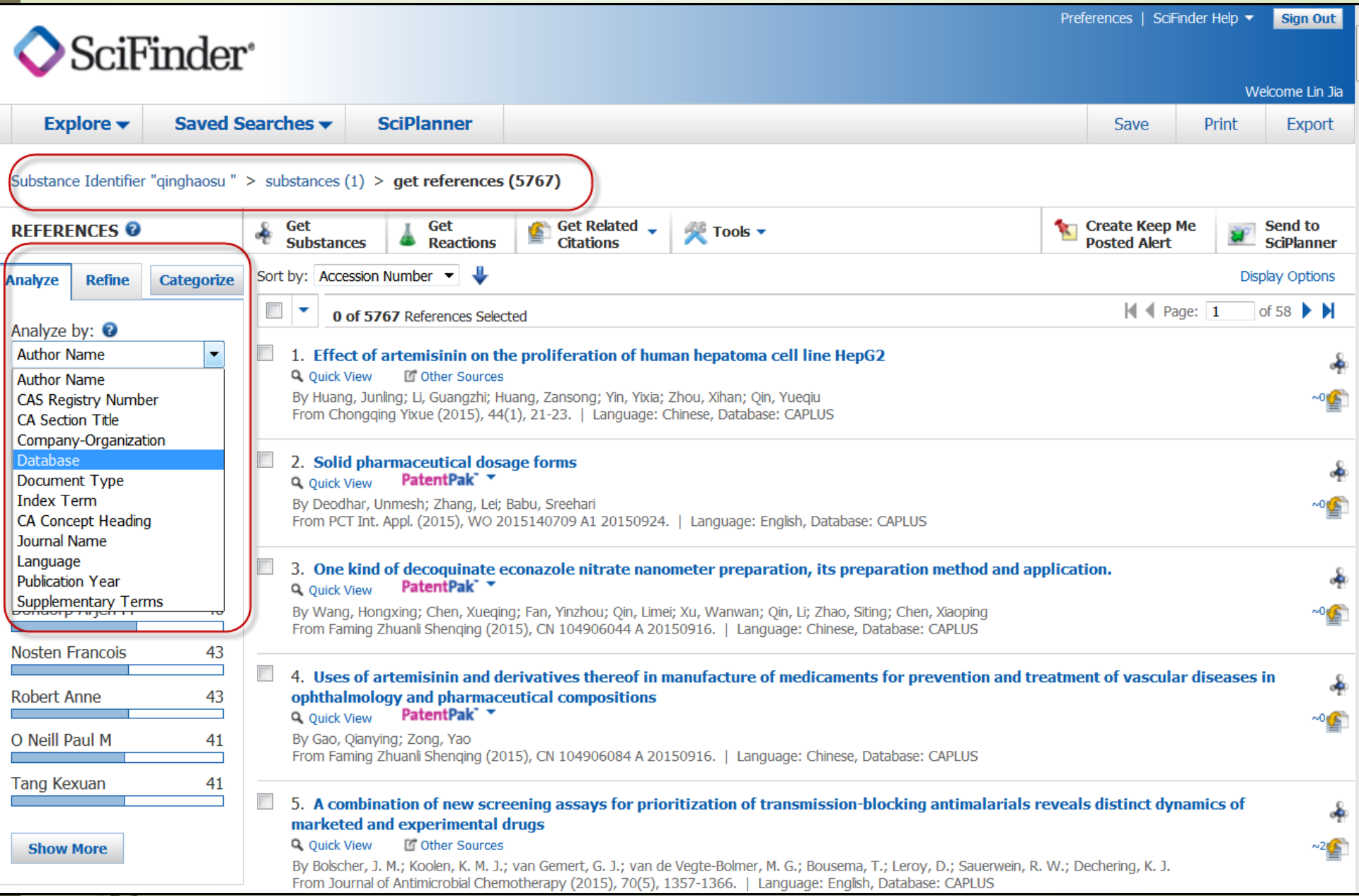
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Journal Name
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Supplementary Terms
Nosten Francois 43
Robert Anne 43
O Neill Paul M 41
Tang Kexuan 41
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Page: 1 of 58
1. Effect of artemisinin on the proliferation of human hepatoma cell line HepG2
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Other Sources
By Huang, Junling; Li, Guangzhi; Huang, Zansong; Yin, Yixia; Zhou, Xihan; Qin, Yueqiu
From Chongqing Yixue (2015), 44(1), 21-23. | Language: Chinese, Database: CAPLUS
2. Solid pharmaceutical dosage forms
Quick View
PatentPak
By Deodhar, Unmesh; Zhang, Lei; Babu, Sreehari
From PCT Int. Appl. (2015), WO 2015140709 A1 20150924. | Language: English, Database: CAPLUS
3. One kind of decoquinate econazole nitrate nanometer preparation, its preparation method and application.
Quick View
PatentPak
By Wang, Hongxing; Chen, Xueqing; Fan, Yinzhou; Qin, Limei; Xu, Wanwan; Qin, Li; Zhao, Siting; Chen, Xiaoping
From Faming Zhuanli Shenqing (2015), CN 104906044 A 20150916. | Language: Chinese, Database: CAPLUS
4. Uses of artemisinin and derivatives thereof in manufacture of medicaments for prevention and treatment of vascular diseases in ophthalmology and pharmaceutical compositions
Quick View
PatentPak
By Gao, Qianying; Zong, Yao
From Faming Zhuanli Shenqing (2015), CN 104906084 A 20150916. | Language: Chinese, Database: CAPLUS
5. A combination of new screening assays for prioritization of transmission-blocking antimalarials reveals distinct dynamics of marketed and experimental drugs
Quick View
Other Sources
By Bolscher, J. M.; Koolen, K. M. J.; van Gemert, G. J.; van de Vegte-Bolmer, M. G.; Bousema, T.; Leroy, D.; Sauerwein, R. W.; Dechering, K. J.
From Journal of Antimicrobial Chemotherapy (2015), 70(5), 1357-1366. | Language: English, Database: CAPLUS

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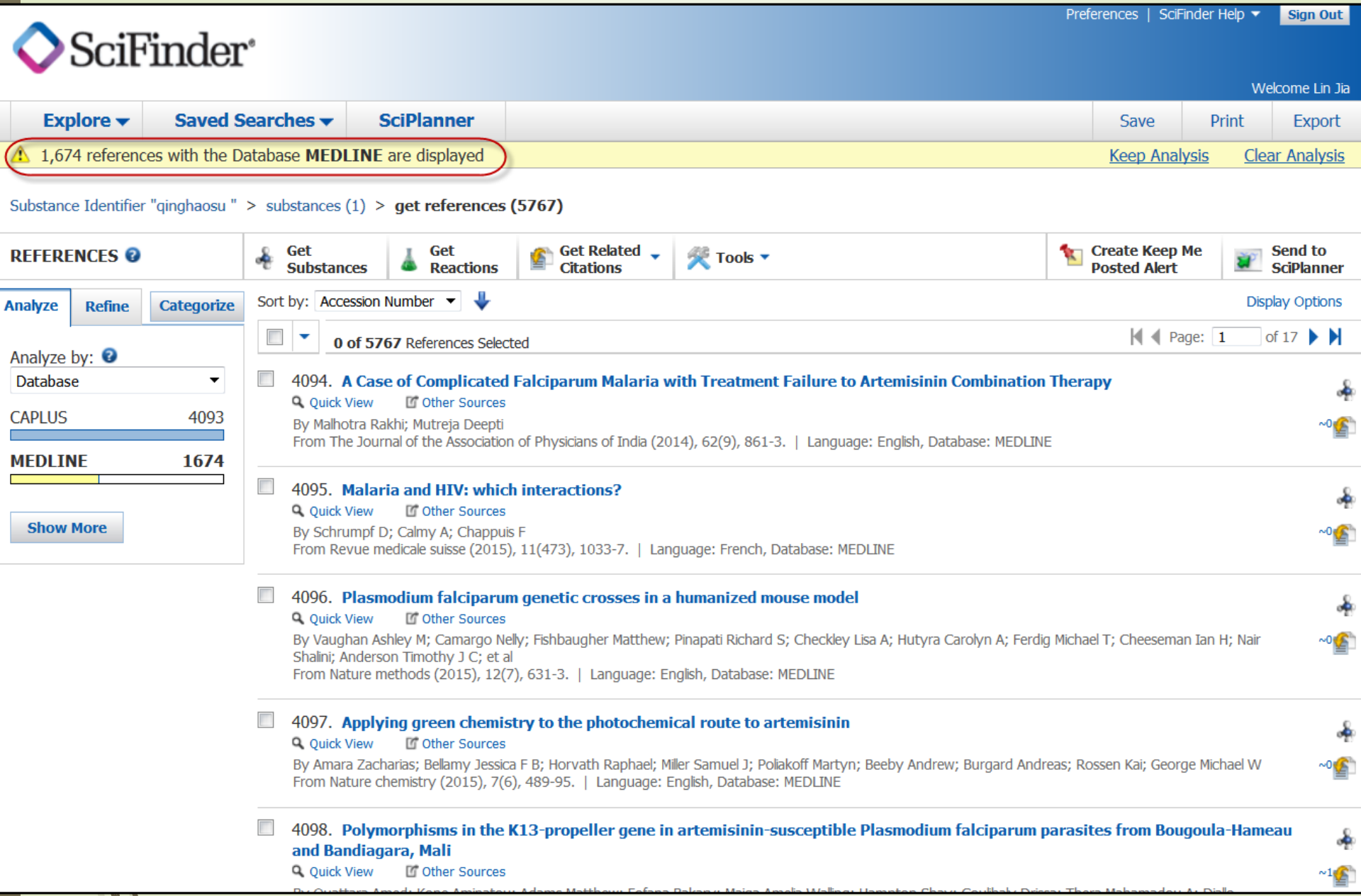
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MEDLINE 1674
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4094. A Case of Complicated Falciparum Malaria with Treatment Failure to Artemisinin Combination Therapy
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Other Sources
By Malhotra Rakhi; Mutreja Deepti
From The Journal of the Association of Physicians of India (2014), 62(9), 861-3. | Language: English, Database: MEDLINE
4095. Malaria and HIV: which interactions?
Quick View
Other Sources
By Schrumpf D; Calmy A; Chappuis F
From Revue medicale suisse (2015), 11(473), 1033-7. | Language: French, Database: MEDLINE
4096. Plasmodium falciparum genetic crosses in a humanized mouse model
Quick View
Other Sources
By Vaughan Ashley M; Camargo Nelly; Fishbaugher Matthew; Pinapati Richard S; Checkley Lisa A; Hutyra Carolyn A; Ferdig Michael T; Cheeseman Ian H; Nair Shalini; Anderson Timothy J C; et al
From Nature methods (2015), 12(7), 631-3. | Language: English, Database: MEDLINE
4097. Applying green chemistry to the photochemical route to artemisinin
Quick View
Other Sources
By Amara Zacharias; Bellamy Jessica F B; Horvath Raphael; Miller Samuel J; Poliakoff Martyn; Beeby Andrew; Burgard Andreas; Rossen Kai; George Michael W
From Nature chemistry (2015), 7(6), 489-95. | Language: English, Database: MEDLINE
4098. Polymorphisms in the K13-propeller gene in artemisinin-susceptible Plasmodium falciparum parasites from Bougoula-Hameau and Bandiagara, Mali
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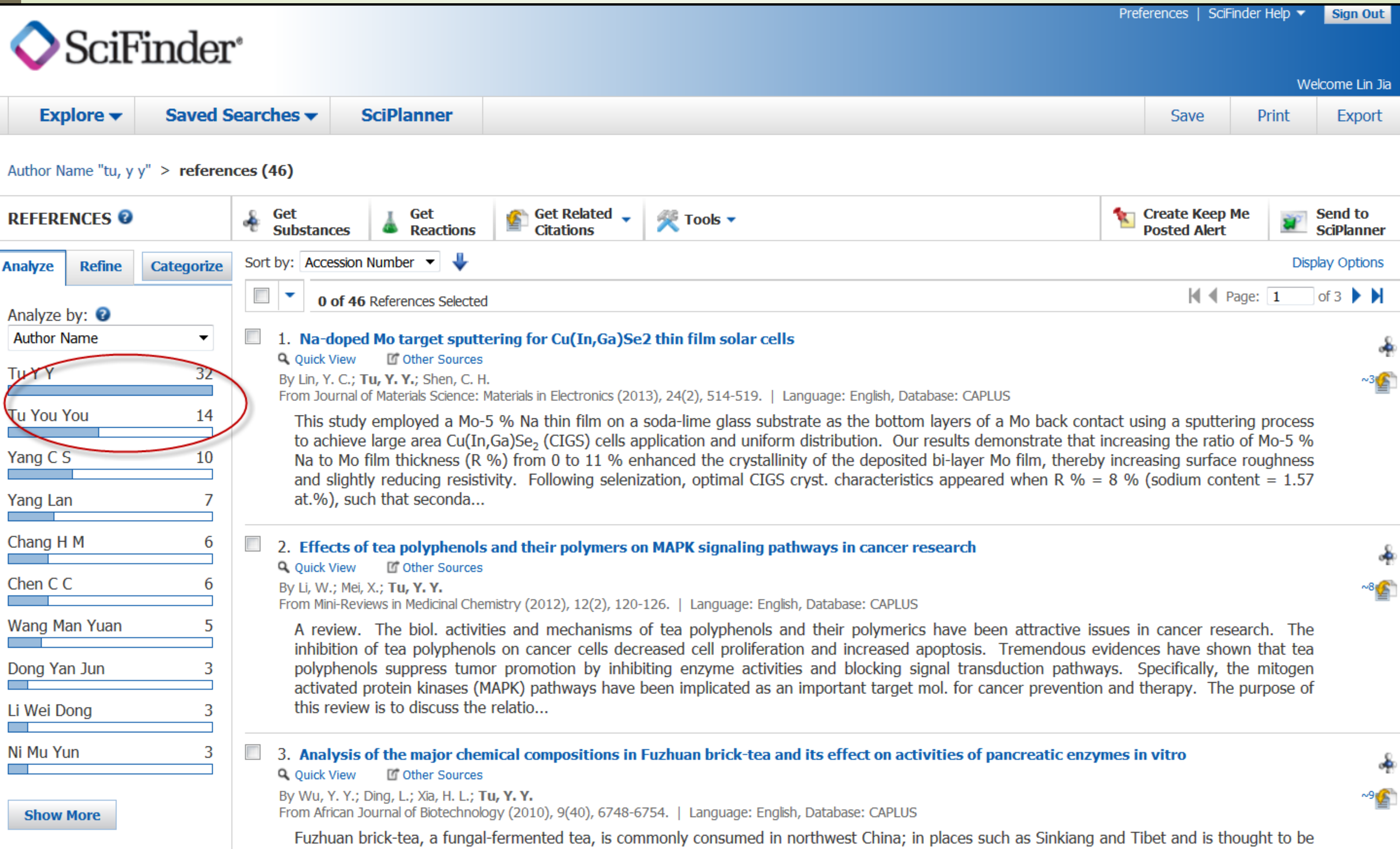

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Tu You You 14
Yang C S 10
Yang Lan 7
Chang H M 6
Chen C C 6
Wang Man Yuan 5
Dong Yan Jun 3
Li Wei Dong 3
Ni Mu Yun 3
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1. Na-doped Mo target sputtering for Cu(In,Ga)Se2 thin film solar cells
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By Lin, Y. C.; Tu, Y. Y.; Shen, C. H.
From Journal of Materials Science: Materials in Electronics (2013), 24(2), 514-519. | Language: English, Database: CAPLUS
This study employed a Mo-5 % Na thin film on a soda-lime glass substrate as the bottom layers of a Mo back contact using a sputtering process to achieve large area Cu(In,Ga)Se2 (CIGS) cells application and uniform distribution. Our results demonstrate that increasing the ratio of Mo-5 % Na to Mo film thickness (R %) from 0 to 11 % enhanced the crystallinity of the deposited bi-layer Mo film, thereby increasing surface roughness and slightly reducing resistivity. Following selenization, optimal CIGS cryst. characteristics appeared when R % = 8 % (sodium content = 1.57 at.%), such that seconda...
2. Effects of tea polyphenols and their polymers on MAPK signaling pathways in cancer research
Quick View Other Sources
By Li, W.; Mei, X.; Tu, Y. Y.
From Mini-Reviews in Medicinal Chemistry (2012), 12(2), 120-126. | Language: English, Database: CAPLUS
A review. The biol. activities and mechanisms of tea polyphenols and their polymerics have been attractive issues in cancer research. The inhibition of tea polyphenols on cancer cells decreased cell proliferation and increased apoptosis. Tremendous evidences have shown that tea polyphenols suppress tumor promotion by inhibiting enzyme activities and blocking signal transduction pathways. Specifically, the mitogen activated protein kinases (MAPK) pathways have been implicated as an important target mol. for cancer prevention and therapy. The purpose of this review is to discuss the relatio...
3. Analysis of the major chemical compositions in Fuzhuan brick-tea and its effect on activities of pancreatic enzymes in vitro
Quick View Other Sources
By Wu, Y. Y.; Ding, L.; Xia, H. L.; Tu, Y. Y.
From African Journal of Biotechnology (2010), 9(40), 6748-6754. | Language: English, Database: CAPLUS
Fuzhuan brick-tea, a fungal-fermented tea, is commonly consumed in northwest China; in places such as Sinkiang and Tibet and is thought to be

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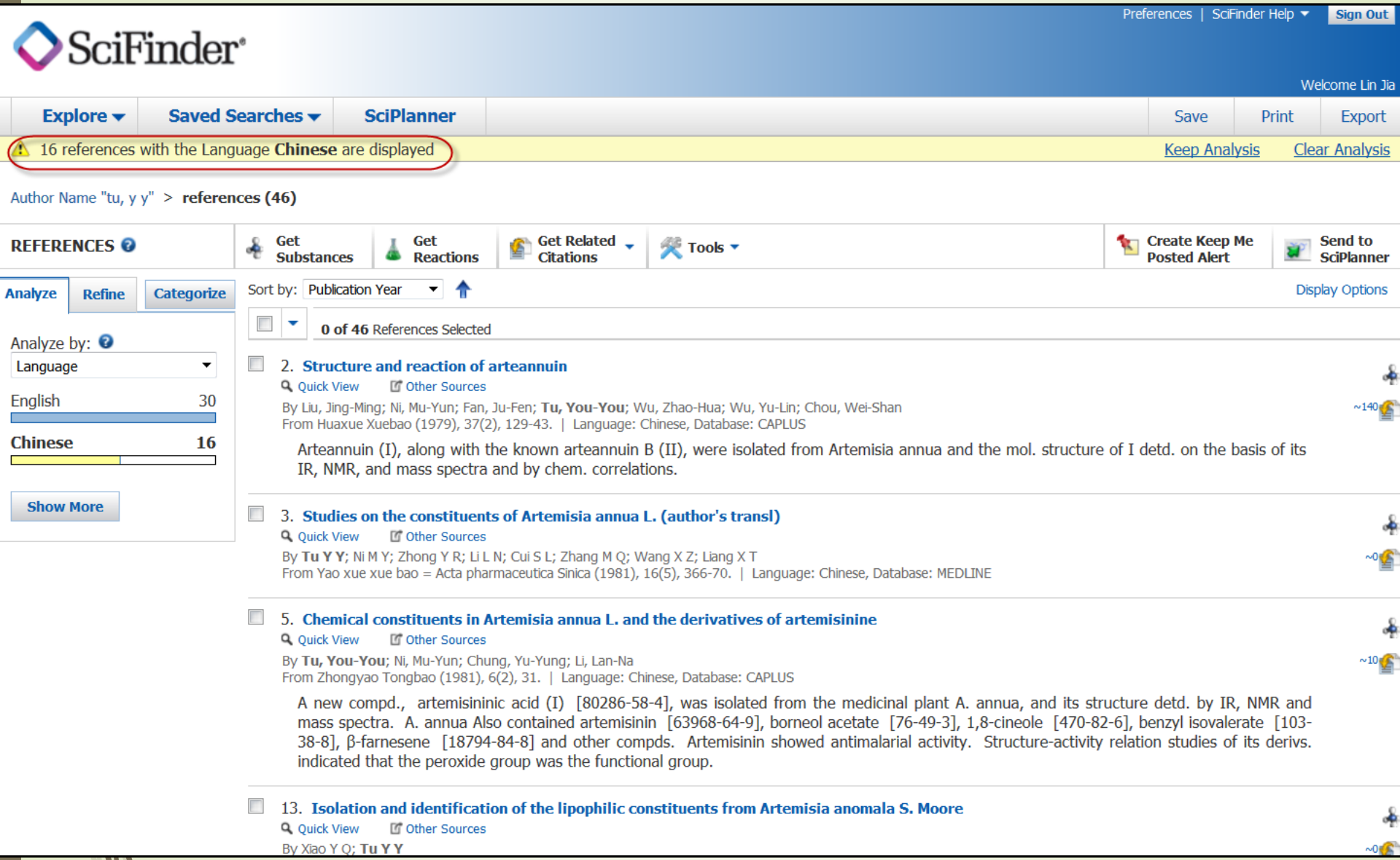
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2. Structure and reaction of arteannuin
Quick View
Other Sources
By Liu, Jing-Ming; Ni, Mu-Yun; Fan, Ju-Fen; Tu, You-You; Wu, Zhao-Hua; Wu, Yu-Lin; Chou, Wei-Shan
From Huaxue Xuebao (1979), 37(2), 129-43. | Language: Chinese, Database: CAPLUS
Arteannuin (I), along with the known arteannuin B (II), were isolated from Artemisia annua and the mol. structure of I detd. on the basis of its IR, NMR, and mass spectra and by chem. correlations.
3. Studies on the constituents of Artemisia annua L. (author's transl)
Quick View
Other Sources
By Tu Y Y; Ni M Y; Zhong Y R; Li L N; Cui S L; Zhang M Q; Wang X Z; Liang X T
From Yao xue xue bao = Acta pharmaceutica Sinica (1981), 16(5), 366-70. | Language: Chinese, Database: MEDLINE
5. Chemical constituents in Artemisia annua L. and the derivatives of artemisinine
Quick View
Other Sources
By Tu, You-You; Ni, Mu-Yun; Chung, Yu-Yung; Li, Lan-Na
From Zhongyao Tongbao (1981), 6(2), 31. | Language: Chinese, Database: CAPLUS
A new compd., artemisininic acid (I) [80286-58-4], was isolated from the medicinal plant A. annua, and its structure detd. by IR, NMR and mass spectra. A. annua Also contained artemisinin [63968-64-9], borneol acetate [76-49-3], 1,8-cineole [470-82-6], benzyl isovalerate [103-38-8], β-farnesene [18794-84-8] and other compds. Artemisinin showed antimalarial activity. Structure-activity relation studies of its derivs. indicated that the peroxide group was the functional group.
13. Isolation and identification of the lipophilic constituents from Artemisia anomala S. Moore
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Other Sources
By Xiao Y Q; Tu Y Y

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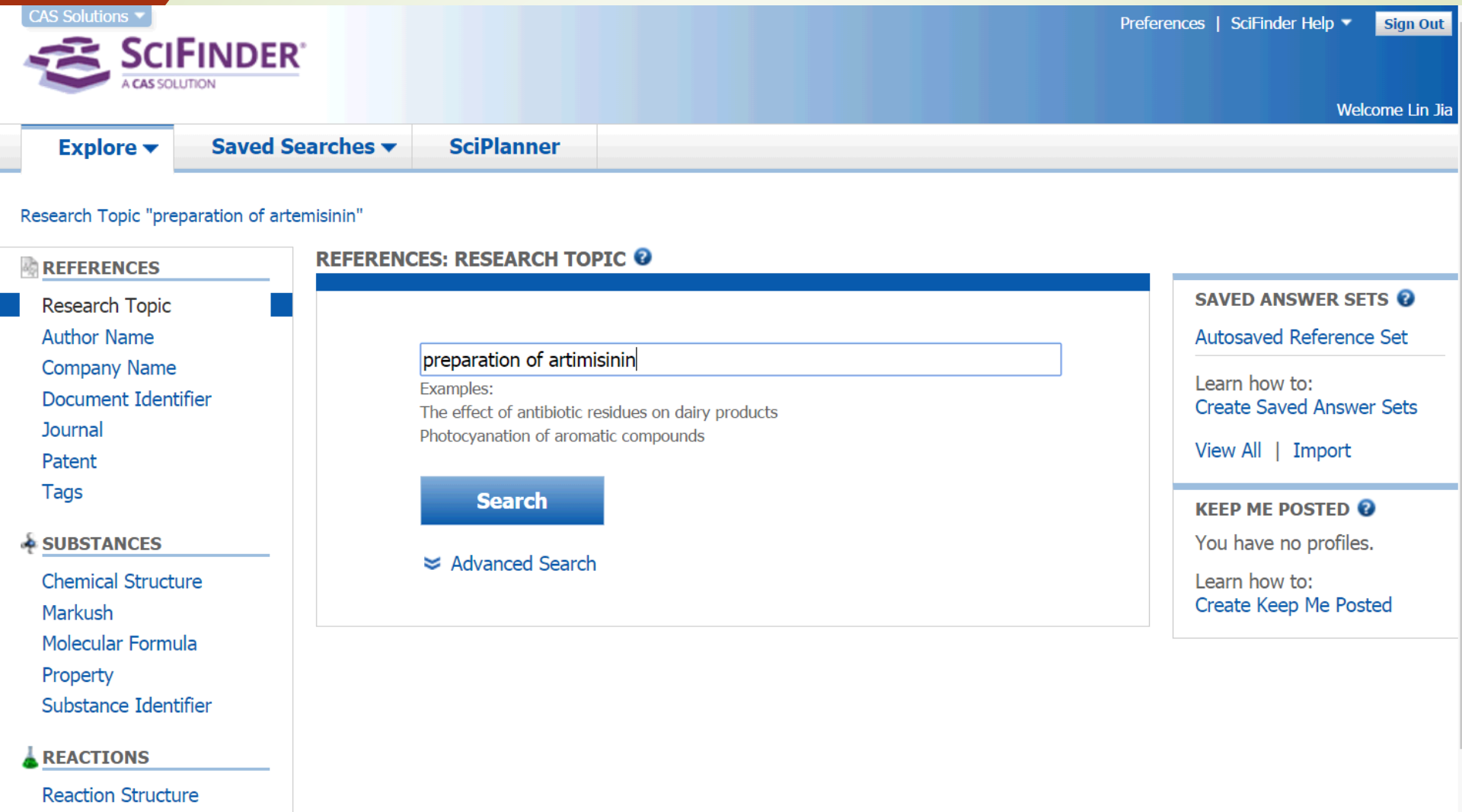
检索方法（Research Topic）



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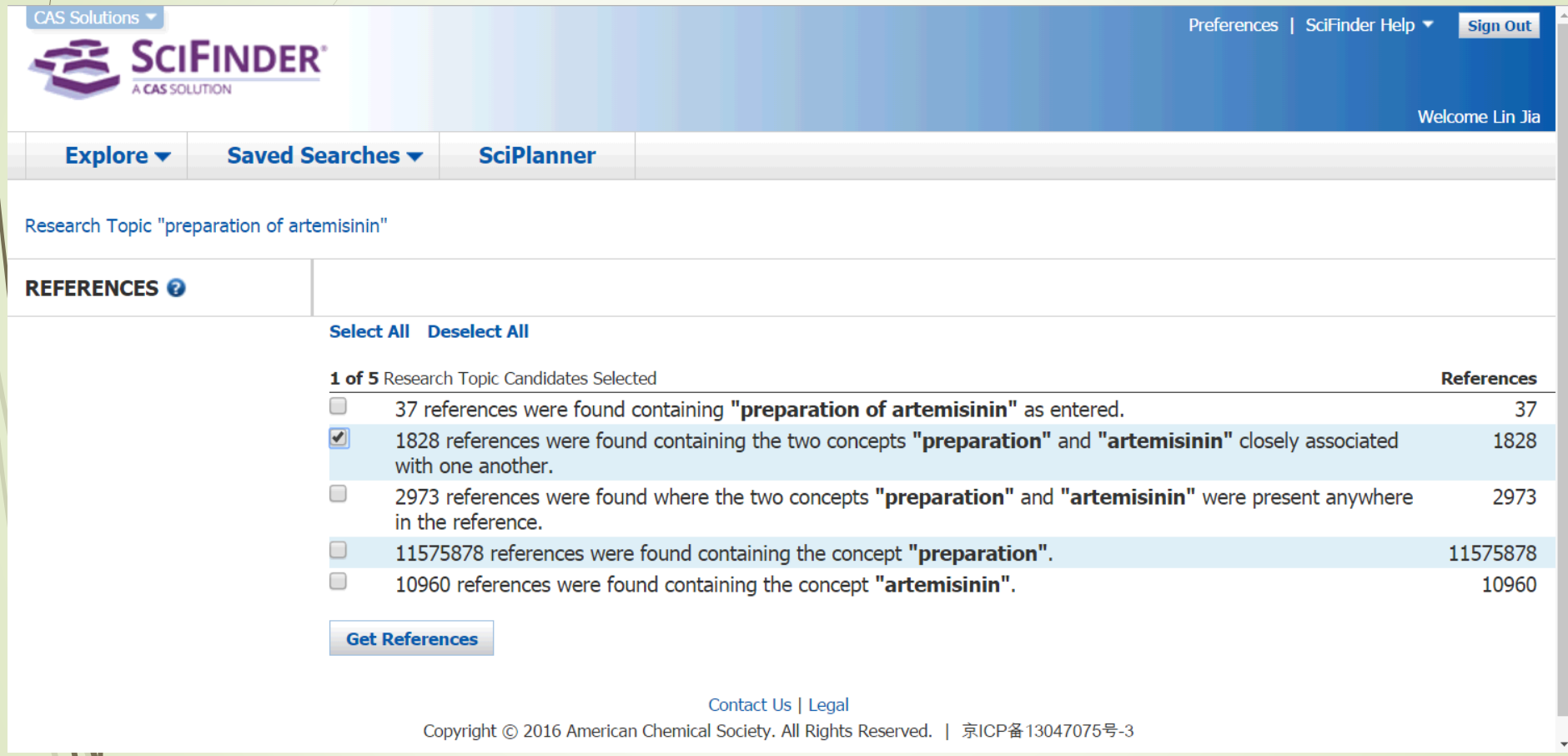
检索方法（Research Topic）



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検索方法（Research Topic）

entering a phrase or sentence in English

- Specify several concepts using plain English.
- Include prepositions and articles to connect the concepts.
- Place acronyms or synonyms in parentheses after the synonymous concept.
- Use "not" or "except" to exclude a particular term.

Note: SciFinder automatically searches related terms and considers alternate spellings and word endings when retrieving results.

检索方法（Research Topic）

- *intramolecular hydroamination of aminoalkenes*
- *reaction kinetics of oxyphosphoranes with alcohols*
- *I am interested in the milk production of cows*

  (检索时系统自动匹配bovines/calf/cattle)
- *human immunodeficiency virus*

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  preparation of artemisinin

- 关于“鸡蛋中大环内酯类抗生素残余物分析”的研究

  Analyses of macrolide antibiotic residues in eggs

- 关于“禽流感病毒”的研究

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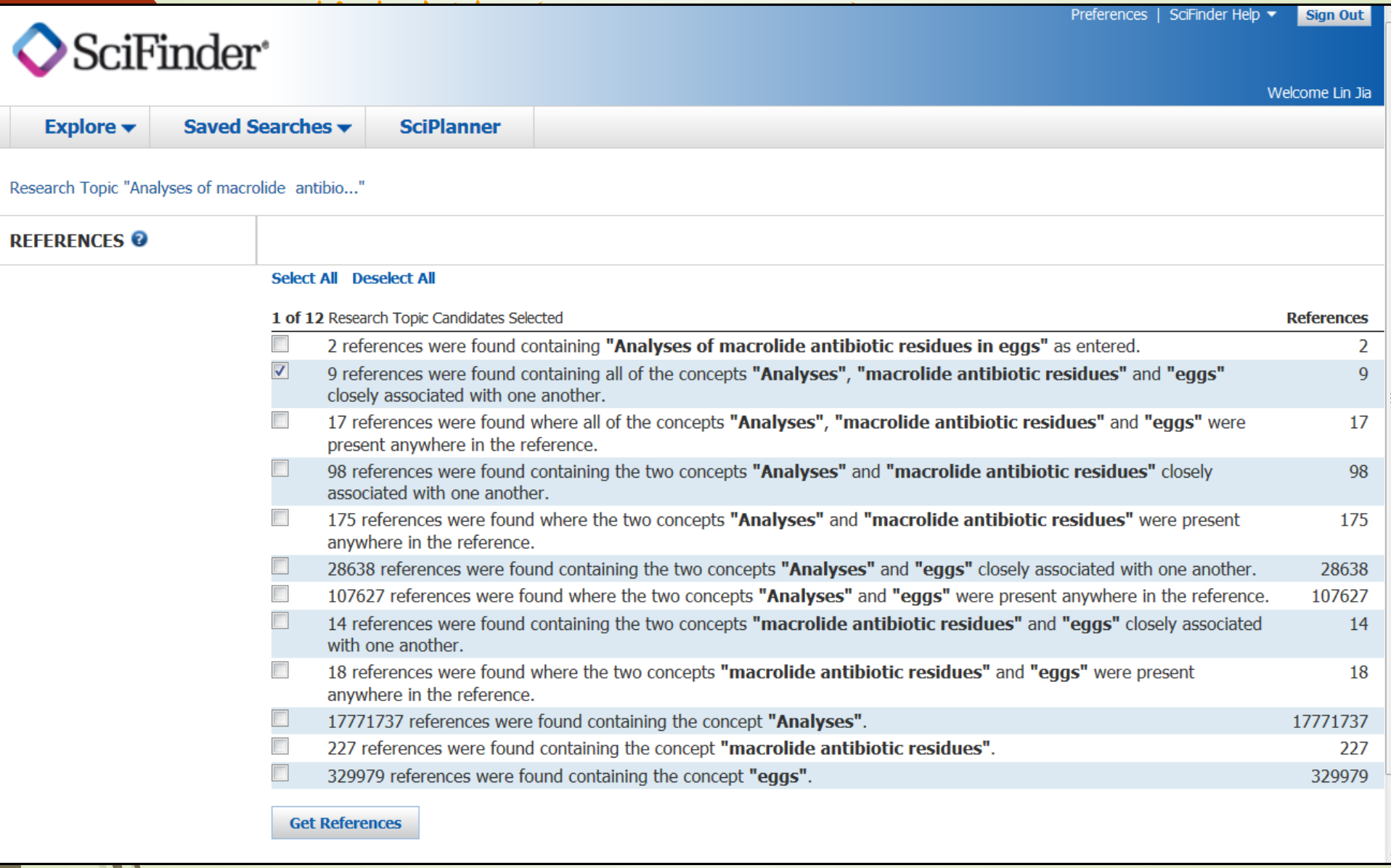
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2 references were found containing "Analyses of macrolide antibiotic residues in eggs" as entered. 2
9 references were found containing all of the concepts "Analyses", "macrolide antibiotic residues" and "eggs" closely associated with one another. 9
17 references were found where all of the concepts "Analyses", "macrolide antibiotic residues" and "eggs" were present anywhere in the reference. 17
98 references were found containing the two concepts "Analyses" and "macrolide antibiotic residues" closely associated with one another. 98
175 references were found where the two concepts "Analyses" and "macrolide antibiotic residues" were present anywhere in the reference. 175
28638 references were found containing the two concepts "Analyses" and "eggs" closely associated with one another. 28638
107627 references were found where the two concepts "Analyses" and "eggs" were present anywhere in the reference. 107627
14 references were found containing the two concepts "macrolide antibiotic residues" and "eggs" closely associated with one another. 14
18 references were found where the two concepts "macrolide antibiotic residues" and "eggs" were present anywhere in the reference. 18
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227 references were found containing the concept "macrolide antibiotic residues". 227
329979 references were found containing the concept "eggs". 329979
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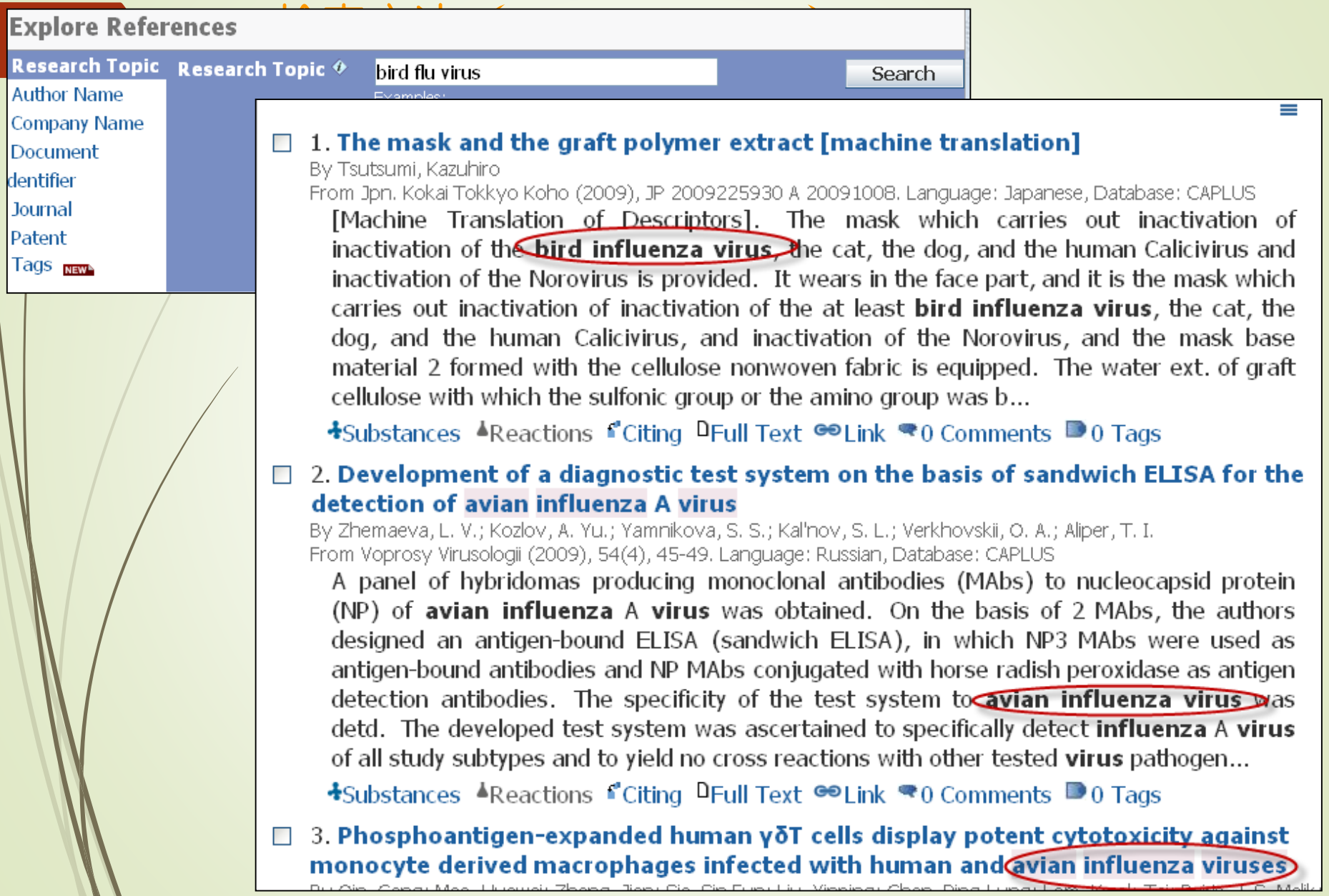
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[Machine Translation of Descriptors]. The mask which carries out inactivation of inactivation of the bird influenza virus, the cat, the dog, and the human Calicivirus and inactivation of the Norovirus is provided. It wears in the face part, and it is the mask which carries out inactivation of inactivation of the at least bird influenza virus, the cat, the dog, and the human Calicivirus, and inactivation of the Norovirus, and the mask base material 2 formed with the cellulose nonwoven fabric is equipped. The water ext. of graft cellulose with which the sulfonic group or the amino group was b...
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2. Development of a diagnostic test system on the basis of sandwich ELISA for the detection of avian influenza A virus
By Zhemaeva, L. V.; Kozlov, A. Yu.; Yamnikova, S. S.; Kal'nov, S. L.; Verkhovskii, O. A.; Aliper, T. I.
From Voprosy Virusologii (2009), 54(4), 45-49. Language: Russian, Database: CAPLUS
A panel of hybridomas producing monoclonal antibodies (MAbs) to nucleocapsid protein (NP) of avian influenza A virus was obtained. On the basis of 2 MAbs, the authors designed an antigen-bound ELISA (sandwich ELISA), in which NP3 MAbs were used as antigen-bound antibodies and NP MAbs conjugated with horse radish peroxidase as antigen detection antibodies. The specificity of the test system to avian influenza virus was detd. The developed test system was ascertained to specifically detect influenza A virus of all study subtypes and to yield no cross reactions with other tested virus pathogen...
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  - (•) on all atoms
- ( ) Similarity

- [ ] Include tautomers
- [ ] Ignore stereo
- [ ] No salts
- [ ] No mixtures
- [ ] No isotopes
- [ ] No charges
- [ ] No radicals
- [ ] No ring closures
- [x] Align results with query

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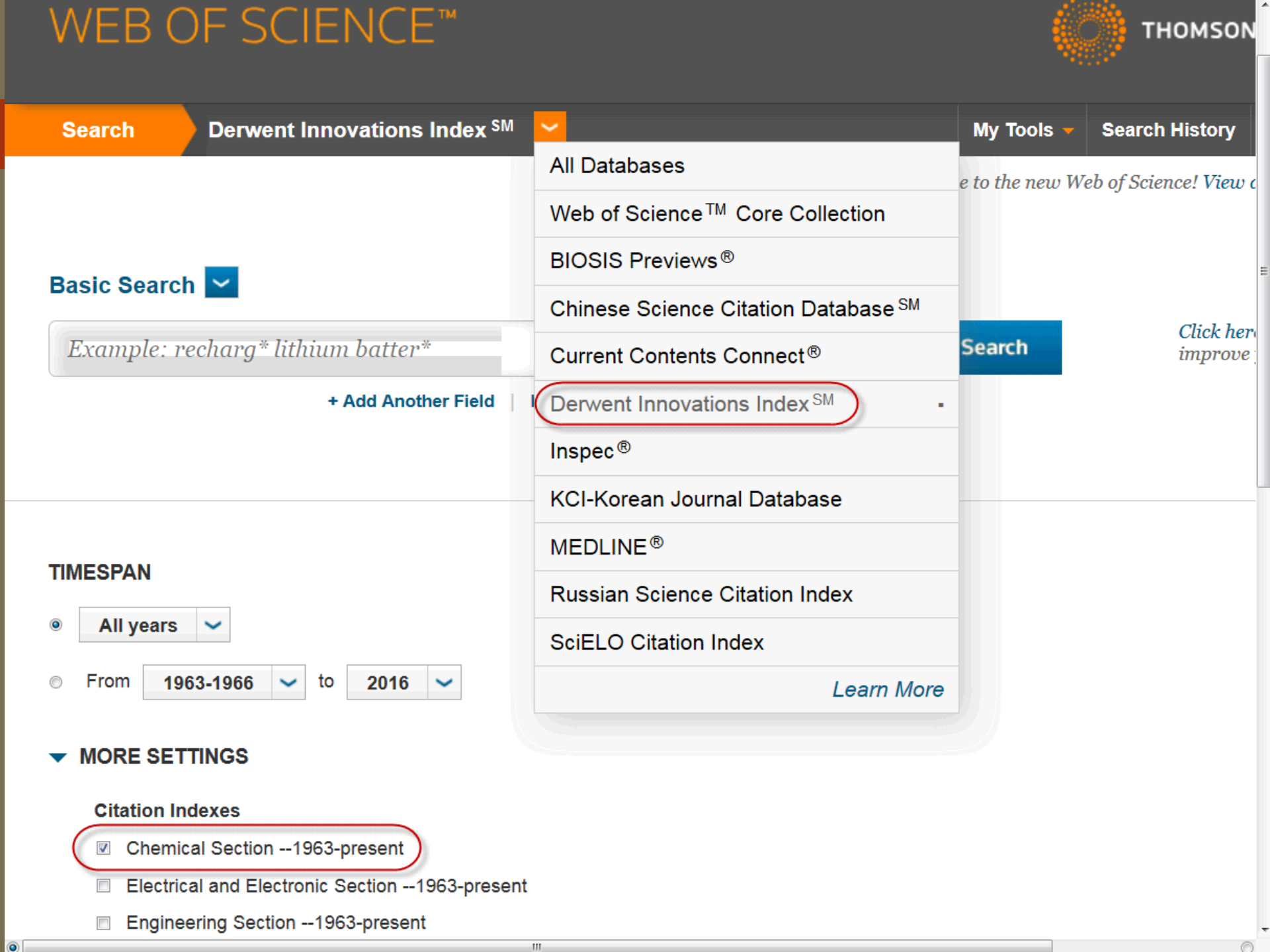
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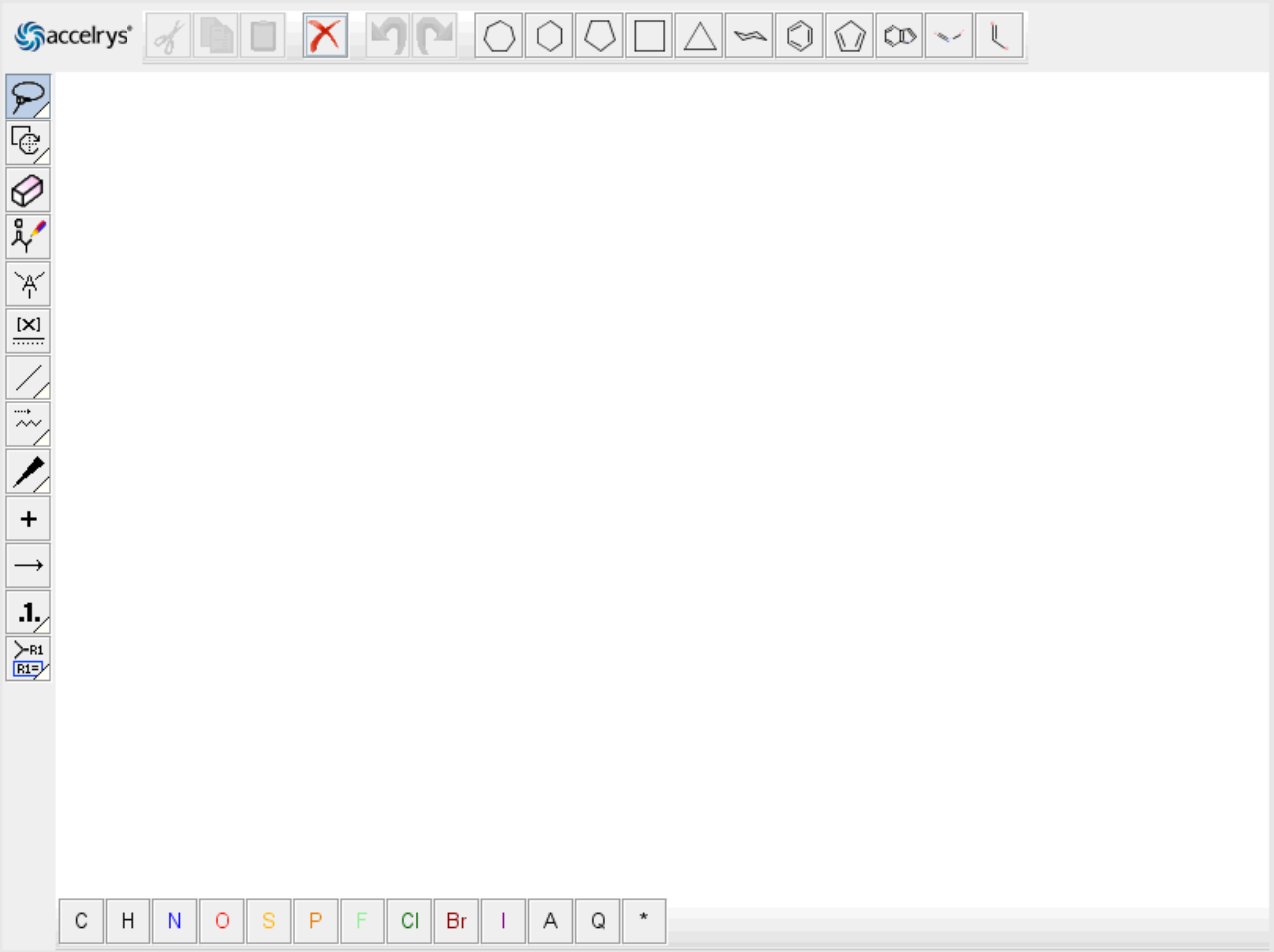

Combine structure and text AND OR

Combine structure and text ◉ AND ○ OR

Compound Name:

◉ Synonyms ○ Systematic ○ Both

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Substance Description: *Select from List*

*Example: ALKALOIDS or PHOSPHAT**

Structure Description:

Example: ISOTOPE LABELLED

Standardized Molecular Formula:

*Example: C2 H8**

Molecular Formula:

Example: C17 H16 N8 O5 S5 . C2 H F3 O2

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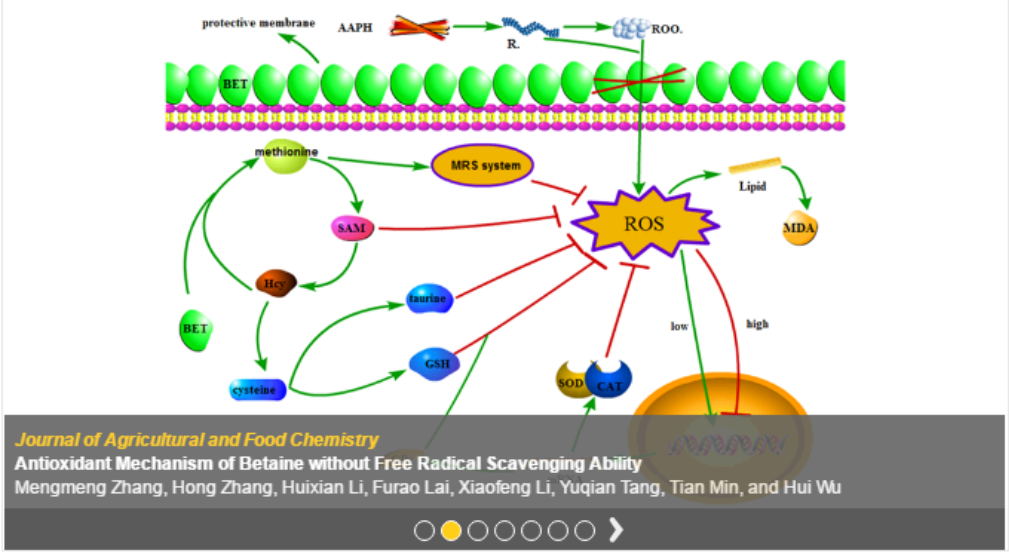

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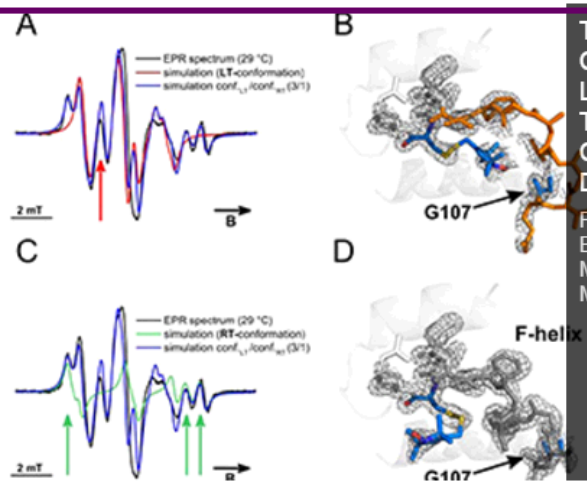

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Philipp Consentius, Ulrich Gohlke, Bernhard Loll, Claudia Alings, Robert Müller, Udo Heinemann, Martin Kaupp, Markus Wahl, and Thomas Risse*

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Observation of Quantum Confinement in Monodisperse Methylammonium Lead Halide Perovskite Nanocrystals Embedded in Mesoporous Silica

Victor Malgras, Satoshi Tominaka, James W. Ryan, Joel Henzie, Toshiaki Takei, Koji Ohara, and Yusuke Yamauchi

Publication Date (Web): September 25, 2016 (Article)

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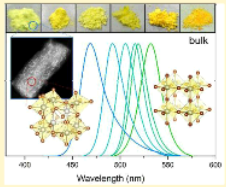
Observation of Quantum Confinement in Monc Methylammonium Lead Halide Perovskite Nanc in Mesoporous Silica

Victor Malgras,[†] Satoshi Tominaka,[†] James W. Ryan,[‡] Joel Henzie,[†] Tos and Yusuke Yamauchi*[,†]

[†]World Premier International (WPI) Research Center for Materials Nanoarchitectonics, N (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan
[‡]International Center for Young Scientists (ICYS), National Institute for Materials Science 305-0044, Japan
[§]Research and Utilization Division, Japan Synchrotron Radiation Research Institute, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan

Supporting Information

ABSTRACT: Hybrid organic–inorganic metal halide perovskites have fascinating electronic properties and have already been implemented in various devices. Although the behavior of bulk metal halide perovskites has been widely studied, the properties of perovskite nanocrystals are less well-understood because synthesizing them is still very challenging, in part because of stability. Here we demonstrate a simple and versatile method to grow monodisperse $CH_3NH_3PbBr_xI_{3-x}$ perovskite nanocrystals inside mesoporous silica templates. The size of the nanocrystal is governed by the pore size of the templates (3.3, 3.7, 4.2, 6.2, and 7.1 nm). In-depth structural analysis shows that the nanocrystals maintain the perovskite crystal structure, but it is slightly distorted. Quantum confinement was observed by tuning the size of the particles via the template. This approach provides an additional route to tune the optical bandgap of the nanocrystal. The level of quantum confinement was modeled taking into account the dimensions of the rod-shaped nanocrystals and their close packing inside the channels of the template. Photoluminescence measurements on CH_3NH_3PbBr clearly show a shift from green to blue as the pore size is decreased. Synthesizing perovskite nanostructures in templates improves their stability and enables tunable electronic properties via quantum confinement. These structures may be useful as reference materials for comparison with other perovskites, or as functional materials in all solid-state light-emitting diodes.



INTRODUCTION

Hybrid organic–inorganic metal halide perovskites exhibit unusual electronic, optical, and crystallographic properties enabling high mobilities[1,2] and long diffusion lengths.[3,4] They are promising candidates for photovoltaic applications and have rapidly achieved outstanding performances.[5−9] The chemical structure obeys the AMX_3 stoichiometry, where A is the organic cation, M is the metal cation (e.g., Pb^{2+}, Sn^{2+}), and X is the halide anion (e.g., Cl^-, Br^-, I^-). The optical bandgap can be tuned by selecting the appropriate A and X components: methylammonium and bromide lead to wider bandgaps than

their size or surface chemistry is useful for various light-emitting applications (e.g., LEDs, lasers). In addition, quantum confinement offers a different angle from which the electronic properties can be studied and manipulated. Many semiconductor nanocrystals display interesting behavior when their radius is less than the exciton Bohr radius, such as bandgap expansion, increased Coulombic attraction of the paired charges, energy level quantization, and slower electron–phonon relaxation.[12−15]

Research on $CH_3NH_3PbX_3$ nanocrystals has been primarily limited to colloidal nanoplatelets[16−19] and nanoparticles,[20−23] through coprecipitation or seeding methods, as well as

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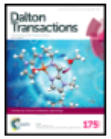

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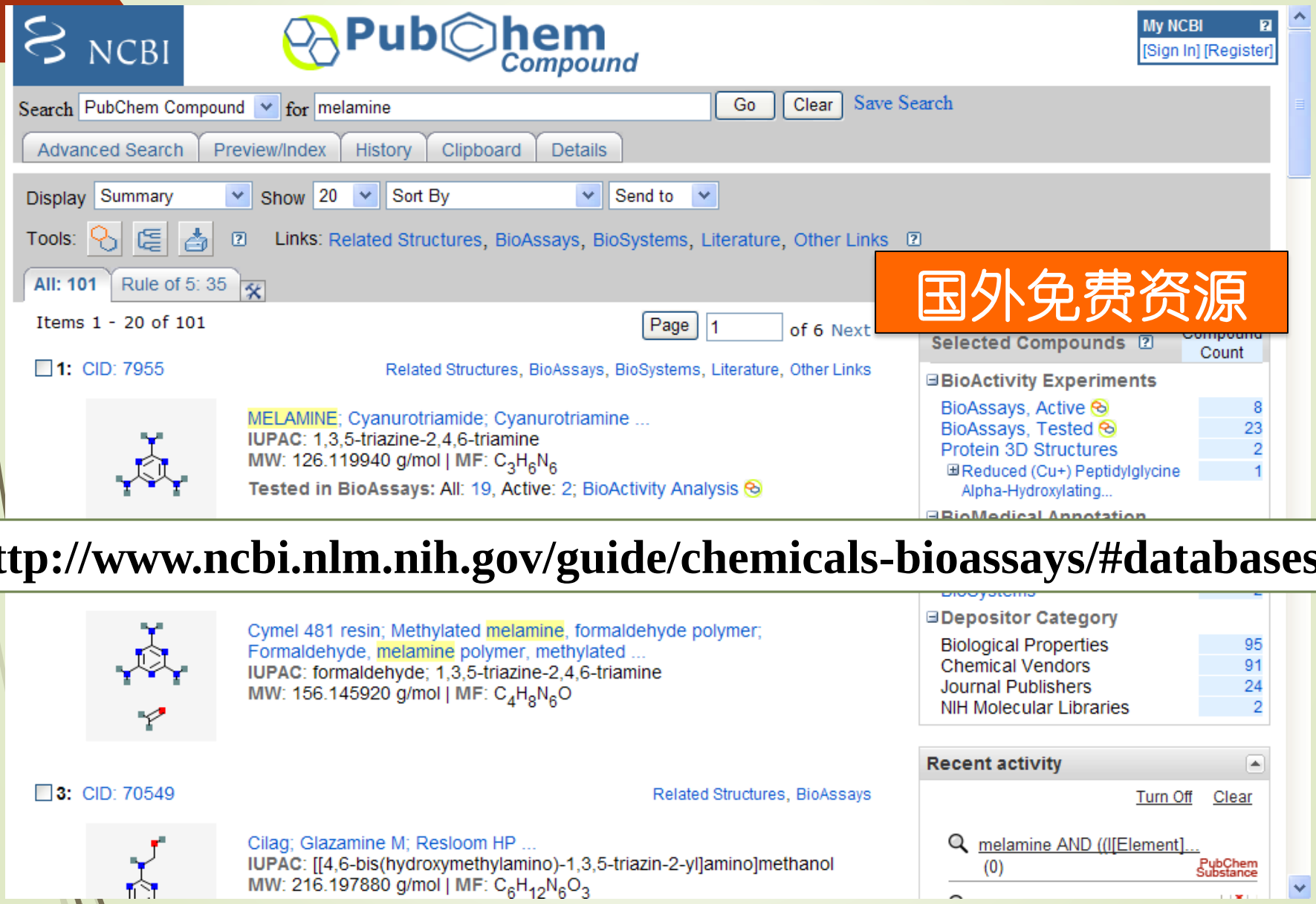

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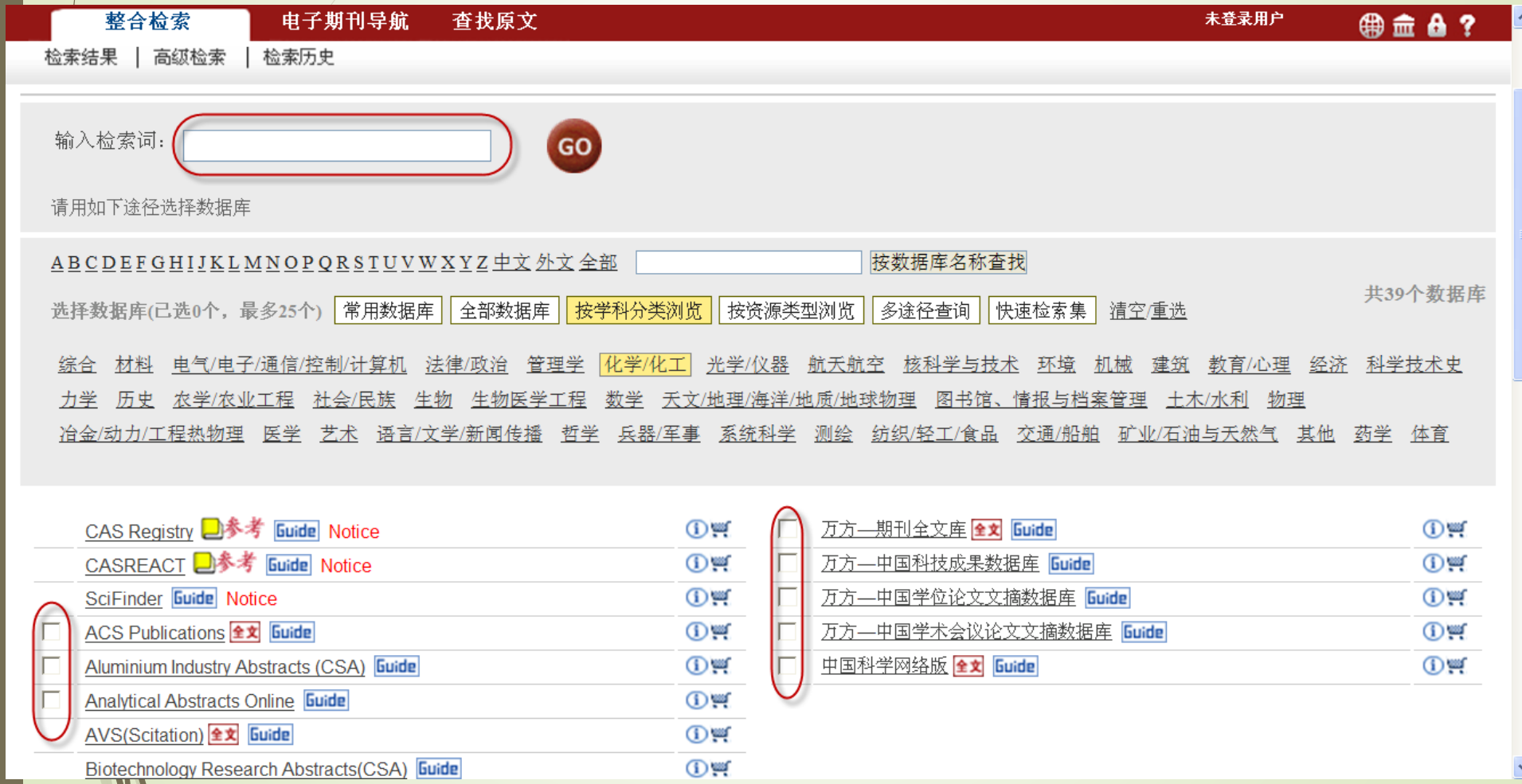

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