化学及相关学科信息资源概述

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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记录内容包含文献基本题录信息和化学特有信息

- **题录信息（基本同其他学科信息资源）**

  标题、责任者、来源、文摘……

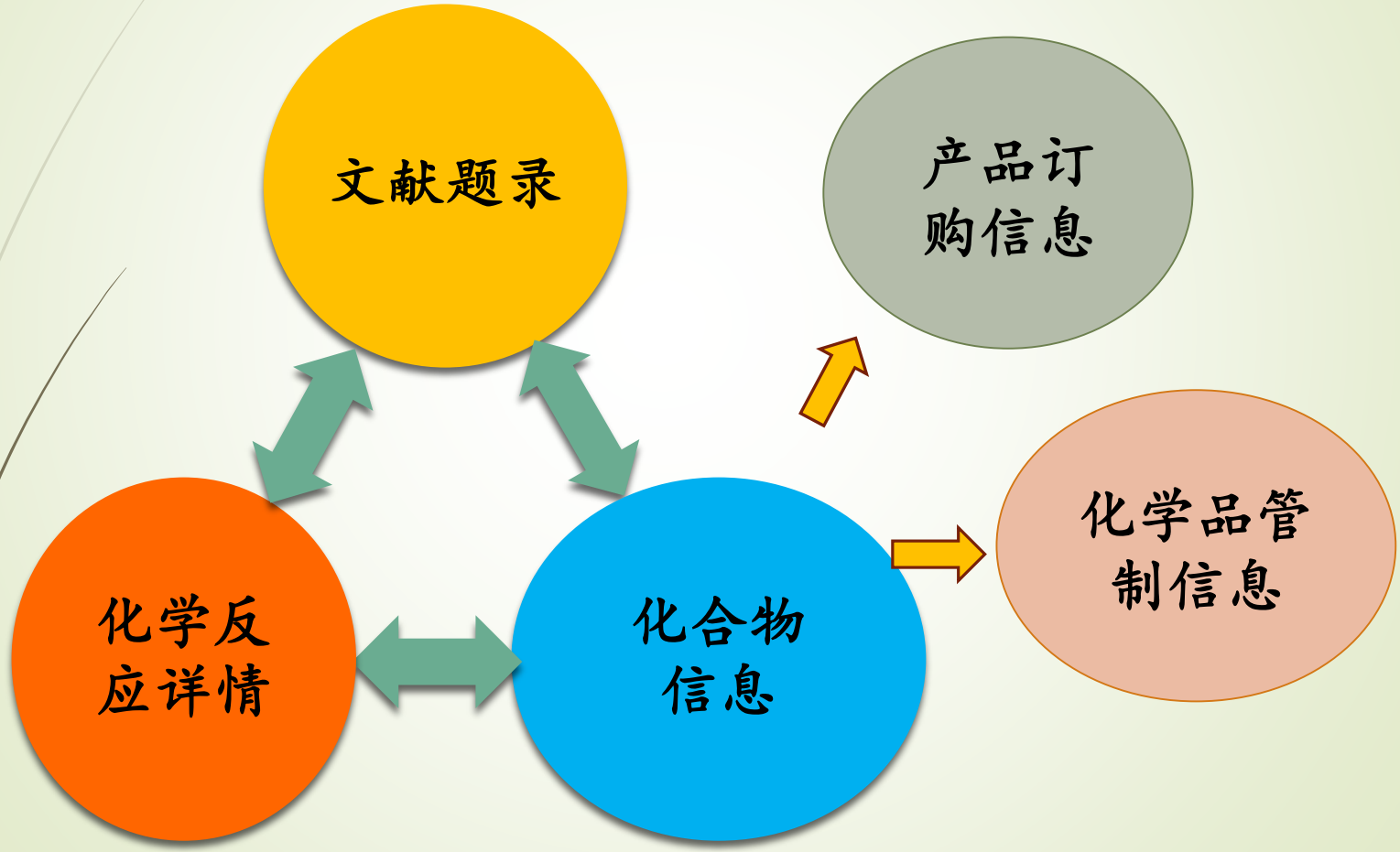
- **反应信息**

  反应式（步骤、条件、中间体、产率……）、反应条件……

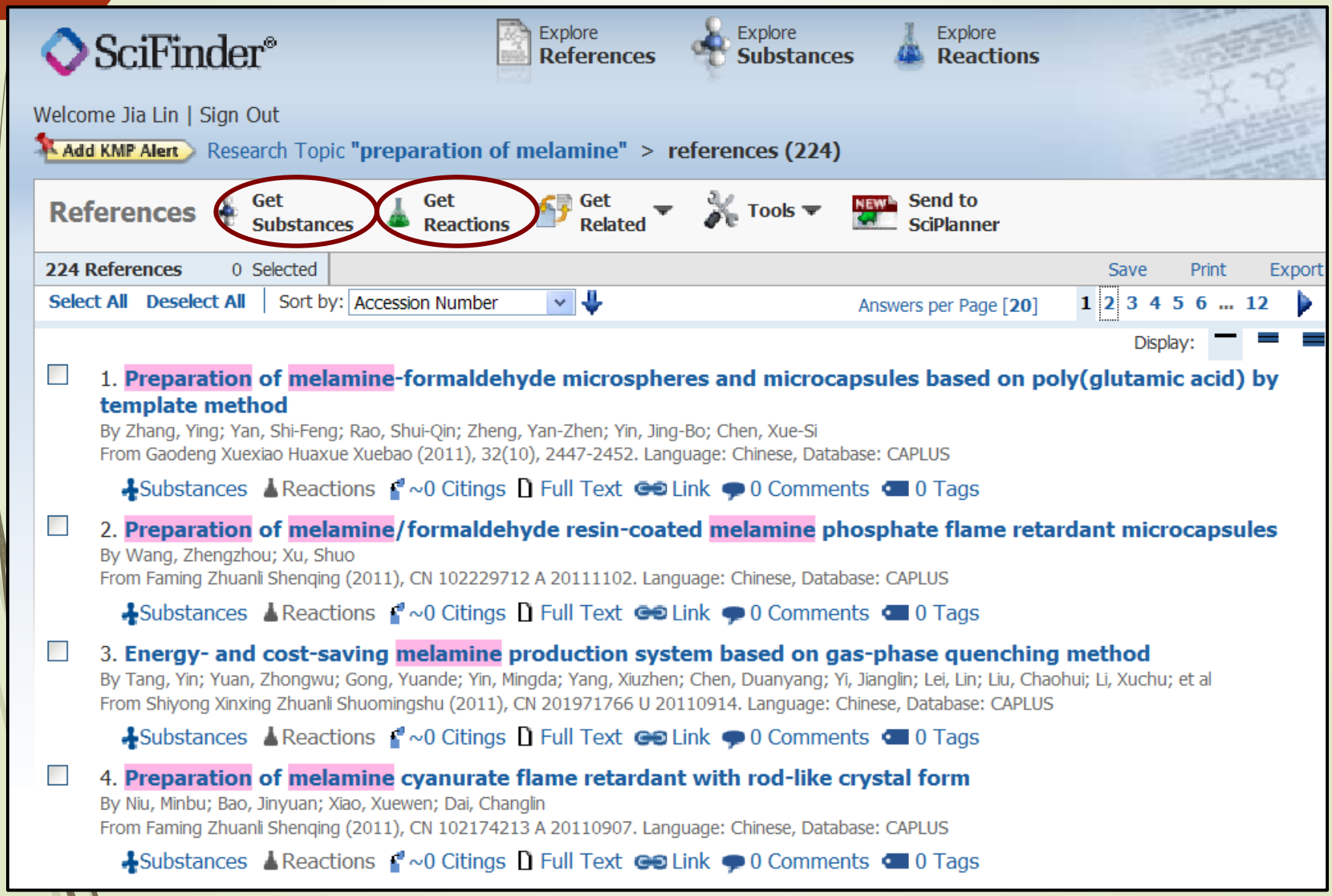
- **化合物信息**

  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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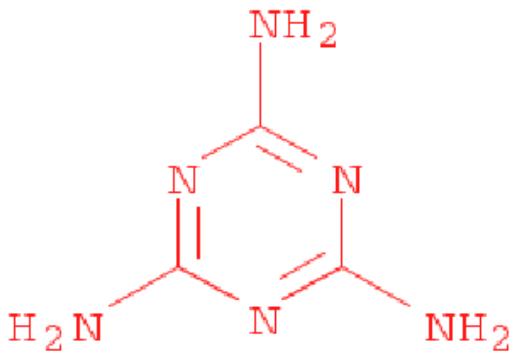
Substances | Get References | Get Reactions | Tools | Send to SciPlanner

31 Substances | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [50]

View:

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

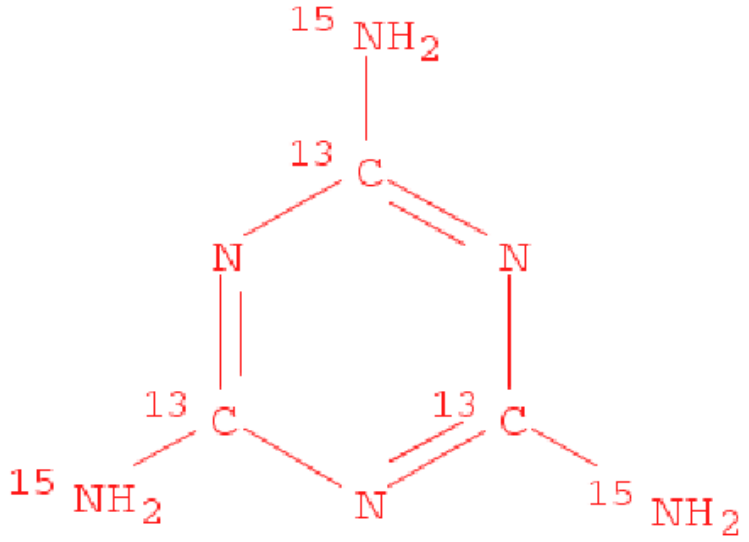


$C_3H_6N_6$

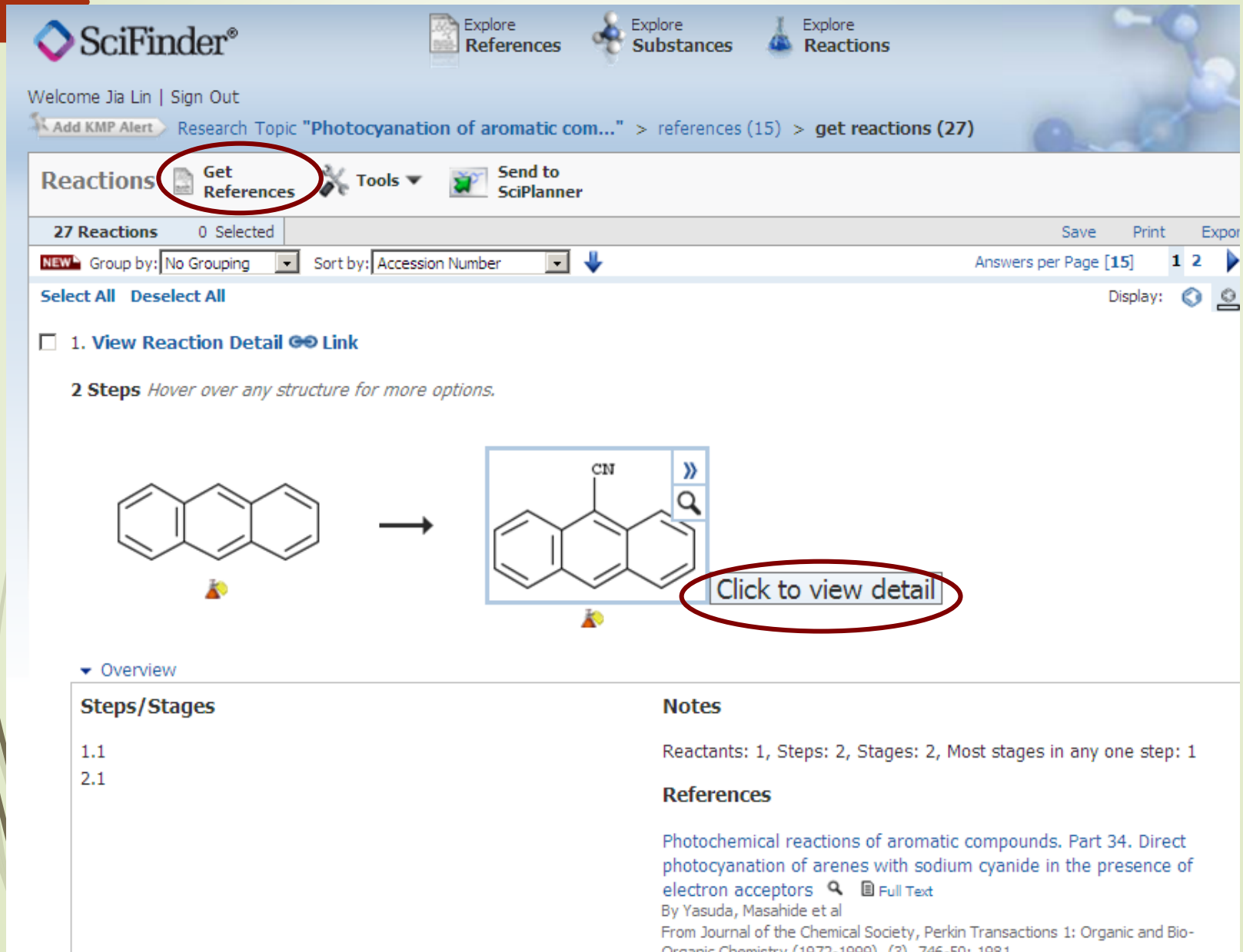
~1 References

Reactions

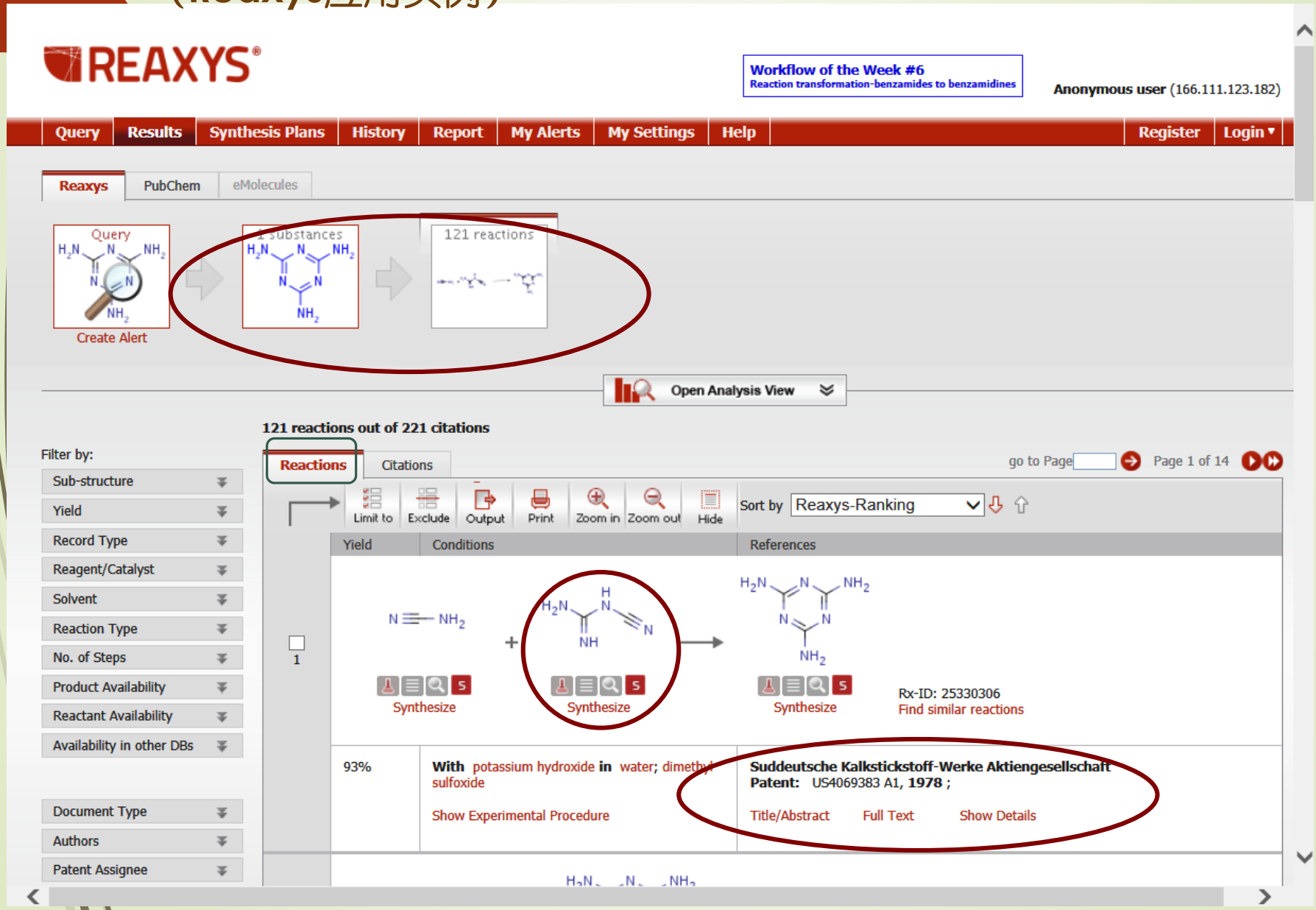
2. **Substance Detail**
   1246816-14-7



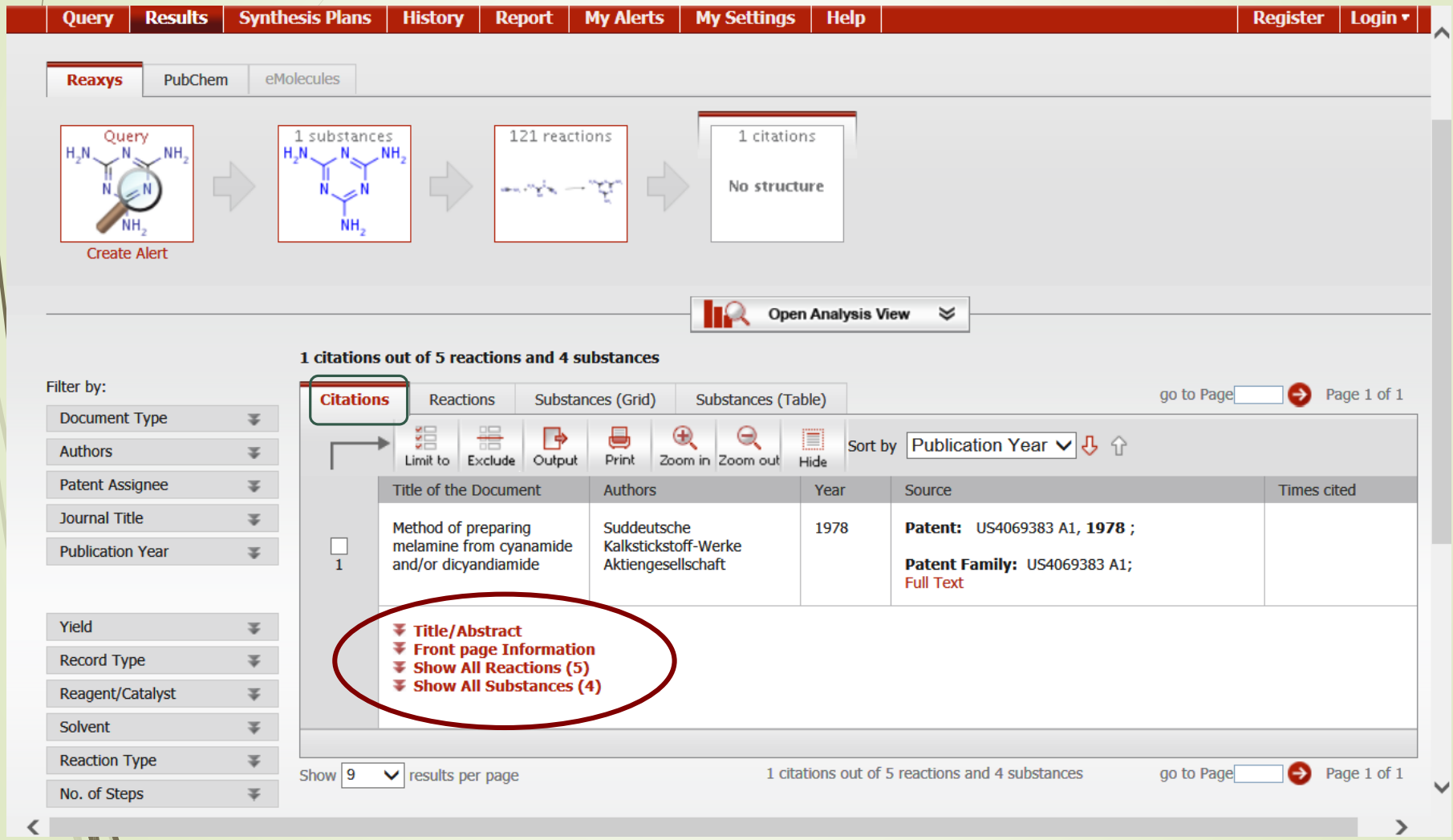
②文献信息、化合物、反应之间无缝链接（SciFinder应用实例）



②文献信息、化合物、反应之间无缝链接（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

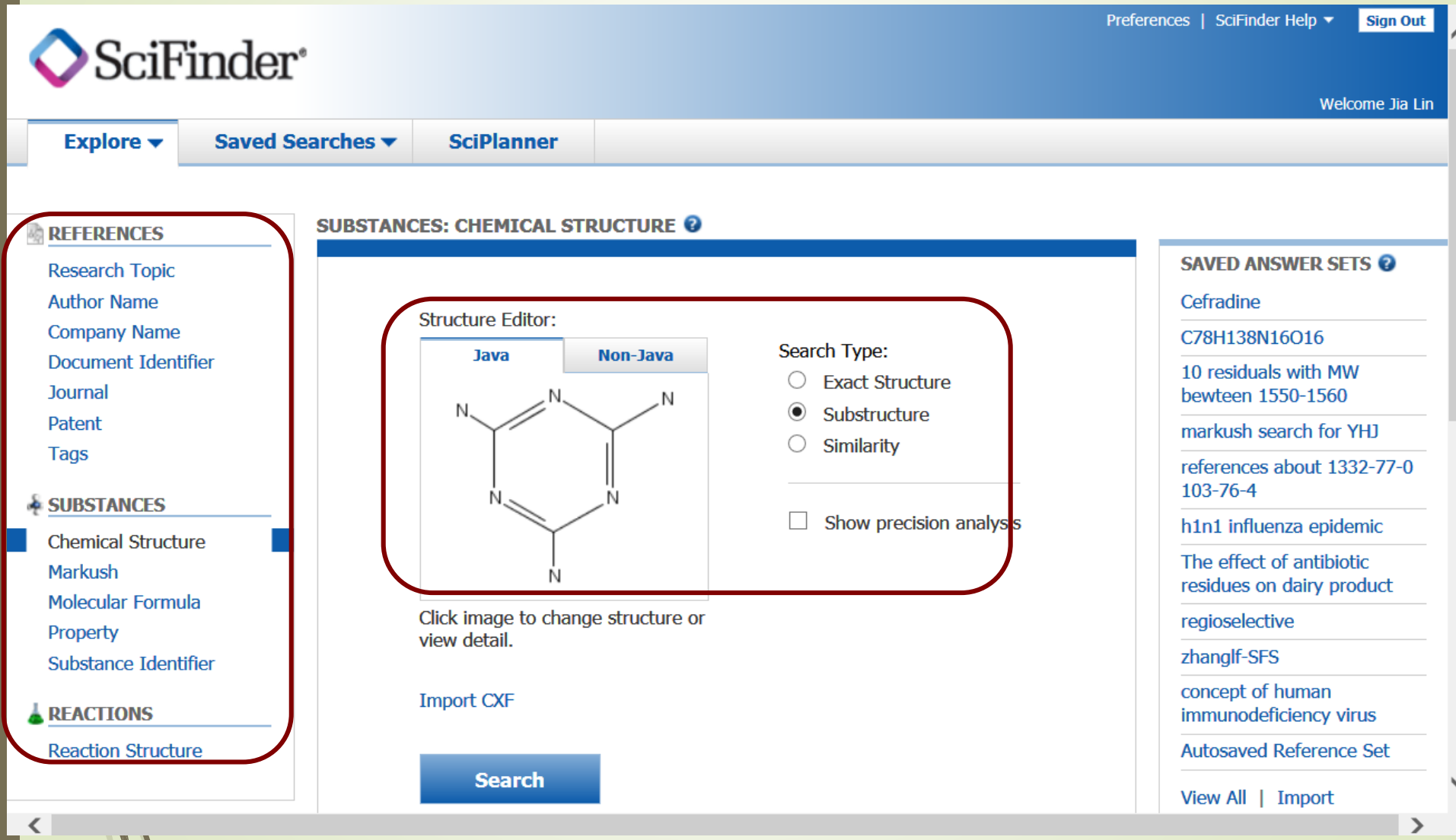
  反应式（完整/部分）、反应条件、产率、反应步骤……

- 化合物信息

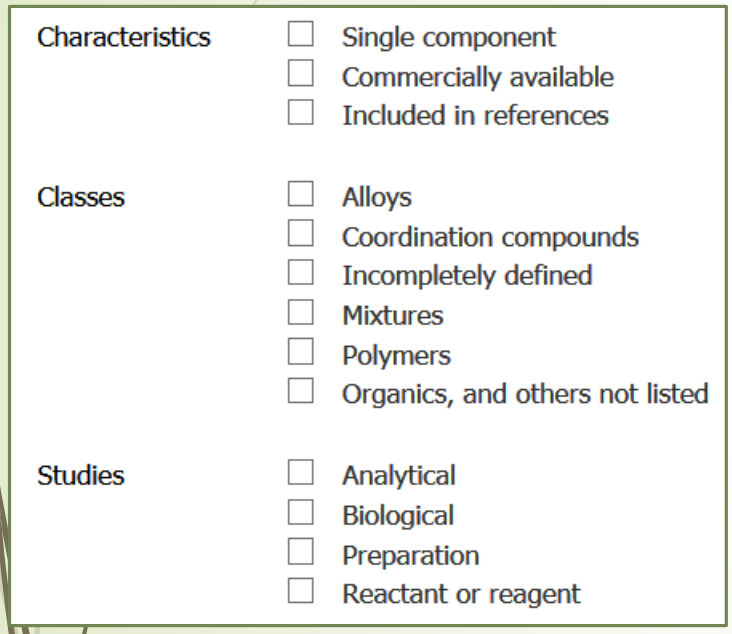
  结构式、名称、代码、物理化学性质

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

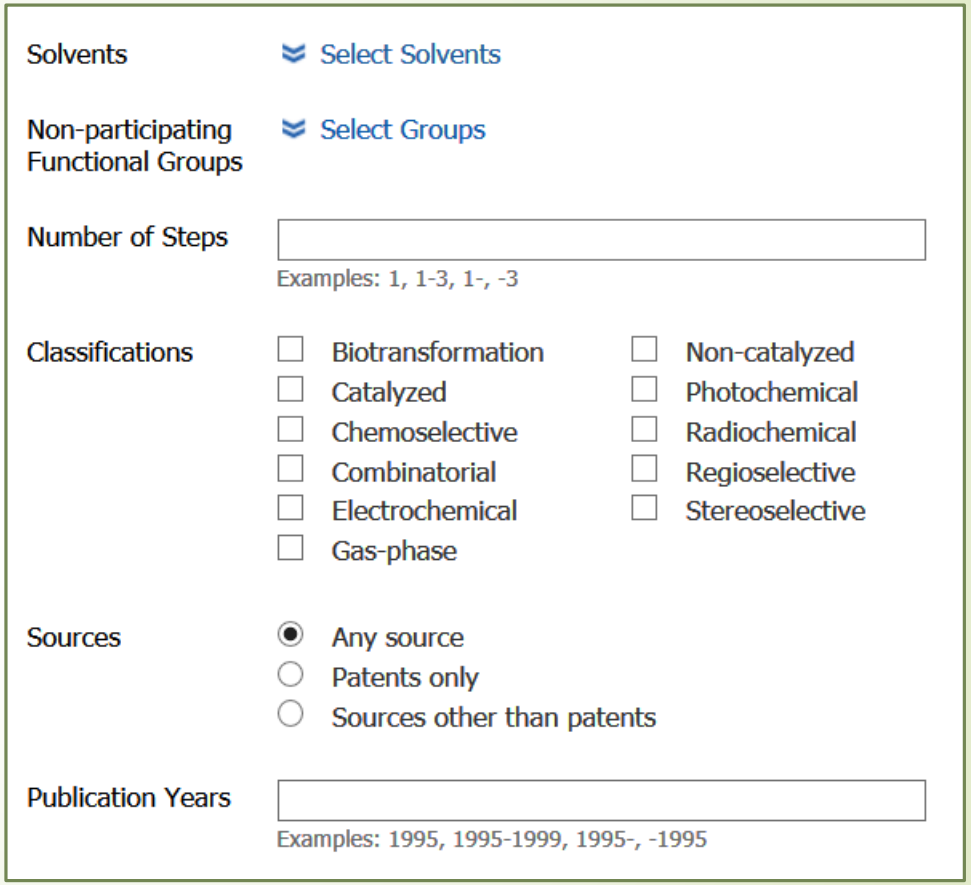
③丰富实用的检索途径、检索字段和检索限定



③丰富实用的检索途径、检索字段和检索限定



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 ——美国化学学会出版物**
- **RSC Publishing——英国皇家化学学会出版物**
- **Knovel-**Chemistry & Chemical Engineering**——交互式参考工具**
- **网络免费资源**
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- 需要注册个人账号（须用……tsinghua.edu.cn邮箱，且在校园网内注册，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）
- **CHEMCATS** (Chemical Suppliers)
- **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	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
	Molecular Formula		
	Markush		
	Property		
	Identifier		
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

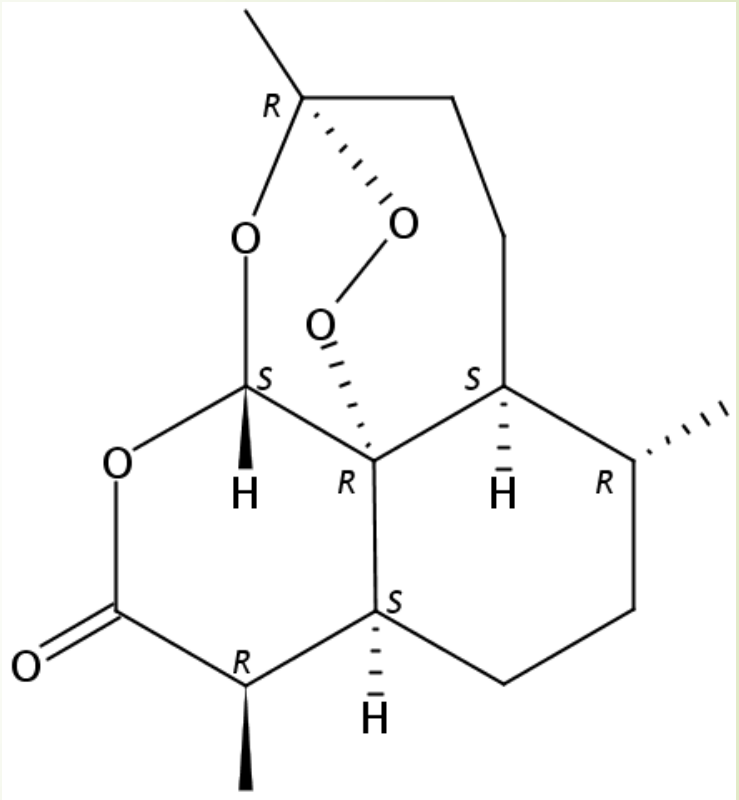
检索实例

2015生理或医学诺奖

屠呦呦

青蒿素

疟疾



关于青蒿素制备的文献

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Substance Identifier "qinghaosu " > substances (1)

SUBSTANCES

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0 of 1 Substance Selected

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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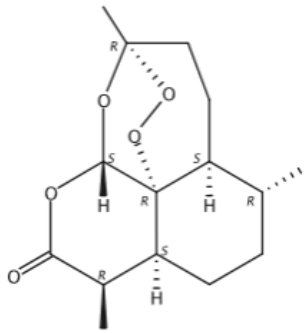
1. 63968-64-9

~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*)-

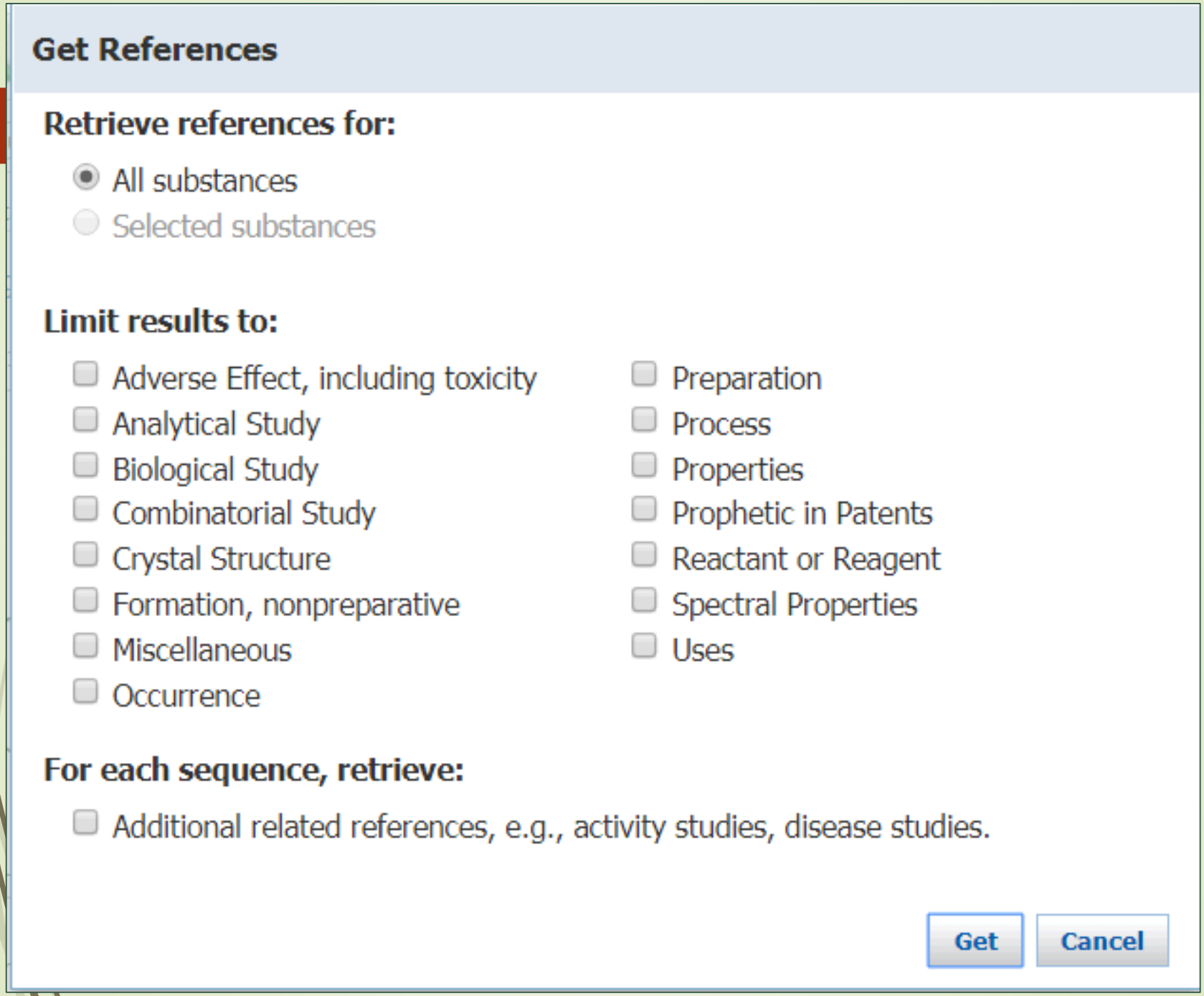
Key Physical Properties

Regulatory Information

Spectra

Experimental Properties

20170928截屏


Get References
Retrieve references for:
All substances
Selected substances
Limit results to:
Adverse Effect, including toxicity
Analytical Study
Biological Study
Combinatorial Study
Crystal Structure
Formation, nonpreparative
Miscellaneous
Occurrence
Preparation
Process
Properties
Prophetic in Patents
Reactant or Reagent
Spectral Properties
Uses
For each sequence, retrieve:
Additional related references, e.g., activity studies, disease studies.
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Substance Identifier "qinghaosu " > substances (1) > get references (6830)

REFERENCES

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Analyze | Refine | Categorize

Analyze by: Author Name

White Nicholas J 97
Tang Kexuan 74
Posner Gary H 73
Dondorp Arjen M 64
Nosten Francois 59
Haynes Richard K 57
Avery Mitchell A 51
Meunier Bernard 49
O Neill Paul M 45
Robert Anne 43

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0 of 6830 References Selected

Page: 1 of 342

1. **Chinese medicine product for treatment of goose teniasis and preparation method thereof**

Quick View PATENTPAK

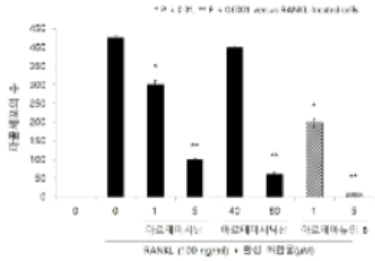
By Wang, Yanlin; Wang, Yanbao; Gao, Yue
From Faming Zhuanli Shenqing (2017), CN 107137620 A 20170908. | Language: Chinese, Database: CAPLUS

The title Chinese medicine product comprises (by wt. parts): Coptis chinensis root 25-45, Pharbitis nil seed 25-50, artemisinin 40-60, Eucalyptus robusta 10-25, Phragmites communis root 10-20, Areca catechu 15-25, Omphalia lapidescens 5-10, Ligusticum chuanxiong 5-12, Gleditsia sinensis 4-9, Zanthoxylum schinifolium 5-9, Morus alba leaf 2-5, chopped garlic 6-9, and pumpkin 8-11. The present invention is made up of pure natural Chinese herbal medicines, has advantages of low price, no side effect, no drug residue, and scientific compatibility, has effects of killing insect, eliminating stagnat...

2. **Pharmaceutical composition including artemisinin B as active ingredient for preventing and treating bone disease**

Quick View PATENTPAK

By Jung, Won Yun; Park, Gwang Gyun; Lee, Seon Gyeong; Kim, Hyeong Geun
From Repub. Korea (2017), KR 1770523 B1 20170823. | Language: Korean, Database: CAPLUS



The present invention relates to a pharmaceutical compn. including artemisinin B as an active ingredient for preventing and treating bone disease. The pharmaceutical compns. including the artemisinin B of the present invention has less side effects and toxicity, since it exhibits a remarkable effect of inhibiting osteoclast formation than artemisinin, another major component of mushroom, it is expected to be widely used in medicine.

3. **Treatment for protozoa borne illness by tinidazole dissolving biofilm in combination with anti-protozoal such as coartem, atovaquone and mefloquine, and Artemisia deriv.**

Quick View PATENTPAK

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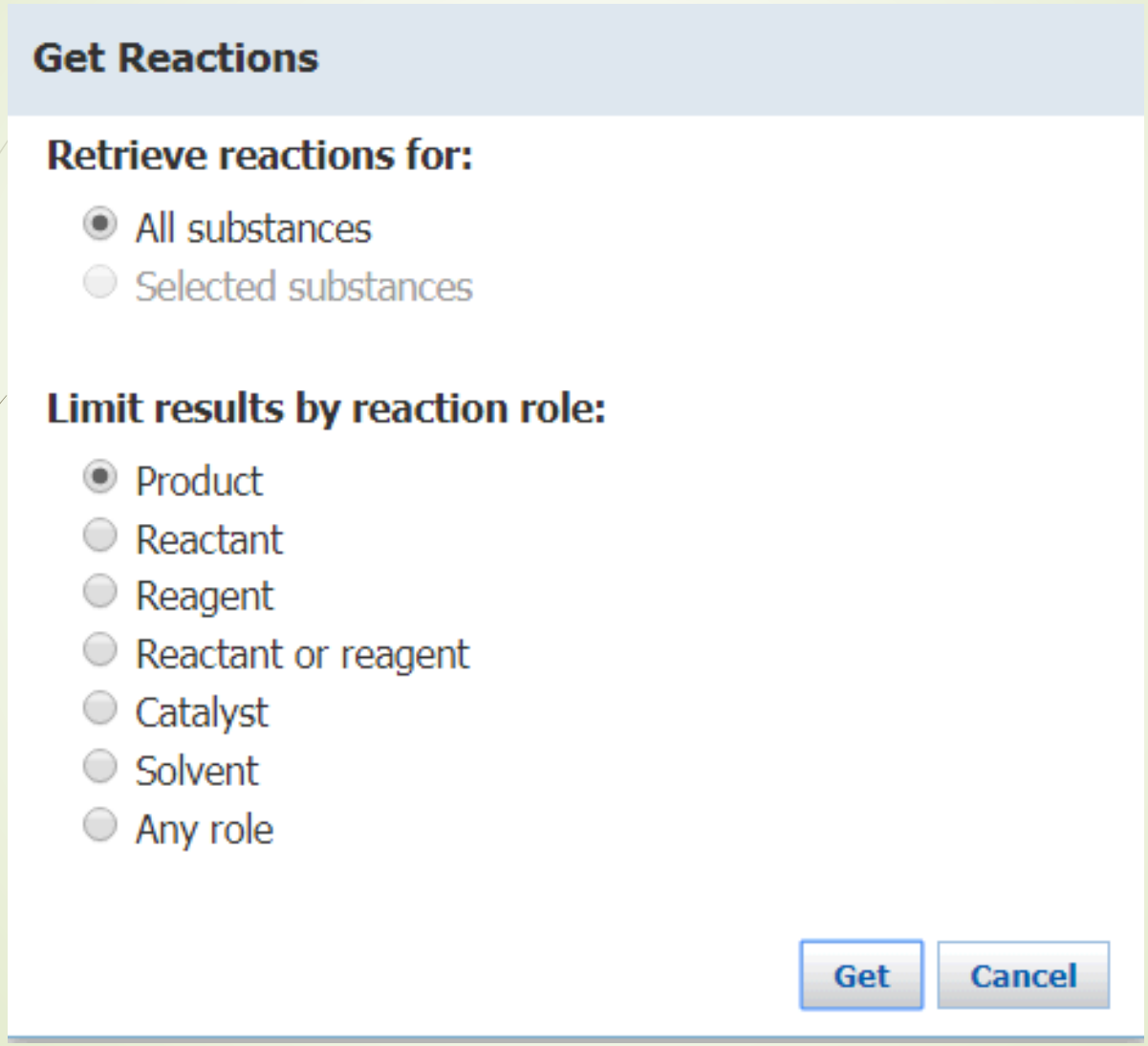
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Retrieve reactions for:
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Selected substances
Limit results by reaction role:
Product
Reactant
Reagent
Reactant or reagent
Catalyst
Solvent
Any role
Get
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Substance Identifier "qinghaosu " > substances (1) > **get reactions (540)**

REACTIONS | Get References | Tools | Send to SciPlanner

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Group by: No Grouping | Sort by: Accession Number | Display Options

0 of 540 Reactions Selected | Page: 1 of 36

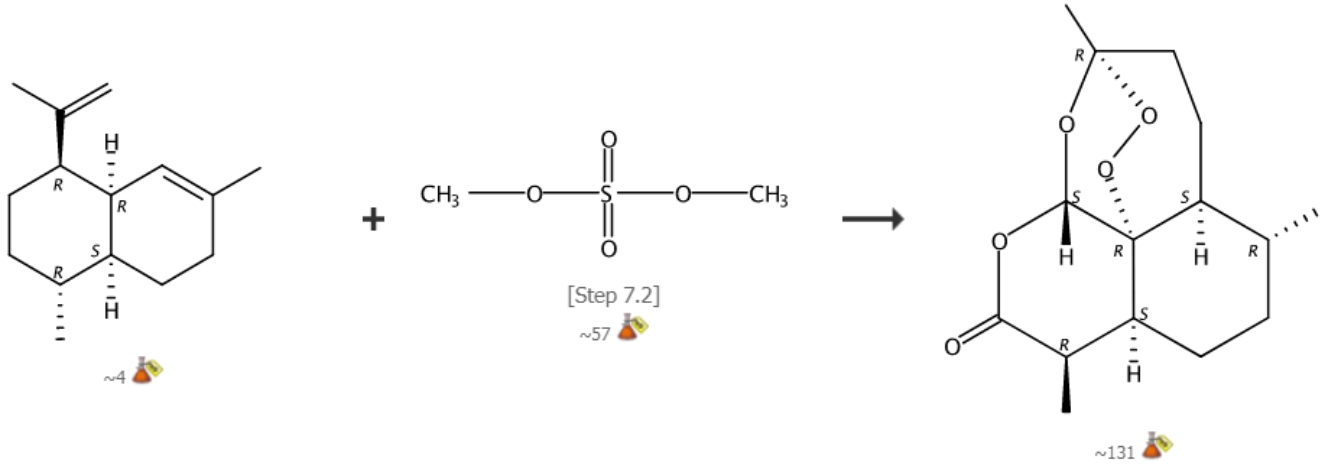
Analyze by: Reagent

O_2	304
H_2O_2	291
HCl	144
Et_3N	140
NaOH	128
$NaIO_4$	125
$NaHCO_3$	95
$PhI(OAc)_2$	70
NaH_2PO_4	67
C_5H_5N	66

Show More

1. **View Reaction Detail Link**

8 Steps *Hover over any structure for more options.*



Overview

Steps/Stages

1.1 C:HCO_2H, 25°C → 30°C
1.2 R:H_2O_2, S:H_2O, 12 h, 30°C; 25 h, 30-34°C; 34°C → 10°C
1.3 R:NaOH, S:H_2O, 5-10°C, pH 7-8
2.1 R:Isocyanuric chloride, S:Cyclohexane, 30 min, 25-30°C; 6-7 h, 25-30°C; 30°C → -5°C; 1 h, -5°C
3.1 R:K_2HPO_4, R:KBr, S:DMSO, 25°C → 85°C; 40-45 h, 80-85°C
3.2 S:H_2O
4.1 R:H_2NSO_3H, R:NaOClO, S:H_2O, S:Me_2CHOH, 3.5 h, 0-5°C, pH 3.7; 1 h, 0-5°C

Notes

1) optimization study, optimized on solvent, optimized on catalyst, optimized on reagent, optimized on temperature, regioselective, 2) optimization study, optimized on reagent, optimized on solvent, optimized on temperature, 3) optimization study, optimized on base, optimized on reagent, optimized on solvent, optimized on temperature, 5) stereoselective, 8) Indion resin used (stage 3), Reactants: 2, Reagents: 14, Catalysts: 2, Solvents: 8, Steps: 8, Stages: 21, Most stages in any one step: 4

References

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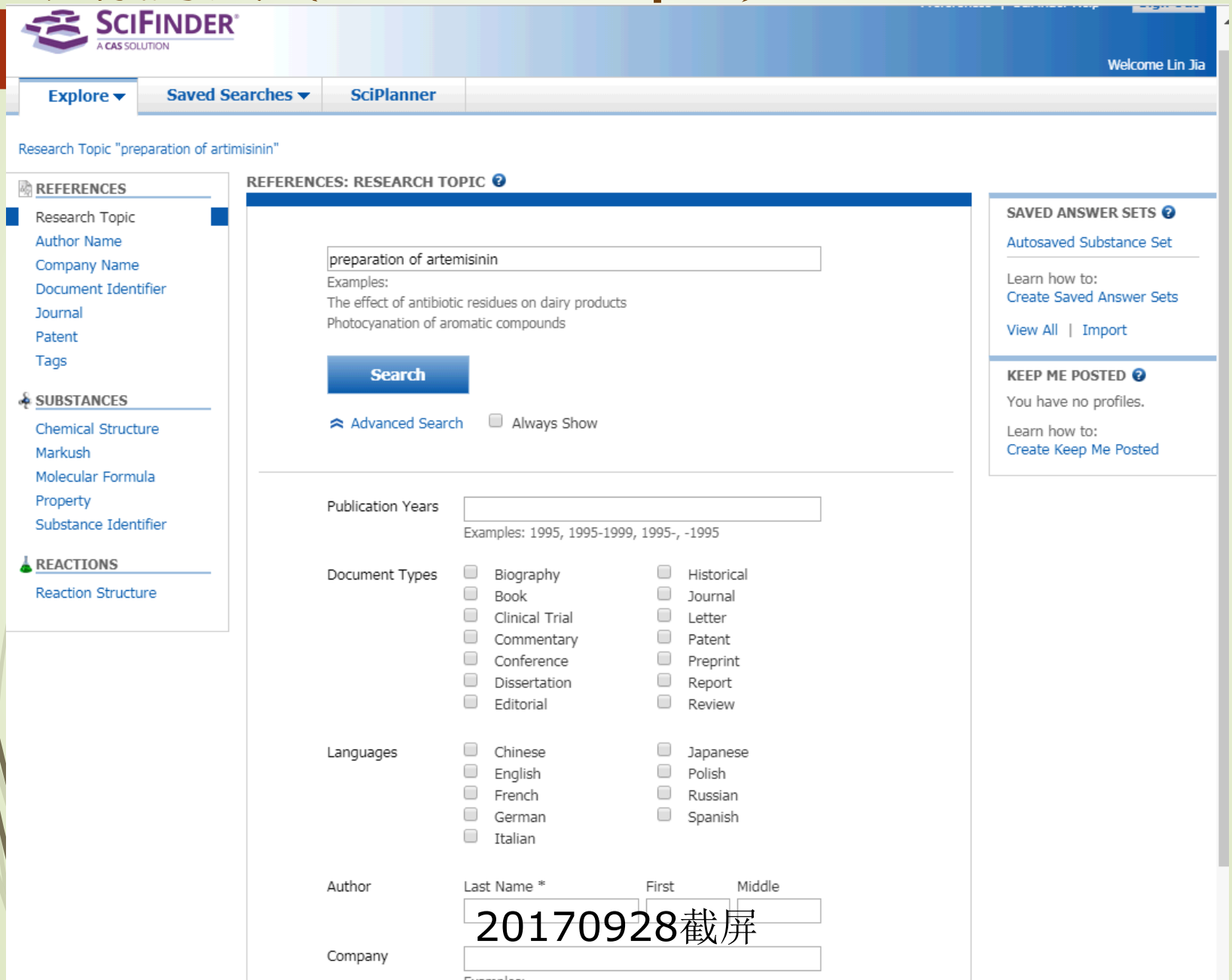
检索方法（Research Topic）



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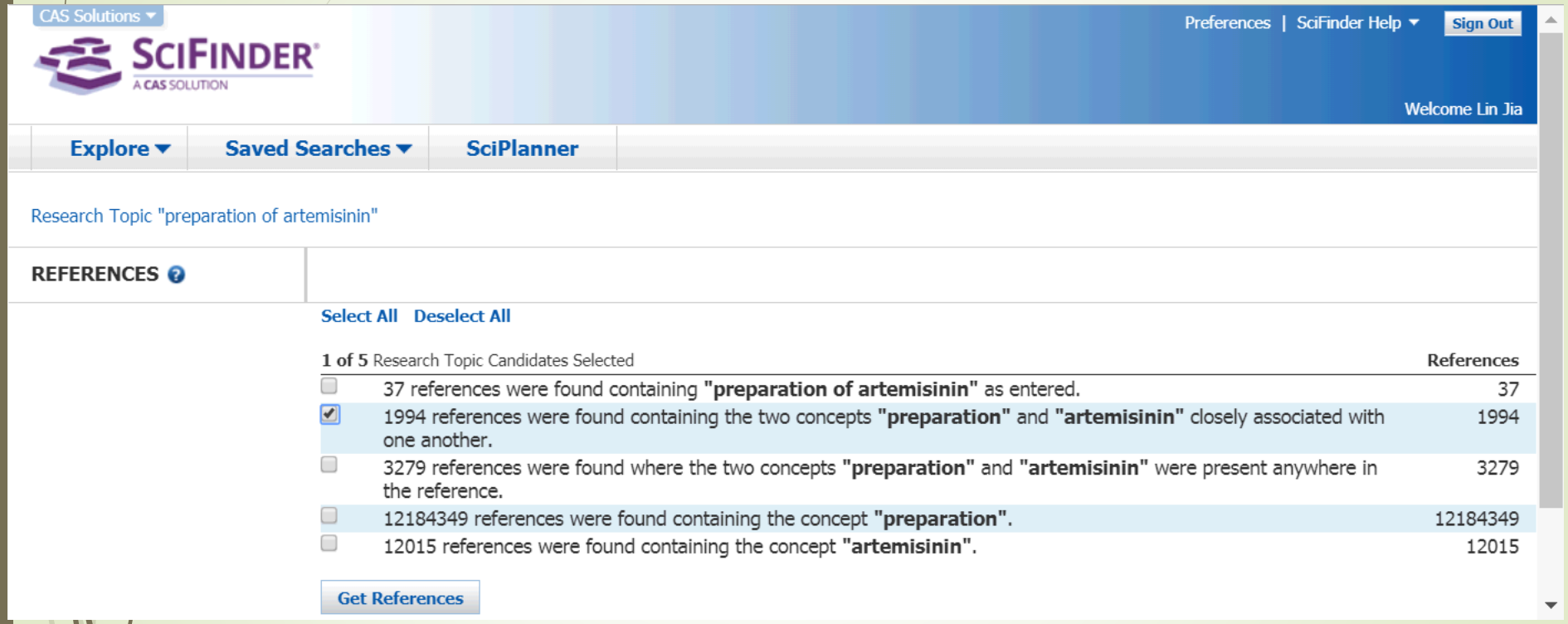
检索方法（Research Topic）



20170928截屏

37. **The interaction of heme with plakortin and a synthetic endoperoxide analogue: new insights into the heme-activated antimalarial mechanism**

Quick View Other Sources

By Persico, Marco; Fattorusso, Roberto; Taglialatela-Scafati, Orazio; Chianese, Giuseppina; de Paola, Ivan; Zaccaro, Laura; Rondinelli, Francesca; Lombardo, Marco; Quintavalla, Arianna; Trombini, Claudio; et al
From Scientific Reports (2017), 7, 45485. | Language: English, Database: CAPLUS

In the present work we performed a combined exptl. and computational study on the interaction of the natural antimalarial endoperoxide plakortin and its **synthetic** analog 4a with heme. Obtained results indicate that the studied compds. produce reactive carbon radical species after being reductively activated by heme. In particular, similarly to **artemisinin**, the formation of radicals prone to inter-mol. reactions should represent the key event responsible for Plasmodium death. To our knowledge this is the first exptl. investigation on the reductive activation of simple antimalarial endoperoxi...

38. **Synthesis of Qinghaosu Analogues from Dihydroqinghao Aldehyde: A Dark Singlet Oxygen Approach**

Quick View Other Sources

By Liu, Xunshen; Chen, Huijun; Xu, Zejun; Wu, Yikang; Liu, Bo
From Chinese Journal of Chemistry (2017), 35(4), 465-476. | Language: English, Database: CAPLUS

A range of **qinghaosu** (**artemisinin**) analogs were **synthesized** from modified dihydroqinghao acid/aldehyde using dark singlet oxygen to trigger off the key step of the trioxane formation. The newly accessed 1,2,4-trioxanes featured a side chain extended from the carbon corresponding to the lactone carbonyl group of **qinghaosu** through a stable carbon-carbon single bond instead of an acetal oxygen-carbon bond in most similar analogs in the literature. Biotin and various amines were also connected to the **qinghaosu** core, resp., through such a linear tether in efforts to develop hybrids and potentiall...

39. **Cancer combination therapies with artemisinin-type drugs**

Quick View Other Sources

By Efferth, Thomas
From Biochemical Pharmacology (Amsterdam, Netherlands) (2017), 139, 56-70. | Language: English, Database: CAPLUS

Artemisia annua L. is a Chinese medicinal plant, which is used throughout Asia and Africa as tea or press juice to treat malaria. The bioactivity of its chem. constituent, **artemisinin** is, however, much broader. We and others found that **artemisinin** and its derivs. also exert profound activity against tumor cells in vitro and in vivo. Should **artemisinin**-type drugs be applied routinely in clin. oncol. in the future, then it should probably be as part of combination therapy regimens rather than as monotherapy. In the present review, I give a comprehensive overview on synergistic and additive e...

40. **AaMYB1 and its orthologue AtMYB61 affect terpene metabolism and trichome development in Artemisia annua and Arabidopsis thaliana**

Quick Vi... Other Sources

Yang, Ke; Tang, Kexuan; ...

20170928截屏

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*

  (检索时系统自动匹配HIV)

检索方法（Research Topic）——实例

- 关于青蒿素制备方法

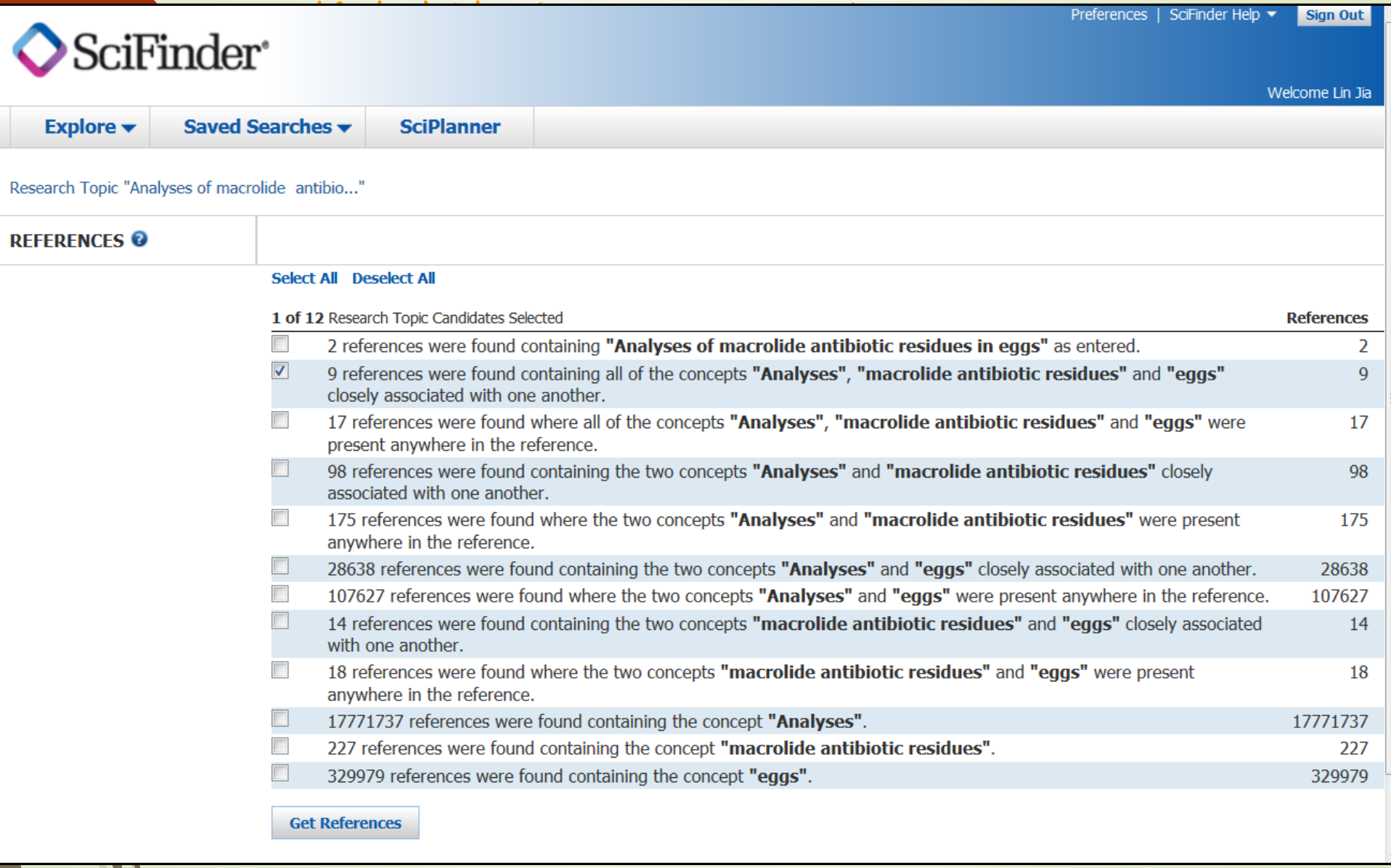
  preparation of artemisinin

- 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

  bird flu virus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Research Topic "Analyses of macrolide antibio..."
REFERENCES
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Deselect All
1 of 12 Research Topic Candidates Selected
References
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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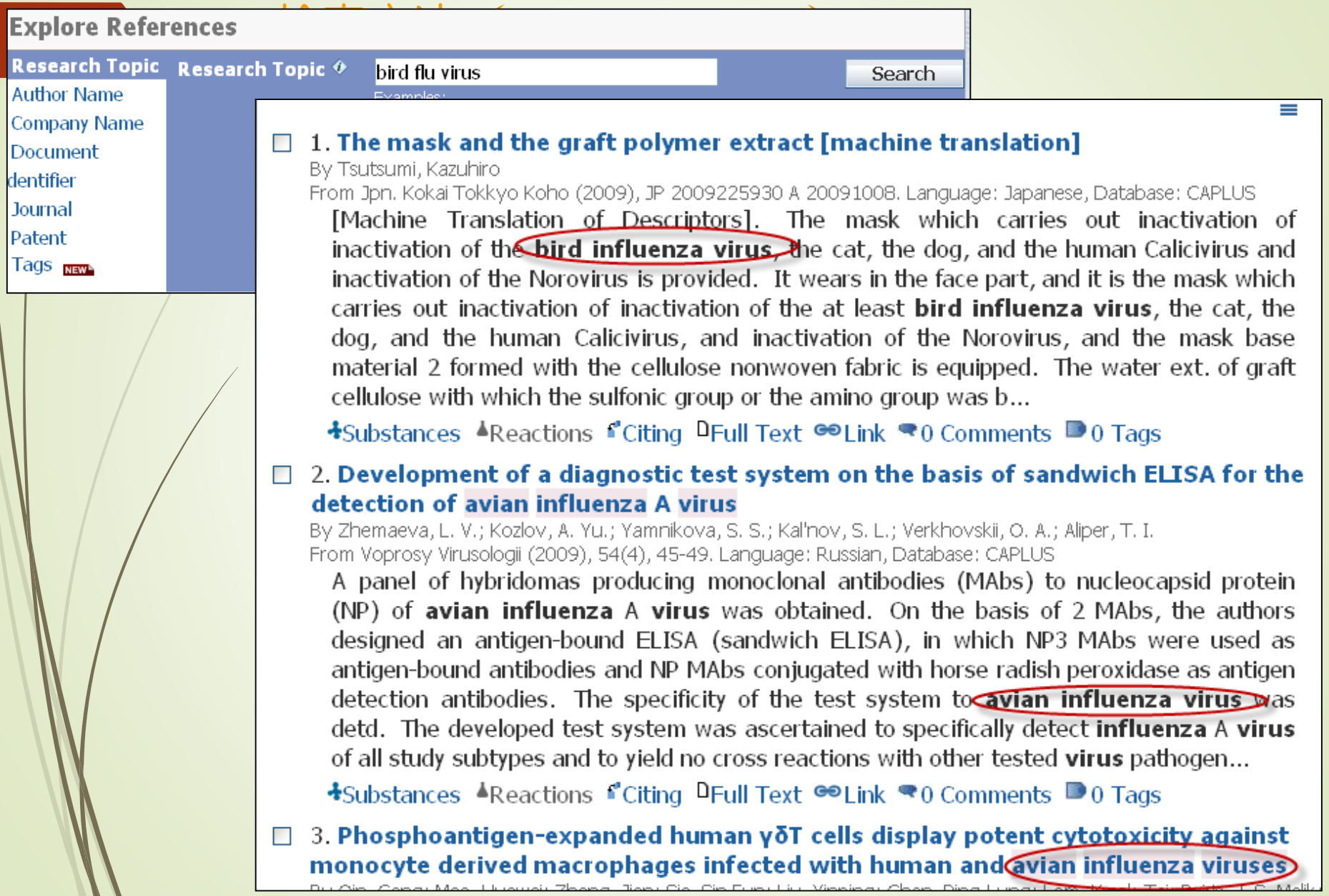
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2. Development of a diagnostic test system on the basis of sandwich ELISA for the detection of avian influenza A virus
By Zhemaeva, L. V.; Kozlov, A. Yu.; Yamnikova, S. S.; Kal'nov, S. L.; Verkhovskii, O. A.; Aliper, T. I.
From Voprosy Virusologii (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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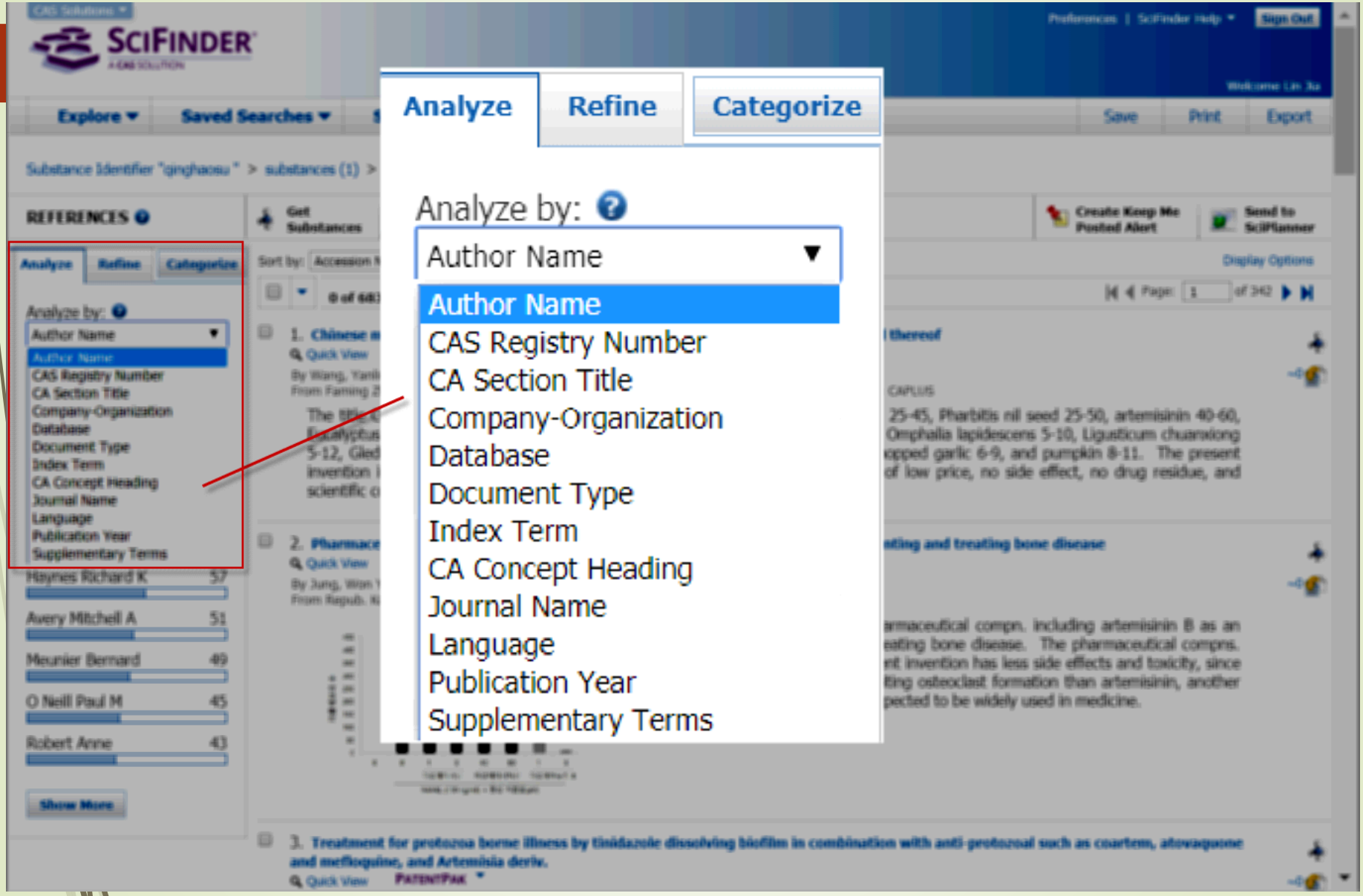
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  - (•) on all atoms
- ( ) Similarity

- [ ] Include tautomers
- [ ] Ignore stereo
- [ ] No salts
- [ ] No mixtures
- [ ] No isotopes
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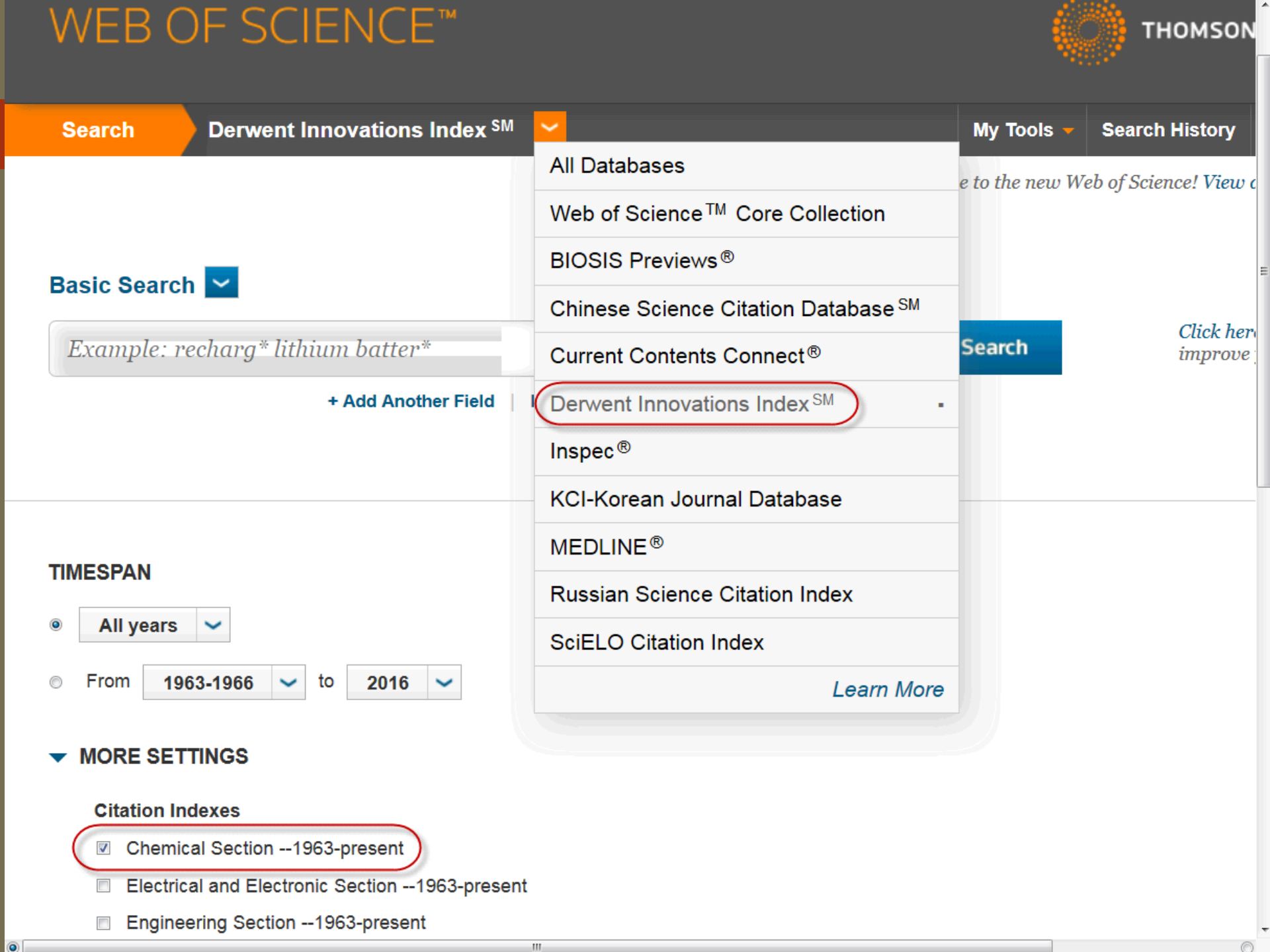
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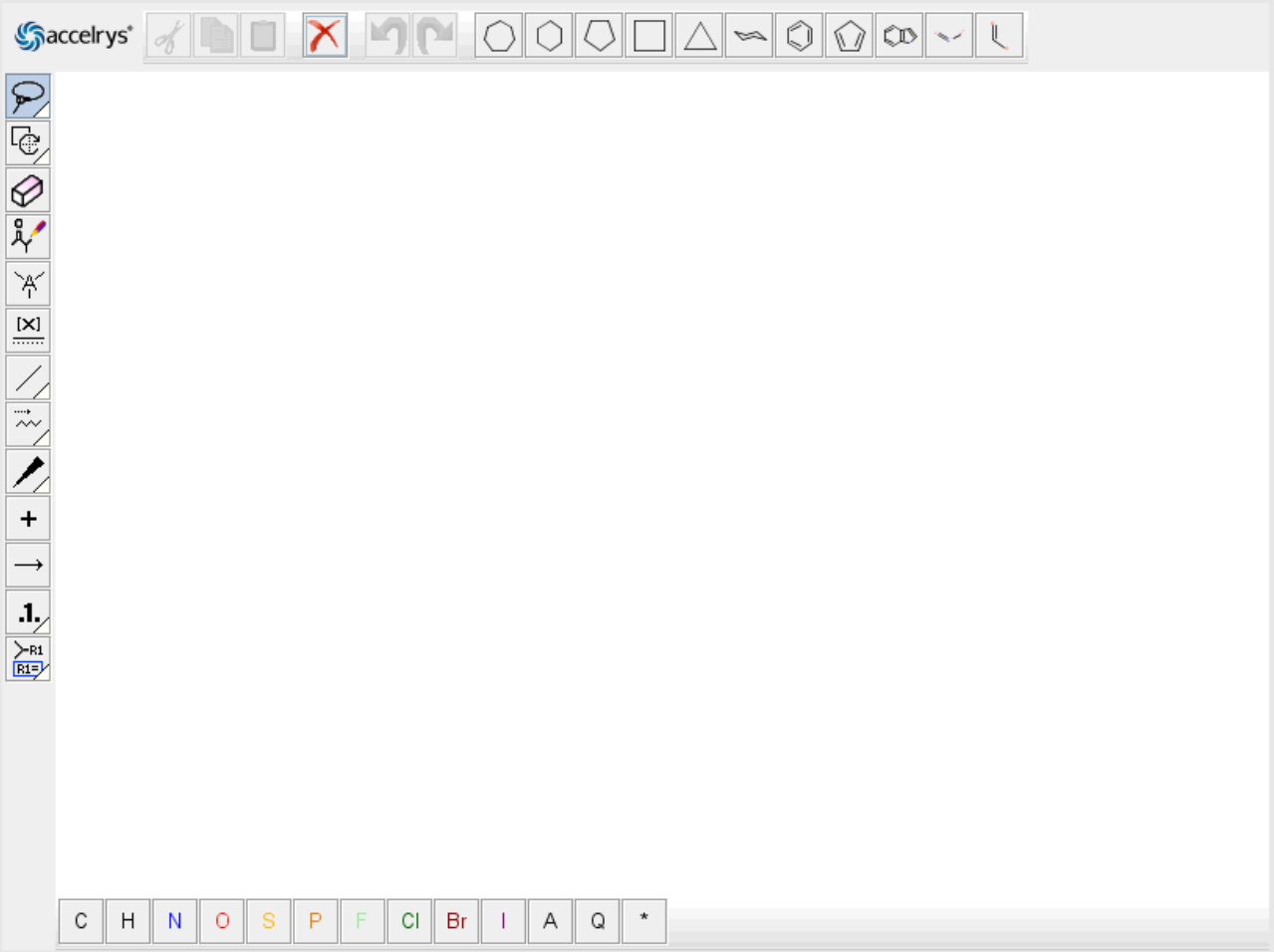

Combine structure and text AND OR

Combine structure and text ◉ AND ○ OR

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◉ Synonyms ○ Systematic ○ Both

*Example: NICKEL or AMINO**

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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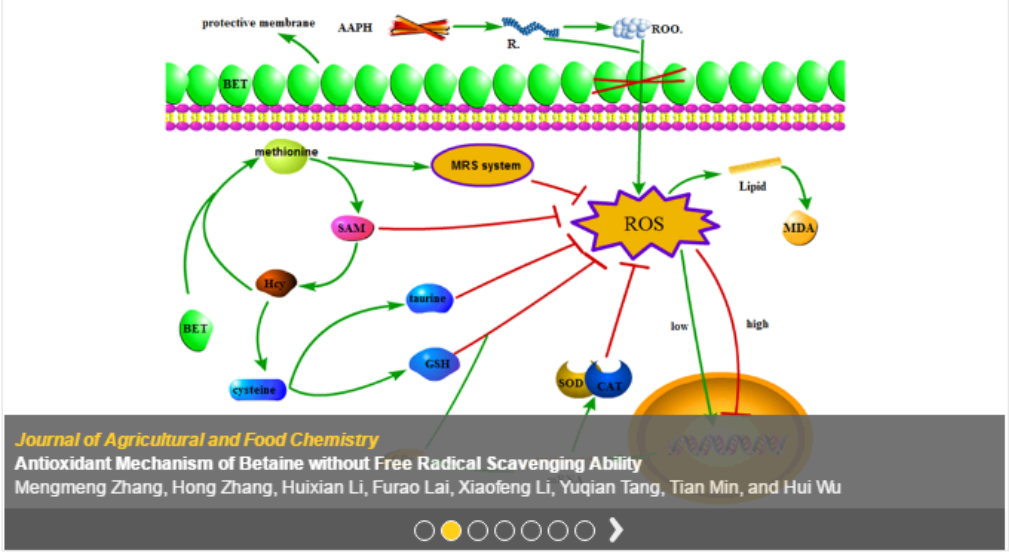

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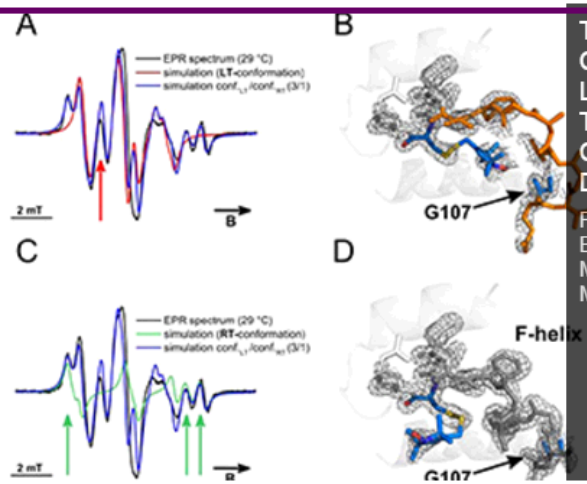

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Observation of Quantum Confinement in Monodisperse Methylammonium Lead Halide Perovskite Nanocrystals Embedded in Mesoporous Silica

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

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References

1. Ponseca, C. S., Jr.; Savenije, T. J.; Abdellah, M.; Zheng, K.; Yartsev, A.; Pascher, T.; Harlang, T.; Chabera, P.; Pullerits, T.; Stepanov, A.; Wolf, J. P.; Sundström, V. *J. Am. Chem. Soc.* **2014**, *136*, 518910.1021/ja412583t [CrossRef] [PubMed] [CAS]

2. Wehrenfennig, C.; Eperon, G. E.; Johnston, M. B.; Snaith, H. J.; Herz, L. M. *Adv. Mater.* **2014**, *26*, 158410.1002/adma.201305172 [CrossRef] [PubMed] [CAS]

3. Xing, G.; Mathews, N.; Sun, S.; Lim, S. S.; Lam, Y. M.; Grätzel, M.; Mhaisalkar, S.; Sum, T. C. *Science* **2013**, *342*, 34410.1126/science.1243167 [CrossRef] [PubMed] [CAS]

4. Stranks, S. D.; Eperon, G. E.; Grancini, G.; Menelaou, C.; Alcocer, M. J. P.; Leijtens, T.; Herz, L. M.; Petrozza, A.; Snaith, H. J. *Science* **2013**, *342*, 34110.1126/science.1243982 [CrossRef] [PubMed] [CAS]

5. Kojima, A.; Teshima, K.; Shirai, Y.; Miyasaka, T. *J. Am. Chem. Soc.* **2009**, *131*, 605010.1021/ja809598r [CrossRef] [PubMed] [CAS]

6. Kim, H.-S.; Lee, C.-R.; Im, J.-H.; Lee, K.-B.; Moehl, T.; Marchioro, A.; Moon, S.-J.; Humphry-Baker, R.; Yum, J.-H.; Moser, J. E.; Grätzel, M.; Park, N.-G. *Sci. Rep.* **2012**, *2*, 59110.1038/srep00591 [PubMed] [CAS]

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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*[,†]

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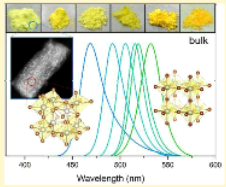
Supporting Information

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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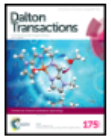

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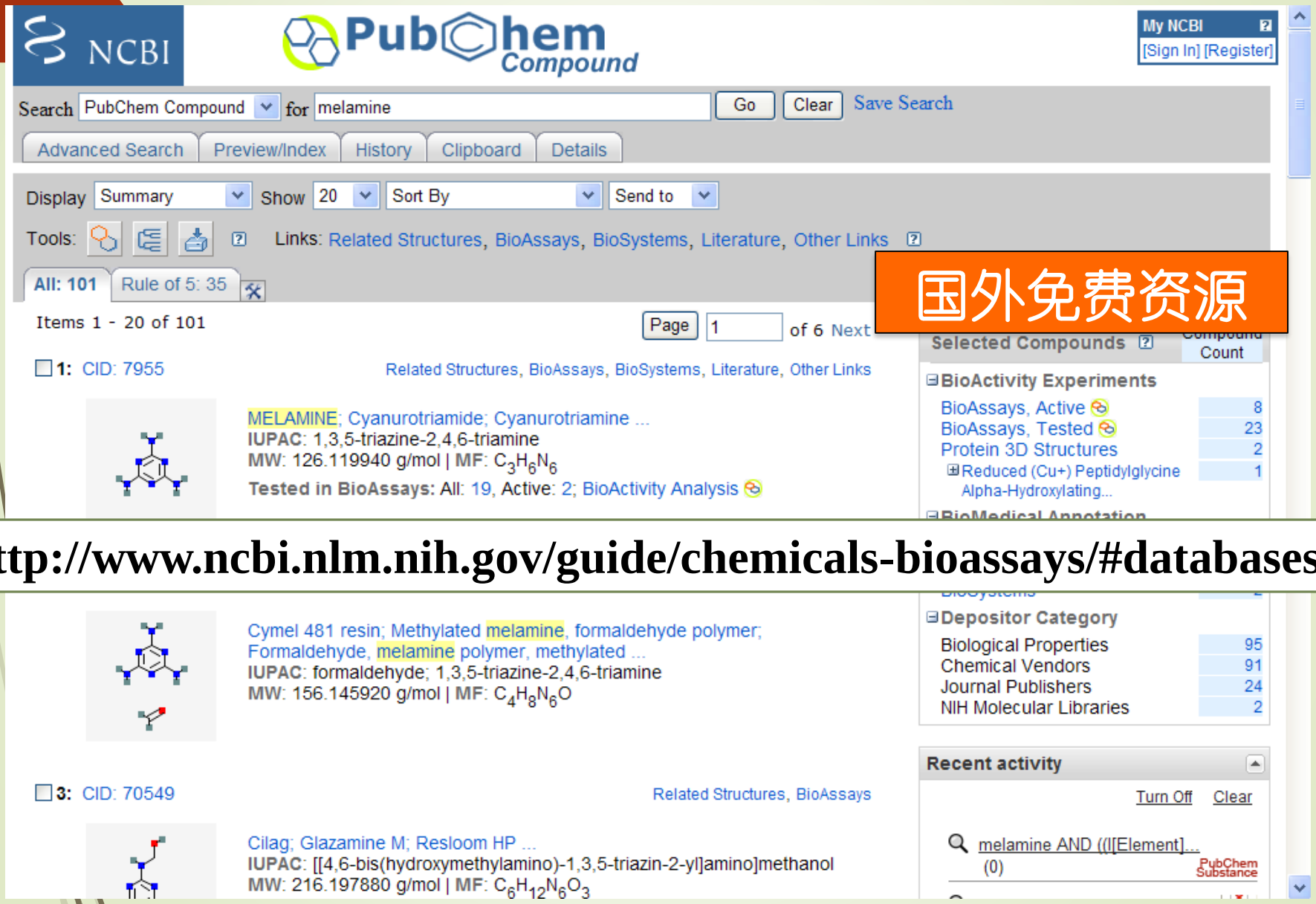

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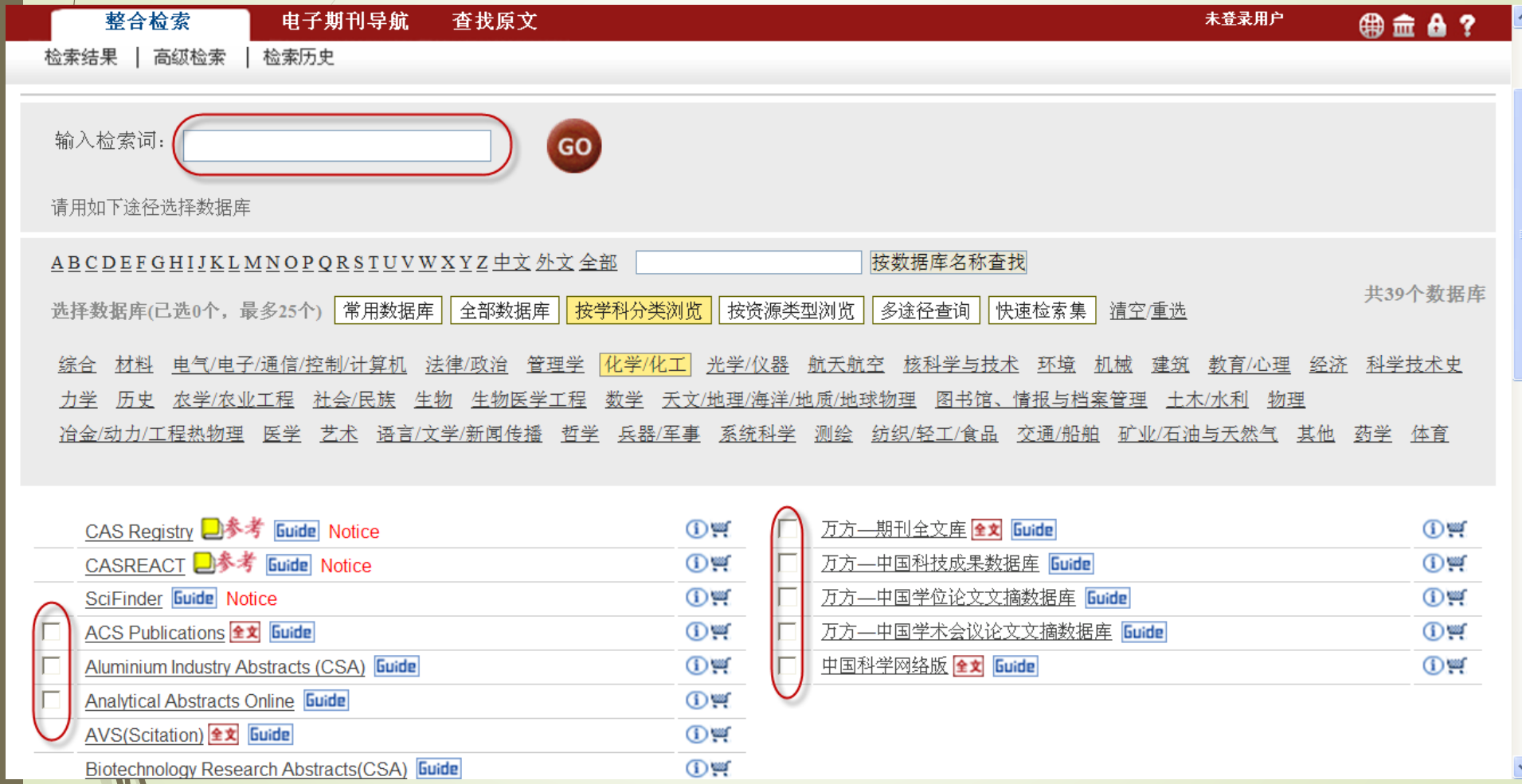

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