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获取化合物理化性质及合成制备数据的途径

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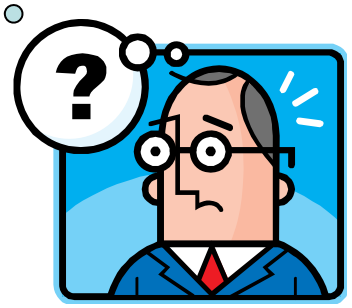
问题1：如何查找一个科学数据？

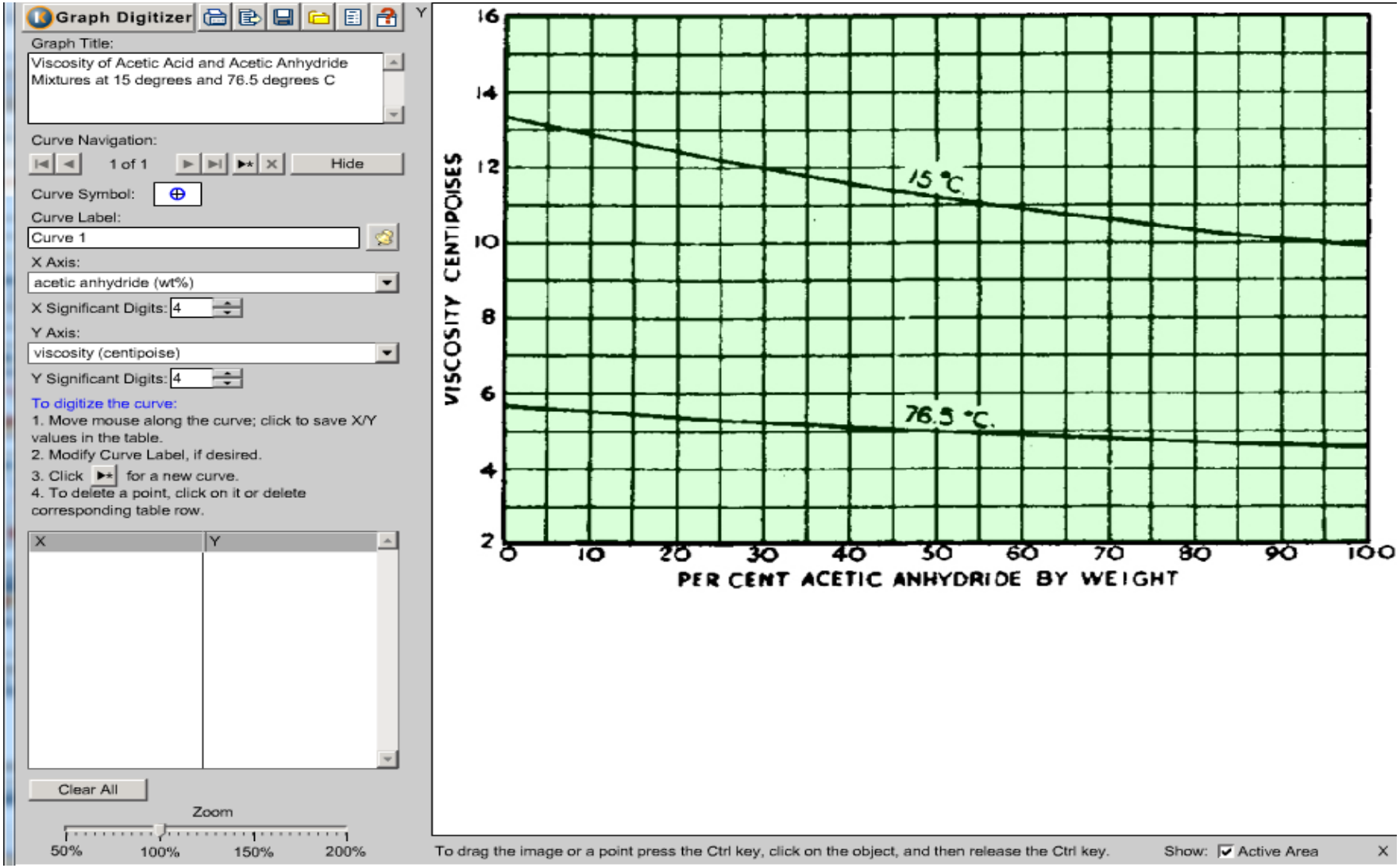
光谱数据
电化学常数
热物理常数
……

How do I filter factual from speculative data?



How much time will it take to filter through all these to find the relevant information?

问题2：如何查找满足现有实验条件的实验数据？



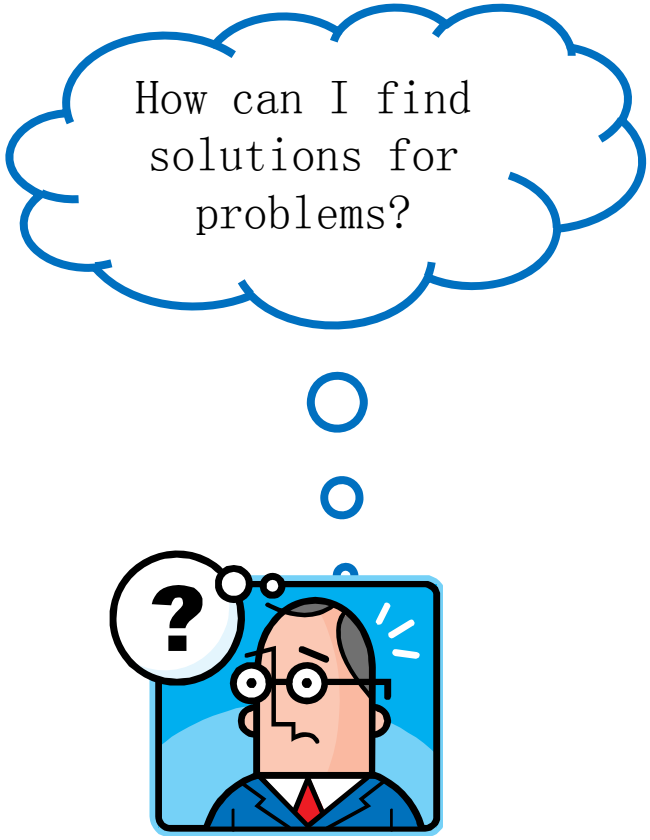
问题3：如何解决学习、研究中的实际问题？

我如何查找国特色类群知植物图谱？

MPA和KSI单位如何转换？

如何提高太阳能的转换效率？

……



一位钢铁厂的冶金学家收到一个制造要求：

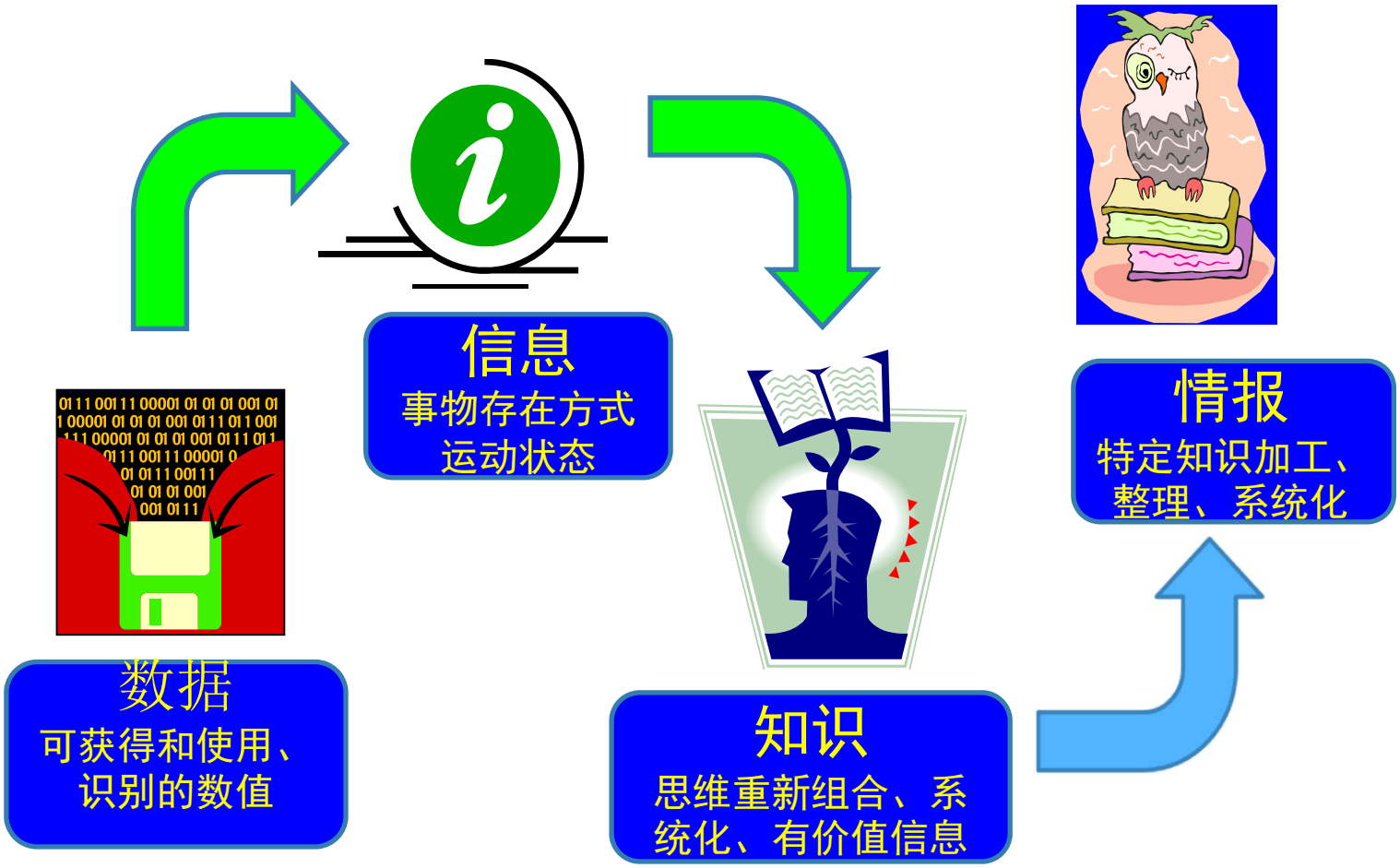
抗张强度至少为415MPa

最大拉伸强度至少为690MPa的碳钢

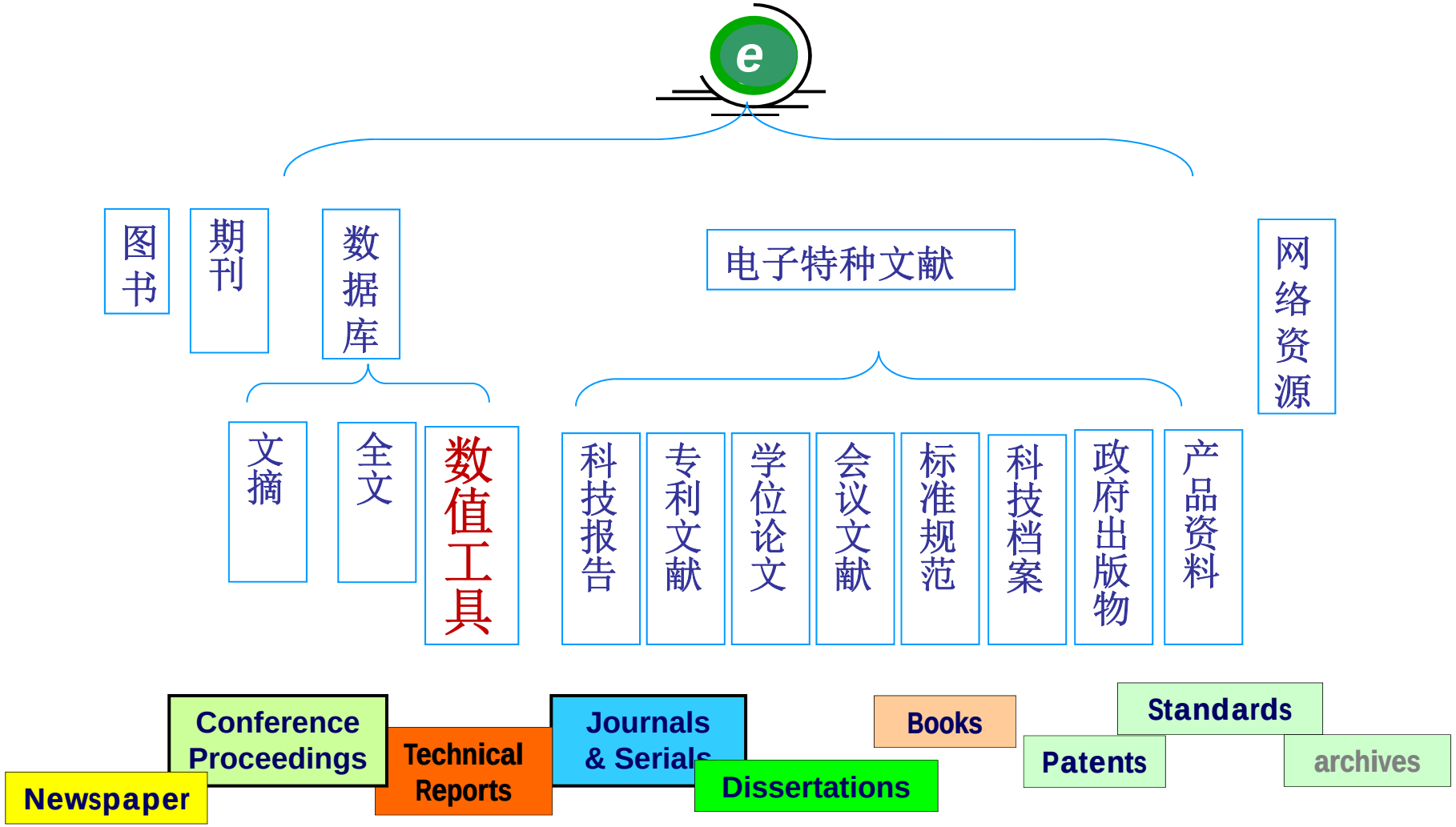
符合要求的条件下，碳钢中碳最佳%…

为什么对查找数据会感觉困难

信息相关的概念——丢失了数据



我们最熟悉的信息获取渠道



——Springer Materials

——Reaxys

- 检索方法
- 实例

1、SpringerMaterials

SpringerMaterials是什么

- 全球上最大的物理和化学科学数据资源
- 包括全部 Landolt Börnstein（LB）印本资料信息

LANDOLT-BÖRNSTEIN inside

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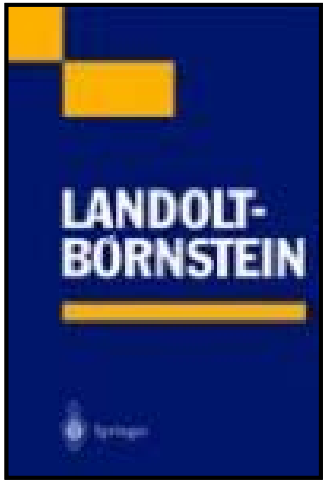
Landolt Börnstein（LB）工具书



- Landolt-Börnstein （LB） 工具书由世界著名的科技出版社— 德国施普林格出版社(Springer-Verlag) 出版。
- 由Hans Landolt 和 Richard Börnstein两位教授在1883年共同创建了这套工具书，迄今已经有130年历史，是一套连续出版科学技术领域重要的数值与事实型工具书。

从夸克到银河系
海量数据！

LB工具书的数据

✓数据来源于全世界千余名物理与工程领域的科学家撰稿的研究期刊全文

✓内容涉及相关科学与技术的数值数据（原始数据、图表、试验数据）

✓函数关系、常用单位以及基本常数等，还有相关论文与评论等文献

✓所有数据都经过严格苛刻的评估和筛选

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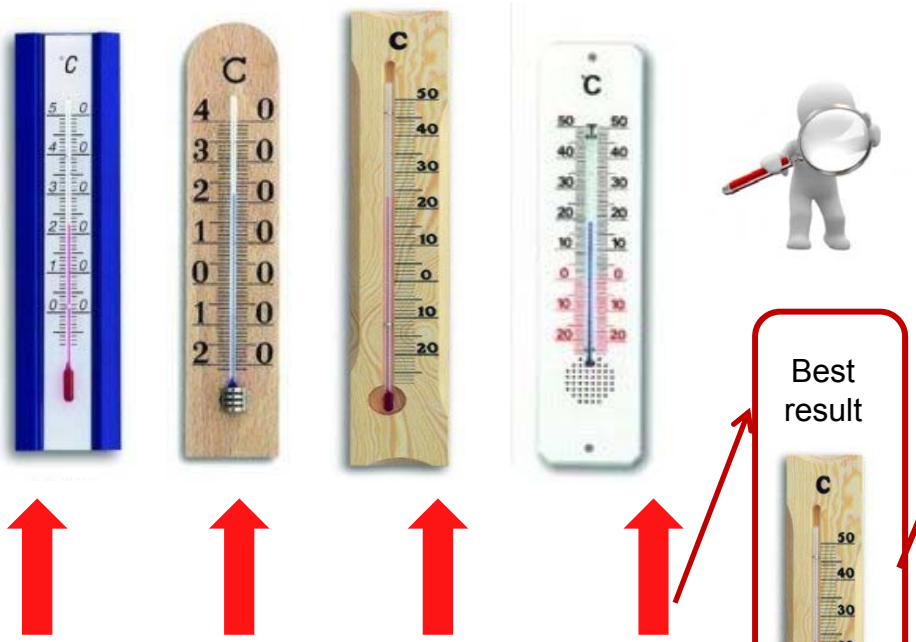
“严格的评估与筛选”意味着什么？

温度

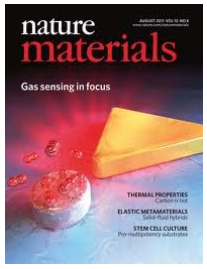


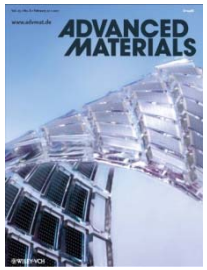
Best result

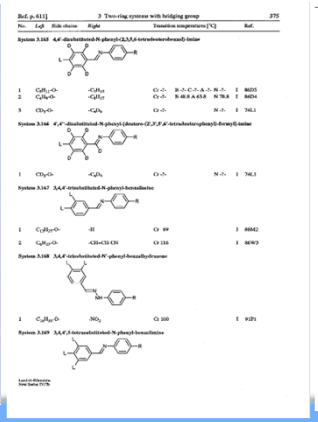
- 数据来自全球各领域的一千多名专家负责对8,000多种经同行评审的期刊原文进行严格苛刻的审阅，评估和筛选，然后将最有效的信息整齐排列和收录。

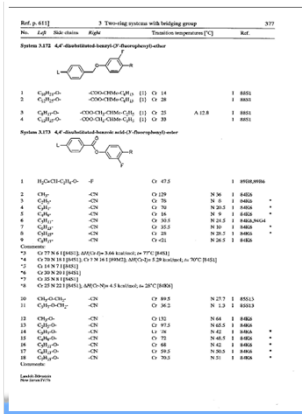
- 挑选最准确，最可靠的数据
- 描述最佳实验方法和最佳实践操作
- 提供充分背景资料

- 提供原始数据、图表、试验数据、还有相关论文与评论等文献；









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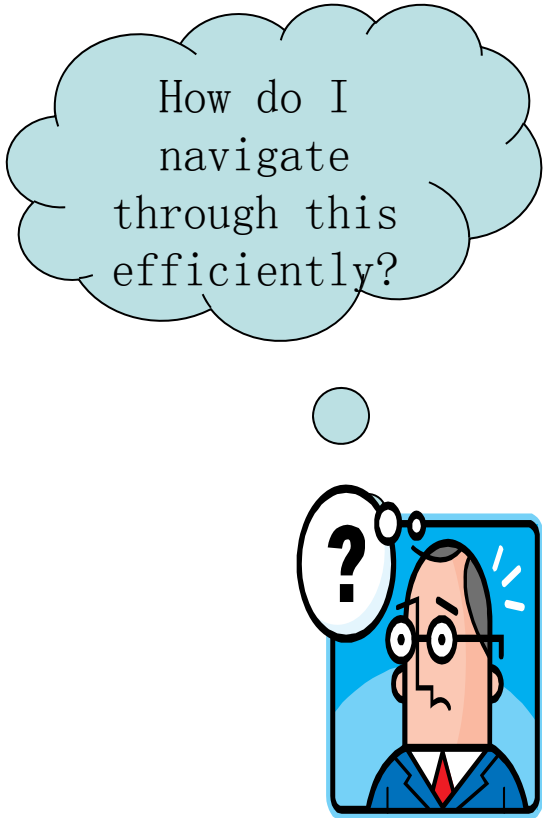
the language of science

ELSEVIER

Landolt-Börnstein 工具书分为8部（group)

Group I – 基本粒子、原子核和原子
(Elementary Particles, Nuclei and Atoms)
Group II – 分子和基团(Molecules and Radicals)
Group III – 聚凝态物质(Condensed Matter)
Group IV – 物理化学(Physical Chemistry)
Group V – 地球物理(Geophysics)
Group VI – 天文学和天体物理学(Astronomy and Astrophysics)
Group VII – 生物物理学(Biophysics)
Group VIII – 先进材料和技术(Advanced Materials and Technologies)



2001年，Springer 推出 Landolt-Börnstein 在线服务
2009年底，Springer 隆重推出 SpringerMaterials 数据库

- **SpringerMaterials（Landolt Börnstein 新丛书系列）**
  - 涵盖250,000多种化学物质与材料的物理和化学数据

- 粒子、核子和原子
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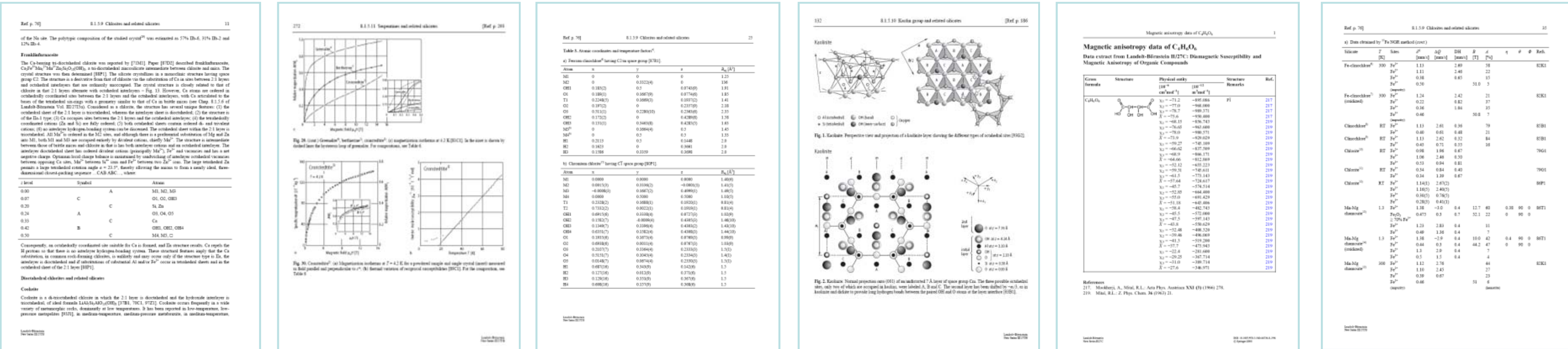
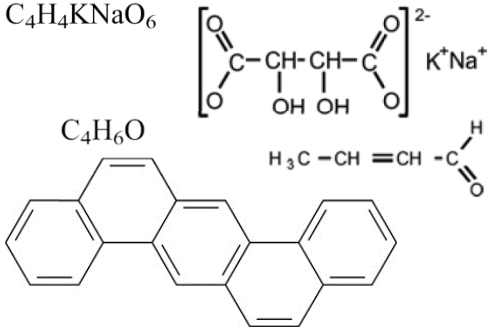
- 电子结构与传输
- 磁学
- 半导体
- 超导体
- 结晶学
- 热力学
- 多相系统
- 先进材料
- 先进技术
- 天体和地球物理学

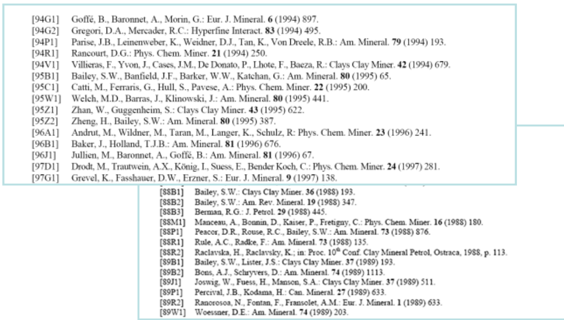
数据类型

- > 195,000 页 | > 90,000 篇在线文献| > 125,000 份各类图表



- > 150,000 种化学物质 | > 1,000,000 参考文献




[94G1] Goffé, B., Baronnet, A., Morin, G.: Eur. J. Mineral. **6** (1994) 897.
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[96B1] Baker, J., Holland, T.J.B.: Am. Mineral. **81** (1996) 676.
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[89J1] Joswig, W., Fuess, H., Manson, S.A.: Clays Clay Miner. **37** (1989) 511.
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[89R2] Ranorosoa, N., Fontan, F., Fransolet, A.M.: Eur. J. Mineral. **1** (1989) 633.
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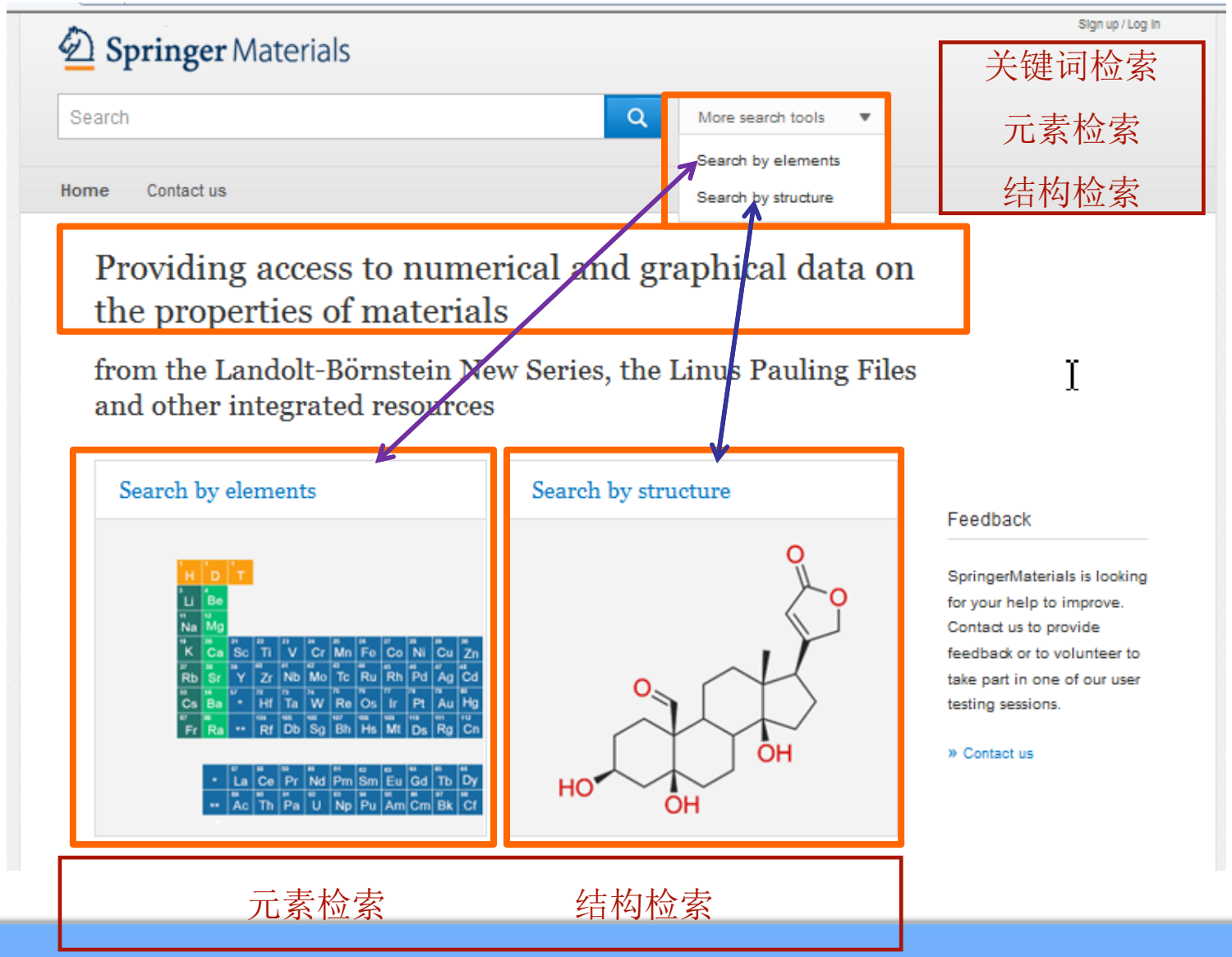

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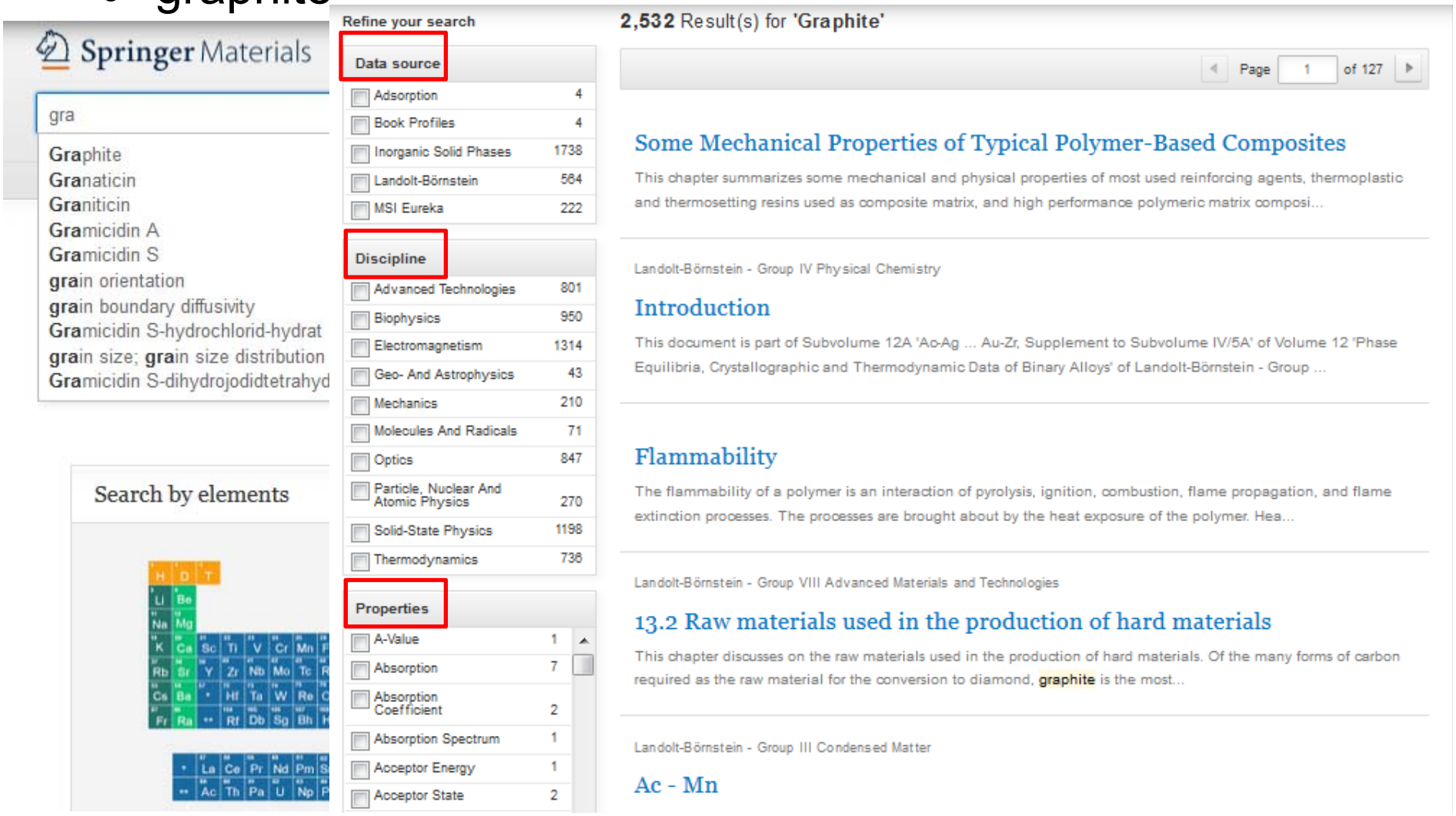
关键词检索

- graphite



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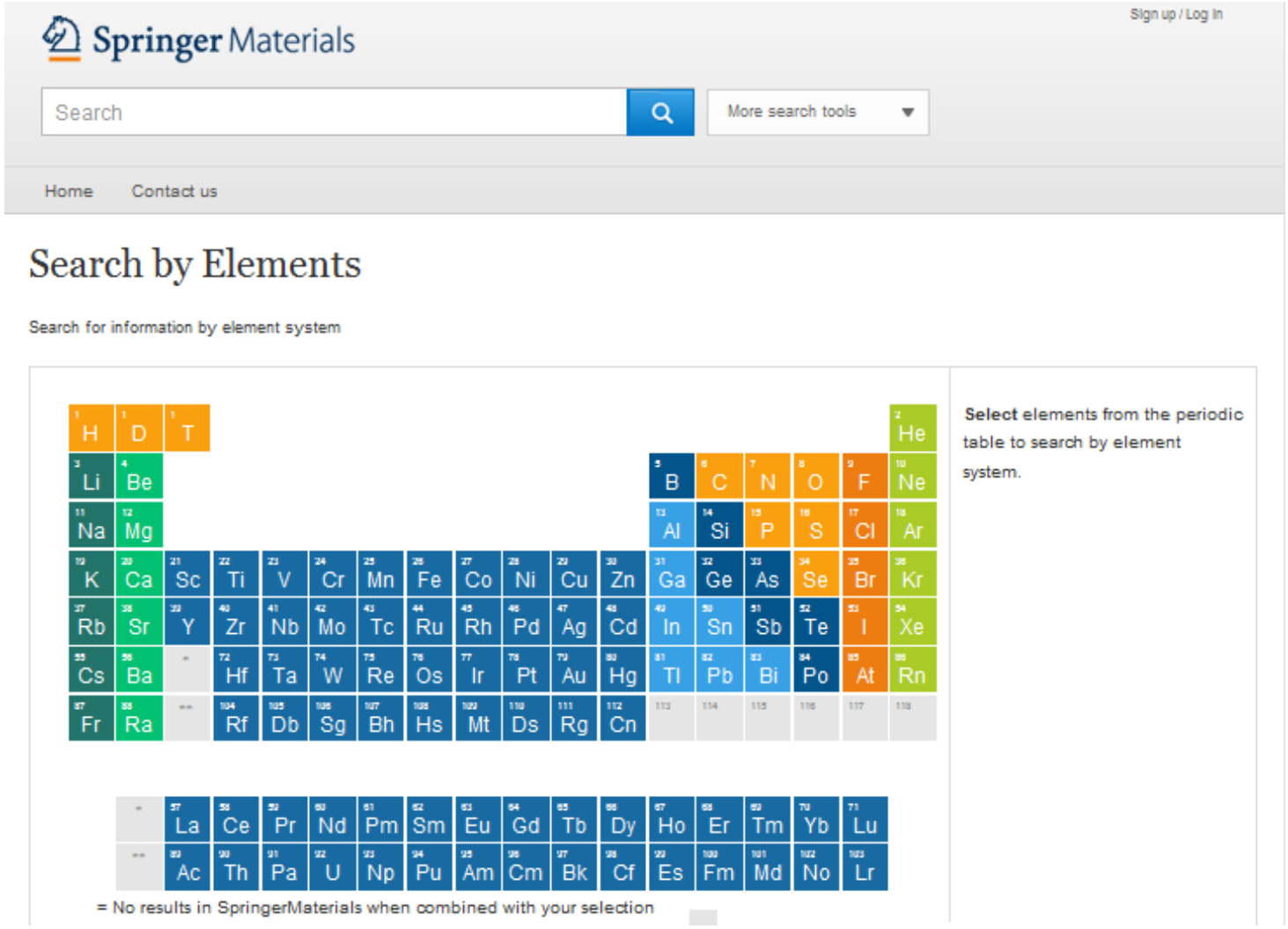
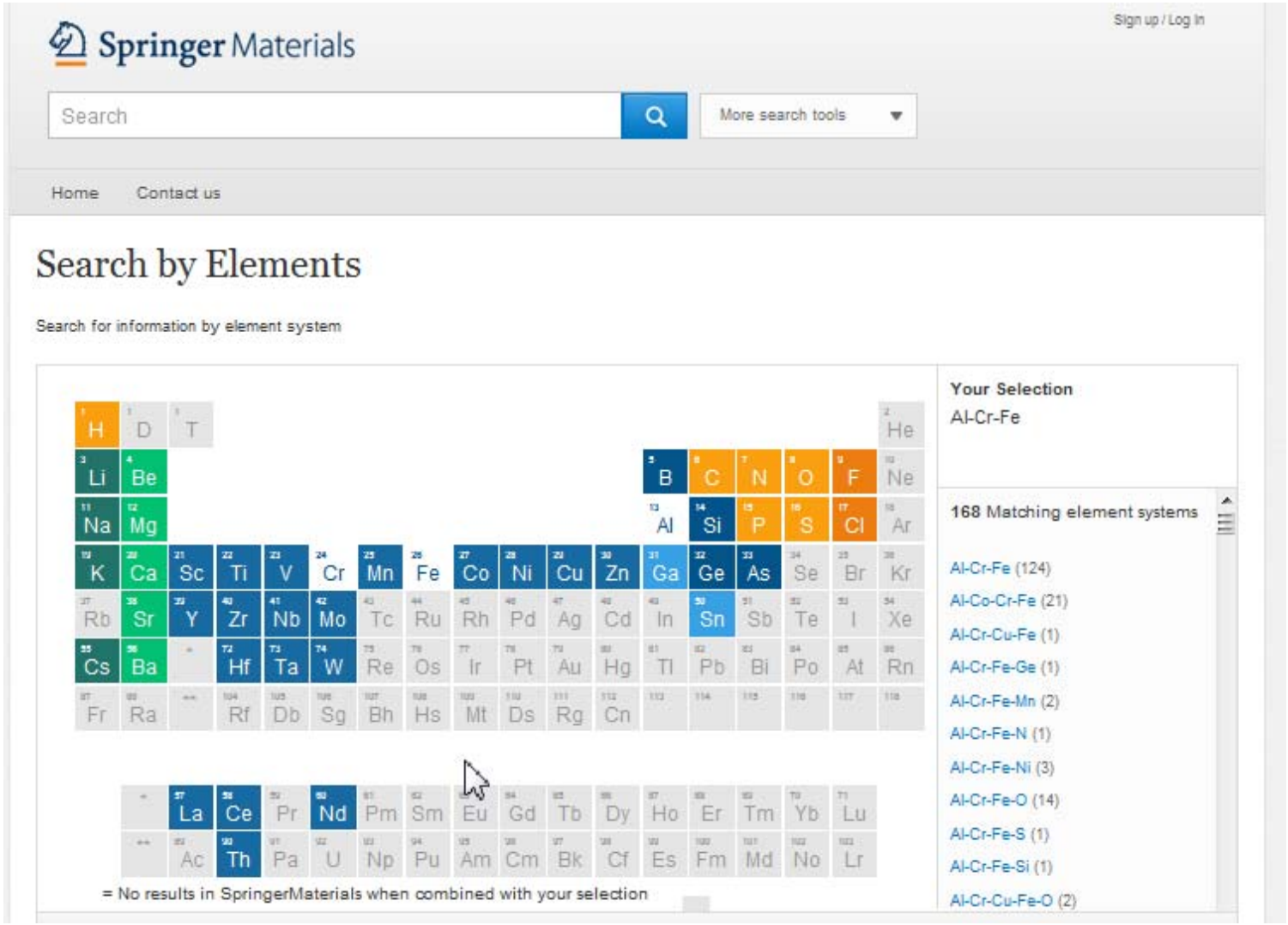
元素检索

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Your Selection
Al-Cr-Fe
168 Matching element systems
Al-Cr-Fe (124)
Al-Co-Cr-Fe (21)
Al-Cr-Cu-Fe (1)
Al-Cr-Fe-Ge (1)
Al-Cr-Fe-Mn (2)
Al-Cr-Fe-N (1)
Al-Cr-Fe-Ni (3)
Al-Cr-Fe-O (14)
Al-Cr-Fe-S (1)
Al-Cr-Fe-Si (1)
Al-Cr-Cu-Fe-O (2)
= No results in SpringerMaterials when combined with your selection

Refine Your Search

Data Source

- Inorganic Solid Phases 62
- Landolt-Börnstein 18
- MSI Eureka 44

Discipline

- Advanced Technologies 23
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Properties

- Activity 1
- Antiferromagnetic Neel Temperature 2
- Arrott Plot 1
- Atomic Environment 17

124 Result(s) for **'Al-Cr-Fe'**

Page 1 of 7

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Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Thermodynamic calculations of the Al corner of the **Al-Cr-Fe** system by Saunders [...)/(αFe)+(γFe) surface in the **Al-Cr-Fe** system, based on the microstructural, hardness,...

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Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Although the **Al-Cr-Fe** system has undergone many investigations, the **Al-Cr-Fe** equilibrium diagram has not been determined in... ...the (γFe)-loop in the **Al-Cr-Fe** system are given...

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Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

...scientific interest in the phase relations in the **Al-Cr-Fe** system, particularly as alloys of this system... ...approximants is also an interesting peculiarity of the **Al-Cr-Fe**

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Isothermal section at 750°C

Temperature: 750 °C

Concentration Range: Fe conc. [0-100 at.%] vs. Al conc. [0-100 at.%] vs. Cr conc. [0-100 at.%]

Part of report on 'Al-Cr-Fe Ternary Phase Diagram Evaluation'

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 Report ID: 10.14873.1.1

Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Materials Science International Team, MSIT ®[1] and Gautam Ghosh

Abstract

This report for the ternary system Al-Cr-Fe discusses binary systems, solid phases, invariant equilibria, liquidus surface, and isothermal sections.

Introduction

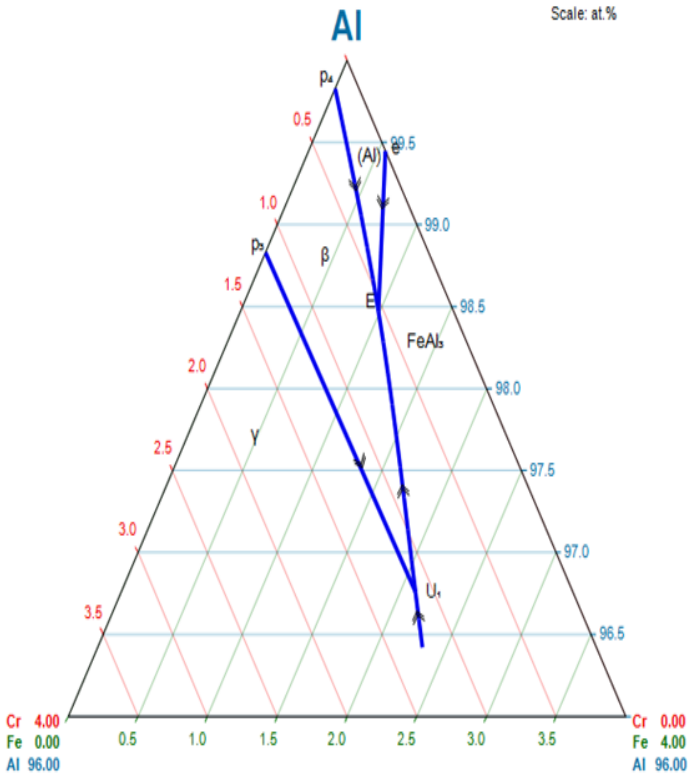
The major part of the work has been investigated by Kornilov [*39Kor*, *40Kor1*, *40Kor2*, *45Kor*] and [*46Kor*] and Kozheurov [*70Koz1*] and [*70Koz2*]. Kornilov used Armco grade Fe (0.25 mass% C, 0.05 mass% Si and traces of Mn), Al pigs (0.1 mass% Si, 0.1 mass% Cu), Al powder (0.1 mass% Si, 0.1 mass% Cu), chromium oxide of unspecified purity and analytically pure iron oxide. The alloys were prepared by the aluminothermic process which was also used by other investigators [*32Tai1*, *32Tai2*, *43Mon*, *51Pra*, *53Cas*, *54Chi*, *55Tag*] and [*58Chu*]. Thermal analysis was performed to monitor the solidification process, in an induction furnace in insulated corundum crucibles and under an inert atmosphere of He-Ar. [*32Tai1*] and [*32Tai2*] used Armco grade Fe (0.14 mass% Si), Al (0.17 mass% Si, 0.6 mass% Fe) and the liquidus surface was determined by thermal analysis. Chubb [*58Chu*] determined isothermal sections using high-purity Al (99.994 mass%), iodide Cr (99.988 mass%) and electrolytic Fe (99.994 mass%) having extremely low levels of interstitial elements C, H, O, N. Alloys were prepared by arc melting, followed by homogenizing treatment at 1000°C for 100 h. Final heat treatments were done under argon atmosphere in silica capsules and quenched into water. Phase analysis was carried out by optical metallography, X-ray diffraction and hardness testing. [*55Tag*] and [*58Tag*] studied the effect of Al addition in Fe-Cr binary alloys on the formation of the σ-phase by means of optical microscopy, X-ray diffraction and hardness measurements.

Tables

Table 1
Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Prototype	Lattice Parameters (pm)	Comments
(Al) ≤660.452	cF4 Cu	a = 404.88	pure Al at 24°C [*V-C*]
(Cr,αFe)			(Cr) and (αFe) completely soluble, Al solubility both in (Cr) and in (αFe) ≈ 46 at.% [*Mas*]
Cr ≤1863	cI2 W	a = 288.4	pure Cr at 27°C [*V-C*]
(αFe)(r) ≤912		a = 286.65	pure Fe at 20°C [*V-C*]

Fig. 2: Liquidus projection of the Al-corner



MSI **Fig. 2: Liquidus projection of the Al-corner**

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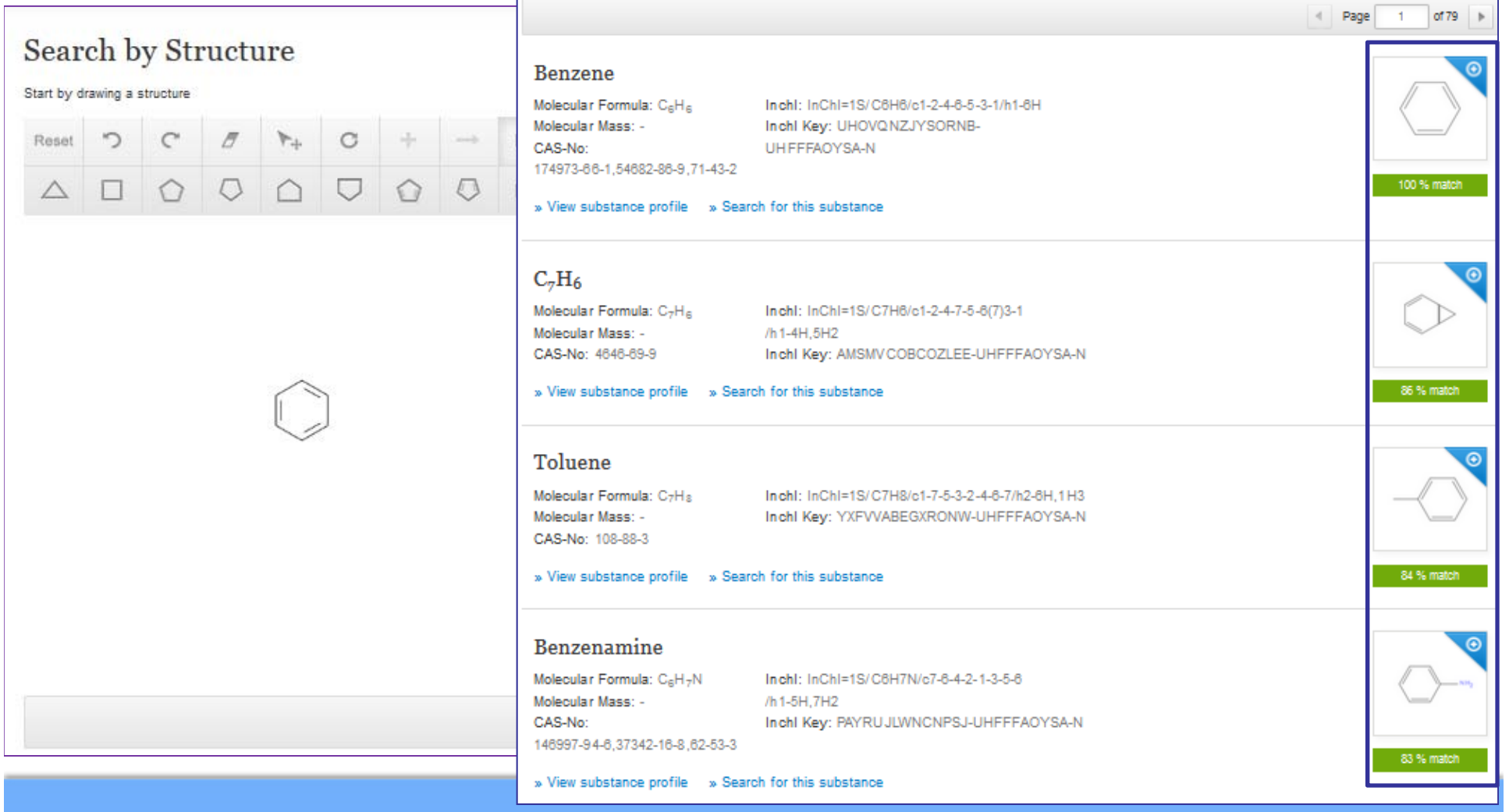
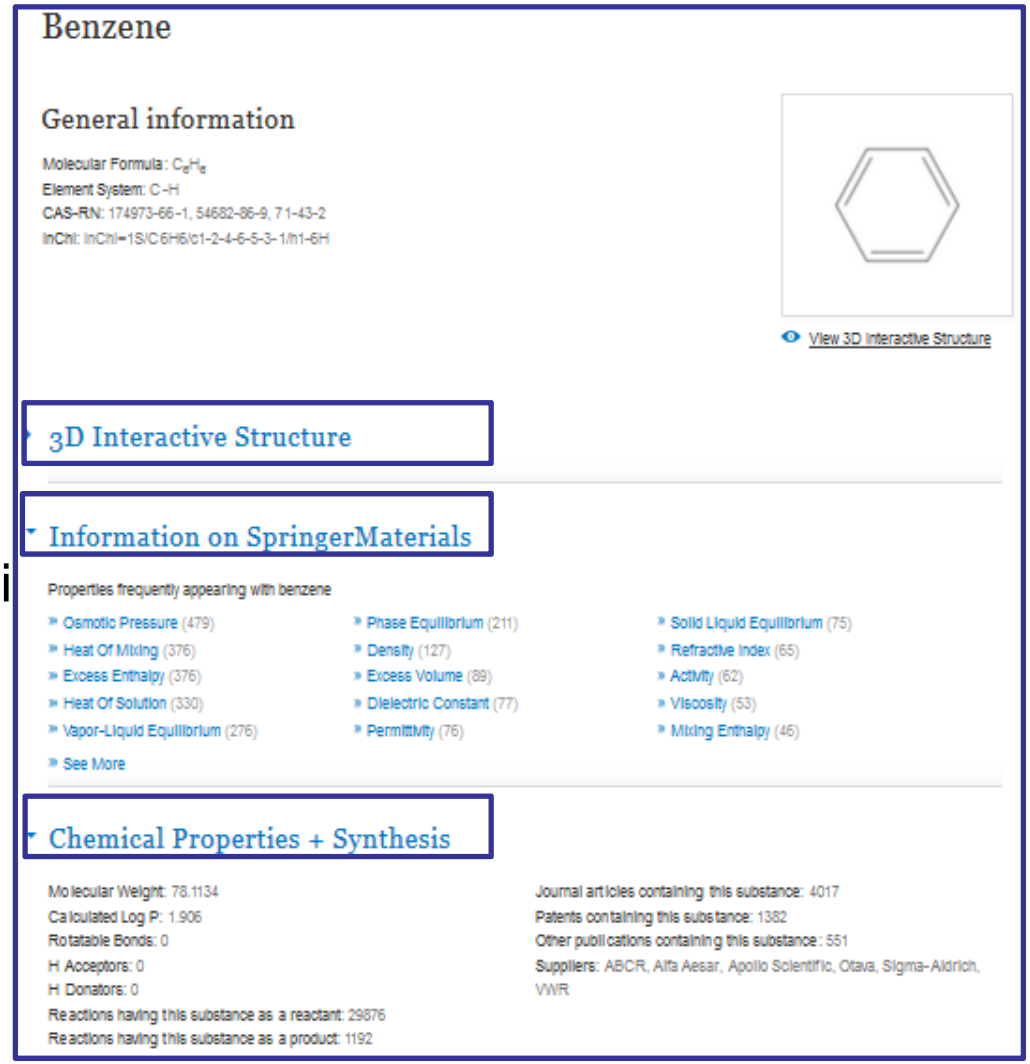
结构检索

- benzene

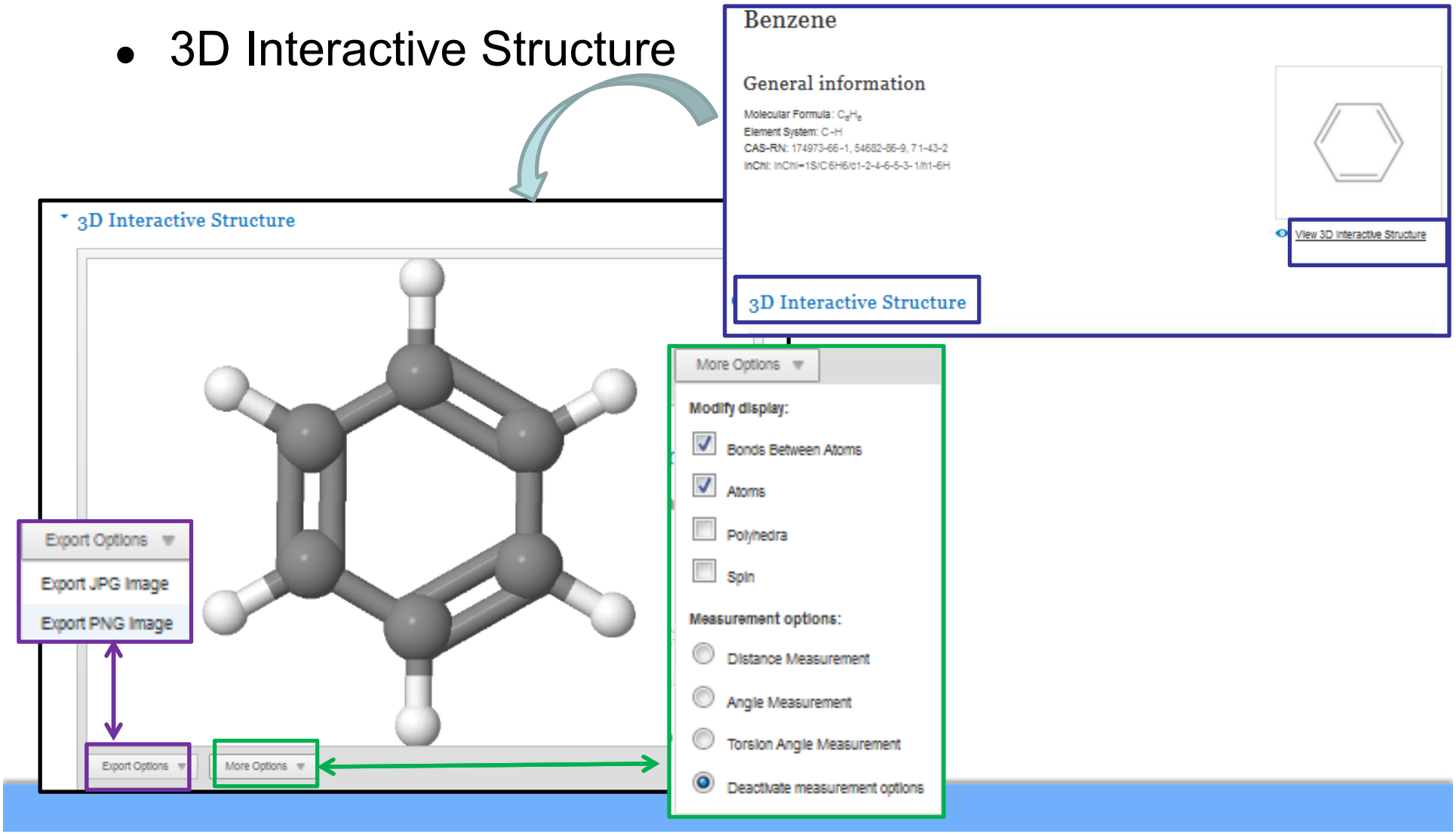


检索结果分类：

- 3D Interactive Structure
- Information on SMs
- Chemical Properties+Synthesi



- 3D Interactive Structure



- Information on SMs——Band gap

Benzene

General information

Molecular Formula: C_6H_6
Element System: C-H
CAS-RN: 174973-66-1, 54682-86-9, 71-43-2
InChI: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

View 3D Interactive Structure

3D Interactive Structure

Information on SpringerMaterials

Properties frequently appearing with benzene

- Osmotic Pressure (479)
- Heat Of Mixing (376)
- Excess Enthalpy (376)
- Heat Of Solution (330)
- Vapor-Liquid Equilibrium (276)
- Phase Equilibrium (211)
- Density (127)
- Excess Volume (89)
- Dielectric Constant (77)
- Permittivity (76)
- Solid Liquid Equilibrium (75)
- Refractive Index (65)
- Activity (62)
- Viscosity (53)
- Mixing Enthalpy (46)

See More

Chemical Properties + Synthesis

Molecular Weight: 78.1134
Calculated Log P: 1.906
Rotatable Bonds: 0
H Acceptors: 0
H Donators: 0
Reactions having this substance as a reactant: 29876
Reactions having this substance as a product: 1192

Journal articles containing this substance: 4017
Patents containing this substance: 1382
Other publications containing this substance: 551
Suppliers: ABCR, Alfa Aesar, Apollo Scientific, Otava, Sigma-Aldrich, VWR

Information on SpringerMaterials

Properties frequently appearing with benzene

- Osmotic Pressure (479)
- Heat Of Mixing (376)
- Excess Enthalpy (376)
- Heat Of Solution (330)
- Vapor-Liquid Equilibrium (276)
- Phase Equilibrium (211)
- Density (127)
- Excess Volume (89)
- Dielectric Constant (77)
- Permittivity (76)
- Solid Liquid Equilibrium (75)
- Refractive Index (65)
- Activity (62)
- Viscosity (53)
- Mixing Enthalpy (46)
- Diffusion (39)
- Chemical Diffusion (38)
- Sound Velocity (36)
- Heat Capacity (32)
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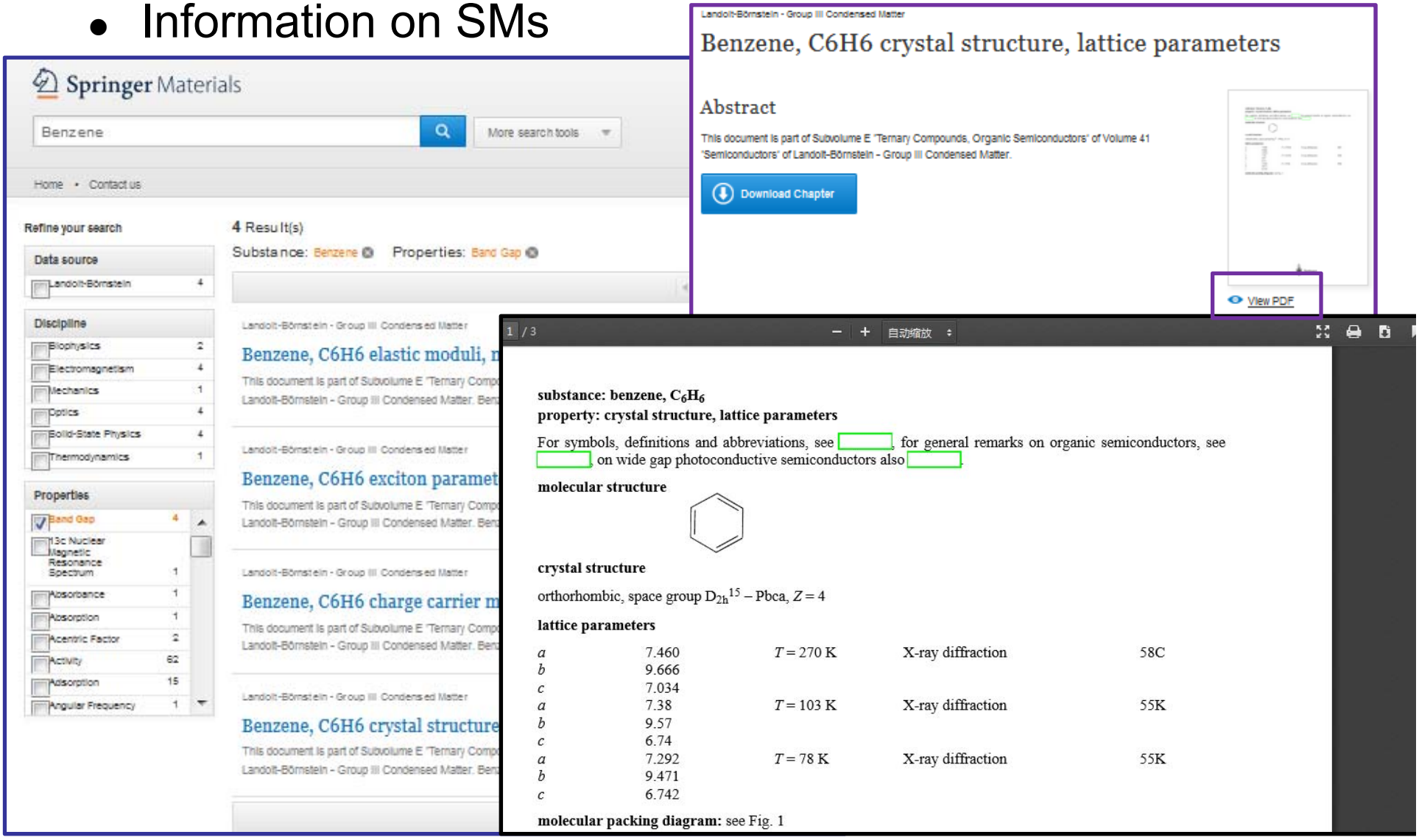
- Solid-Liquid Phase Equilibrium (28)
- Composition (16)
- Chemical Composition (16)
- Adsorption (15)
- Virial Coefficient (14)
- Polarization Degree (13)
- Luminescence Emission Linewidth (13)
- Luminescence (13)
- Heat Conductivity (12)
- Thermal Conductivity (12)
- Dilution Enthalpy (10)
- Crystal Structure (7)
- Band Structure (7)
- Isentropic Compressibility (6)
- Compressibility (5)
- Effective Mass (4)
- Unit Cell Parameter (4)
- Melting Temperature (4)
- Hole g-Factor (4)
- Band Gap (4)
- Mobility (4)
- Dielectricity (3)
- Electronic Structure (3)
- Photoemission Spectroscopy (3)
- Internuclear Distance (3)
- Phase Transition (3)
- Photoemission (3)
- Quadrupole Coupling (3)
- Core Level Transition (3)
- Valence Band (3)
- Critical Point (3)
- Nuclear Quadrupole Coupling (2)
- Space Group (2)
- Acentric Factor (2)
- Transition Enthalpy (2)
- Differential Scanning Calorimetry (2)
- Rotational Excitation Cross Section (2)
- Heat Of Fusion (2)
- Boiling Point (2)
- Magnetic Susceptibility (2)
- Centrifugal Distortion (2)
- Rotation-Vibration Spectrum (2)
- Liquid-Liquid Equilibrium (2)
- Molar Heat Capacity (2)
- Diamagnetic Susceptibility (2)
- Formula Unit (2)
- Vapor Pressure (2)
- Dipole Moment (2)
- Point Group (2)
- Unit Cell (2)
- Phonon Wavenumber (1)
- Expansion Coefficient (1)
- Coupling Constant (1)
- Piezooptic Effect (1)
- Enthalpy (1)
- Excitation Data (1)
- 13c Nuclear Magnetic Resonance Spectrum (1)
- Phase Diagram (1)
- Magnetic Susceptibility Exaltation (1)
- Angular Frequency (1)
- Absorbance (1)
- Exciton Fine Structure (1)
- Grain Size (1)
- Phase Transition Temperature (1)
- Magnetic Anisotropy (1)
- Gibbs Energy (1)
- Piezooptic Constant (1)
- Molar Mass (1)
- Self-Diffusion (1)
- Equilibrium Structure (1)
- Diffusion Of Impurities (1)
- Absorption (1)
- Charge Carrier Mobility (1)
- Impurity Concentration (1)
- Formation Entropy (1)
- Elastic Coefficients (1)
- Diamagnetic Susceptibility Exaltation (1)
- Migration Energy (1)
- Chemical Shift (1)
- Dispersion (1)
- Transition Entropy (1)
- Structure Data (1)
- Formation Enthalpy (1)
- Reaction Coordinate (1)
- Radical Ion State (1)
- Potential Energy (1)
- Creep (1)
- Formation Energy (1)
- Dunham Energy Parameter (1)
- Nuclear Quadrupole Resonance Spectroscopy (1)
- Latent Heat (1)
- Heat Of Sublimation (1)
- Heat Of Transition (1)
- Entropy (1)
- Coriolis Coupling (1)
- Tracer Diffusion (1)
- Shock Waves (1)
- Asymmetry Parameter (1)
- Nuclear Magnetic Resonance (1)
- Melting Curve (1)

- Information on SMs



适用的行业

- Chemicals 化工产品
- IT & Semiconductors 计算机&半导
- Optics 光学
- Photovoltaics 光伏材料
- Glass & Ceramics 玻璃和制陶业
- Metals & Mining 冶金和矿产
- Engineering 工程
- Petrochemistry 石油化工
- Automotive 汽车业
- Electronics 电子工业
- Aerospace & Defence 航空与国防
- Energy 能源
- Oil & Gas 石油

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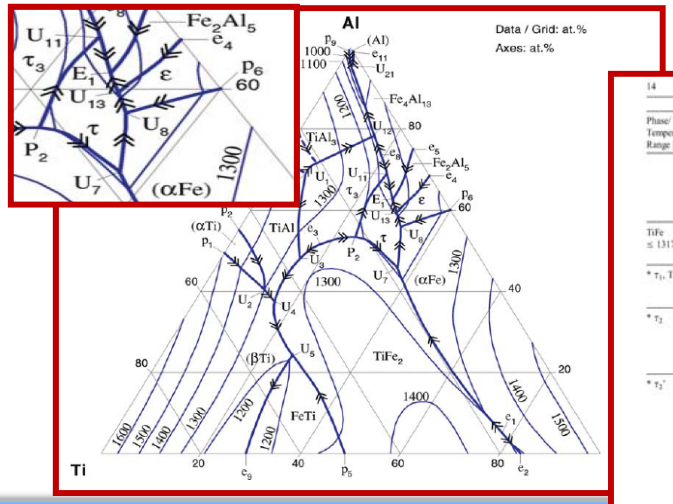
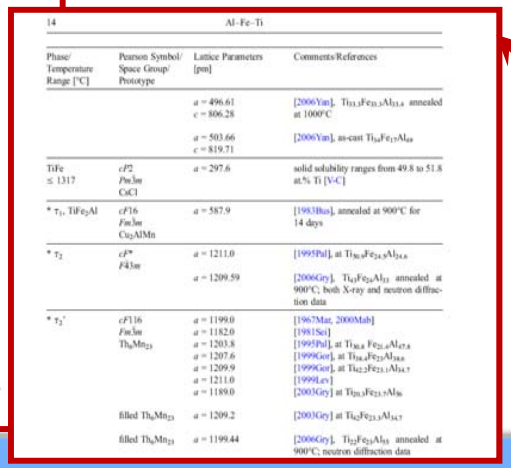
利用Springer Materials准备课题或者对试验结果进行分析

例如：利用Springer Materials查找材料参数

- 利用专业知识库进行可靠的新材料设计
- 为研究项目找出哪种材料能够提供最可靠的匹配参数
- 在实际测量完毕以后与已知的材料参数进行对比、评估与证实试验所获得的数据





14 Al–Fe–Ti

Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
		a = 496.61 c = 806.28	[2006Yan], $Ti_{13.3}Fe_{33.3}Al_{53.4}$, annealed at 1000°C
		a = 503.66 c = 819.71	[2006Yan], as-cast $Ti_{16}Fe_{17}Al_{67}$
TiFe ≤ 1317	$cP2$ $Pm\bar{3}m$ CsCl	a = 297.6	solid solubility ranges from 49.8 to 51.8 at.% Ti [V-C]
* τ_1, $TiFe_2Al$	$cF16$ $Fm\bar{3}m$ Cu_2AlMn	a = 587.9	[1983Hus], annealed at 900°C for 14 days
* τ_2	cF^* $F\bar{4}3m$	a = 1211.0 a = 1209.59	[1995Pal], at $Ti_{30.3}Fe_{25.8}Al_{43.8}$ [2006Gry], $Ti_{19}Fe_{29}Al_{52}$ annealed at 900°C; both X-ray and neutron diffraction data
* τ_2'	$cF116$ $Fm\bar{3}m$ Th_6Mn_{23}	a = 1199.0 a = 1182.0 a = 1203.8 a = 1207.6 a = 1209.9 a = 1211.0 a = 1189.0	[1967Mat, 2000Mah] [1981Sei] [1995Pal], at $Ti_{46.4}Fe_{32.4}Al_{47.8}$ [1999Ger], at $Ti_{34.4}Fe_{32}Al_{33.6}$ [1999Ger], at $Ti_{42.2}Fe_{23.1}Al_{34.7}$ [1999Lev] [2003Gry] at $Ti_{20.3}Fe_{23.3}Al_{56}$
	filled Th_6Mn_{23}	a = 1209.2	[2003Gry] at $Ti_{32}Fe_{23.3}Al_{34.7}$
	filled Th_6Mn_{23}	a = 1199.44	[2006Gry], $Ti_{22}Fe_{33}Al_{55}$ annealed at 900°C; neutron diffraction data

飞机设计师需要寻找制作高强度机翼的新型铝合金材料，例如： Al-Fe-Ti

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SpringerMaterials包含的材料种类

Metals
金属

Ceramics
陶瓷

Nuclear physics
原子物理

Semiconductors
半导体

Thin Films
薄膜

Nano Powders
纳米粉

Biomaterials
生物材料

Nanotubes
纳米管

Organic Materials
有机材料

Composite Materials
复合材料

Nanomaterials
纳米材料

内容：

大型的 全面的 重要的 系统的 权威的 可信的

使用： *方便的 快捷的*

全院开通 免费

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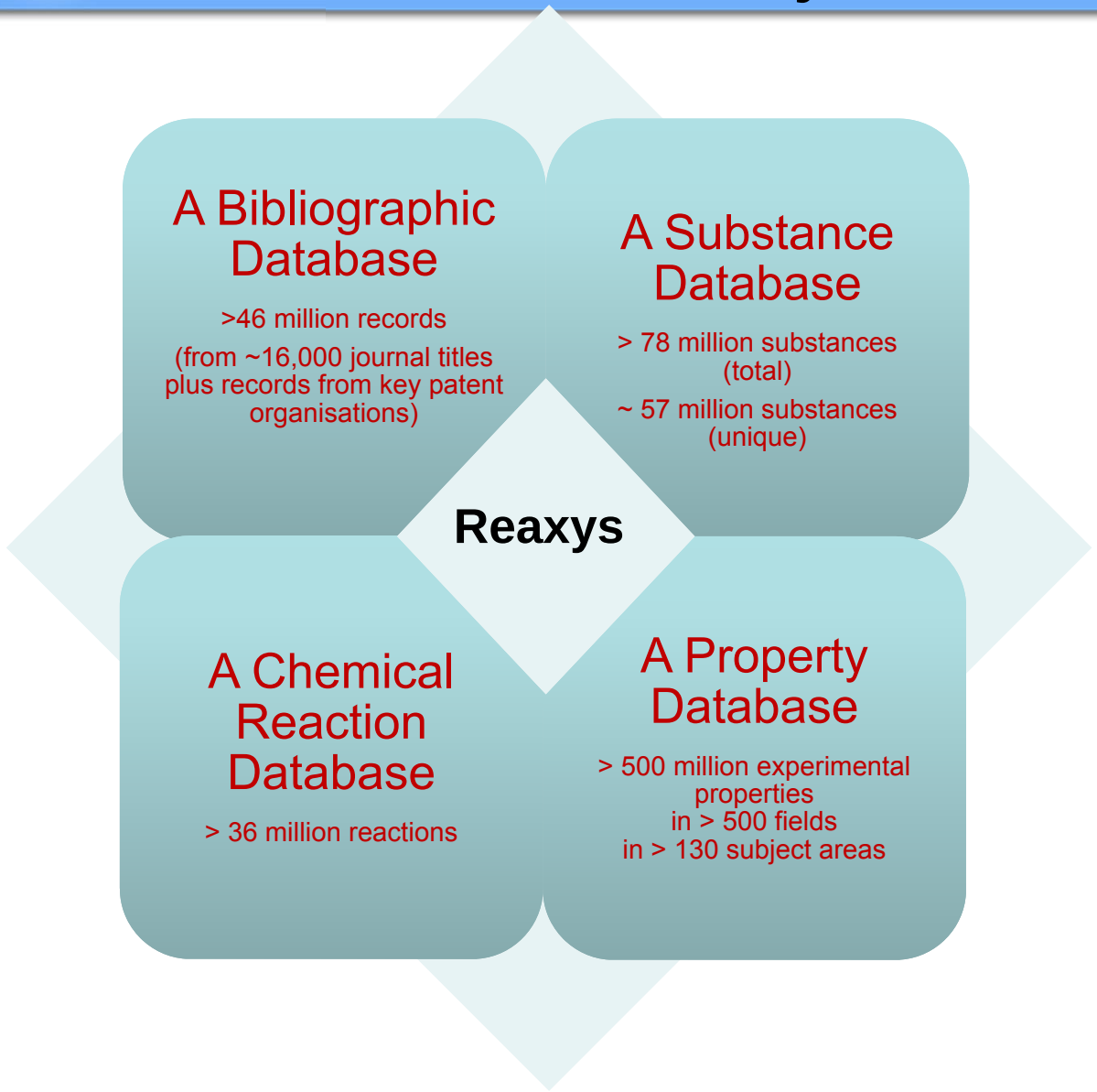
- Reaxys组成

Beilstein	Gmelin	PCD
有机化学（始于1771）	**无机化学**（始于1772）	**化学专利**（始于1976）
全球最全的有机化学数值和事实库 化学结构相关的化学、物理等方面的性质；化学反应相关的各种数据 详细的药理学，环境病毒学，生态学等信息资源	当今最全面的无机与金属有机化学数值与事实数据库 详细的理化性质，地质学，矿物学，冶金学，材料学等方面的信息资源	化学专利数据库 世界知识产权组织，美国专利局，欧洲专利局专利信息

☺ Reaxys数据



INTEGRATED DATABASES

PubChem
BioAssay | Compound | Substance

eMolecules
Linking researchers needs to supplier capabilities

INTEROPERABILITY WITH

Scopus

ScienceDirect

☺ Reaxys数据

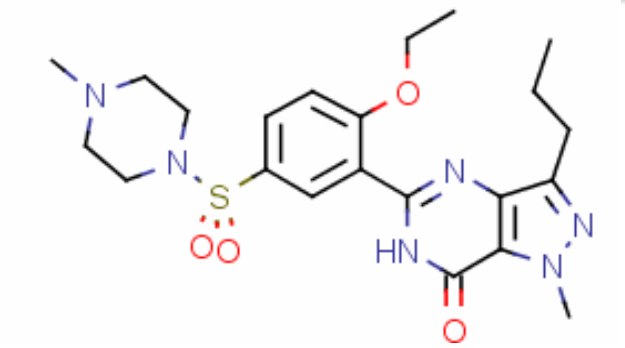
- ***~57.0 Million unique Substances***
- ***~36.6 Million Reactions***
- ***~500 Million experimental properties***
- ***~16,000 Journal Titles***

(Life Science, Chemistry&Engineering, Pharmacology, Enviromental Science, Books, Conference proceedings, Editorials etc.)

- ***~46 Million Bibliographic Records***
- ***> 500 Search fields(through querylet)***

解决的问题

1. **是什么?**
   - 新物质？专利保护?
   - 物化性质(密度，粘度，折射率，生成焓等)?



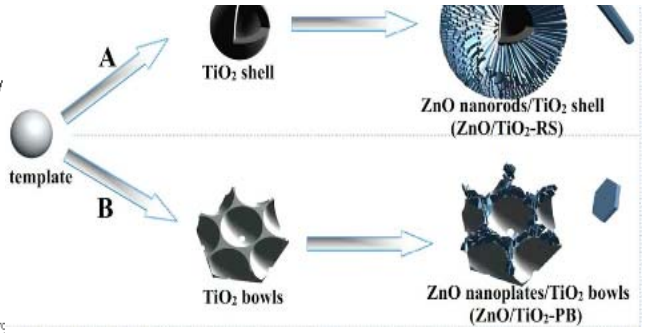
2. **什么用途?**
   - 反应物？溶剂？催化剂?
   - 生物活性？药理性质？
   - 毒性?

Fabrication of Ordered ZnO/TiO_2 Heterostructures via a Templating Technique

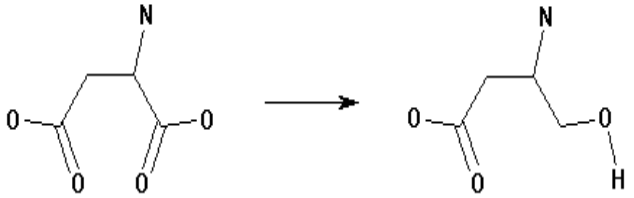
Jian F. Lei *†, Li B. Li †, Xue H. Shen ‡, Kai Du †, Jing Ni †, Chao J. Liu †, and Wei S. Li §
† School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China
‡ College of Life Science, Tarim University, Alar 843300, China
§ School of Chemistry and Environment, South China Normal University, Guangzhou 510006, China

Langmuir, Article ASAP
DOI: 10.1021/la4027859
Publication Date (Web): October 16, 2013

*E-mail: leijianfei9966@163.com. Telephone and fax: 86-37



3. **怎样得到?**
   - 已知制备方法?
   - 对制备方法进行改进?



Reaxys专门服务于从事有机化学、无机化学、有机金属化学及相关学科的

- 药物化学家
- 合成化学家
- 过程工程师
- 化工工程师
- 材料化学家

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检索

REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION

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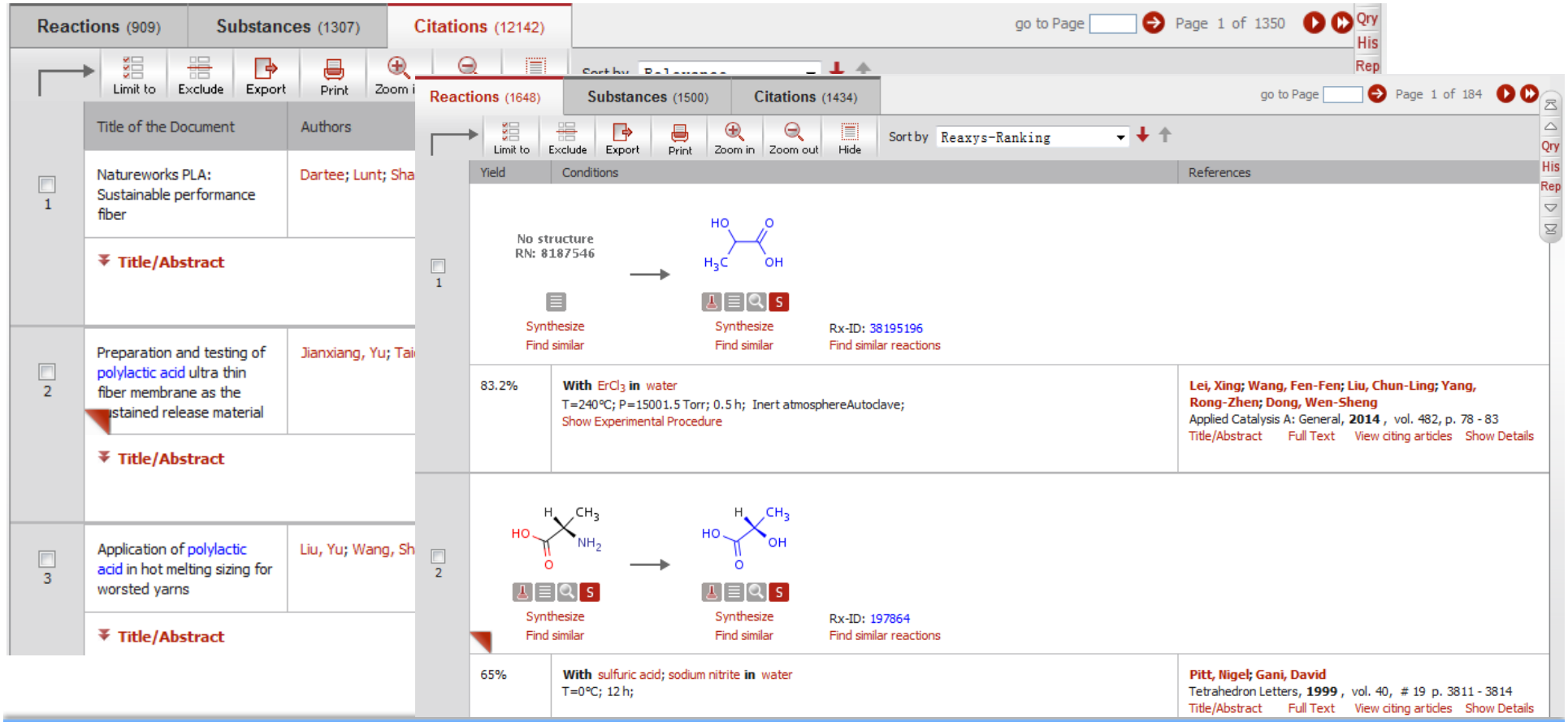
快速智能检索

- “publications about polylactic acid”
- “preparation of polylactic acid”



反应检索


Structure
selected query editor:
MarvinSketch
by ChemAxon
PASTE
STRUCTURE EDITOR
As drawn
Substructure
on heteroatoms
on all atoms
Similarity
结构限定
Include tautomers
Ignore stereo
No isotopes
No charges
No radicals
No ring closures
Ignore atom mappings
Align results with query
Keep fragments
separate
together
化学结构其他
检索条件限定
Create Structure Template from Name
Please select role
Product
Starting material
Reagent / Catalyst
Any role
反应角色限定
Reaction Data
Yield (numerical)
Solvent
Reagent/Catalyst
Time (h)
Temperature (°C)
Pressure (Torr)
Reaction Type
Lookup
反应数据限定
Search Reactions

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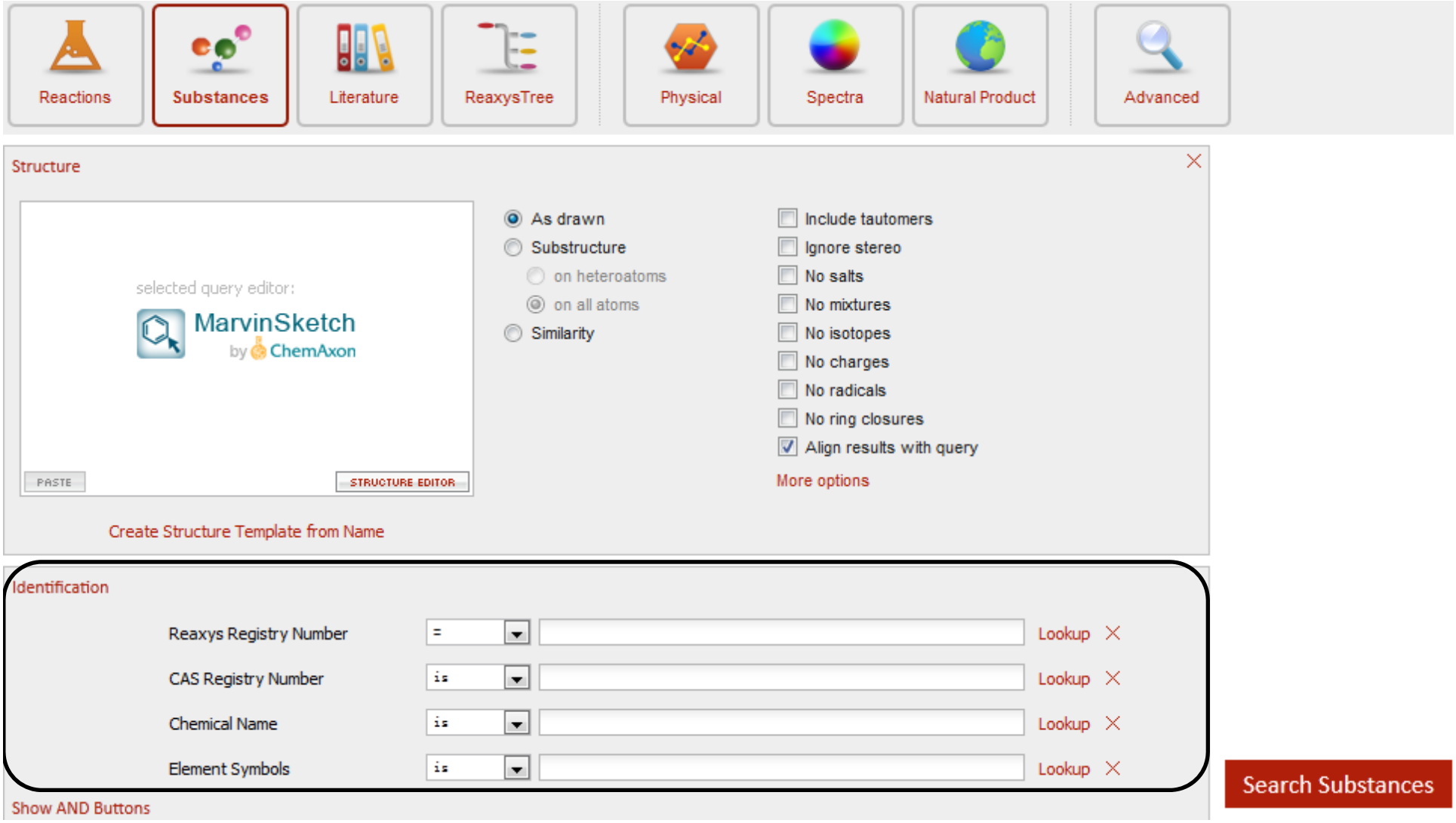
物质检索



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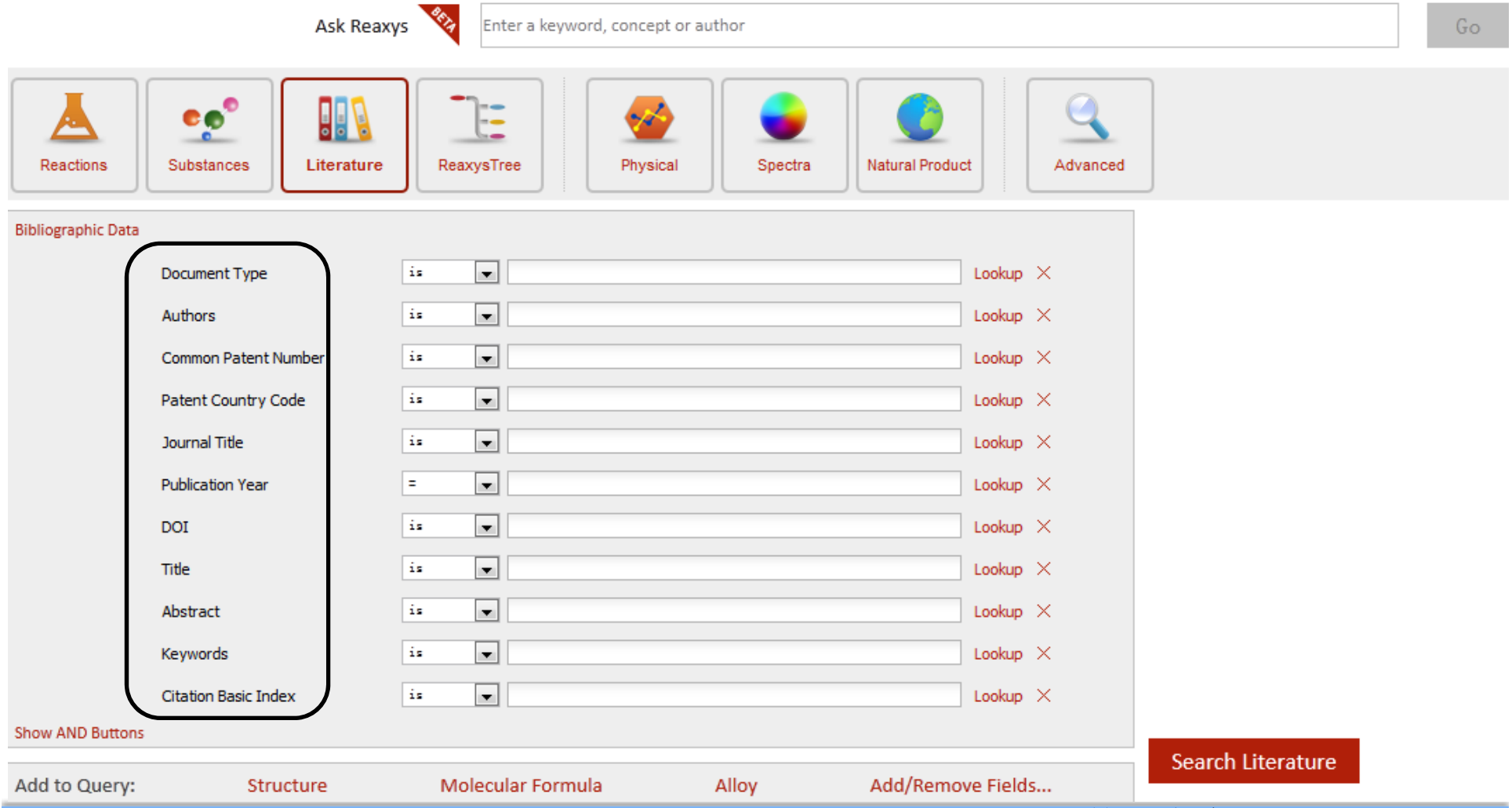
文献检索



Reaxys数据库介绍

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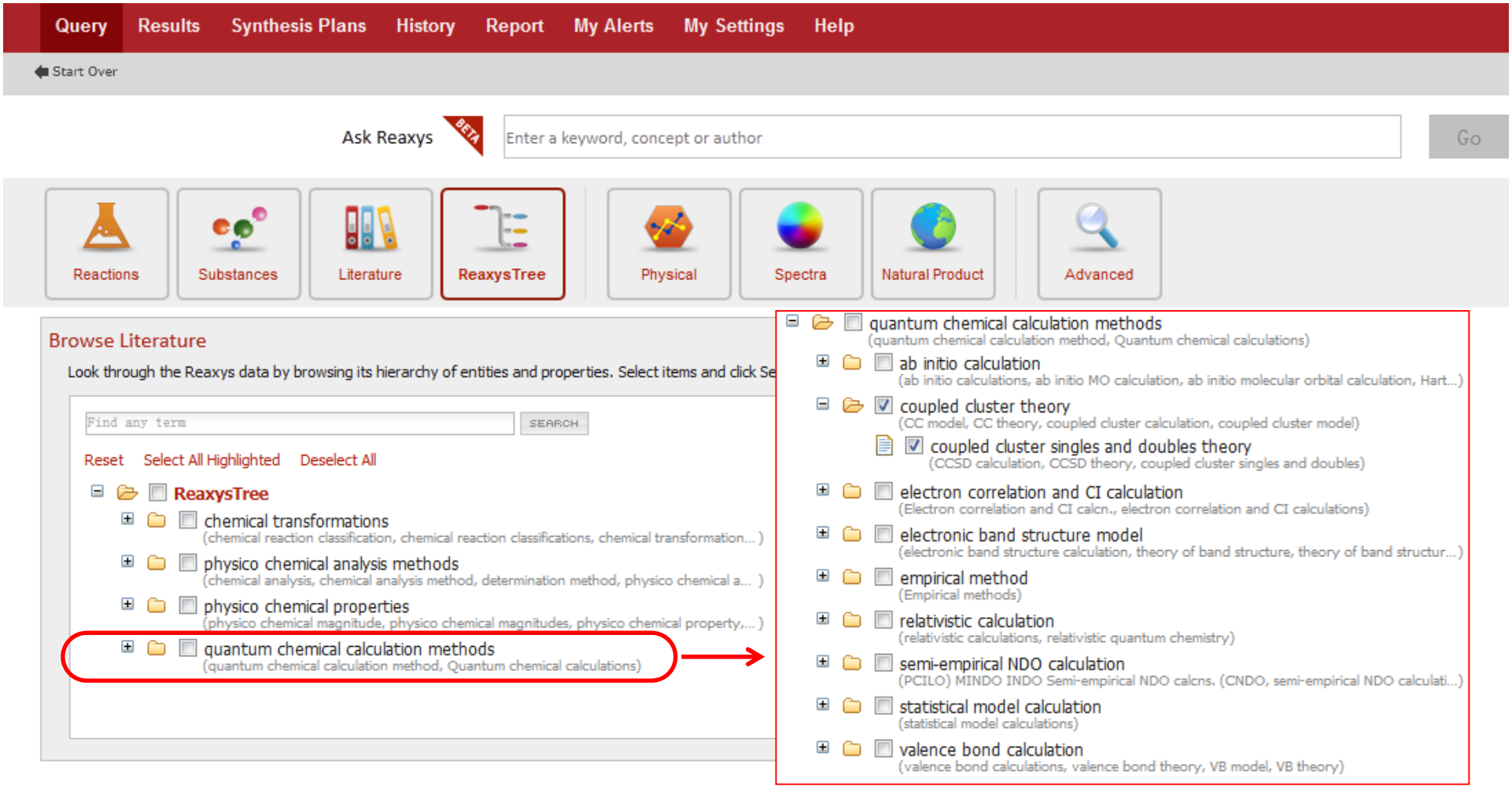
ReaxysTree检索

按Reaxys数据库的系统分类，进行选择、检索



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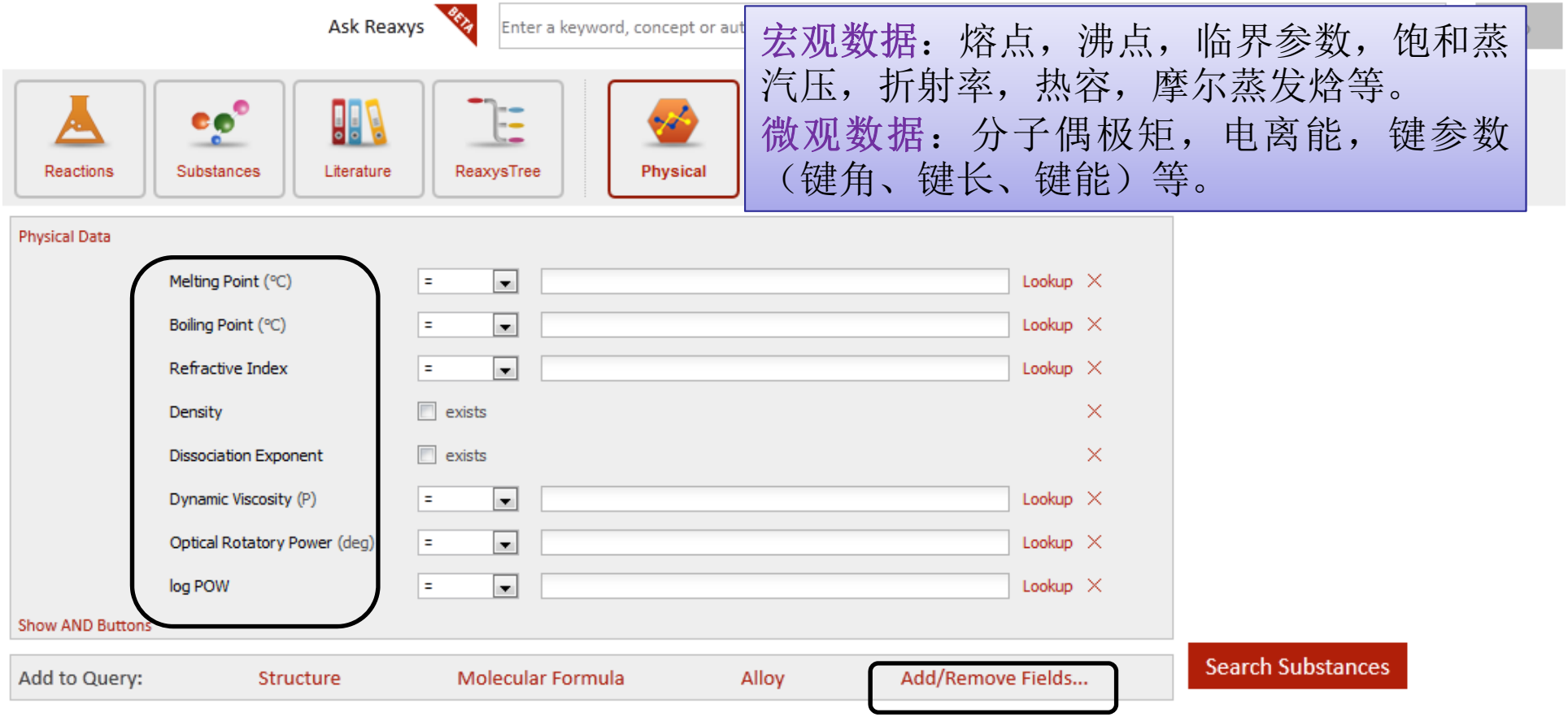
物理检索

宏观数据：熔点，沸点，临界参数，饱和蒸汽压，折射率，热容，摩尔蒸发焓等。
微观数据：分子偶极矩，电离能，键参数（键角、键长、键能）等。



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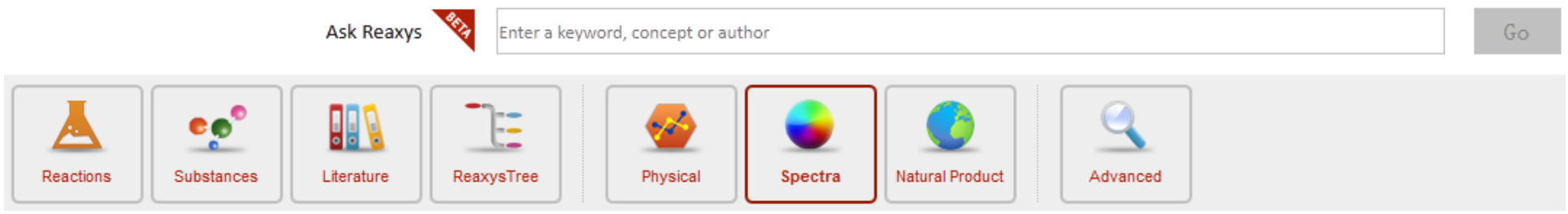
图谱检索



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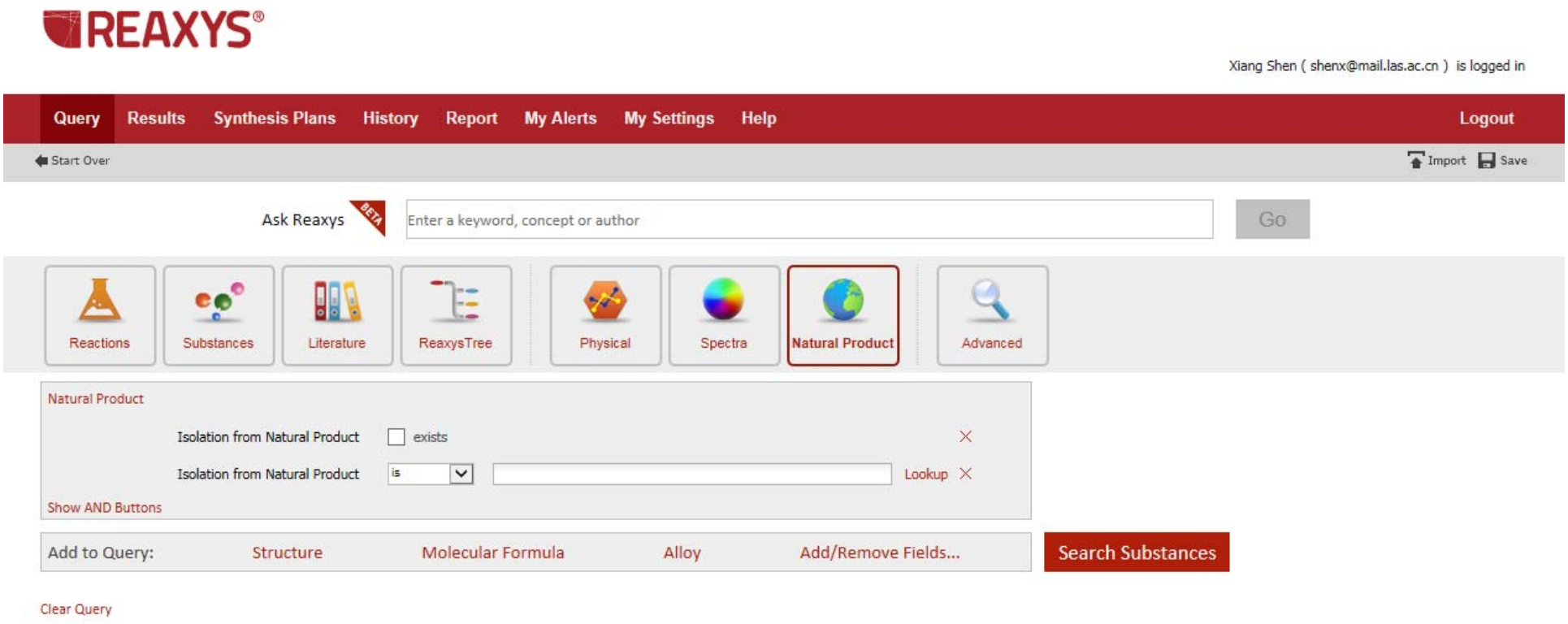
天热产物检索



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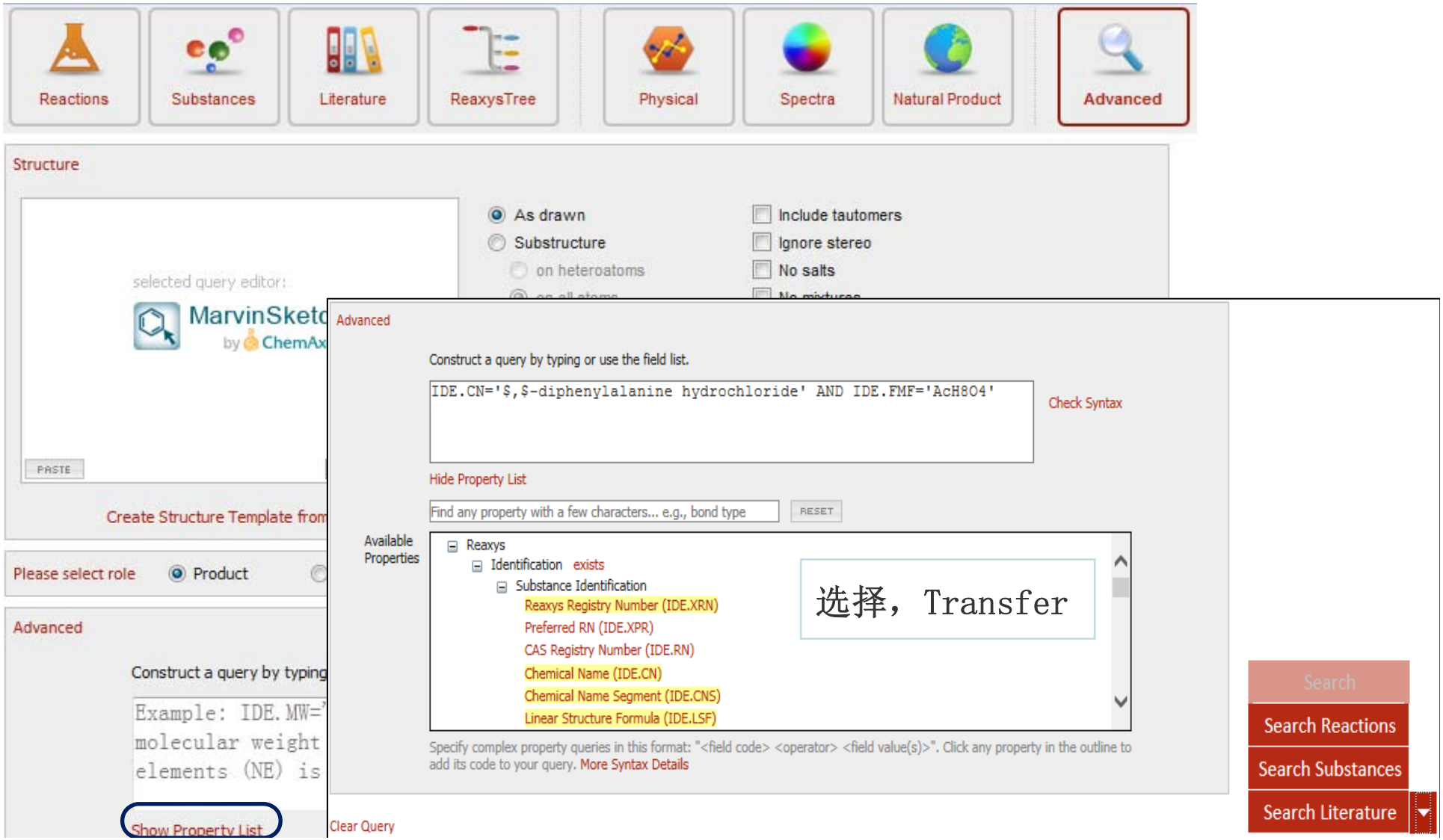
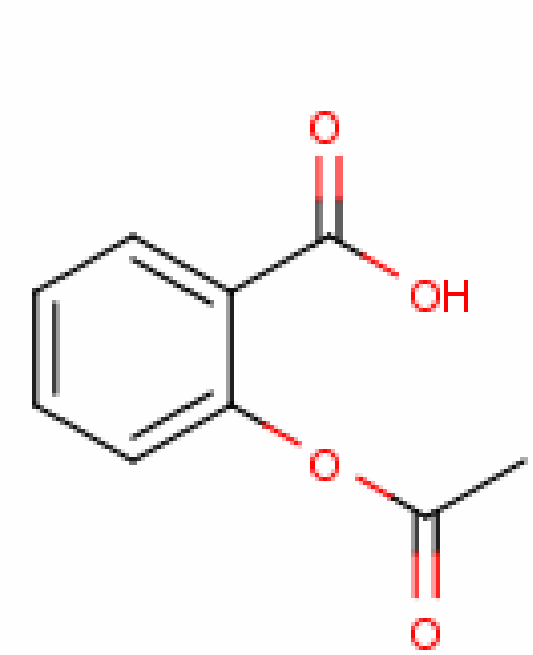
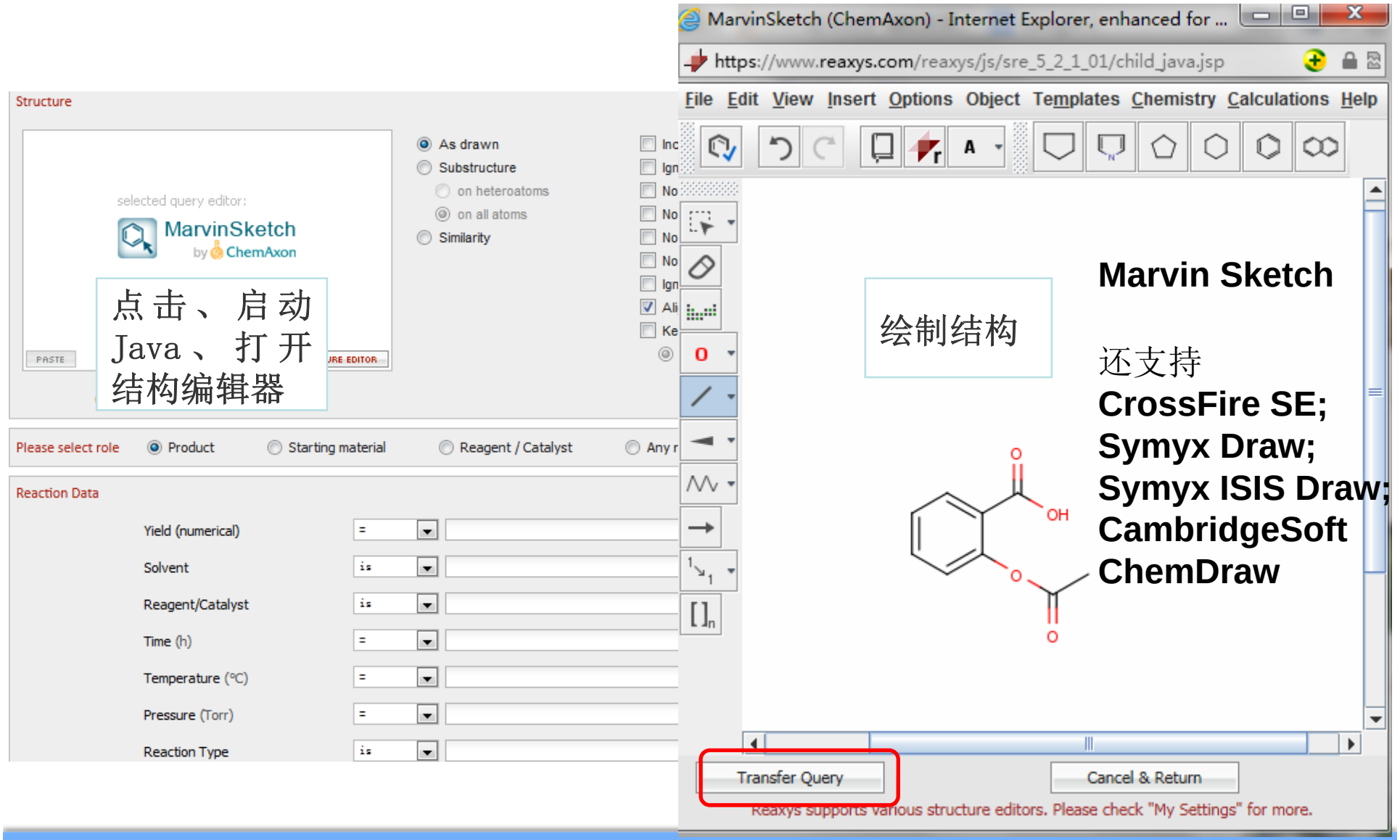
高级检索



检索示例



检索反应
设计合成路线


MarvinSketch (ChemAxon) - Internet Explorer, enhanced for ...
https://www.reaxys.com/reaxys/js/sre_5_2_1_01/child_java.jsp
File Edit View Insert Options Object Templates Chemistry Calculations Help
Structure
selected query editor:
MarvinSketch
by ChemAxon
点击、启动Java、打开结构编辑器
As drawn
Substructure
on heteroatoms
on all atoms
Similarity
Please select role
Product
Starting material
Reagent / Catalyst
Reaction Data
Yield (numerical)
Solvent
Reagent/Catalyst
Time (h)
Temperature (°C)
Pressure (Torr)
Reaction Type
绘制结构
Marvin Sketch
还支持
CrossFire SE;
Symyx Draw;
Symyx ISIS Draw;
CambridgeSoft ChemDraw
Transfer Query
Cancel & Return
Reaxys supports various structure editors. Please check "My Settings" for more.

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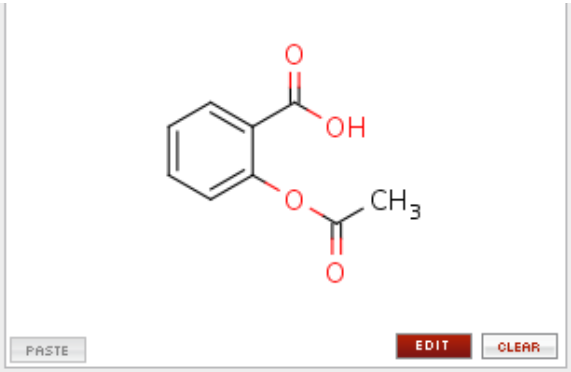

As drawn
Substructure
on heteroatoms
on all atoms
Similarity

Create Structure Template from Name

Please select role: Product | Starting material | Reagent / Catalyst

Reaction Data

Yield (numerical)	=	
Solvent		ethan
Reagent/Catalyst		
Time (h)	=	
Temperature (°C)	=	
Pressure (Torr)	=	
Reaction Type	is	
Reaction Basic Index	is	

= < <= > >=

is starts with ends with contains

Lookup

Show AND Buttons

Add to Query: Structure Molecu... Alloy Add/Remove Fields...

Search Reactions

Select index items and click 'Transfer'

Reaxys

Search for: ethan

可多选

ethanbol (1)
ethane (5)
ethane 1,2-dithiol (2)
ethane-1,2-diamine (5)
ethane-1,2-diol (52)
ethane-1,2-dithiol (9)
ethanedioic acid dihydrate (1)
ethanediol methyl ether (2)
ethanedithiol; 1,2- (1)
ethanesulfonic acid (1)
ethanethioamide (3)
ethanethiol (1623)
ethanethiolic acid (20)
ethanl (2)
ethanlo (1)
ethanno (2)
ethannol (4)
ethano (4)
ethano; (1)
ethanol (4111556)

Transfer
Reset
Cancel

Page 312 of 572

ethanbol
ethane
ethane 1,2-dithiol
ethane-1,2-diamine
ethane-1,2-diol
ethane-1,2-dithiol
ethanedioic acid dihydrate
ethanediol methyl ether
ethanedithiol; 1,2-
ethanesulfonic acid
ethanethioamide
ethanethiol
ethanethiolic acid

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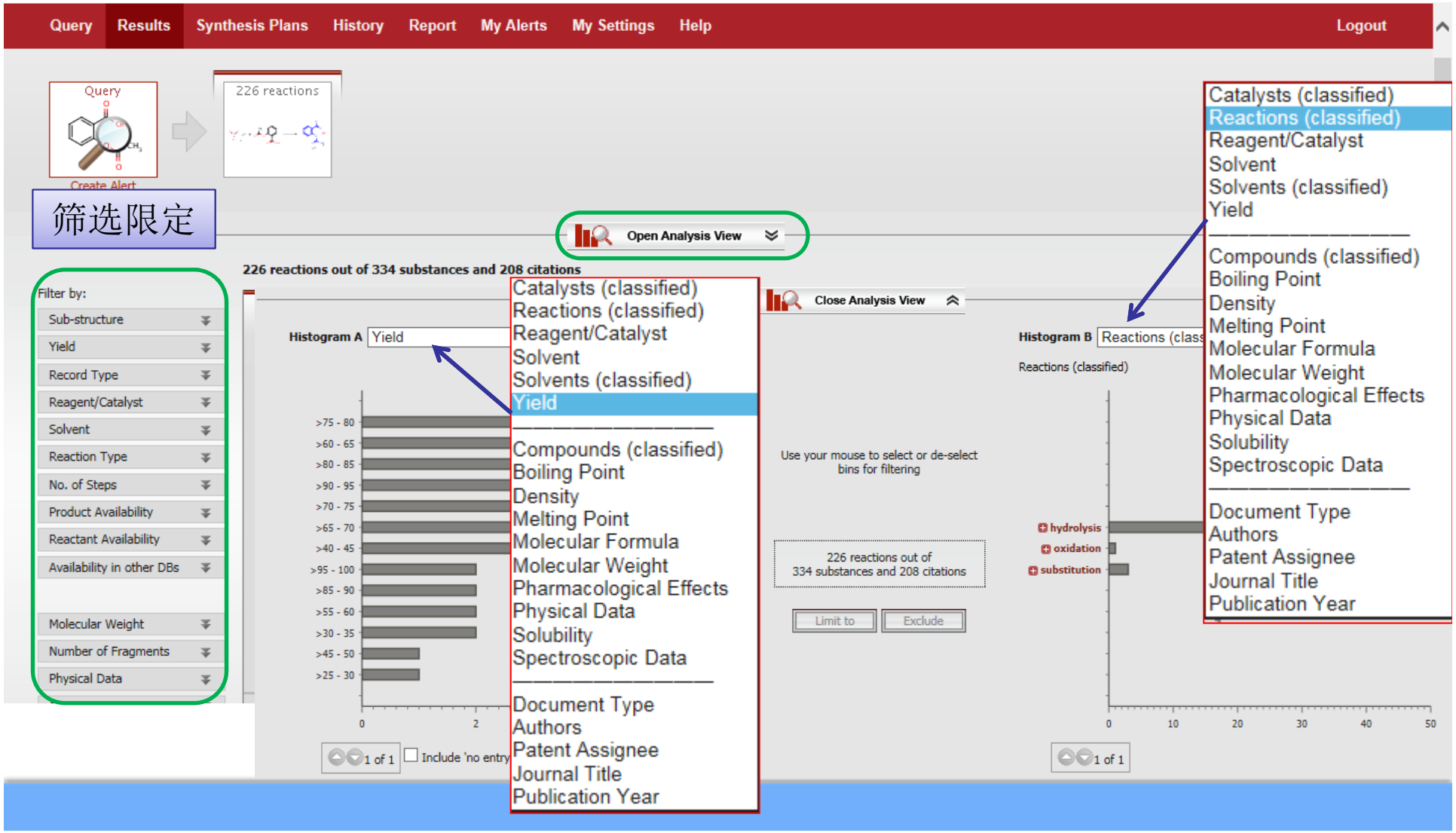
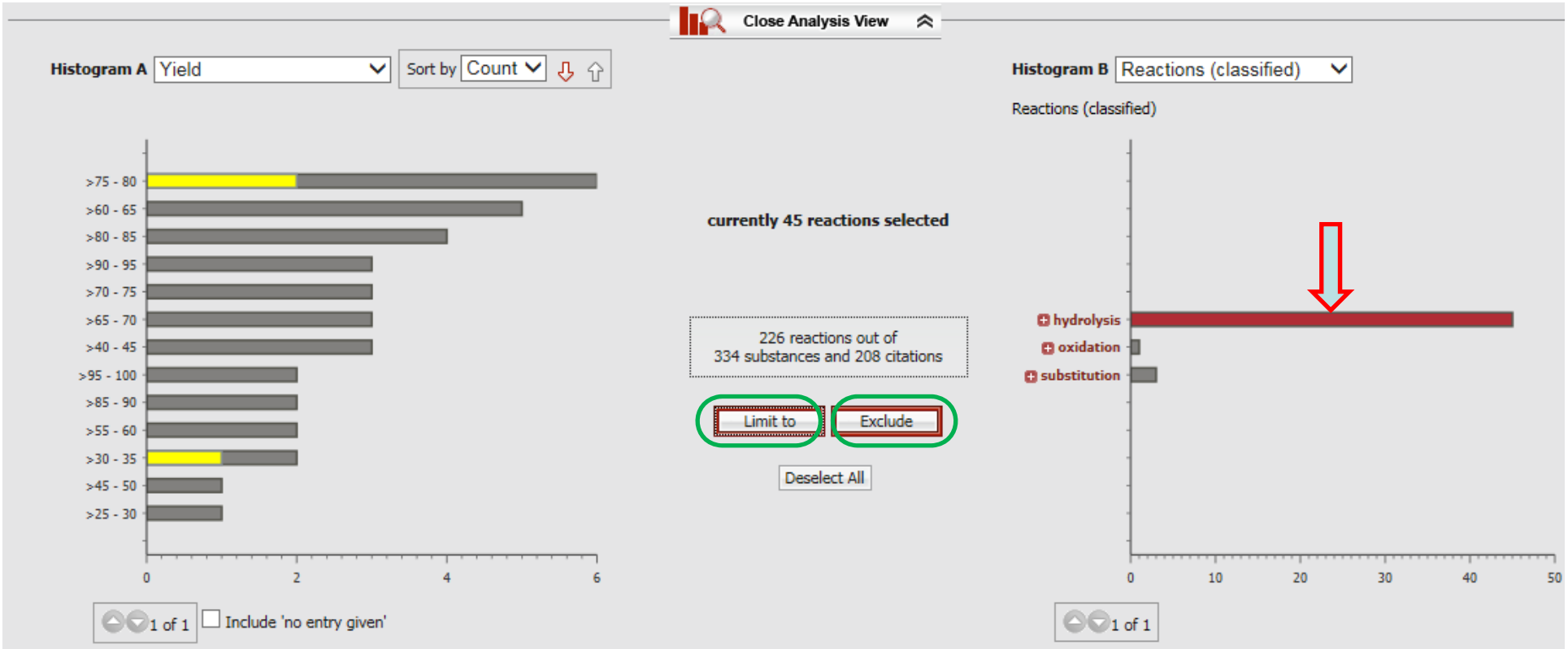
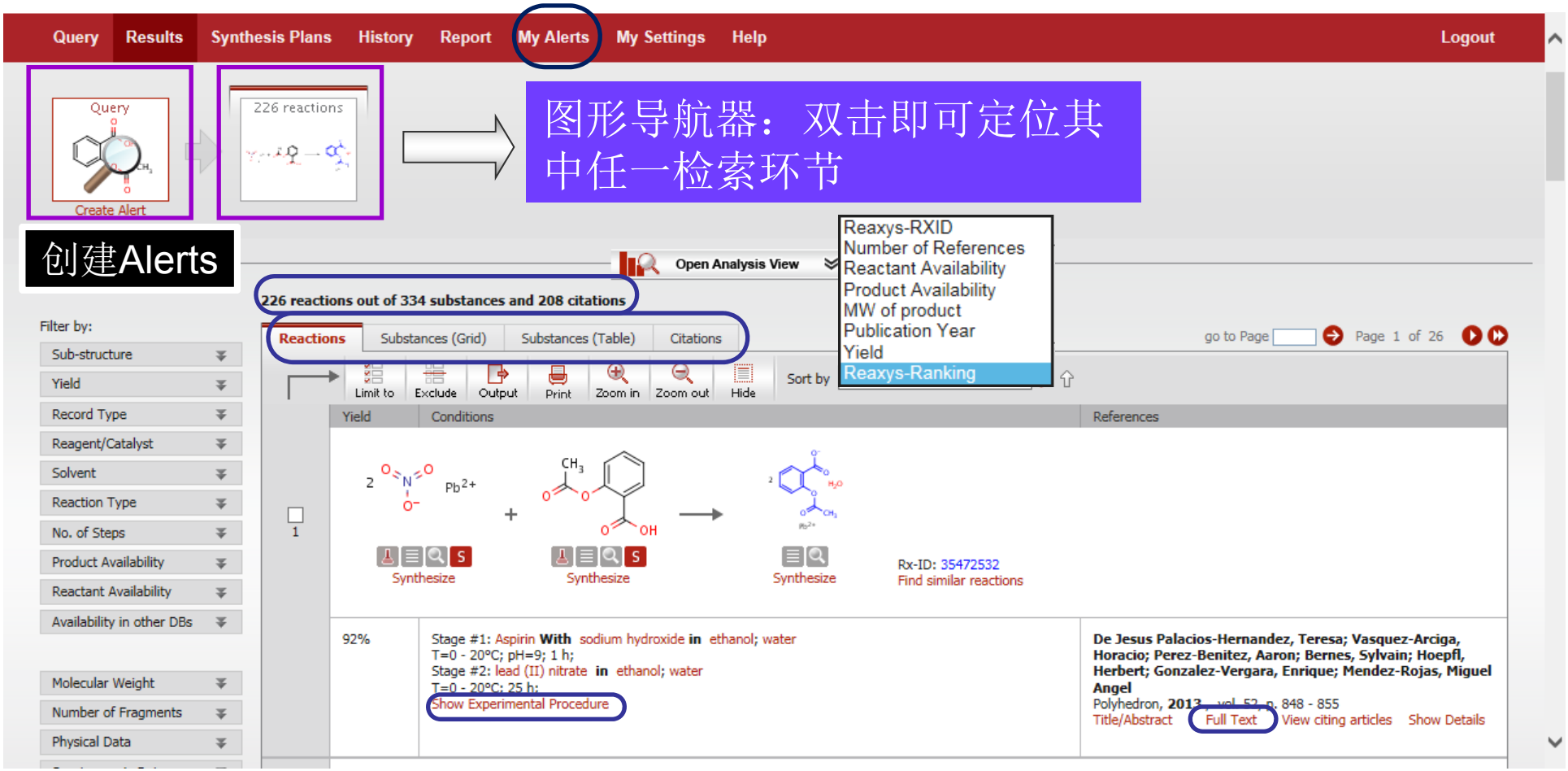
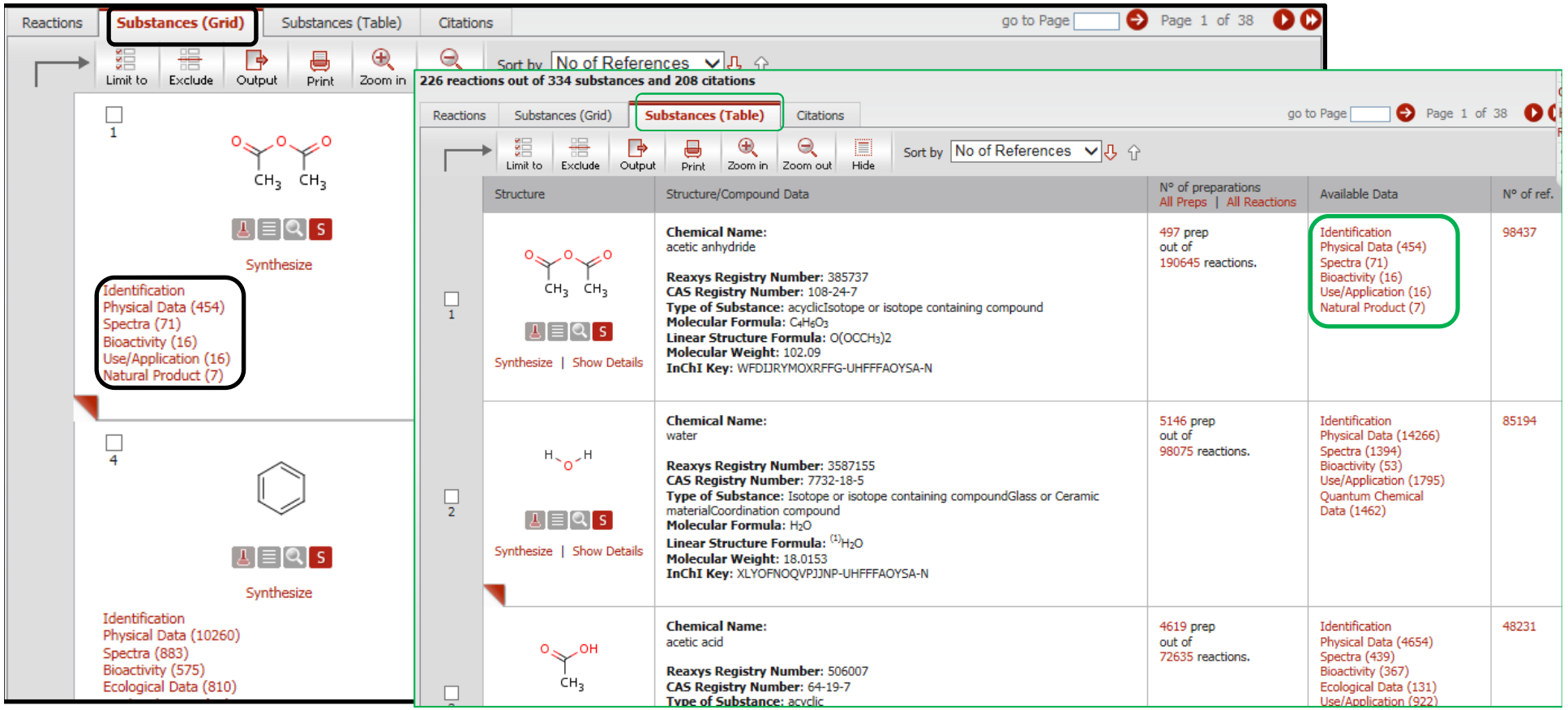



Close Analysis View
Histogram A
Yield
Sort by
Count
>75 - 80
>60 - 65
>80 - 85
>90 - 95
>70 - 75
>65 - 70
>40 - 45
>95 - 100
>85 - 90
>55 - 60
>30 - 35
>45 - 50
>25 - 30
0
2
4
6
1 of 1
Include 'no entry given'
currently 45 reactions selected
226 reactions out of
334 substances and 208 citations
Limit to
Exclude
Deselect All
Histogram B
Reactions (classified)
Reactions (classified)
hydrolysis
oxidation
substitution
0
10
20
30
40
50
1 of 1


Query
Results
Synthesis Plans
History
Report
My Alerts
My Settings
Help
Logout
Query
Create Alert
226 reactions
图形导航器：双击即可定位其中任一检索环节
创建Alerts
Open Analysis View
Reaxys-RXID
Number of References
Reactant Availability
Product Availability
MW of product
Publication Year
Yield
Reaxys-Ranking
226 reactions out of 334 substances and 208 citations
Reactions
Substances (Grid)
Substances (Table)
Citations
go to Page
Page 1 of 26
Filter by:
Sub-structure
Yield
Record Type
Reagent/Catalyst
Solvent
Reaction Type
No. of Steps
Product Availability
Reactant Availability
Availability in other DBs
Molecular Weight
Number of Fragments
Physical Data
Limit to
Exclude
Output
Print
Zoom in
Zoom out
Hide
Sort by
Yield
Conditions
References
Synthesize
Synthesize
Synthesize
Rx-ID: 35472532
Find similar reactions
92%
Stage #1: Aspirin With sodium hydroxide in ethanol; water
T=0 - 20°C; pH=9; 1 h;
Stage #2: lead (II) nitrate in ethanol; water
T=0 - 20°C; 25 h;
Show Experimental Procedure
De Jesus Palacios-Hernandez, Teresa; Vasquez-Arciga, Horacio; Perez-Benitez, Aaron; Bernes, Sylvain; Hoepfl, Herbert; Gonzalez-Vergara, Enrique; Mendez-Rojas, Miguel Angel
Polyhedron, 2013
Title/Abstract
Full Text
View citing articles
Show Details

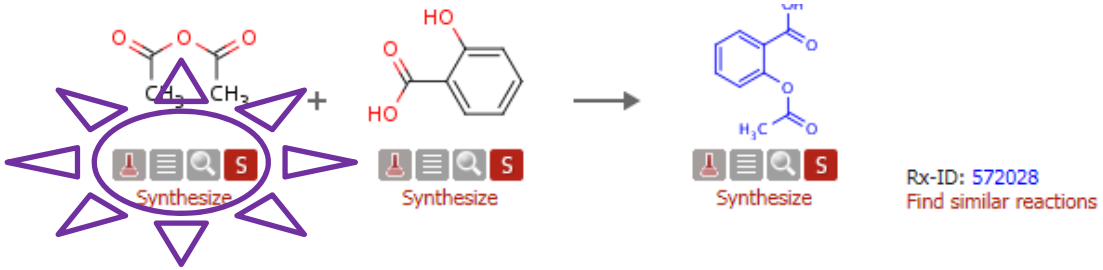

Reactions
Substances (Grid)
Substances (Table)
Citations
go to Page
Page 1 of 38
Limit to
Exclude
Output
Print
Zoom in
Sort by No of References
1
Synthesize
Identification
Physical Data (454)
Spectra (71)
Bioactivity (16)
Use/Application (16)
Natural Product (7)
4
Synthesize
Identification
Physical Data (10260)
Spectra (883)
Bioactivity (575)
Ecological Data (810)
226 reactions out of 334 substances and 208 citations
Zoom out
Hide
Structure
Structure/Compound Data
N° of preparations
All Preps | All Reactions
Available Data
N° of ref.
Chemical Name: acetic anhydride
Reaxys Registry Number: 385737
CAS Registry Number: 108-24-7
Type of Substance: acyclicIsotope or isotope containing compound
Molecular Formula: C4H6O3
Linear Structure Formula: O(OCCH3)2
Molecular Weight: 102.09
InChI Key: WFDIJRYMOXRFFG-UHFFFAOYSA-N
497 prep out of 190645 reactions.
98437
Synthesize | Show Details
Chemical Name: water
Reaxys Registry Number: 3587155
CAS Registry Number: 7732-18-5
Type of Substance: Isotope or isotope containing compoundGlass or Ceramic materialCoordination compound
Molecular Formula: H2O
Linear Structure Formula: (1)H2O
Molecular Weight: 18.0153
InChI Key: XLYOFNOQVPJJNP-UHFFFAOYSA-N
5146 prep out of 98075 reactions.
Identification
Physical Data (14266)
Spectra (1394)
Bioactivity (53)
Use/Application (1795)
Quantum Chemical Data (1462)
85194
Chemical Name: acetic acid
Reaxys Registry Number: 506007
CAS Registry Number: 64-19-7
Type of Substance: acyclic
4619 prep out of 72635 reactions.
Identification
Physical Data (4654)
Spectra (439)
Bioactivity (367)
Ecological Data (131)
Use/Application (922)
48231

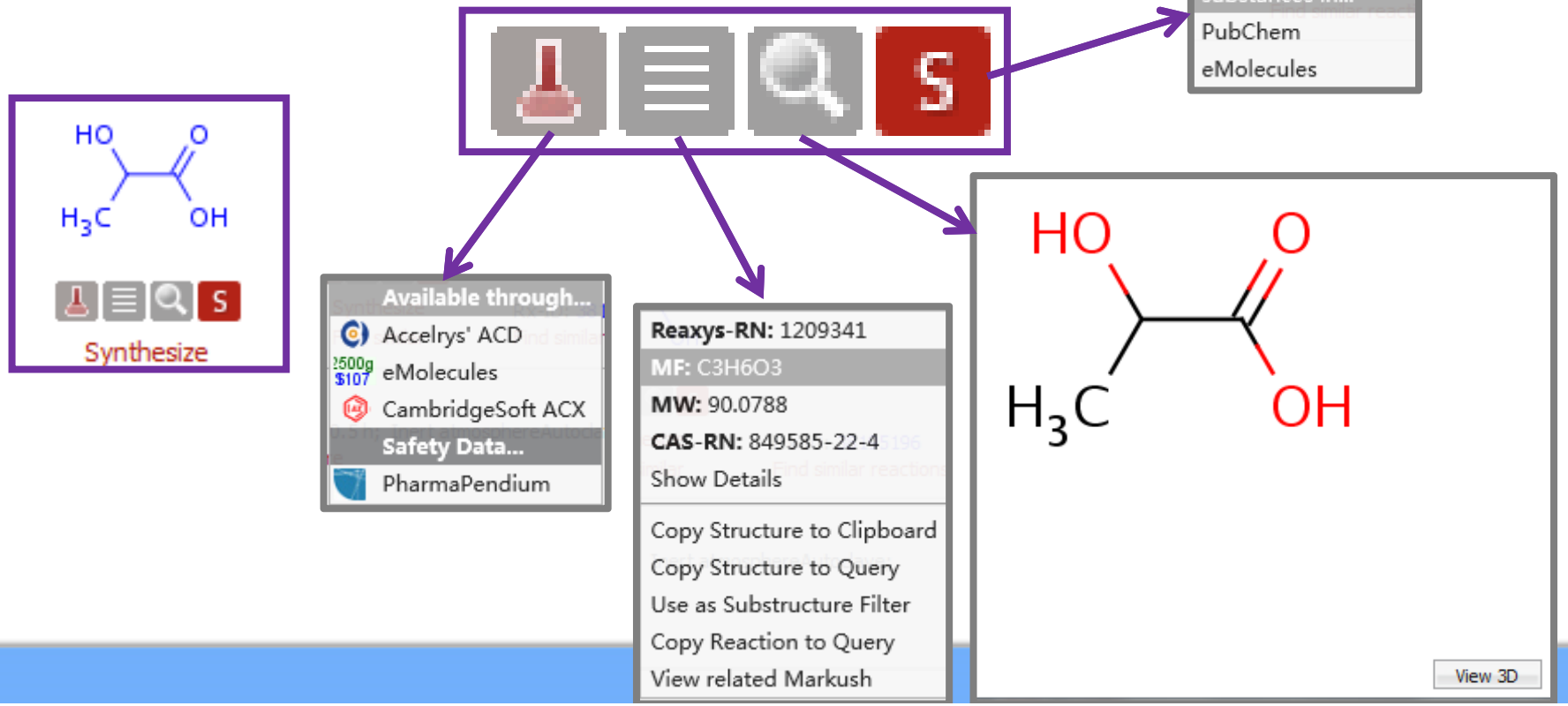
记录该反应的详细文献题录信息

Show All Reactions： 显示该文献中的所有化学反应信息

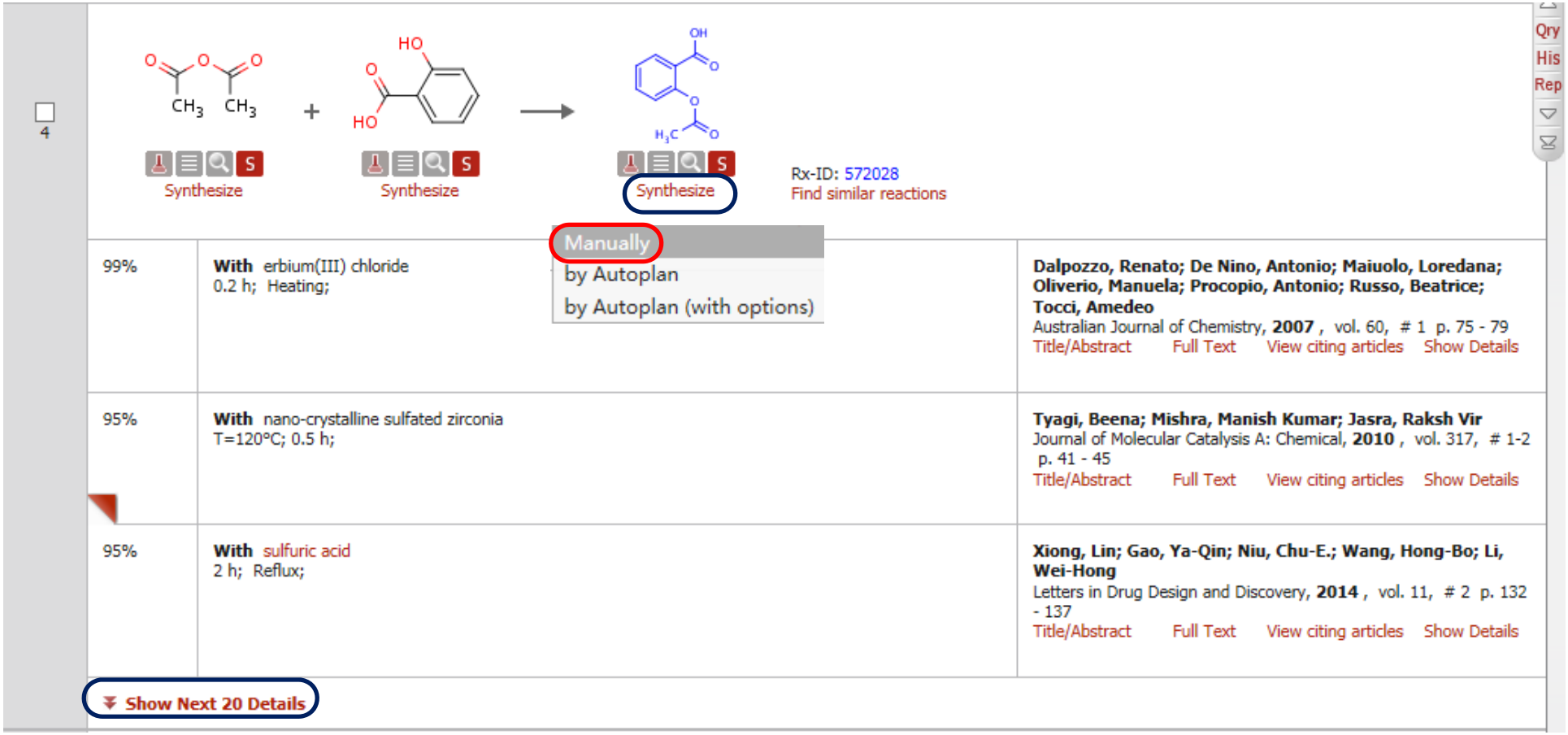
Hit Reactions in this article： 只显示该文献中与检索条件匹配的化学反应

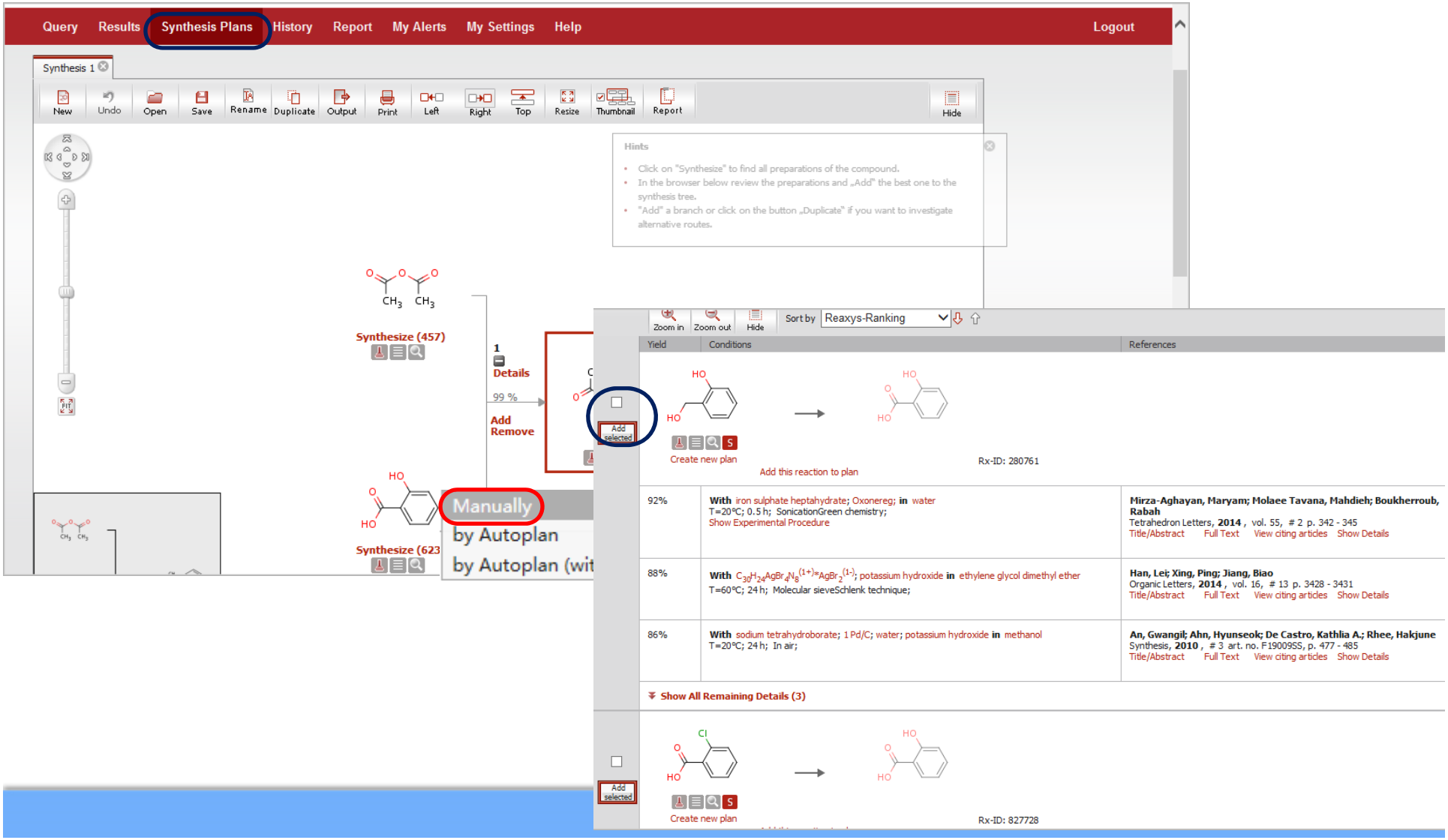
Show All Substances： 显示该文献中所有的化学物质


Synthesize
Synthesize
Synthesize
Rx-ID: 572028
Find similar reactions

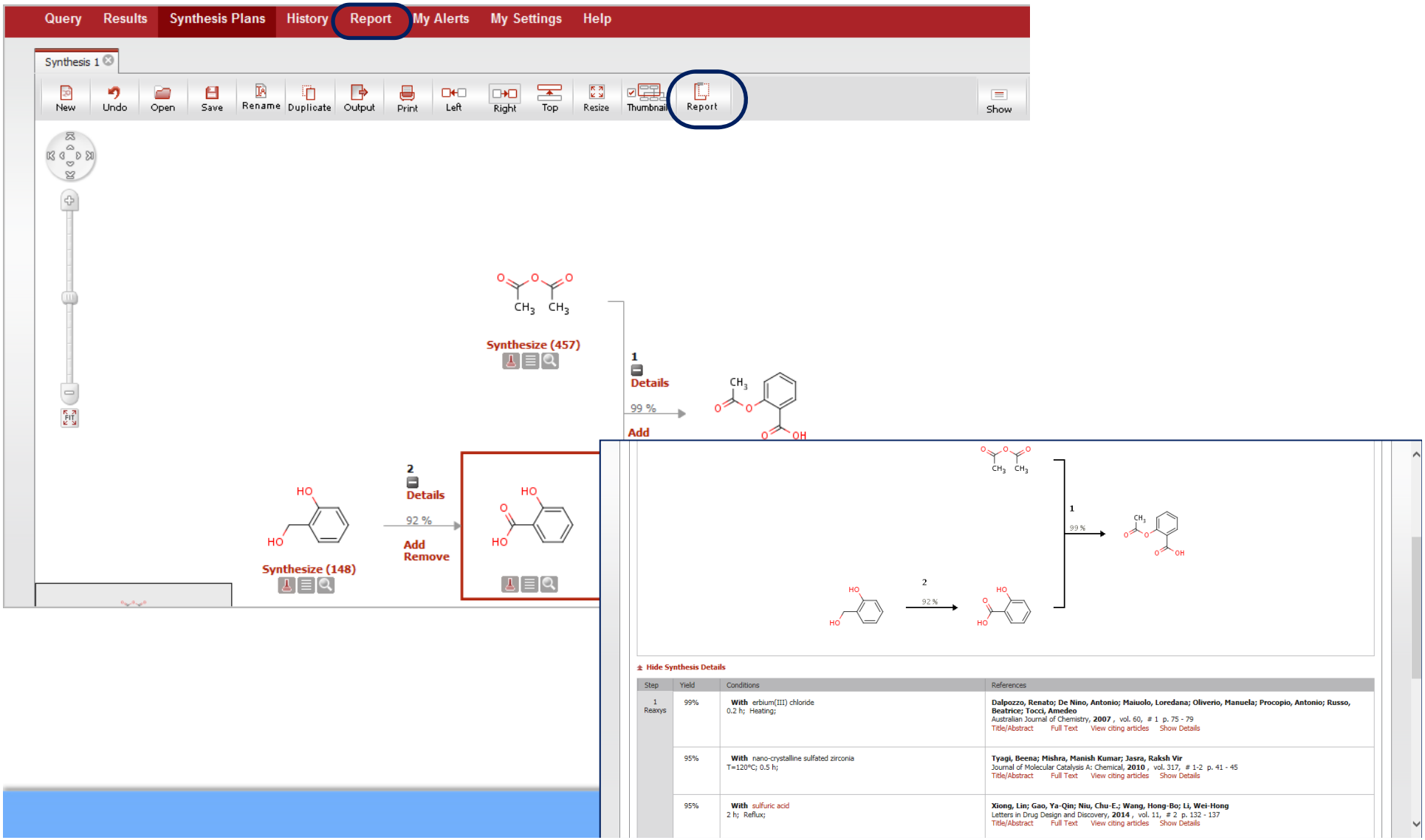

Show corresponding substances in...
PubChem
eMolecules
Synthesize
Available through...
Accelrys' ACD
eMolecules
CambridgeSoft ACX
Safety Data...
PharmaPendium
Reaxys-RN: 1209341
MF: C3H6O3
MW: 90.0788
CAS-RN: 849585-22-4
Show Details
Copy Structure to Clipboard
Copy Structure to Query
Use as Substructure Filter
Copy Reaction to Query
View related Markush
View 3D

Synthesis Plans：设计合成路线图



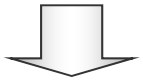

Query
Results
Synthesis Plans
History
Report
My Alerts
My Settings
Help
Logout
Synthesis 1
New
Undo
Open
Save
Rename
Duplicate
Output
Print
Left
Right
Top
Resize
Thumbnail
Report
Hide
Hints
Click on "Synthesize" to find all preparations of the compound.
In the browser below review the preparations and „Add" the best one to the synthesis tree.
"Add" a branch or click on the button „Duplicate" if you want to investigate alternative routes.
Synthesize (457)
1
Details
99 %
Add
Remove
Synthesize (623
Manually
by Autoplan
by Autoplan (wit
Zoom in
Zoom out
Hide
Sort by
Reaxys-Ranking
Yield
Conditions
References
Add selected
Create new plan
Add this reaction to plan
Rx-ID: 280761
92%
With iron sulphate heptahydrate; Oxonereg; in water
T=20°C; 0.5 h; SonicationGreen chemistry;
Show Experimental Procedure
Mirza-Aghayan, Maryam; Molaee Tavana, Mahdieh; Boukherroub, Rabah
Tetrahedron Letters, 2014 , vol. 55, # 2 p. 342 - 345
Title/Abstract Full Text View citing articles Show Details
88%
With C30H24AgBr4N8(1+)*AgBr2(1-); potassium hydroxide in ethylene glycol dimethyl ether
T=60°C; 24 h; Molecular sieveSchlenk technique;
Han, Lei; Xing, Ping; Jiang, Biao
Organic Letters, 2014 , vol. 16, # 13 p. 3428 - 3431
Title/Abstract Full Text View citing articles Show Details
86%
With sodium tetrahydroborate; 1 Pd/C; water; potassium hydroxide in methanol
T=20°C; 24 h; In air;
An, Gwangil; Ahn, Hyunseok; De Castro, Kathlia A.; Rhee, Hakjune
Synthesis, 2010 , # 3 art. no. F19009SS, p. 477 - 485
Title/Abstract Full Text View citing articles Show Details
Show All Remaining Details (3)
Add selected
Create new plan
Rx-ID: 827728

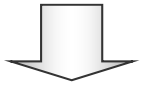
Report


Query
Results
Synthesis Plans
History
Report
My Alerts
My Settings
Help
Synthesis 1
New
Undo
Open
Save
Rename
Duplicate
Output
Print
Left
Right
Top
Resize
Thumbnails
Report
Show
Synthesize (457)
1
Details
99 %
Add
Synthesize (148)
2
Details
92 %
Add
Remove
Hide Synthesis Details
Step
Yield
Conditions
References
1
Reaxys
99%
With erbium(III) chloride
0.2 h; Heating;
Dalpozzo, Renato; De Nino, Antonio; Maiuolo, Loredana; Oliverio, Manuela; Procopio, Antonio; Russo, Beatrice; Tocci, Amedeo
Australian Journal of Chemistry, 2007 , vol. 60, # 1 p. 75 - 79
Title/Abstract Full Text View citing articles Show Details
95%
With nano-crystalline sulfated zirconia
T=120°C; 0.5 h;
Tyagi, Beena; Mishra, Manish Kumar; Jasra, Raksh Vir
Journal of Molecular Catalysis A: Chemical, 2010 , vol. 317, # 1-2 p. 41 - 45
Title/Abstract Full Text View citing articles Show Details
95%
With sulfuric acid
2 h; Reflux;
Xiong, Lin; Gao, Ya-Qin; Niu, Chu-E.; Wang, Hong-Bo; Li, Wei-Hong
Letters in Drug Design and Discovery, 2014 , vol. 11, # 2 p. 132 - 137
Title/Abstract Full Text View citing articles Show Details

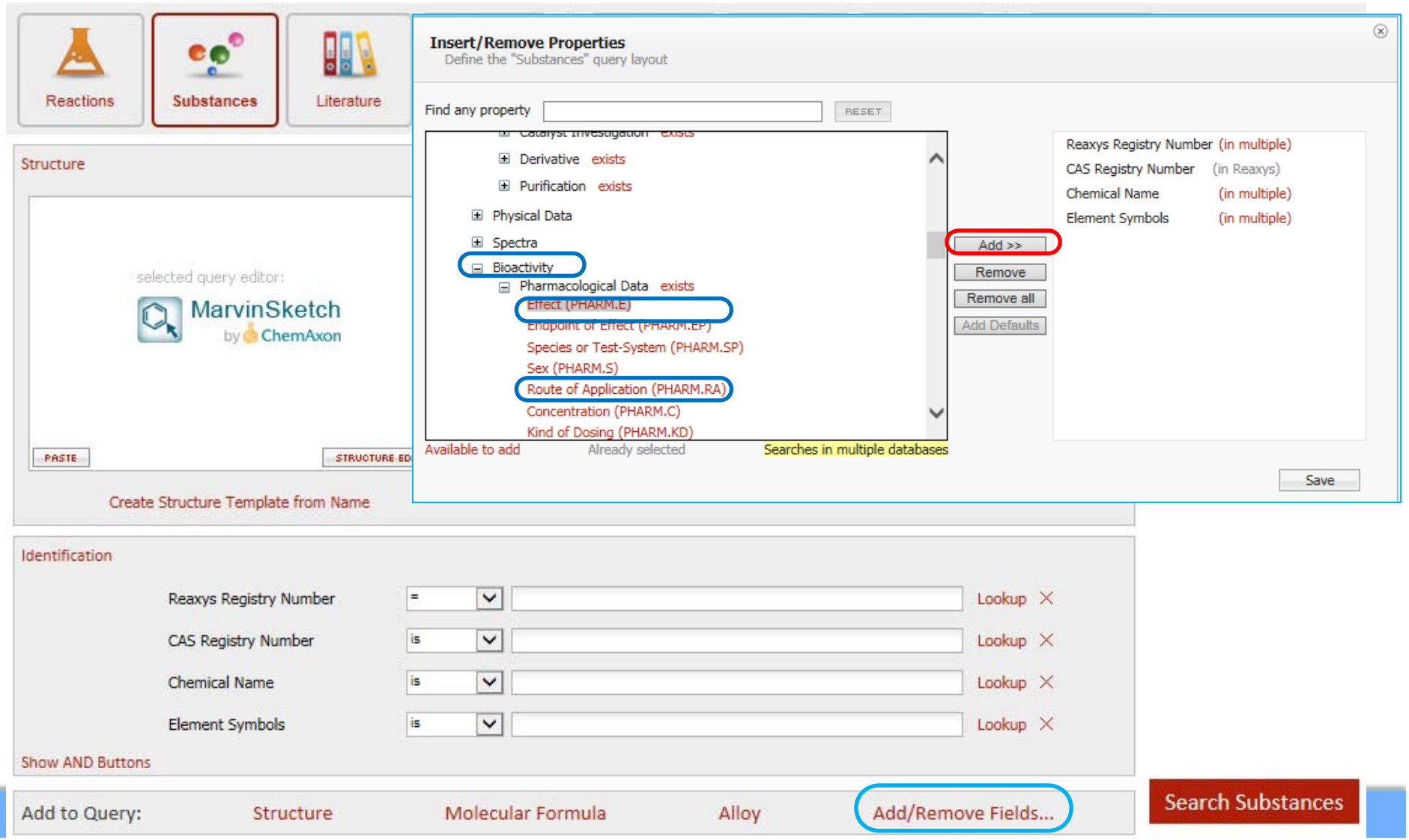
检索示例2：
物质检索

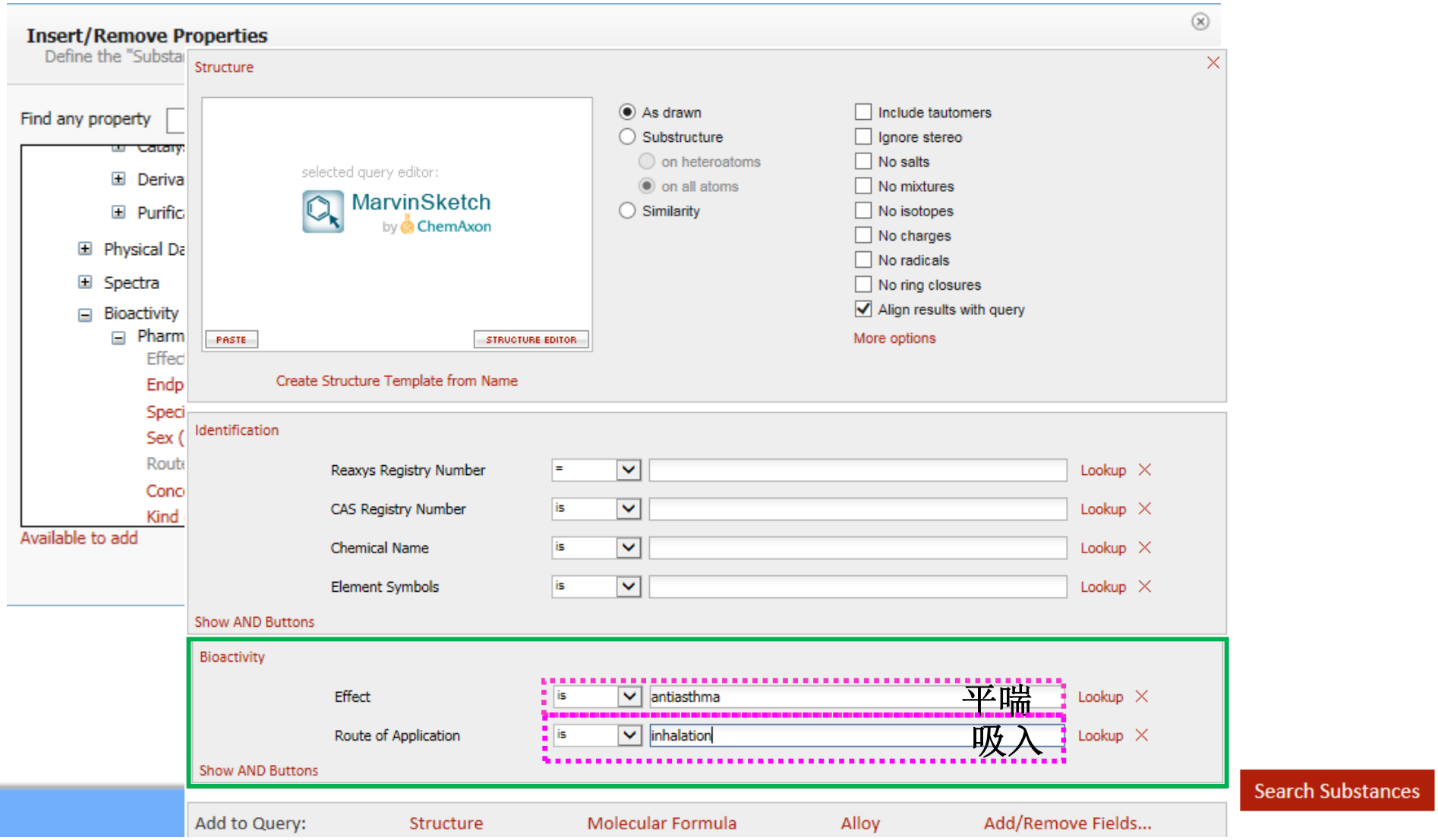
检索吸入时有平喘疗效的化合物

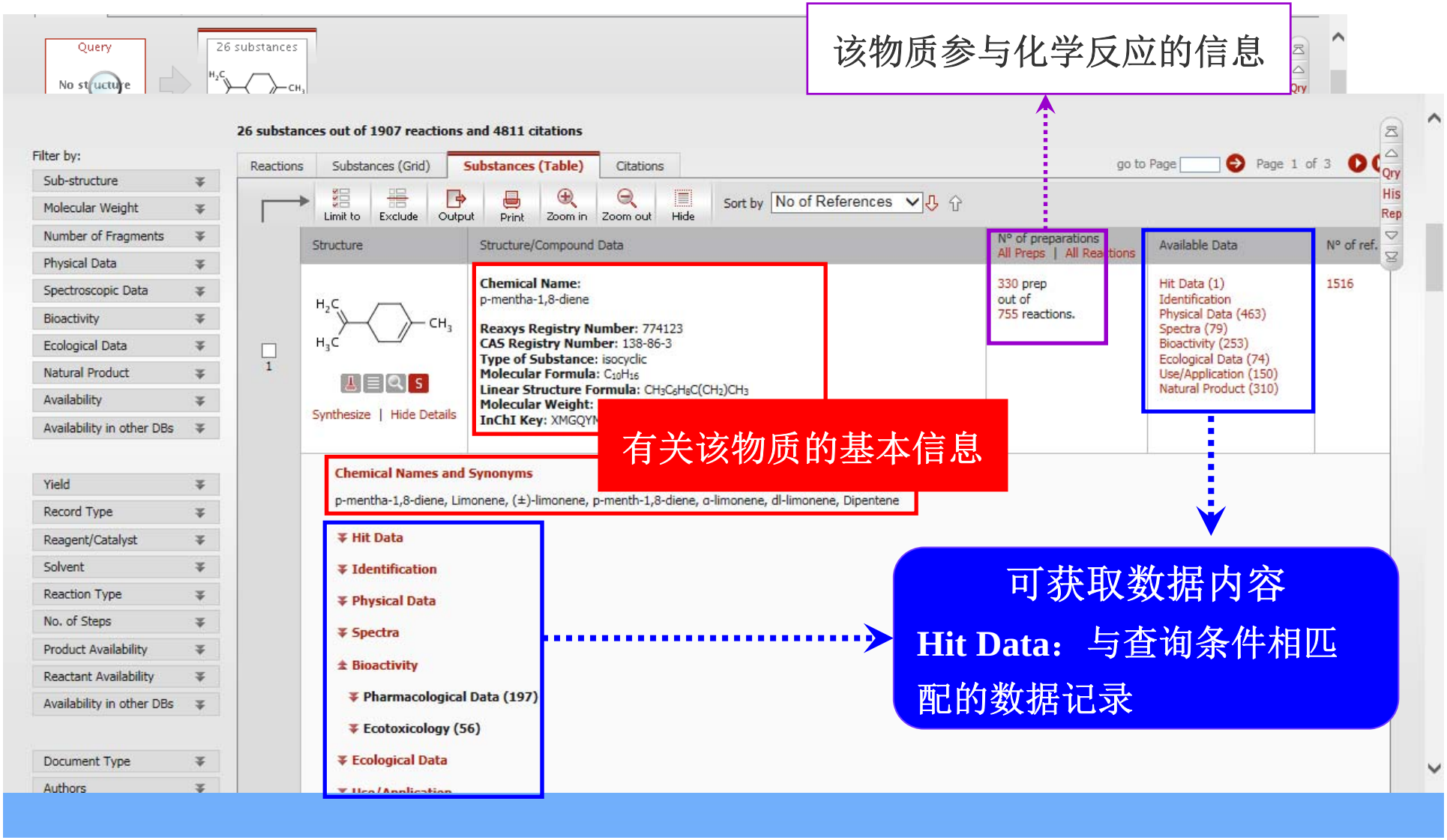




通过物质的药理学性质
查找合适的化合物


Reactions
Substances
Literature
Structure
selected query editor:
MarvinSketch
by ChemAxon
PASTE
STRUCTURE ED
Create Structure Template from Name
Insert/Remove Properties
Define the "Substances" query layout
Find any property
RESET
Derivative exists
Purification exists
Physical Data
Spectra
Bioactivity
Pharmacological Data exists
Effect (PHARM.E)
Species or Test-System (PHARM.SP)
Sex (PHARM.S)
Route of Application (PHARM.RA)
Concentration (PHARM.C)
Kind of Dosing (PHARM.KD)
Add >>
Remove
Remove all
Add Defaults
Reaxys Registry Number (in multiple)
CAS Registry Number (in Reaxys)
Chemical Name (in multiple)
Element Symbols (in multiple)
Available to add
Already selected
Searches in multiple databases
Save
Identification
Reaxys Registry Number
CAS Registry Number
Chemical Name
Element Symbols
Lookup
Show AND Buttons
Add to Query:
Structure
Molecular Formula
Alloy
Add/Remove Fields...
Search Substances


Insert/Remove Properties
Define the "Substa
Find any property
Deriva
Purific
Physical Da
Spectra
Bioactivity
Pharm
Effec
Endp
Speci
Sex (
Route
Conc
Kind
Available to add
Structure
selected query editor:
MarvinSketch
by ChemAxon
PASTE
STRUCTURE EDITOR
As drawn
Substructure
on heteroatoms
on all atoms
Similarity
Include tautomers
Ignore stereo
No salts
No mixtures
No isotopes
No charges
No radicals
No ring closures
Align results with query
More options
Create Structure Template from Name
Identification
Reaxys Registry Number
CAS Registry Number
Chemical Name
Element Symbols
Lookup
Show AND Buttons
Bioactivity
Effect
antiasthma
平喘
Route of Application
inhalation
吸入
Lookup
Show AND Buttons
Add to Query:
Structure
Molecular Formula
Alloy
Add/Remove Fields...
Search Substances


该物质参与化学反应的信息
Query
No structure
26 substances
26 substances out of 1907 reactions and 4811 citations
Filter by:
Sub-structure
Molecular Weight
Number of Fragments
Physical Data
Spectroscopic Data
Bioactivity
Ecological Data
Natural Product
Availability
Availability in other DBs
Yield
Record Type
Reagent/Catalyst
Solvent
Reaction Type
No. of Steps
Product Availability
Reactant Availability
Availability in other DBs
Document Type
Authors
Reactions
Substances (Grid)
Substances (Table)
Citations
go to Page
Page 1 of 3
Limit to
Exclude
Output
Print
Zoom in
Zoom out
Hide
Sort by
No of References
Structure
Structure/Compound Data
N° of preparations
All Preps | All Reactions
Available Data
N° of ref.
Chemical Name:
p-mentha-1,8-diene
Reaxys Registry Number: 774123
CAS Registry Number: 138-86-3
Type of Substance: isocyclic
Molecular Formula: C10H16
Linear Structure Formula: CH3C6H8C(CH2)CH3
Molecular Weight:
InChI Key: XMGQYM
330 prep
out of
755 reactions.
Hit Data (1)
Identification
Physical Data (463)
Spectra (79)
Bioactivity (253)
Ecological Data (74)
Use/Application (150)
Natural Product (310)
1516
Synthesize | Hide Details
有关该物质的基本信息
Chemical Names and Synonyms
p-mentha-1,8-diene, Limonene, (±)-limonene, p-menth-1,8-diene, α-limonene, dl-limonene, Dipentene
Hit Data
Identification
Physical Data
Spectra
Bioactivity
Pharmacological Data (197)
Ecotoxicology (56)
Ecological Data
Use/Application
可获取数据内容
Hit Data：与查询条件相匹配的数据记录
Qry
His
Rep

Chemical Names and Synonyms

p-mentha-1,8-diene, Limonene, (±)-limonene, p-menth-1,8-diene, α-limonene, dl-limonene, Dipent

每条记录都有对浓度、用量、使用方法以及效果等方面的详细数据

Hit Data

Pharmacological Data (1 Hits out of 197 view all)

1 of 1	**Effect**	antiasthma
	Species or Test-System	Brown Norway rat
	Sex	male
	Route of Application	inhalation
	Concentration	125 ppm
	Kind of Dosing	in air; animals breathed continuou
	Method	4-week-old rats sensitized on d 0; received title comp.; Penh value me
	Further Details	OVA: ovalbumin; sensitization by heat killed organisms in saline; non ... is
	Results	title comp. treatment resulted in significant decrease in Penh values close to that in control (1.71 and 1.70, resp.) in comparison with non-treated sensitized rats (2.34); after title comp. treatment minimal to mild pathological changes in lungs found
	Reference	**Keinan, Ehud; Alt, Aaron; Amir, Gail; Bentur, Lea; Bibi, Haim; Shoseyov, David** Bioorganic and Medicinal Chemistry, 2005 , vol. 13, # 2 p. 557 - 562 Title/Abstract Full Text View citing articles Show Details

Title/Abstract： *超链接访问文献记录*

Full Text： *链接到文献全文*

View citing articles： *链接到Scopus数据库中的该文献记录，查看该文献被引用情况*

Show Details: *详细的文献题录信息*

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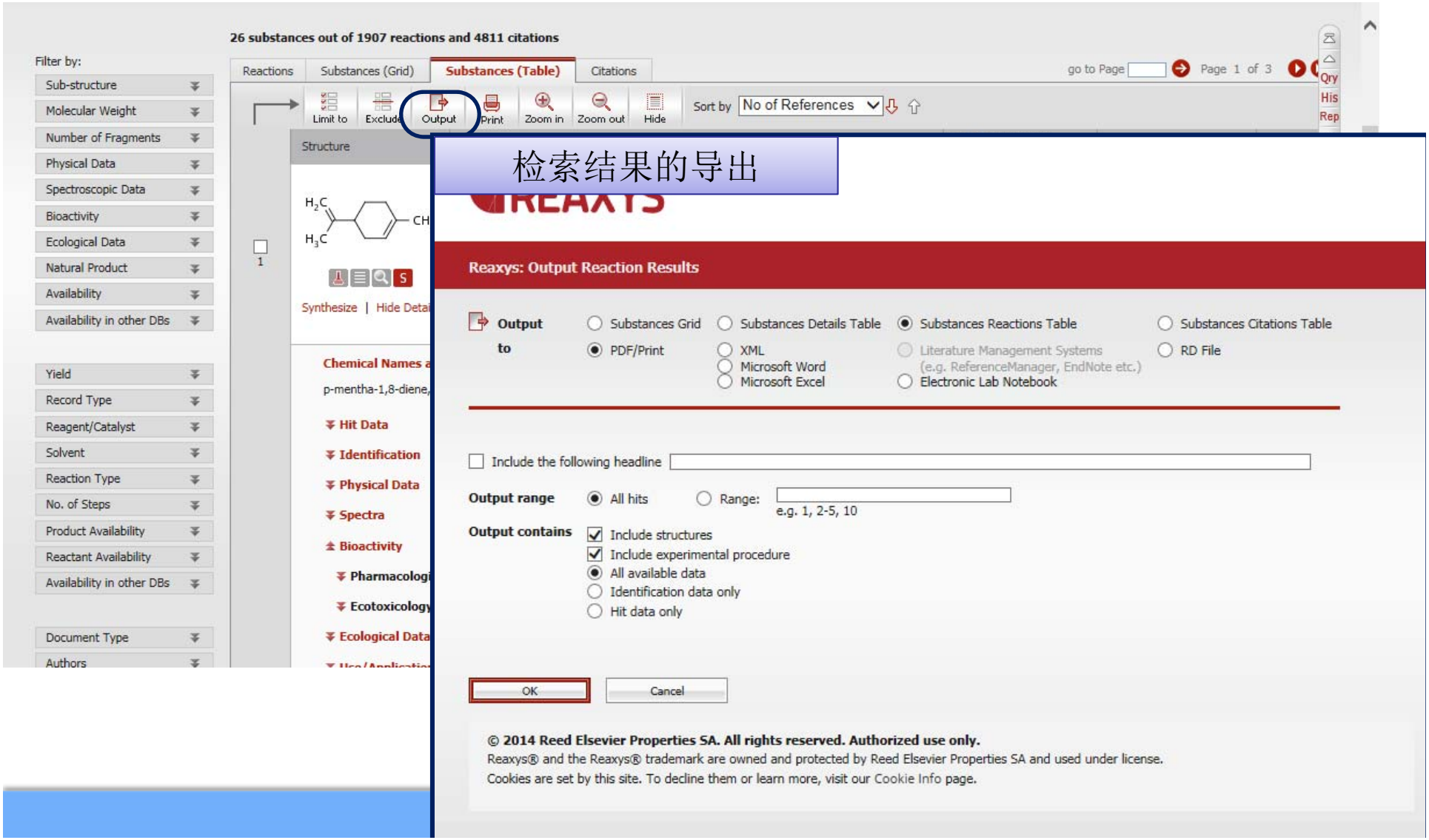
中国科学院国家科学图书馆



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中国科学院国家科学图书馆

Reaxys 平台优势

领域：有机化学、无机化学、金属有机化学

内容：反应、物质、文献

功能：实验步骤、全文、精炼、合成路线设计

提供经过确认的可靠的实验数据

- 科研杂志——物化数据；生物活性；自然产物；反应产率，反应条件，反应物/溶剂；催化剂；商品等；
- 专利——实验过程和光谱信息数据(NMR; IR; MS; UV/VIS)。

化学反应路线合成：

- 设计多步骤反应，比较可供选择的反应路线，帮您做出快速而准确的判断。

Reaxys排序，过滤和分析工具：

- 很容易找到、过滤和分析所得到数据，效率很高。

轻松访问：

- 总是能找到您所需要的信息。

谢谢！