

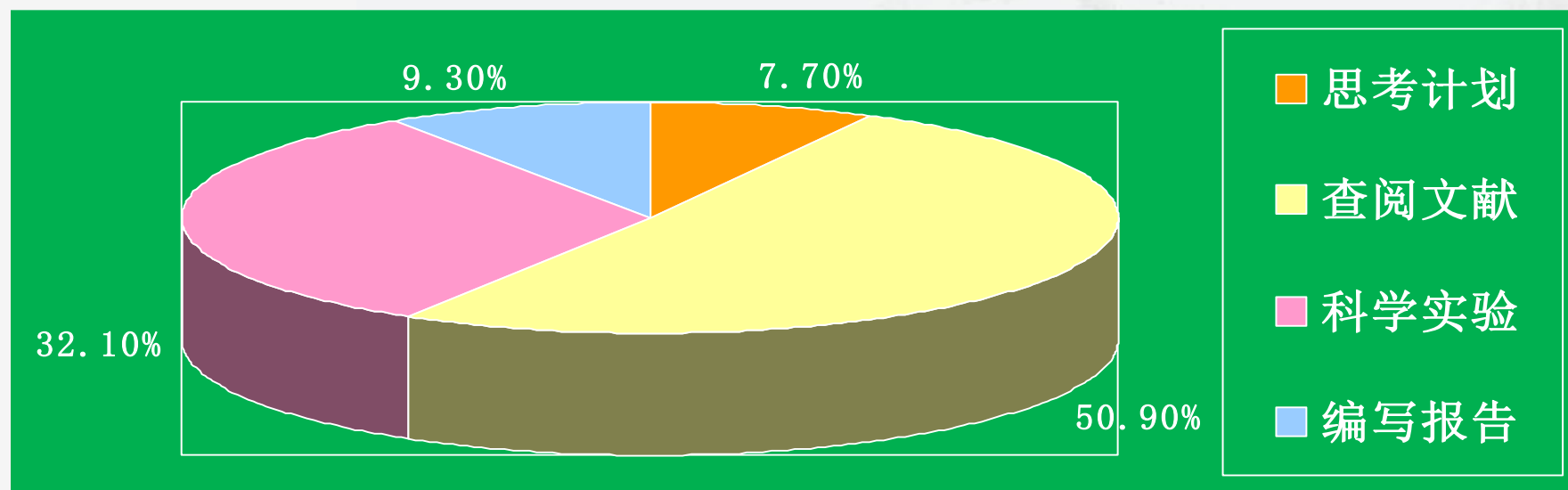


西安交通大学
XI'AN JIAOTONG UNIVERSITY

文献检索及立体异构的计算机模拟

少年班《有机化学实验》教学组

美国国家基金会在化工部的调查统计表明，科研人员工作时间分配：计划思考**7.70%**，信息收集**50.90%**，实验研究**32.10%**，数据处理占**9.30%**。



学习文献检索的目的：

- 增强文献信息检索与利用的意识；
- 熟悉文献信息检索与利用的基本工具；
- 掌握文献信息检索与利用的基本方法；
- 为继续学习和终生学习打下良好的基础。



现实意义：

- 利用文献跟踪学术动态
- 寻找科研课题
- 撰写毕业论文和科技论文
- 申请专利
-



文献类型：

（一）根据载体形式划分

印刷型:印刷在纸张上的文献

缩微型:通过缩微摄影技术将文献存储在胶片上

视听型:记录声音和图像的文献

电子型:以数字形式存储在磁带、磁盘、光盘等介质上,
并通过计算机、网络等读取的文献



(二) 根据加工深度划分

一次文献:原始文献,

包括:期刊论文、会议论文、学位论文、研究报告、专利文献、标准文献等

二次文献:用于查找一次文献线索的工具。

包括:目录、题录、索引、文摘等

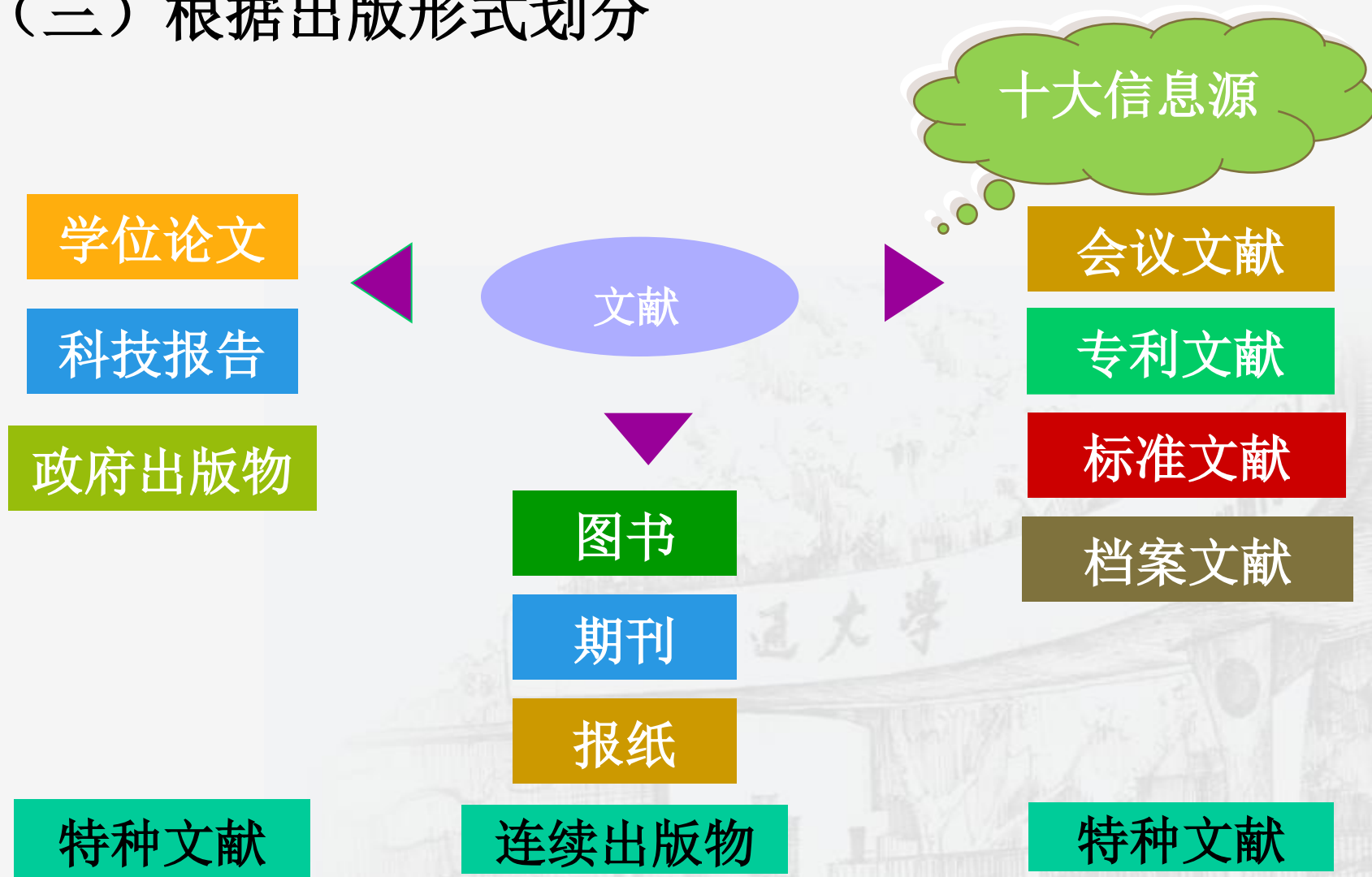
三次文献:对大量的一次文献进行阅读、分析、归纳、整理、概括而成,提供某一学科或专题的历史、现状、发展动态。

包括:综述、述评、进展、动态、指南等。



文献类型：

（三）根据出版形式划分



文献检索工具

题录(Title)

索引(Index)

文摘(Abstract)

文献数据库(Database)

事实数值检索工具

词典
百科全书
手册
年鉴
图表
指南
名录
等



一、重要的参考工具书

字典、辞典、手册、百科全书、年鉴等



常用的化学化工手册、百科全书：

综合性的：

1、CRC Handbook of Chemistry and Physics,

《CRC化学和物理手册》 R. C. Weast, CRC Press

1913年第一版，以后几乎每年一版，

内容不断更新，修订，目前已出到92版



68卷前:

A. Mathematics Tables;

B. The Elements and Inorganic Compounds;

C. Organic Compounds

D. General Chemical Tables

E. General Physical Constants

F. Miscellaneous

****Keywords Index**



2、International Critical Tables of Numerical Data, Physics, Chemistry and Technology

《国际物理、化学及工艺学数据判定表》

1924年以前数据，按主题分为300个项目，每个项目分别由各国专家执笔，数据经过严格审定。数据资料虽嫌陈旧，但仍有很大参考价值。



3、The Sadtler Standard Spectra Collections

《萨特勒标准光谱图集》

内容： 标准红外光谱（棱镜）
标准红外光谱（光栅）
标准紫外光谱
标准NMR

还有某些专业性图集如：**Raman**光谱、荧光光谱、差热分析等，每个图谱注明样品来源、纯度和使用技术（如溶剂、浓度、吸收池厚度等）



4、Atlas of Spectra Data and Physical Constants for Organic Compounds

《有机化合物的光谱数据与物理常数图谱集》

共收21000种有机化合物的光谱数据，包括质谱、NMR、
IR UV四方面，分装六册



3、专业性的--有机化学

(1) Beilstein Handbuch der Organische Chemie

《拜尔施泰因有机化学大全》

目前世界上有机化学方面资料收集得最为齐全的工具书。



第一版由在德国工作的德籍俄国著名化学家
F.K.Beilstein于1882年间编辑出版的。

1918年出第四版

1940年出完正版(H)，共31卷。

1928年开始出版补编

1972年起出版第四补编。



本书基本上收集了所有已经发表的有关有机化合物的文献资料数据。这些资料数据都经过严格的核对和精确验证，因而比较可靠。

本书资料来源于各种科学期刊、专利文献、重要的学位论文和会议报告等。每卷卷首列有所引用的期刊及其它出版物的全称和缩写，还附有缩写词的汇总表。



每个化合物记载的内容包括：

- (i)组成和结构；
- (ii)天然存在及从天然产物中提取的方法；
- (iii)制备方法、生成及提纯方法；
- (iv)分子结构及能量参数；
- (v)物理性质；
- (vi)化学性质；
- (vii)鉴定与分析；
- (viii) 盐及各种生成物。



(2) Dictionary of Organic Compounds

1934—1937年 第一版

1965年 第四版，正编五卷，15个补编

1985年 第五版

本书提供了有机化合物及衍生物的化学结构、物理性质和其它性质，以及有关参考文献及CA登记号。

全书共七卷，后两卷为化合物名称索引和分子式索引、杂原子索引和CA登记号索引。

本书第三版有中译本，书名为《汉译海氏有机化合物辞典》，共四卷，1966年由科学出版社出版。



(3) Comprehensive Organic Chemistry

《综合有机化学》 Pergamon, 1979

这是一本较新的有机化学参考工具书，书名副标题为有机化合物的合成与反应，第六卷为索引。

(4) Reagents for Organic Synthesis

《有机合成试剂》 WILEY, 1967

这是一本有机合成方面的重要参考工具书，收录了大量的有机合成用的重要试剂和催化剂资料，介绍了它们的结构式、分子量、物理常数、合成方法、提纯方法、商品来源和用途。



(5) The Merck Index, An Encyclopedia of Chemicals and Drugs

《化学品与药品的百科全书》 9th, ed. 1979, 11th ed. 1989

第九版收录了近万种化学制品和药品的制备方法，并列出了几万种有关的化学结构式。

该书按化学品和药品的名称顺序排列，并在每个名称前有流水号和CA登记号，每个名称后面列出了由IUPAC命名的名称、分子式、物理和化学性质、用途及参考文献等。还附有可借用的化学名称、药物编号、各种商品名称、分子量、结构式、标题化合物的衍生物等。



二、重要期刊（仅限于英文和中文）



小资料——核心期刊

核心期刊指的是刊载与某一学科（或专业）有关的信息较多，且水平较高，能够反映该学科最新成果和前沿动态，受到该学科读者特别关注的那些期刊。

中文核心期刊



例如：《西安交通大学学报》

外文期刊

我们一般认定被SSCI、SCI、A&HCI、EI等几大索引收录的期刊为外文核心期刊。



核心期刊国内评选体系：

- 北京大学图书馆“中文核心期刊”
- 南京大学“中文社会科学引文索引（CSSCI）来源期刊”
- 中国科学技术信息研究所“中国科技论文统计源期刊”（又称“中国科技核心期刊”）
- 中国社会科学院文献信息中心“中国人文社会科学核心期刊”
- 中国人文社会科学学报学会“中国人文社科学报核心期刊”
- 中国科学院文献情报中心“中国科学引文数据库（CSCD）来源期刊”
- 万方数据股份有限公司建设的“中国核心期刊遴选数据库”——中国期刊库。



期刊的影响因子（IF: Impact Factor）——

E. Carfield 1972年提出期刊的影响因子是国际通行的衡量期刊质量的一个定量指标。通常，期刊的影响因子越大，它的学术影响力和作用也就越大。

期刊的影响因子：

该刊前2年发表论文在统计当年被引用的总次数

前2年发表论文总数

外文期刊的影响因子



《期刊引用报告》JCR (Journal Citation Reports)

中文期刊的影响因子



中国科学引文库（中科院文献情报中心）



一、常用数据库

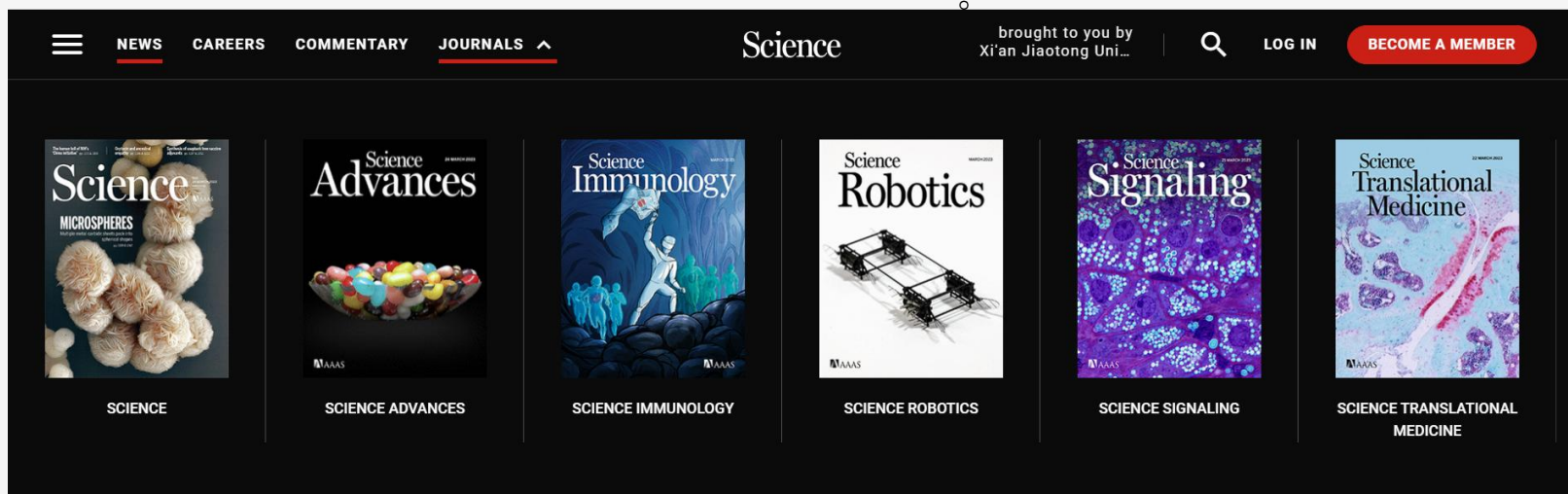
- 1、科学（Science）及其子刊（综合类）
- 2、自然（Nature）及其子刊（综合类）
- 3、美国化学会（ACS，化学类）
- 4、皇家化学会（RSC，化学类）
- 5、Wiley（综合类）
- 6、爱思唯尔（Elsevier， ScienceDirect， 综合类）
- 7、斯普林格（Springer， 综合类）
- 8、其它，如Taylor&Francis， Thieme-Connect等（综合类）
- 9、欧洲专利局（综合类）
- 10、中国知网（综合类）



科学 (Science) 及其子刊

<http://www.sciencemag.org/>

Science是1880年在美国发明家托马斯·爱迪生的资助下创办，现已成为世界领先的尖端研究、论述与科学新闻刊物



Science (IF: 63.714, 2022年) :

<http://www.sciencemag.org/>

Science Advances (IF: 14.957, 2022年) : 科学进展

【开放获取】<http://advances.sciencemag.org/>

Science Immunology: 免疫学 Science Robotics: 机器人学

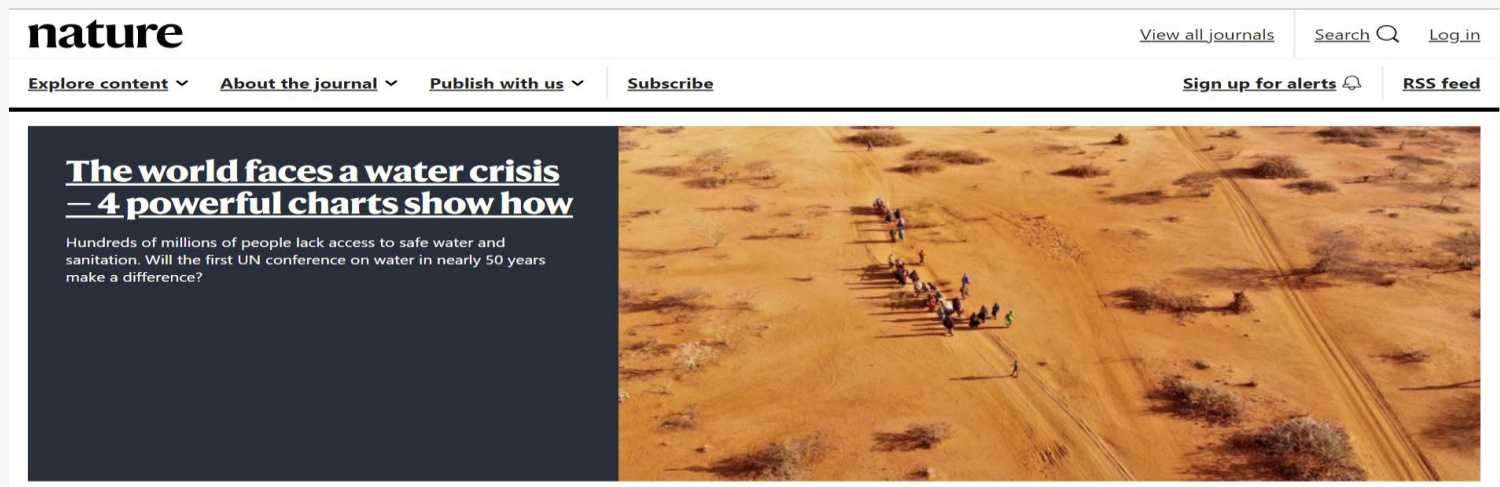
Science Signaling: 信号传递 Science Translational Medicine: 转化医学



自然 (Nature) 及化学领域重要子刊

<http://www.nature.com/>

《自然》创刊于1869年，由英国麦克米伦出版公司创办



Nature: <http://www.nature.com/> (IF: 69.504)

Nature Chemistry:

<http://www.nature.com/nchem/index.html>

Nature Communications (*Open access*):

<http://www.nature.com/ncomms/>



美国化学会 (ACS)

<http://pubs.acs.org/>

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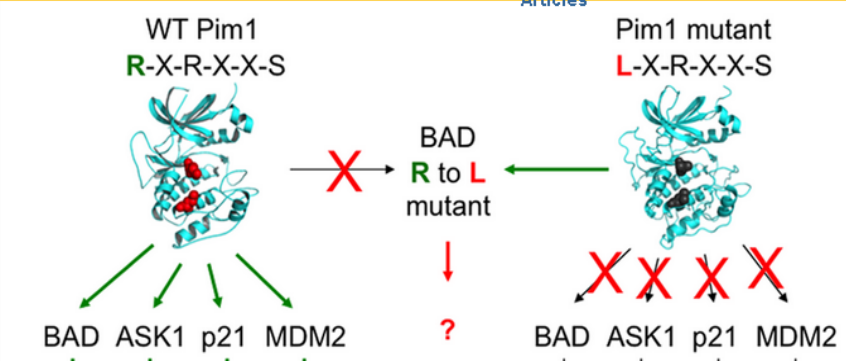
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WT Pim1
R-X-R-X-X-S



Pim1 mutant
L-X-R-X-X-S

BAD R to L mutant

BAD ASK1 p21 MDM2

No effect

ACS Chemical Biology
Rational Redesign of a Functional Protein Kinase-Substrate Interaction
Catherine Chen, Wutigri Nimlamool, Chad J. Miller, Hua Jane Lou, and Benjamin E. Turk

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I

Industrial & Engineering Chemistry
Industrial & Engineering Chemistry Research
Inorganic Chemistry

J

Journal of the American Chemical Society
Journal of Agricultural and Food Chemistry
Journal of Chemical & Engineering Data
Journal of Chemical Education
Journal of Chemical Information and Modeling
Journal of Chemical Theory and Computation
Journal of Medicinal Chemistry
Journal of Natural Products
The Journal of Organic Chemistry
The Journal of Physical Chemistry A
The Journal of Physical Chemistry B
The Journal of Physical Chemistry C
The Journal of Physical Chemistry Letters
Journal of Proteome Research

L

Langmuir

M

Macromolecules
Molecular Pharmaceutics

N

Nano Letters

O

Organic Letters
Organic Process Research & Development
Organometallics



皇家化学会 (RSC)

<http://www.rsc.org/>



The image shows the top section of the Royal Society of Chemistry (RSC) website. At the top left is the RSC logo, a stylized 'C' made of colored segments. To its right is the text 'ROYAL SOCIETY OF CHEMISTRY'. Further right are links for 'Members' area' and 'Support us'. Below this is a horizontal navigation bar with seven categories: 'About us', 'Membership & professional community', 'Campaigning & outreach', 'Journals, books & databases', 'Resources & tools', 'News & events', and 'Locations & contacts'. The main hero section features a large, vibrant image of a coral-like chemical structure in red, white, and yellow. Overlaid on the left side of this image is a dark blue semi-circular area containing the text 'Royal Society of Chemistry', 'We promote, support and celebrate chemistry', and 'The world's leading chemistry community, advancing excellence in the chemical sciences'. A 'Find out more' button is located at the bottom left of this blue area.

ROYAL SOCIETY OF CHEMISTRY

[Members' area](#) | [Support us](#)

About us | Membership & professional community | Campaigning & outreach | Journals, books & databases | Resources & tools | News & events | Locations & contacts

Royal Society of Chemistry

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Learn more about our journals

Find out about the scope, editorial boards and specific authors guidelines of our journals.

Journals are listed under relevant subject areas as a guide. Some may feature under multiple subject areas to reflect their multi-disciplinary content. Click on 'Browse journals' to view them all, sorted A–Z.

Browse journals
A–Z

Analytical

Biological

Catalysis

**Chemical biology &
Medicinal**

Energy

Environmental

Food

General chemistry

Inorganic

Materials

Nanoscience

Organic

Physical



皇家化学会 (RSC) :

旗舰刊物

Chemical Communications (老牌):

<http://pubs.rsc.org/en/journals/journalissues/cc>

Chemical Science (开放获取, 但不收版面费):

<http://pubs.rsc.org/en/journals/journalissues/sc>

Chemical Society Reviews (综述):

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其它明星刊物

Green Chemistry; **Nanoscale**;

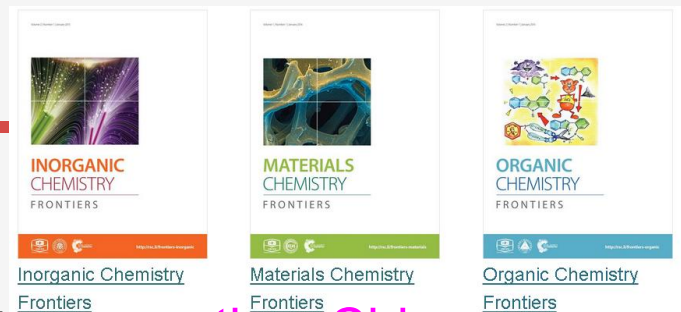
Journal of Materials Chemistry A;

Materials Horizons;

Energy & Environmental Science;

Natural Product Reports .





含有中国元素的Frontiers系列

A unique not-for-profit society partnership between the Chinese Chemical Society (CCS) and the Royal Society of Chemistry will deliver a collection of journals that combine high quality content and fast publication with trusted values of ethical publishing.

Organic Chemistry Frontiers

Editor-in-chief: Shengming Ma,
Shanghai Institute of Organic Chemistry

Inorganic Chemistry Frontiers

Editor-in-chief: Song Gao, Peking University

Materials Chemistry Frontiers

Editor in chief: Ben Zhong Tang,
Hong Kong University of Science and Technology

to be continued...



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Earth, Space & Environmental Sciences

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Life Sciences

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Medicine

Nursing, Dentistry & Healthcare

Physical Sciences & Engineering

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化学类旗舰刊物

Angewandte Chemie International Edition (德国应化):

[http://onlinelibrary.wiley.com/journal/10.1002/\(ISSN\)1521-3773](http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1521-3773)

**Chemistry-A European Journal;
Advanced Synthesis & Catalysis.**

化学类学科交叉系列新期刊

**ChemSusChem; ChemCatChem; ChemElectroChem;
ChemPhysChem; ChemMedChem; ChemBioChem;
ChemPlusChem; ChemNanoMat; ChemPhotoChem**



其它明星刊物（以有机化学为例）

Chemistry – An Asian Journal;

European Journal of Organic Chemistry;

Asian Journal of Organic Chemistry.

中国期刊

Chinese Journal of Chemistry

Editor-in-Chief: Guozhen Ji (计国桢), Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences

Journal of the Chinese Chemical Society

Editor-in-Chief: Jye-Shane Yang, Institute of Chemistry, Academia Sinica, Taipei

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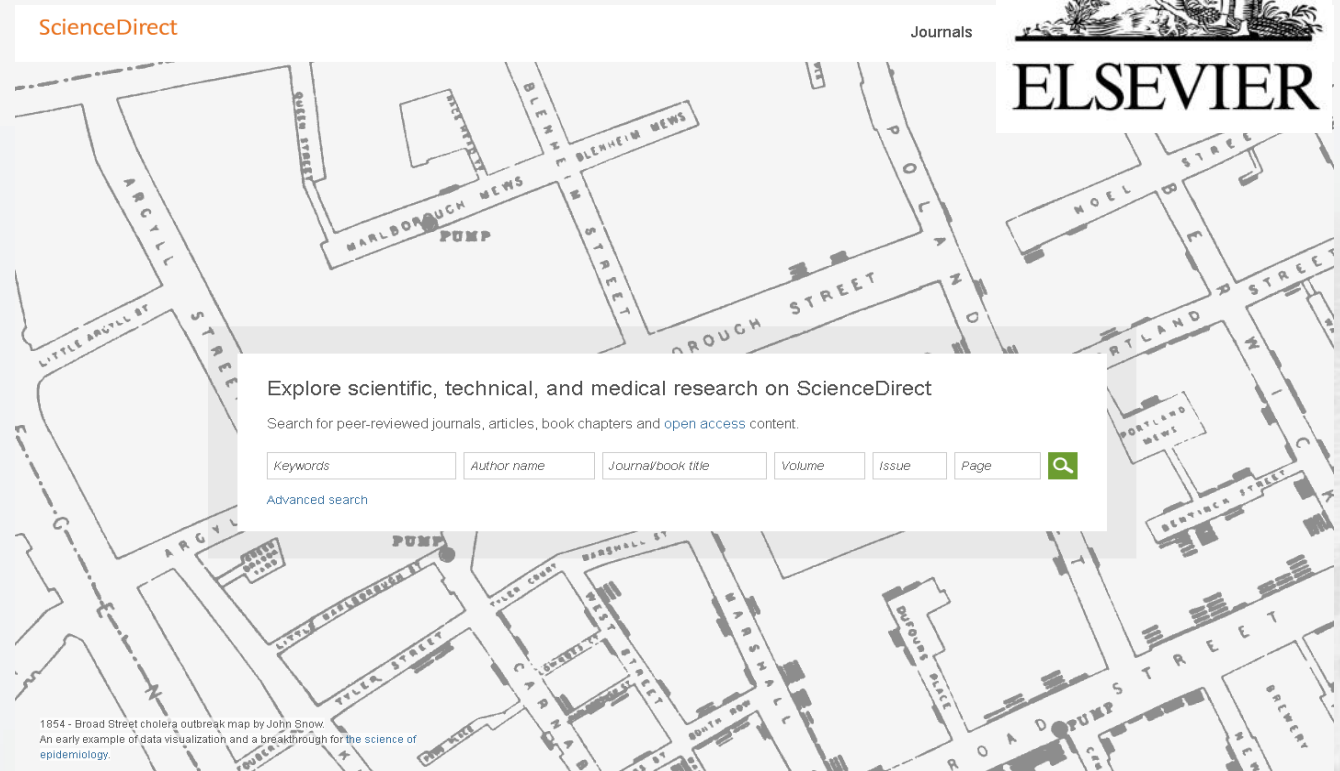
ChemistryOpen



Elsevier

<http://www.sciencedirect.com/>

Elsevier是一家荷兰的国际化多媒体出版集团，主要为科学家、研究人员、学生、医学以及信息处理的专业人士提供信息产品和革新性工具。



1854 - Broad Street cholera outbreak map by John Snow.
An early example of data visualization and a breakthrough for the science of epidemiology.



Elsevier ——期刊众多，少数出彩

化学相关旗舰刊物（主要集中在能源、材料领域）

Journal of Catalysis; **Materials Today**; **Nano Today**;
Applied Catalysis B: Environmental; **Carbon**

有机经典期刊

Tetrahedron; **Tetrahedron Letters**; **Tetrahedron:**
Asymmetry; **Journal of Fluorine Chemistry**.

中国期刊

Chinese Chemical Letters;
Chinese Journal of Catalysis (催化学报);
Chinese Journal of Chemical Engineering ;
Chinese Journal of Analytical Chemistry.

开放获取

如: **Analytical Chemistry Research**



Springer

<https://link.springer.com/>

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Taylor&Francis

<http://www.tandfonline.com/>

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文献全部分类



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W Xue, ZW Qu, S Grimme... - Journal of the American ... , 2016 - ACS Publications
... Juni 115, 10623 Berlin, Germany. ‡ Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Beringstrasse 4, 53115 Bonn, Germany. *J. Am. Chem. Soc.* ...
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Copper-Catalyzed Cross-Coupling of Silicon Pronucleophiles with Unactivated Alkyl Electrophiles Coupled with Radical Cyclization

Weichao Xue[†], Zheng-Wang Qu[‡], Stefan Grimme^{*†}, and Martin Oestreich^{*†}

[†] Institut für Chemie, Technische Universität Berlin, Strasse des 17. Juni 115, 10623 Berlin, Germany

[‡] Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Beringstrasse 4, 53115 Bonn, Germany

J. Am. Chem. Soc., **2016**, 138 (43), pp 14222–14225

DOI: 10.1021/jacs.6b09596

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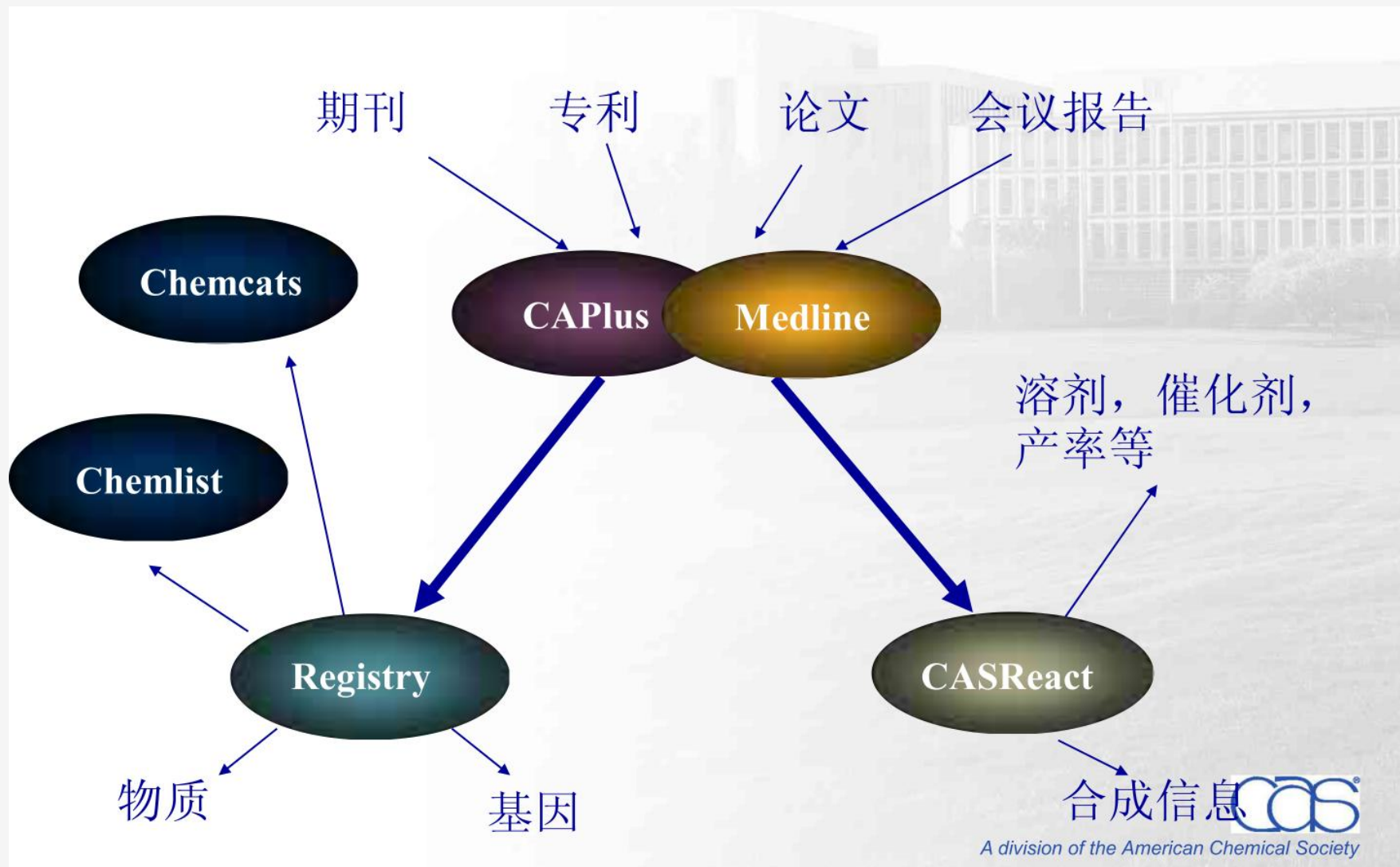


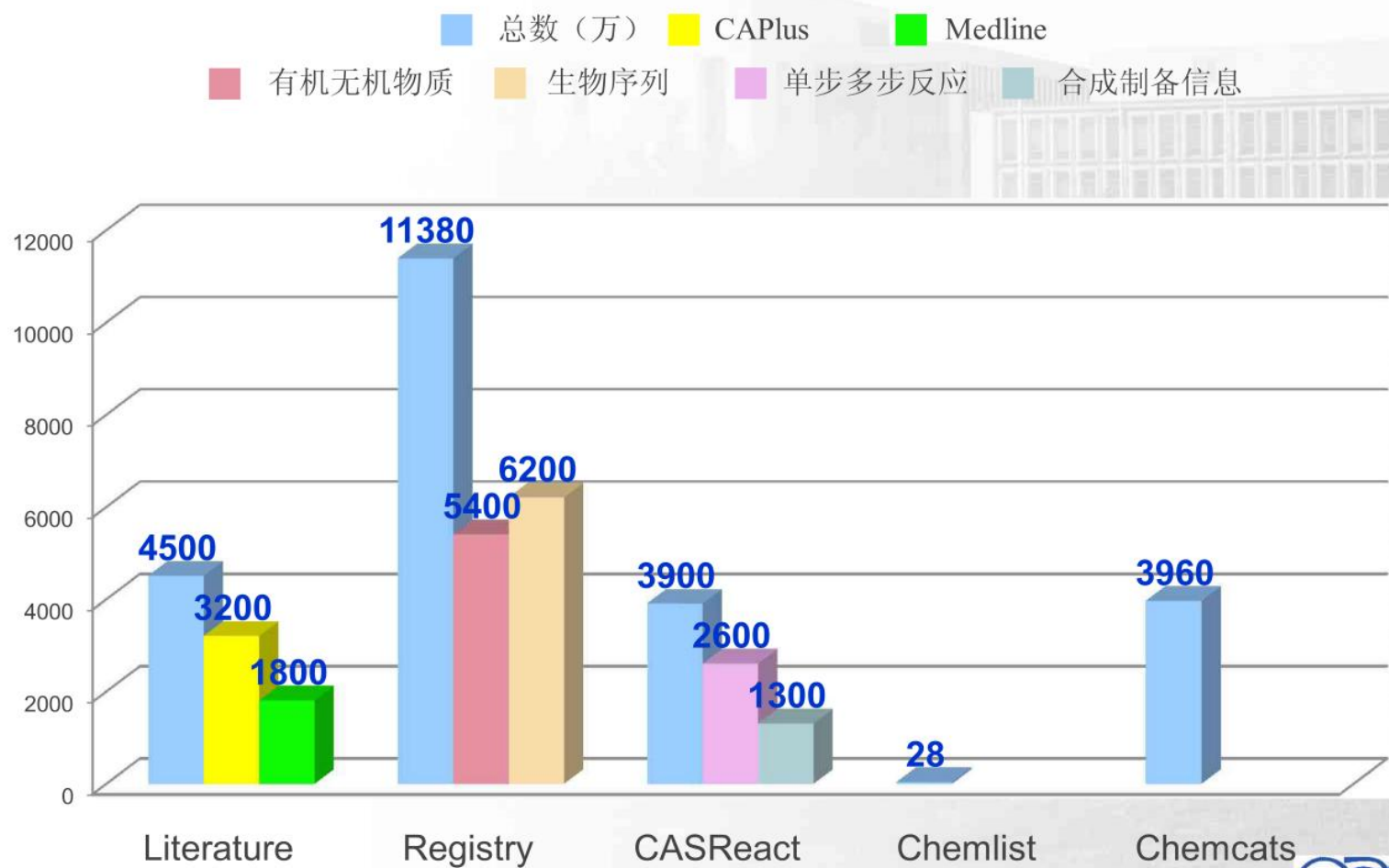
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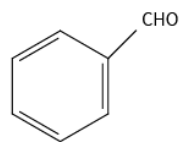
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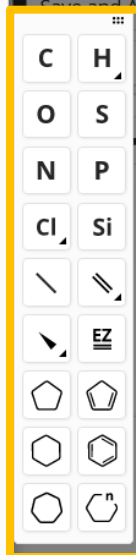
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Molecular Formula: C₇H₆O (106.12)

CHO

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31-614-CAS-35688522

Steps: 1 Yield: 1%

1.1 Reagents: [Hydrogen peroxide](#)Catalysts: [Copper](#), [\[3-\[\[bis\[\(2-pyridinyl-κN\)methyl\]amino-κN\)methyl\]-2-\(hydroxy-κO\)-5-methyl...](#)Solvents: [Acetonitrile](#), [Water](#); 3 h, 50 °C

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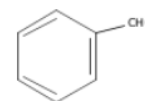
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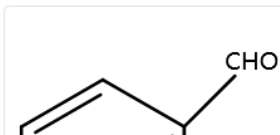
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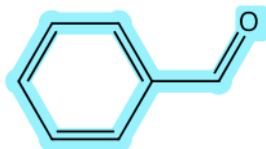
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100-52-7



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Benzaldehyde

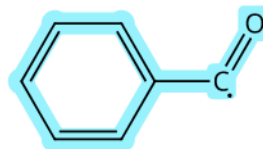
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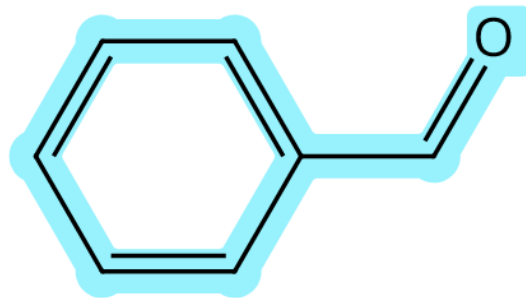
Reactions (239,773)

Scheme 1 (1 Reaction)

Steps: 1 Yield: 100% ...

CAS number,
物质数字识别号码





C_7H_6O

Benzaldehyde (7CI, 8CI, 9CI, ACI)

Key Physical Properties	Value	Condition
Molecular Weight	106.12	-
Melting Point (Experimental)	-26 °C	-
Boiling Point (Experimental)	179 °C	-
Density (Experimental)	1.050 g/cm ³	Temp: 15 °C

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By: Sheldon, Roger A.

Chemical Society Reviews (2012), 41(4), 1437-1451 | Language: English, Database: CAPLUS and MEDLINE

A review. In this tutorial review, the fundamental concepts underlying the principles of green and sustainable chem. - atom and step economy and the E factor - are presented, within the general context of efficiency in organic synthesis. The importance of waste minimisation through the widespread application of catalysis in all its forms - homogeneous, heterogeneous, organocatalysis and biocatalysis - is discussed. These general principles are illustrated with simple practical examples, such as alc. oxidation and carbonylation and the asym. reduction of ketones. The latter reaction is exemplif...

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By: Enache, Dan I.; Edwards, Jennifer K.; Landon, Philip; Solsona-Espriu, Benjamin; Carley, Albert F.; Herzing, Andrew A.; Watanabe, Masashi; Kiely, Christopher J.; Knight, David W.; Hutchings, Graham J.

Science (Washington, DC, United States) (2006), 311(5759), 362-365 | Language: English, Database: CAPLUS and MEDLINE

The oxidation of alcs. to aldehydes with O₂ in place of stoichiometric oxygen donors is a crucial process for the synthesis of fine chems. However, the catalysts that have been identified so far are relatively inactive with primary alkyl alcs. We showed that Au/Pd-



Fundamentals of green chemistry: efficiency in reaction design

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Keywords: review green chem

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Abstract

In this *tutorial review*, the fundamental concepts underlying the principles of green and sustainable chemistry - atom and step economy and the E factor - are presented, within the general context of efficiency in organic synthesis. The importance of waste minimisation through the widespread application of catalysis in all its forms – homogeneous, heterogeneous, organocatalysis and biocatalysis – is discussed. These general principles are illustrated with simple practical examples, such as alcohol oxidation and carbonylation and the asymmetric reduction of ketones. The latter reaction is exemplified by a three enzyme process for the production of a key intermediate in the synthesis of the cholesterol lowering agent, atorvastatin. The immobilisation of enzymes as cross-linked enzyme aggregates (CLEAs) as a means of optimizing operational performance is presented. The use of immobilised enzymes in catalytic cascade processes is illustrated with a trienzymatic process for the conversion of benzaldehyde to (*S*)-mandelic acid using a combi-CLEA containing three enzymes. Finally, the transition from fossil-based chemicals manufacture to a more sustainable biomass-based production is discussed.

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PDF (3633K)

Article information

<https://doi.org/10.1039/C1CS15219J>

Article type	Tutorial Review
Submitted	15 Aug 2011
First published	28 Oct 2011
Citation	Chem. Soc. Rev. , 2012, 41 , 1437-1451



Reactions for 100-52-7

References ▾



Save and Alert

Filter Behavior

Filter by

Exclude

Substance Role

☒ Product (24K)

☐ Reactant (213K)

☐ Reagent (6,072)

☐ Catalyst (596)

☐ Solvent (198)

Yield

☐ 90-100% (3,845)

☐ 80-89% (1,808)

☐ 70-79% (1,186)

☐ 50-69% (1,624)

☐ 30-49% (1,219)

[View All](#)

Number of Steps

☐ 1 (18K)

☐ 2 (2,012)

☐ 3 (1,113)

Filtering:

Substance Role: Product X

[Clear All Filters](#)

☐ 24,331 Results

Group: By Document

Sort: Relevance

View: Expanded

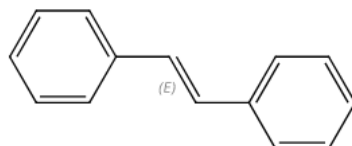
☐ 1

Microreactor-controlled product selectivity in photosensitized energy transfer versus energy transfer pathways

By: Fu, Xiao-Gang; Zhang, Li-Ping; Wu, Li-Zhu; Tung, Chen-Ho
Journal of Photoscience (2003), 10(1), 175-180 | Language: English, Database

Full Text ▾

[View 7 Related Reactions](#)



Double bond geometry shown

Suppliers (62)

Suppliers (66)

31-486-CAS-4380920

Steps: 1 Yield: 100%



Filter Behavior

Filter by

Exclude

Substance Role

- ☐ Product (24K)
- ☒ Reactant (213K)
- ☐ Reagent (6,072)
- ☐ Catalyst (596)
- ☐ Solvent (198)

Yield

- ☐ 90-100% (43K)
- ☐ 80-89% (36K)
- ☐ 70-79% (26K)
- ☐ 50-69% (33K)
- ☐ 30-49% (15K)

[View All](#)

Number of Steps

- ☐ 1 (213K)

Non-Participating Functional Groups

- ☐ Alkene (35K)
- ☐ Ketone (31K)
- ☐ Halide (26K)

Filtering:

Substance Role: Reactant X

[Clear All Filters](#)

☐ 213,877 Results

Group: By Document

Sort: **Publication Date: Newest**

View: Expanded

☐ 1

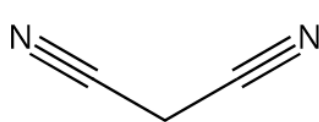
Photochemical synthesis of pyrano[2,3-d]pyrimidine scaffold using eosin Y as direct hydrogen atom transfer (HAT) photocatalyst under air atmosphere

By: Mohamadpour, Farzaneh

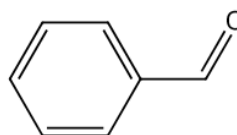
BMC Chemistry (2023), 17(1), 2 | Language: English, Database: CAPLUS and M

Full Text

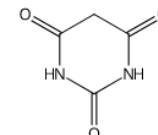
[View 2 Related Reactions](#)



+



+

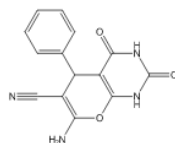


→

Suppliers (61)

Suppliers (66)

Suppliers (89)



搜索特定合成路径

CAS Draw

Return to Home

Draw or change atoms or bonds.

reactant

product

Molecular Formula: C_7H_6O (106.12) · $C_7H_6O_2$ (122.12)

C

Zoom: 100%

OK Cancel

Filter Behavior

Filter by Exclude

Reaction Role

Product (1)

$C_7H_6O_2 \cdot x C_7H_6O \cdot x (C_2H_4O)_x$

Components: 3

Ethenol, homopolymer, benzoate, cyclic acetal with benzaldehyde

$(C_8H_{12}N_2 \cdot C_7H_6O_2 \cdot C_7H_6O \cdot C_6H_{11}N)_x$

Components: 4

Benzoic acid, polymer with benzaldehyde, 1,6-diisocyanohexane and 1,6-hexanediamine...



Structure Match

As Drawn (888)

Substructure (84K)

Similarity (25K)

Filter Behavior

Filter by

Exclude

Yield

☒ 90-100% (199)

☐ 80-89% (102)

☐ 70-79% (58)

☐ 50-69% (69)

☐ 30-49% (35)

[View All](#)

Number of Steps

☐ 1 (199)

Reaction Mapping

☐ Mapping Data Available (199)

Experimental Protocols

☐ Synthetic Methods (94)

Filtering: Yield: 90-100% X

[Clear All Filters](#)

☐ 199 Results

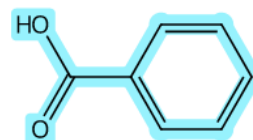
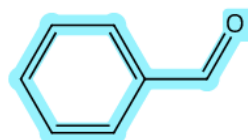
Group: By Document ▾ Sort: Publication Date: Newest ▾ View: Expanded ▾

☐ 1

Light-Promoted Chlorine-Radical-Mediated Oxidation of Benzylic C(sp³)-H Bonds utilizing Air as Oxidant

By: Xu, Ning; Peng, Xiaoqing; Luo, Can; Huang, Lei; Wang, Chaodong; et al
Advanced Synthesis & Catalysis (2023), 365(2), 142-147 | Language: English, Database: CAplus

Full Text ▾



Suppliers (66)

Suppliers (153)

31-614-CAS-35375420

Steps: 1 Yield: 95%

- 1.1 Reagents: [Oxygen](#)
Catalysts: [Hydrochloric acid](#), [6-Bromobenzothiazole](#)
Solvents: [Acetonitrile](#), [Water](#); 24 h, 60 °C
- 1.2 Reagents: [Sodium bicarbonate](#)
Solvents: [Water](#)



SciFinder 检索练习



查找一个自己感兴趣的化学结构，看看是否有文献报道。



通过Sci-Finder查找一个自己感兴趣的反应并对反应进行条件分析。



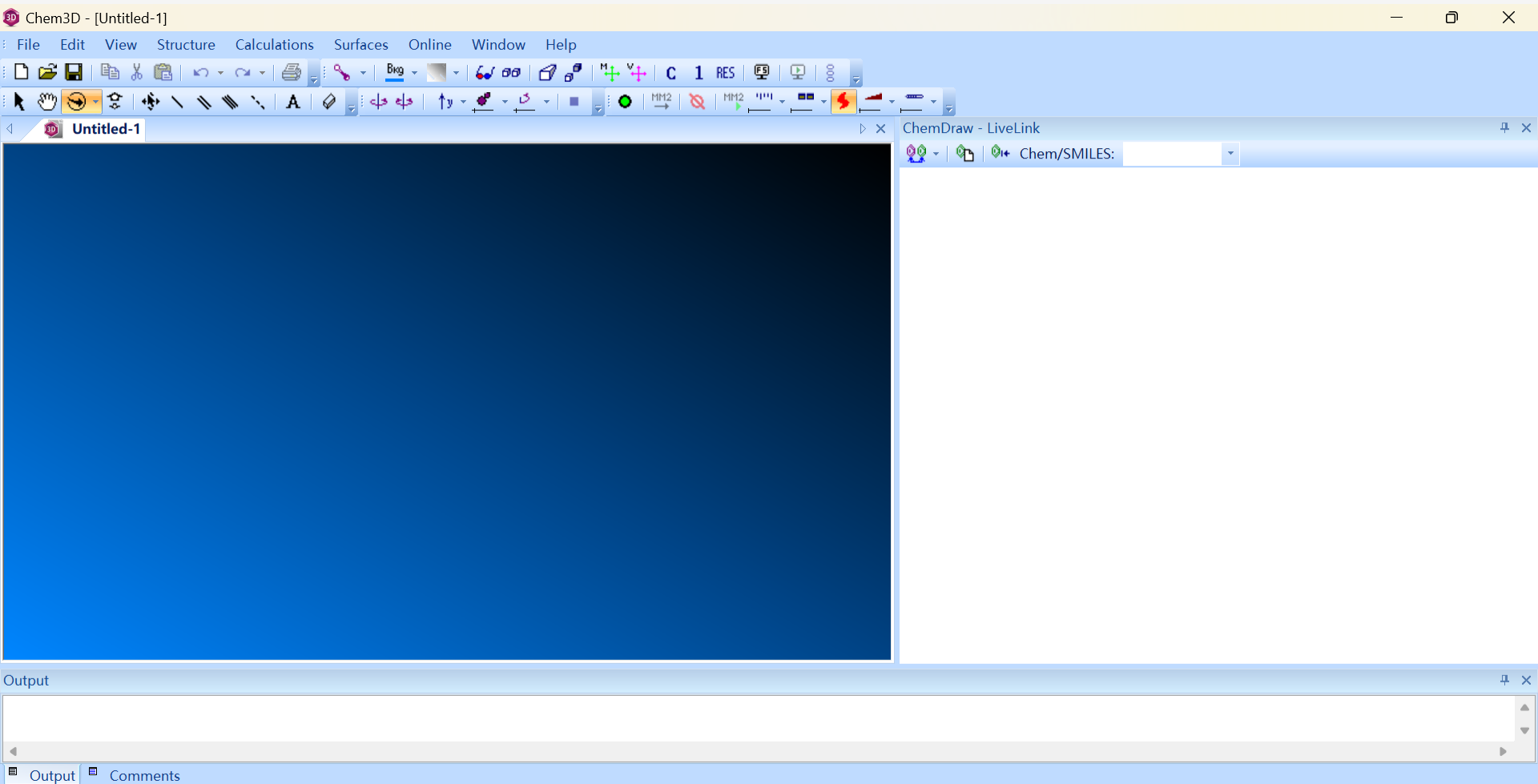
利用Sci-Finder查找阿司匹林的创新合成路径，并设计创新合成方案。



四、Chem3D 模拟化合物立体异构



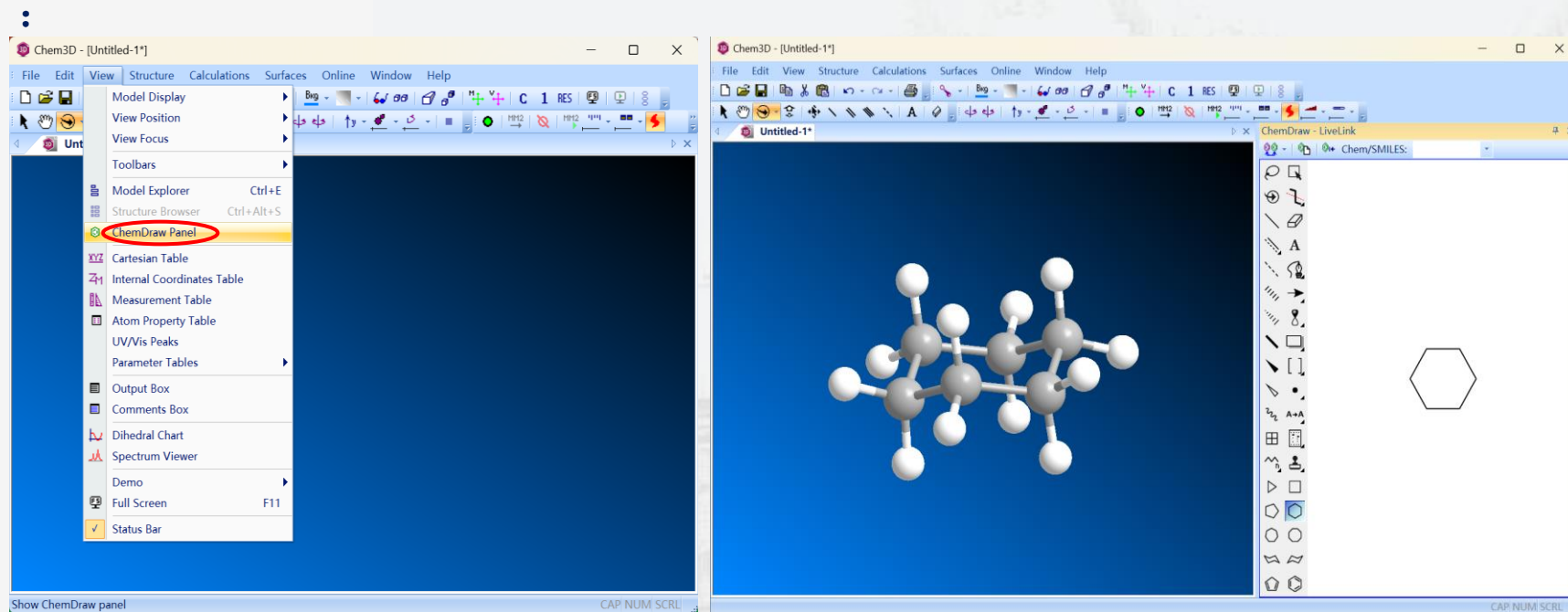
Chem3D 打开后的页面状态:



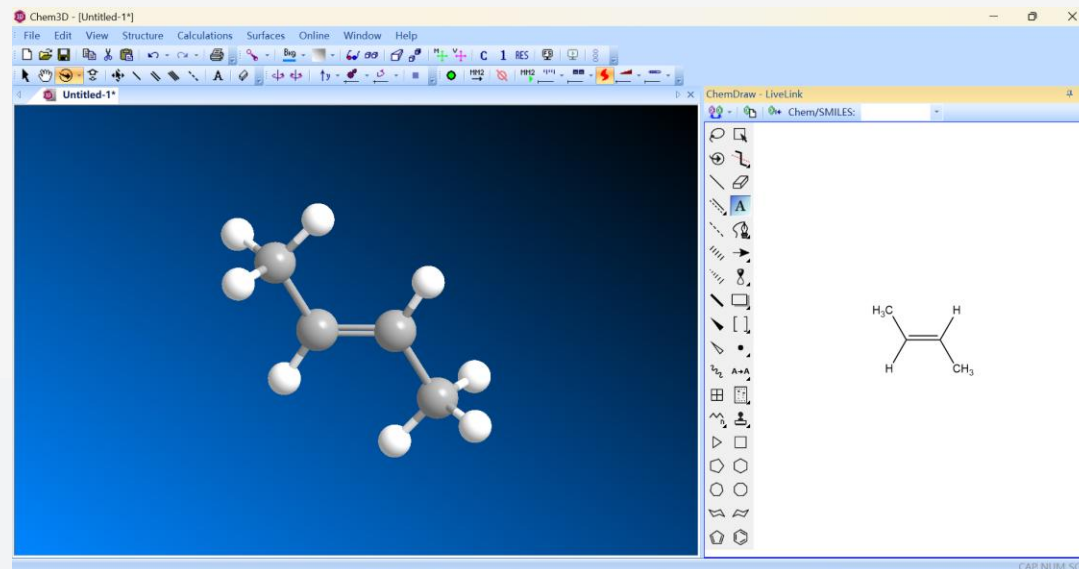
方法一：使用ChemDraw Panel面板

单击View菜单并选择ChemDraw Panel命令可以在Chem 3D中打开ChemDraw面板，因为ChemDraw创建平面结构所以绘制过程比较清晰也更容易掌握。

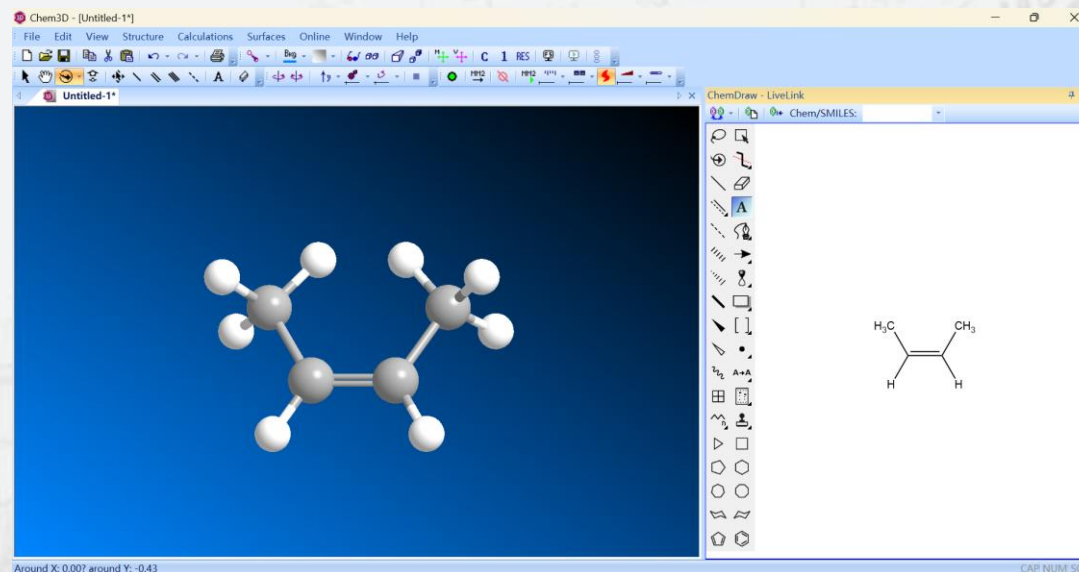
创建分子构型的方法是：只要在ChemDraw Panel中单击就会出现工具栏，然后选择工具绘制需要的结构即可，Chem 3D窗口会同步显示对应的立体模型，这样的绘制方法比较好的是绘制者可以同时观察平面和立体结构。绘制效果如下图所示：



反-2-丁烯:



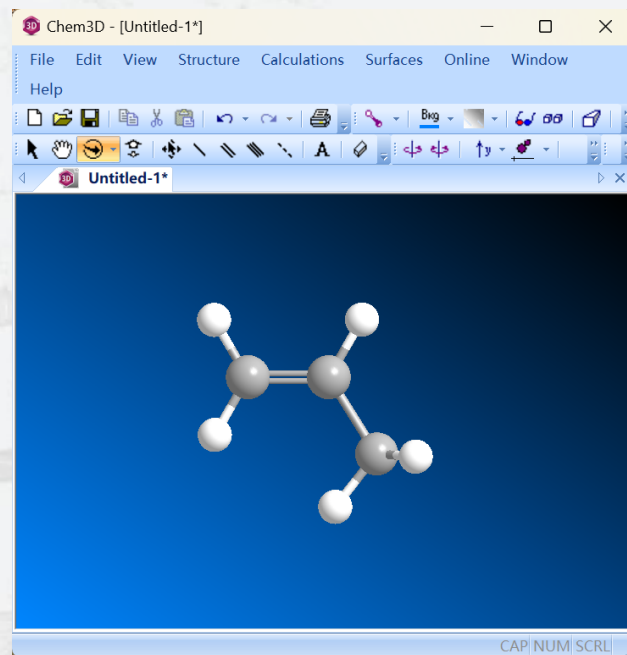
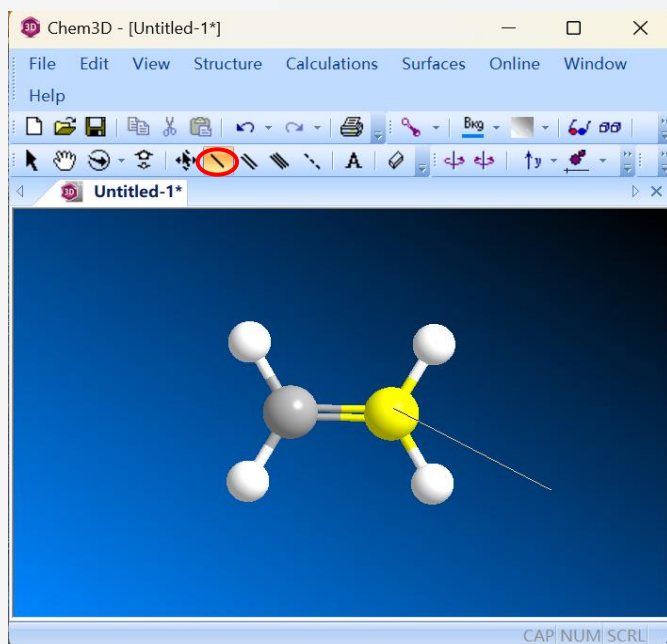
顺-2-丁烯:



方法二：使用键工具

利用Chem 3D的Building工具条中单键、双键、叁键工具就可以创建分子立体模型，这要求绘制者要对化学立体模型比较熟悉。

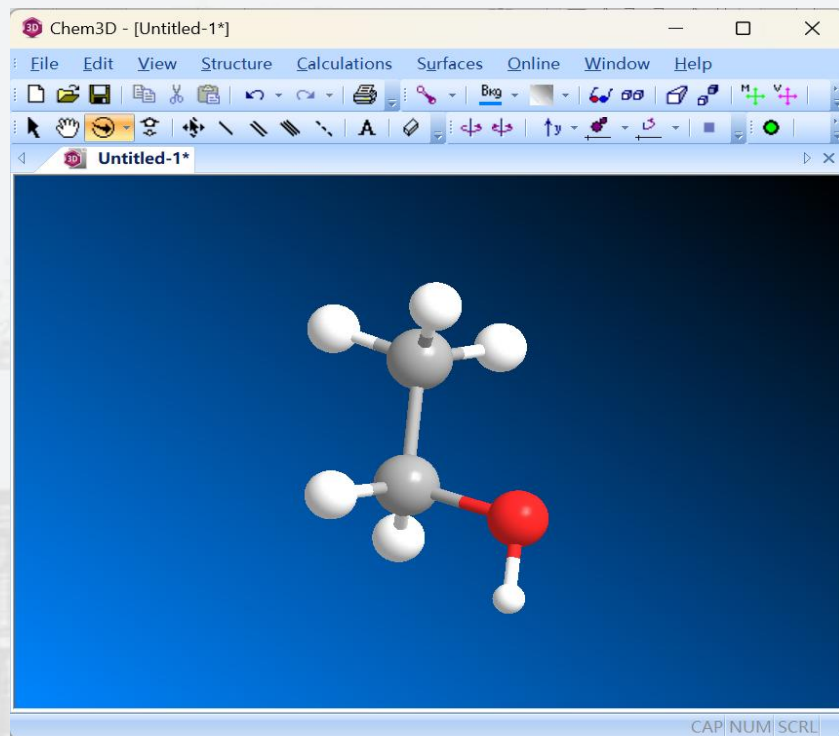
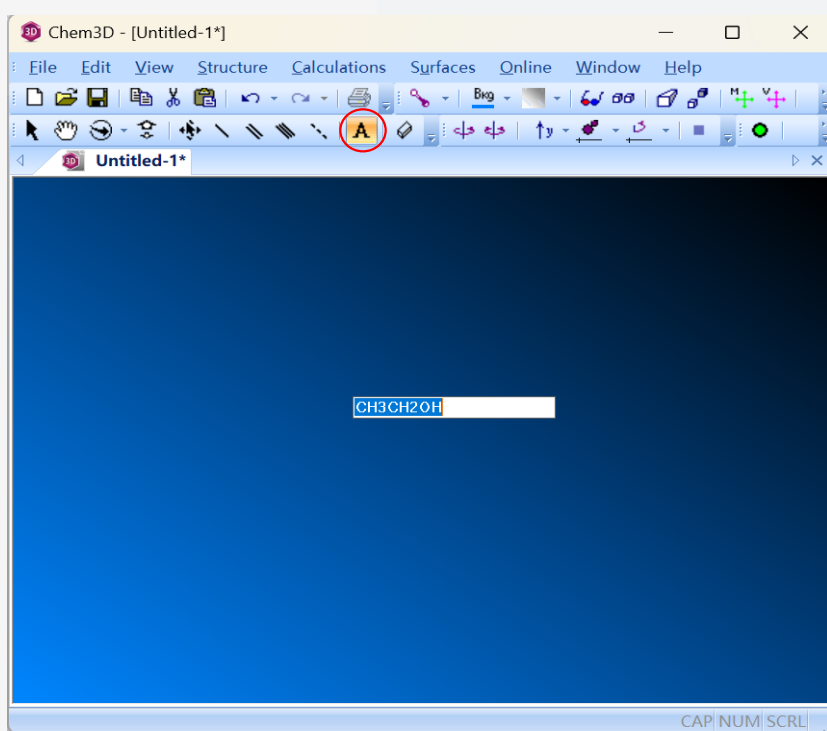
创建方法是：单击键工具，然后在绘制窗口拖动鼠标，绘制完一根C-C键后释放鼠标按钮，然后再以其中一个C原子为起点，继续绘制其它键，最后根据需要修改原子或基团类型。



方法三：使用文本工具

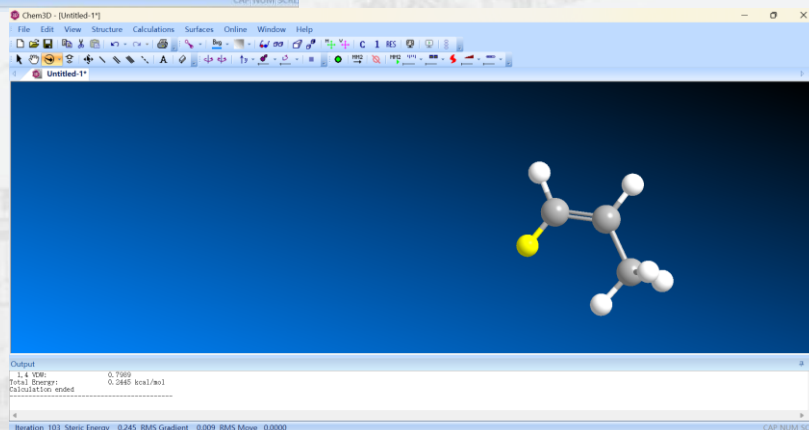
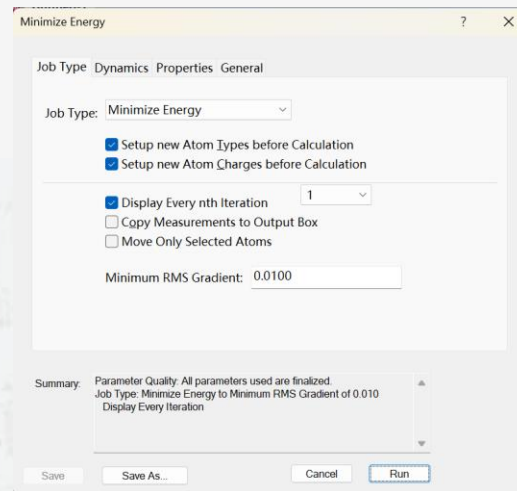
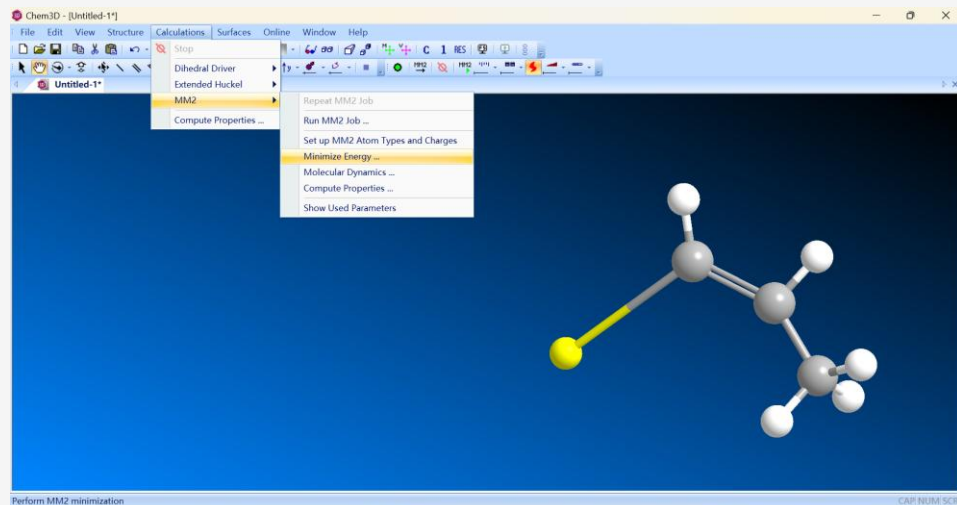
使用Building工具条中的文本工具创建立体模型需要绘制者对该分子构型的化学式尤为清楚。

创建方法是：选择文本工具后在下方窗口单击生成文本输入框，然后在文本区域内键入原子符号及数量(即化学式)，比如创建乙醇的立体模型记载输入框中，最后按下回车键即可，效果图如下所示：



计算化合物构象能量最低值（MM2）

打开软件，点击Calculations——MM2——Minimize Energy（图1），此时会出现图2界面，直接点击右下角Run运行即可。



利用检索工具设计阿司匹林的合成路径，以小组的形式进行汇报。讨论之前的阿司匹林合成路径的不同，优缺点等等。





西安交通大学
XI'AN JIAOTONG UNIVERSITY

谢谢各位同学！



少年班《有机化学实验》教学组