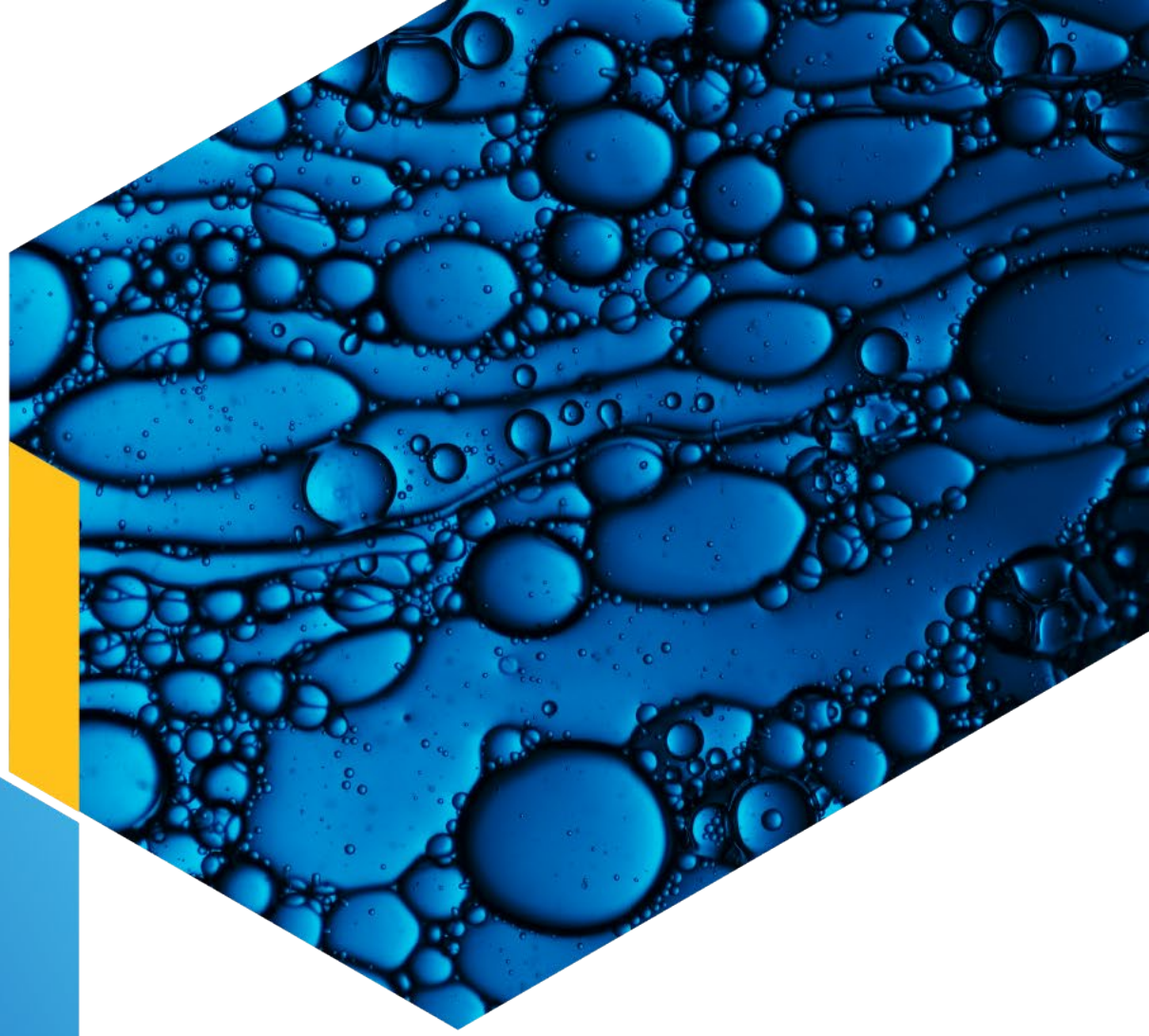
CAS SciFinder

全程助力科学研究突破



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大纲

- **CAS SciFinder介绍**
- **文献相关信息的获取策略**
  - 文献检索方法
  - 文献结果分析、精炼和详情
- **物质相关信息的获取策略**
  - 物质检索方法
  - 如何检索无机化合物、配位化合物和聚合物
  - 物质结果分析、精炼和详情
- **反应相关信息的获取策略**
  - 反应的获取方法
  - 反应结果分析、精炼及详情

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CAS致力于提高创新效率

CAS的数据和服务是基于对以往知识经验的回顾，对当代前沿研究的洞察，以及对未来发展趋势的前瞻

HINDSIGHT

Connecting past discoveries
to build a better future

连接前人的发现，建设更美好的未来

INSIGHT

Revealing unseen relationships that spark ideas and speed discovery

揭示能激发想法和加速发现的，未预见的联系

FORESIGHT

Identifying trends and emerging opportunities to accelerate growth

确定加速增长的趋势和新机遇

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CAS具有最全面的学科连接内容合集

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CAS SciFinder覆盖的学科

- **生物化学：**
  - 农化产品管控信息、生化遗传学、发酵、免疫化学、药理学
- **有机化学各领域：**
  - 氨基酸、生物分子、碳水化合物、有机金属化合物、类固醇
- **大分子化学各领域：**
  - 纤维素、木质素、造纸；涂料、墨水
  - 染料、有机颜料； 合成橡胶； 纺织品、纤维
- **应用化学各领域：**
  - 大气污染、陶瓷、精油、化妆品、化石燃料、黑色金属、合金
- **物理、无机、分析化学各领域：**
  - 表面化学、催化剂、相平衡、核现象、电化学

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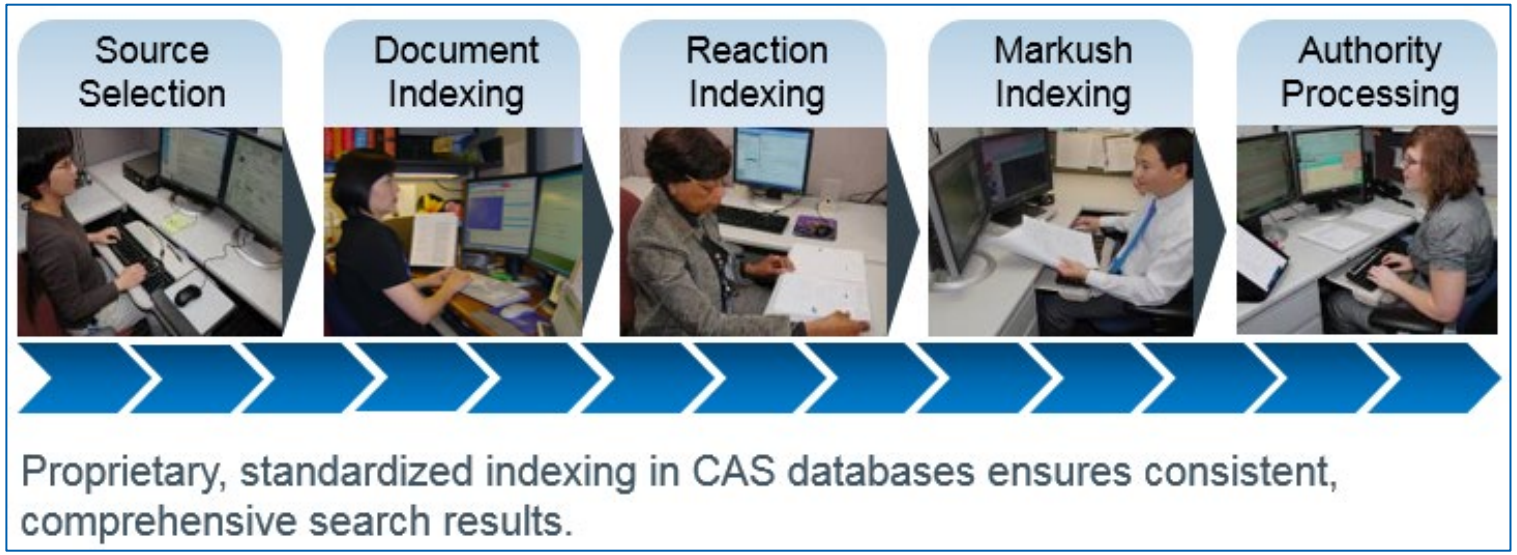
CAS科学家的智力标引



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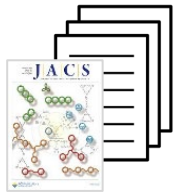
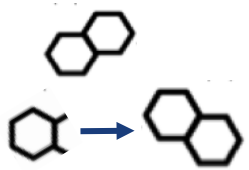
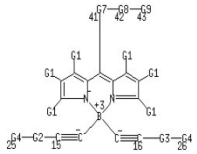


1990
Smith, M.
anthracene





Androst-4-en-3-one, 17-hydroxy-17-methyl-, (17β)-

CAS科学家利用人类智慧对公开内容进行揭示，使相关信息更容易被挖掘

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CAS解决方案与服务

DISCOVERY
发现

CAS SciFinder Discovery Platform™

Get discoveries to market faster and optimize margins by giving researchers the information they need

INTELLECTUAL PROPERTY
知识产权

STN IP Protection Suite™

Ensure that your intellectual property is protected and find opportunities to extend into new markets

CUSTOM SOLUTIONS
定制服务

CAS Custom Services℠

Customized data, analytics and insights to maximize the value of information assets and fuel digitalization success

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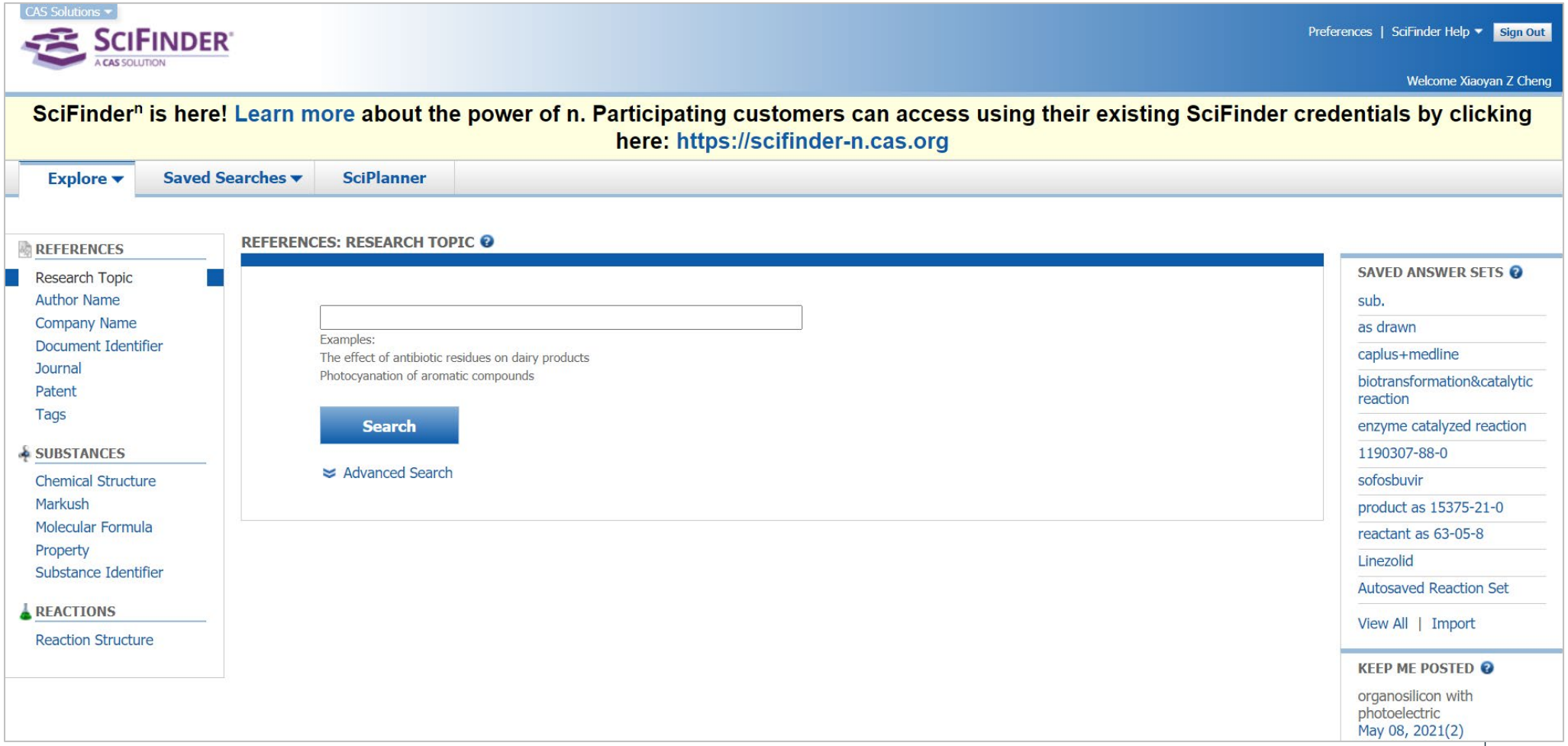
检索界面



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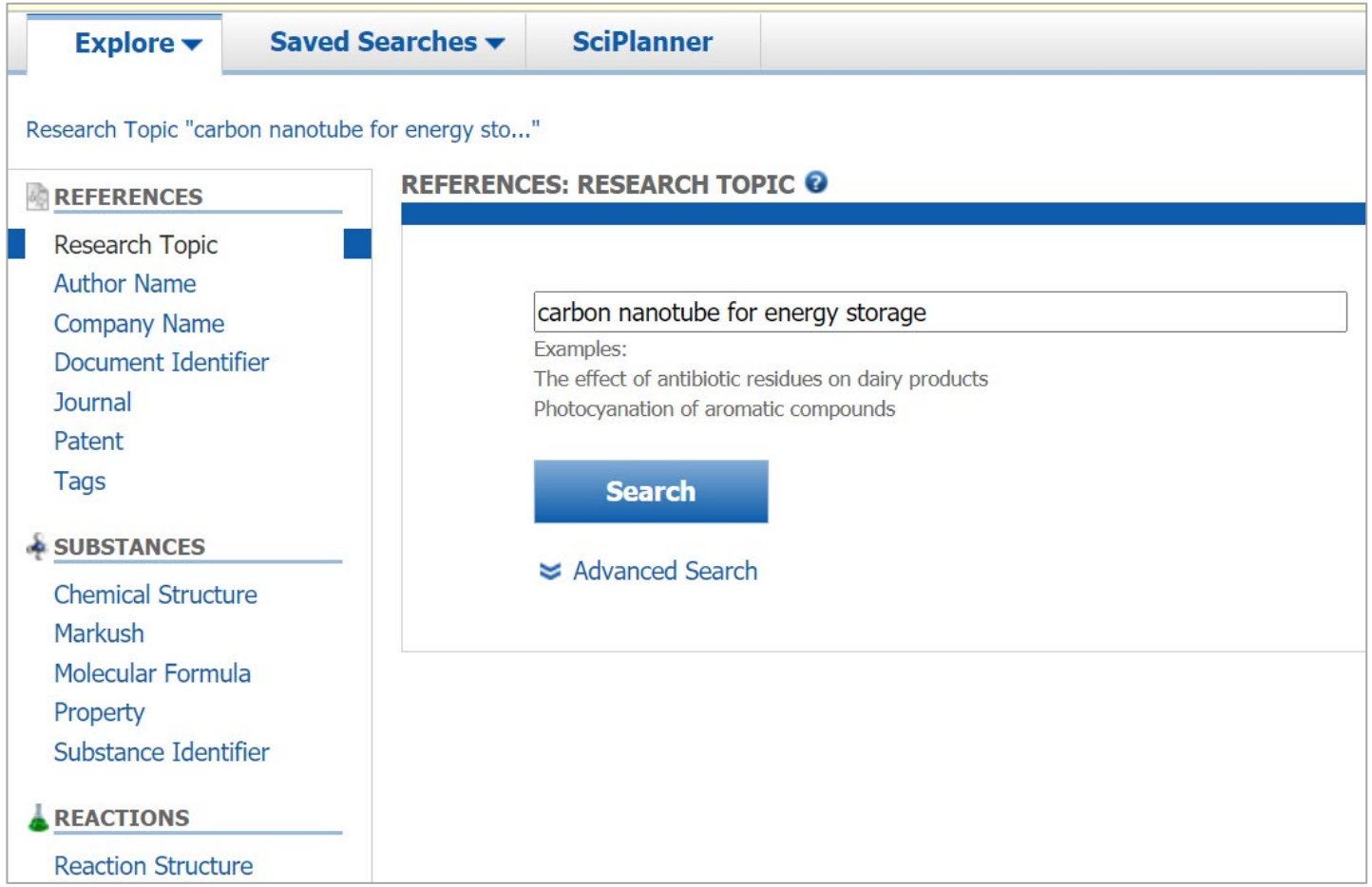
文献检索

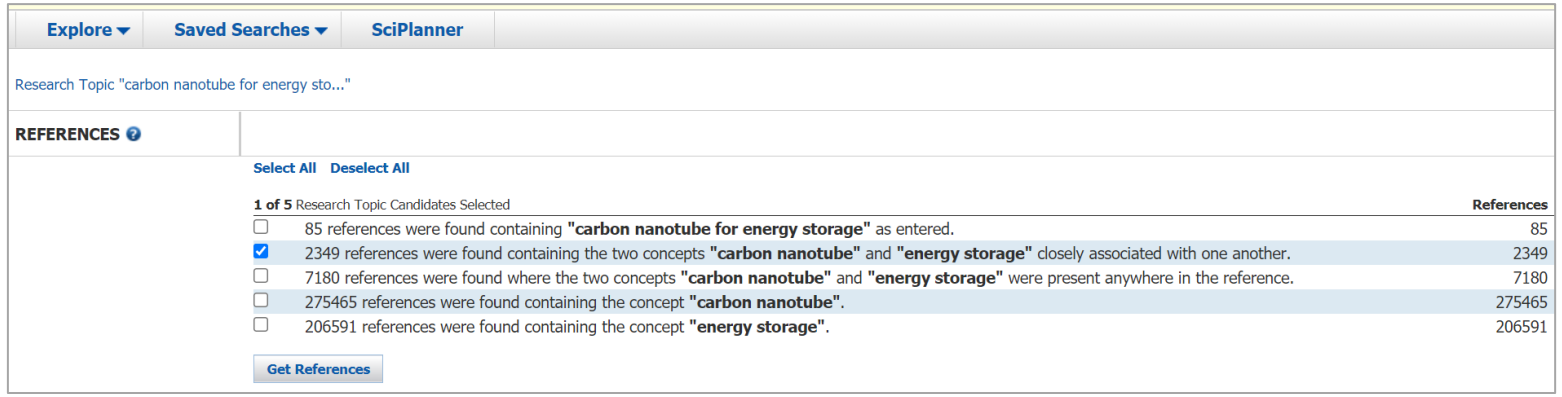
- 文献检索方法
  - 主题检索
  - 作者名检索
  - 机构名检索
  - 文献标识符检索
  - 期刊名称和专利信息（公开号，申请号等）
  - 从物质，反应获得文献

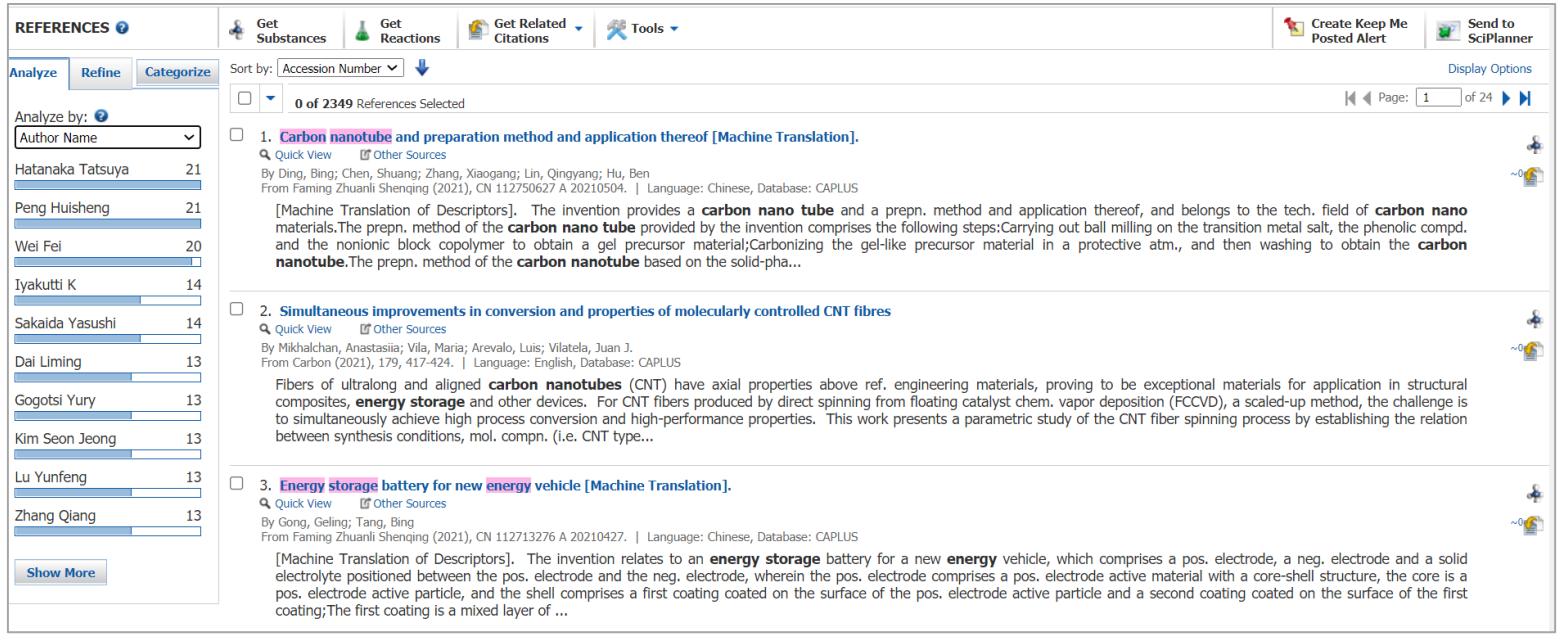
- 检索策略推荐
  - 关注某特定领域的文献：主题检索
  - 关注物质有关的文献：先获得物质，再获得文献
  - 关注某科研人员的文献：作者名检索
  - 关注某机构科研进展：机构名检索

文献主题检索



文献结果候选项





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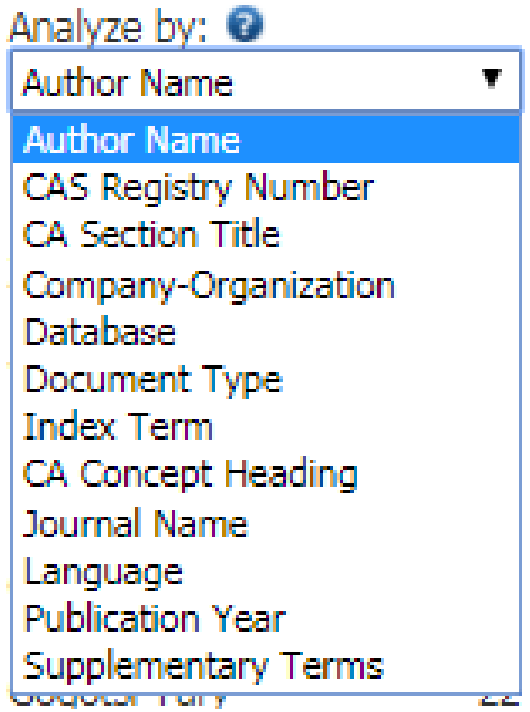
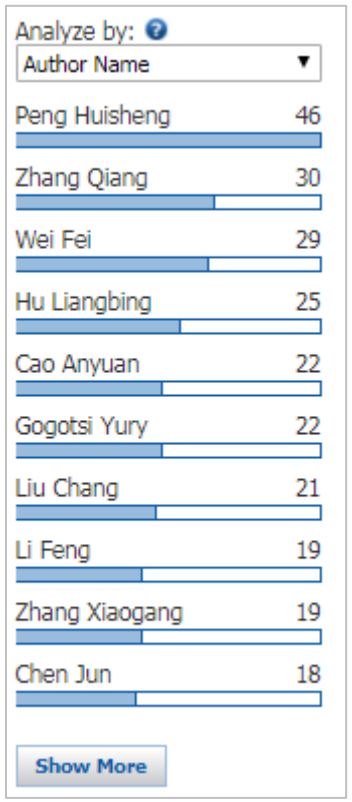
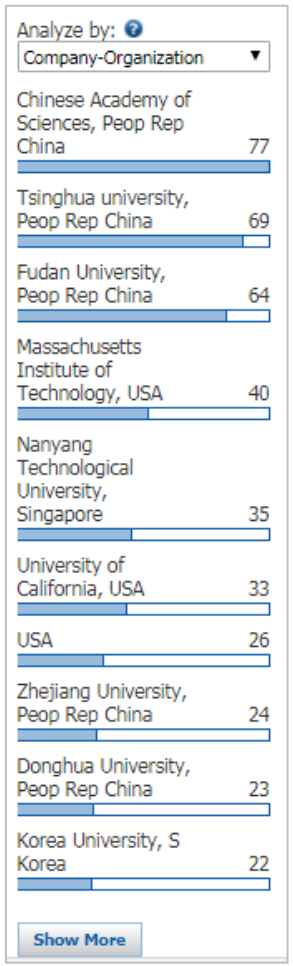
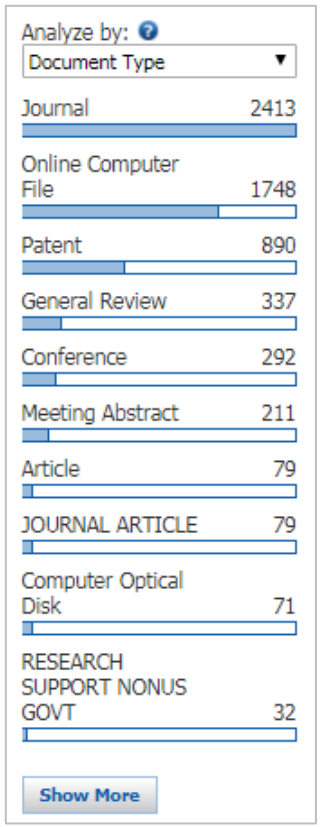
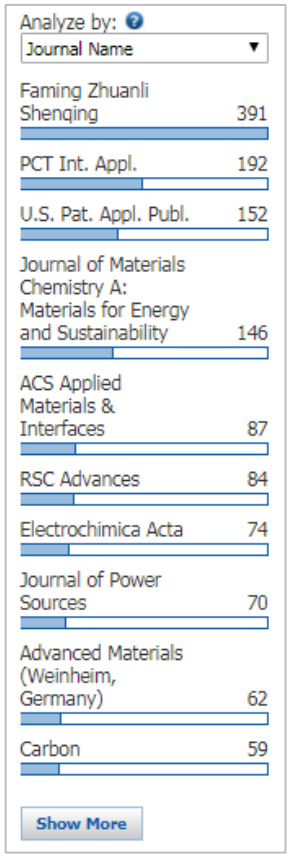
文献结果分析



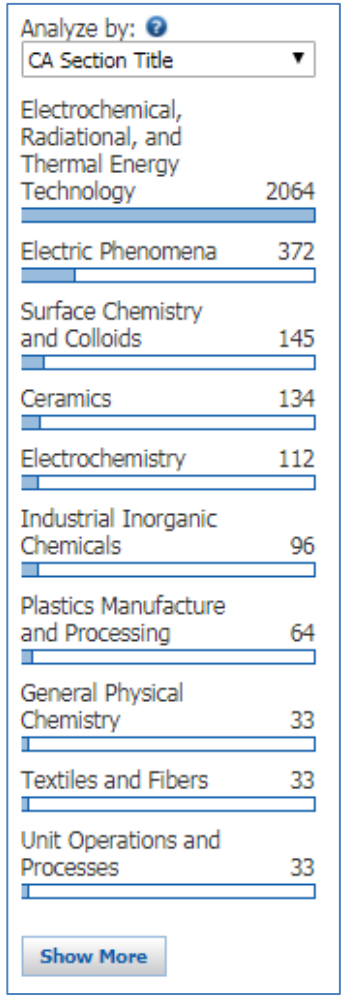


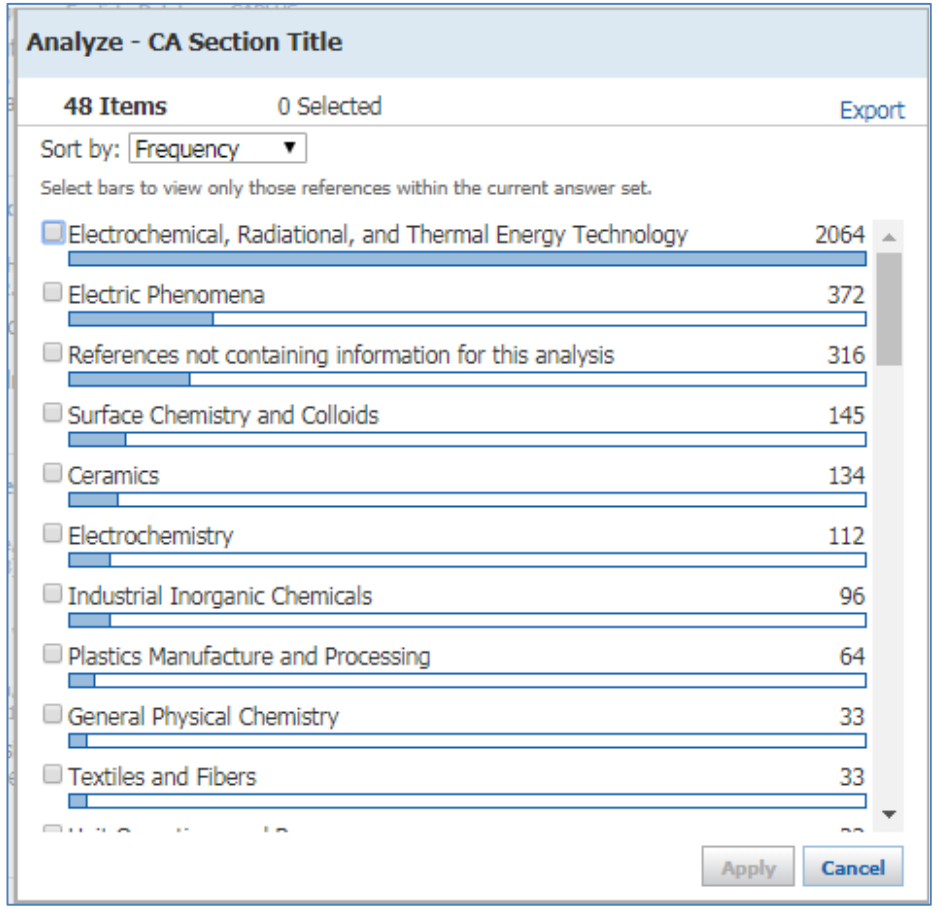






文献检索结果分析：CA Section Title





电化学、放射及热能技术

电现象

表面化学和胶体

硅酸盐

电化学

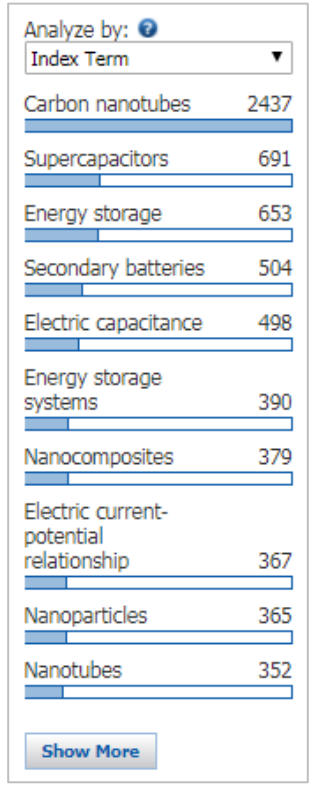
工业无机化合物

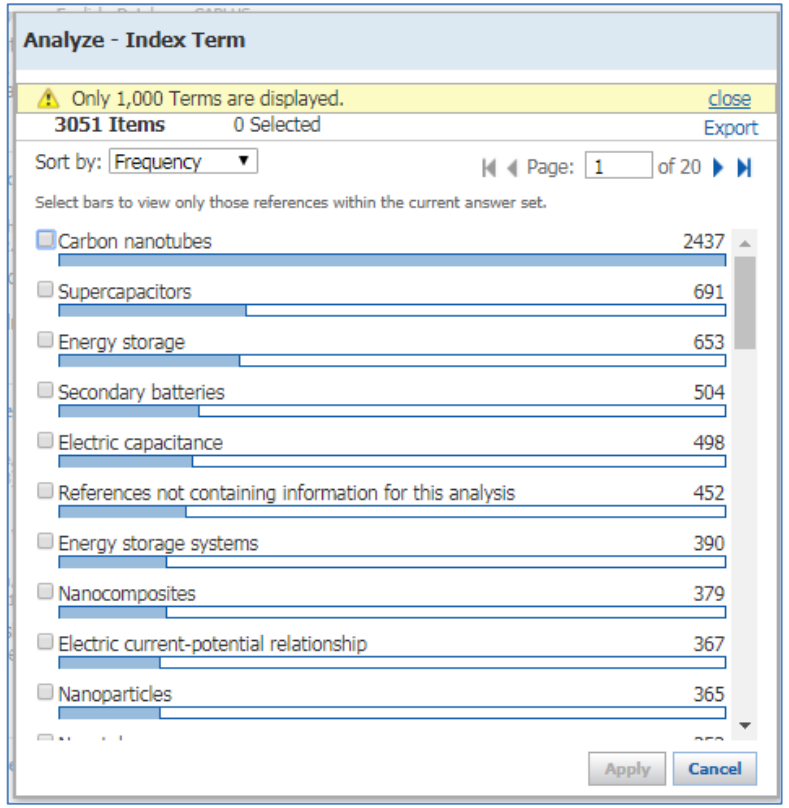
塑料制备和加工

普通物理化学

织物和纤维

通过Index Term，可纵览或精炼研究点信息





碳纳米管

超级电容器

能量储蓄

蓄电池

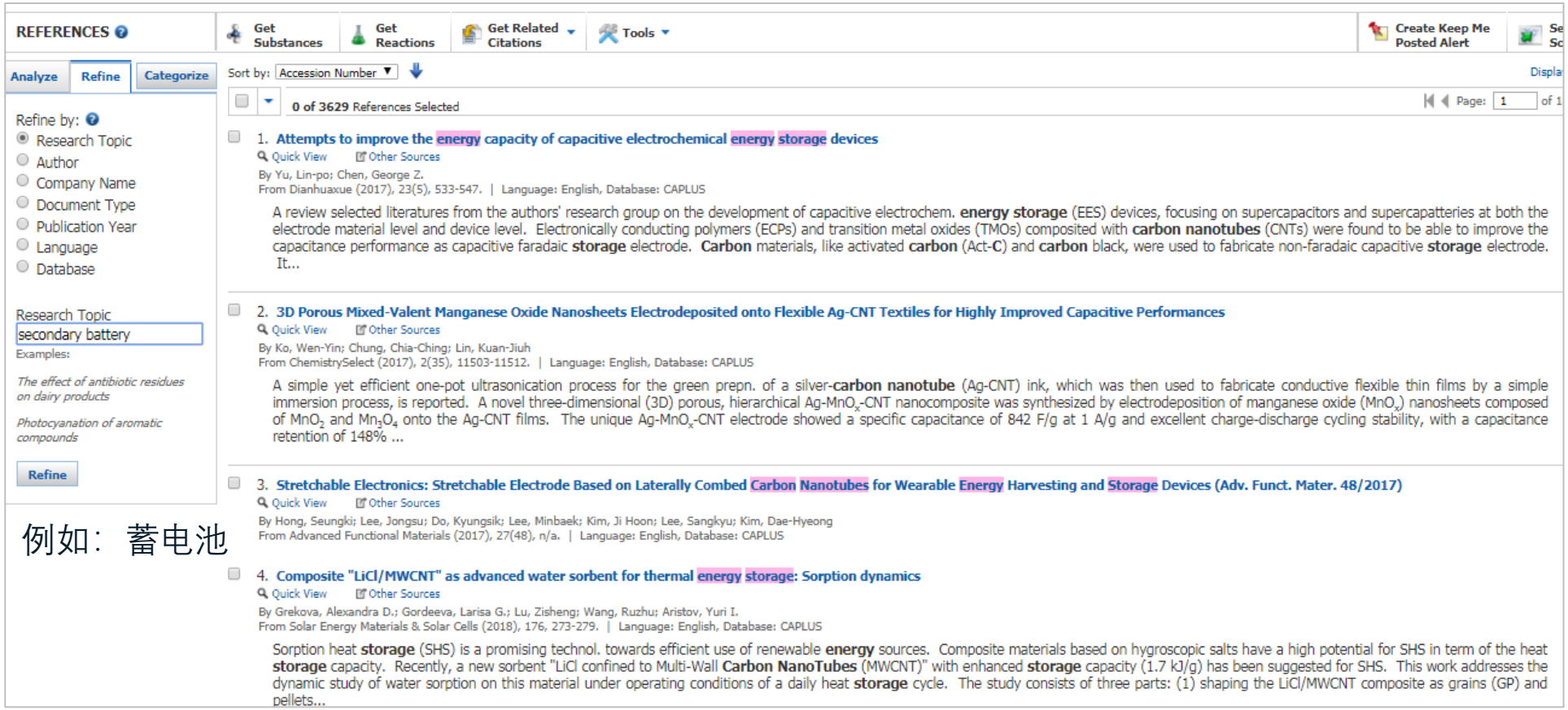
电容

能量储蓄系统

电流-电位关系

纳米粒子

也可通过Refine，筛选感兴趣的主题、作者、机构等



例如：蓄电池

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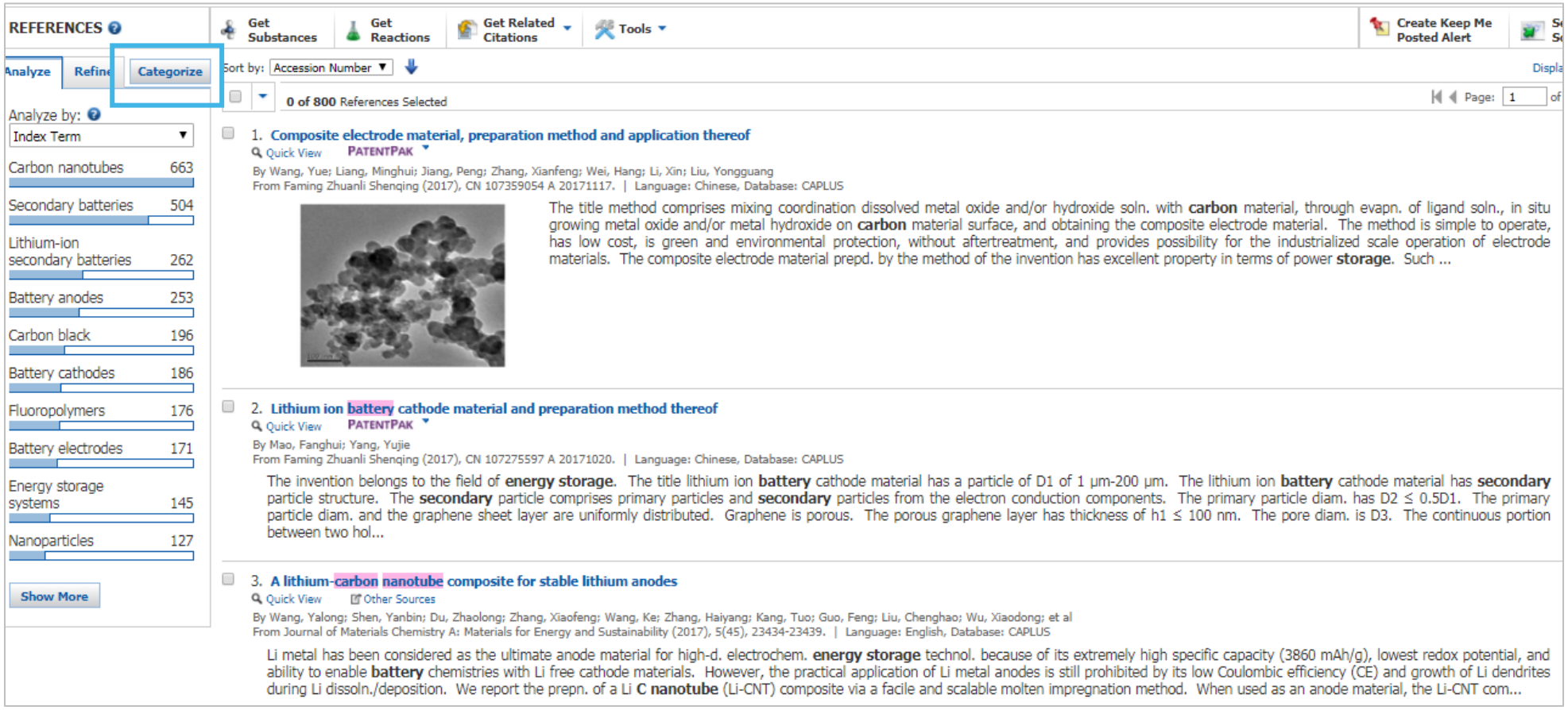
通过Categorize，可精准获取特定的研究信息



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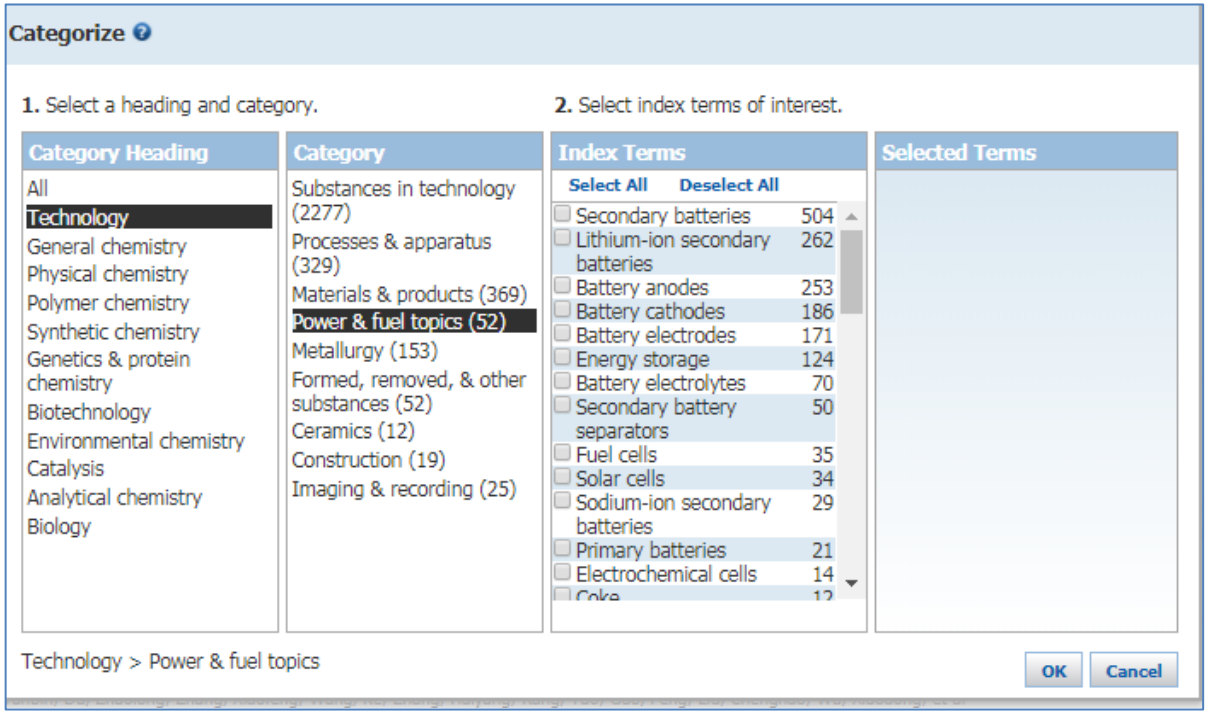
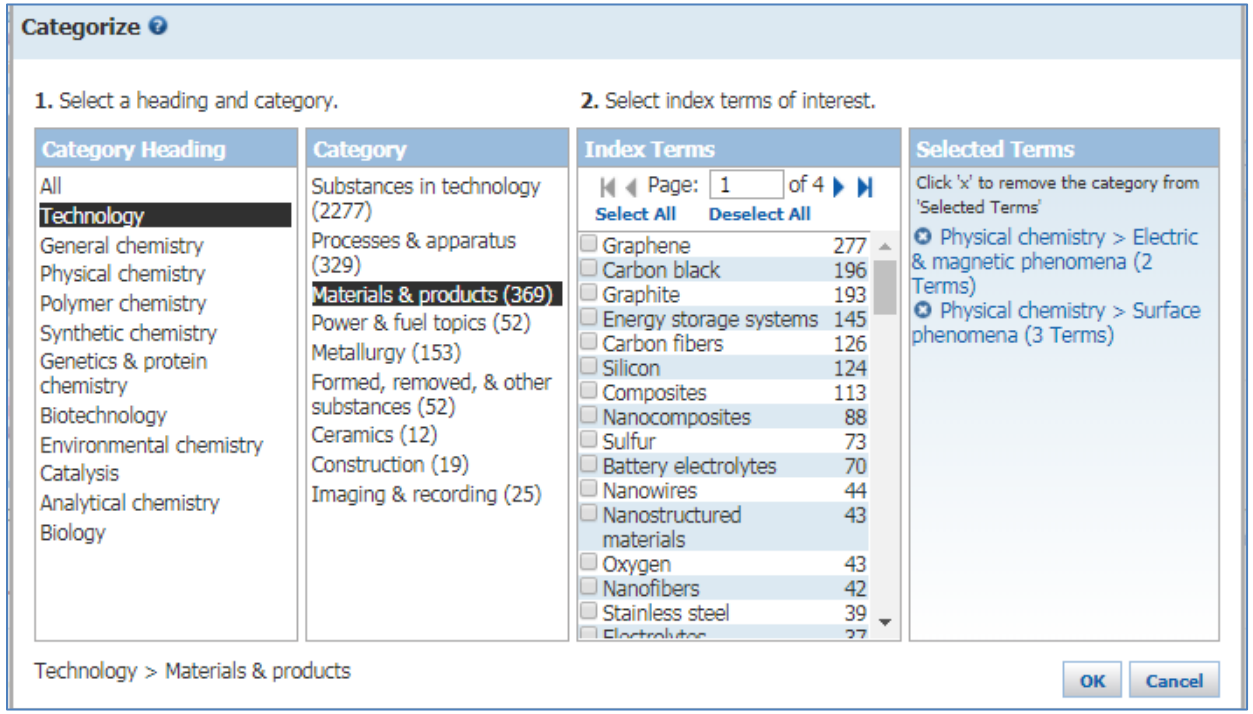
通过Technology，精准获取制备的能源&燃料，材料&产品等信息





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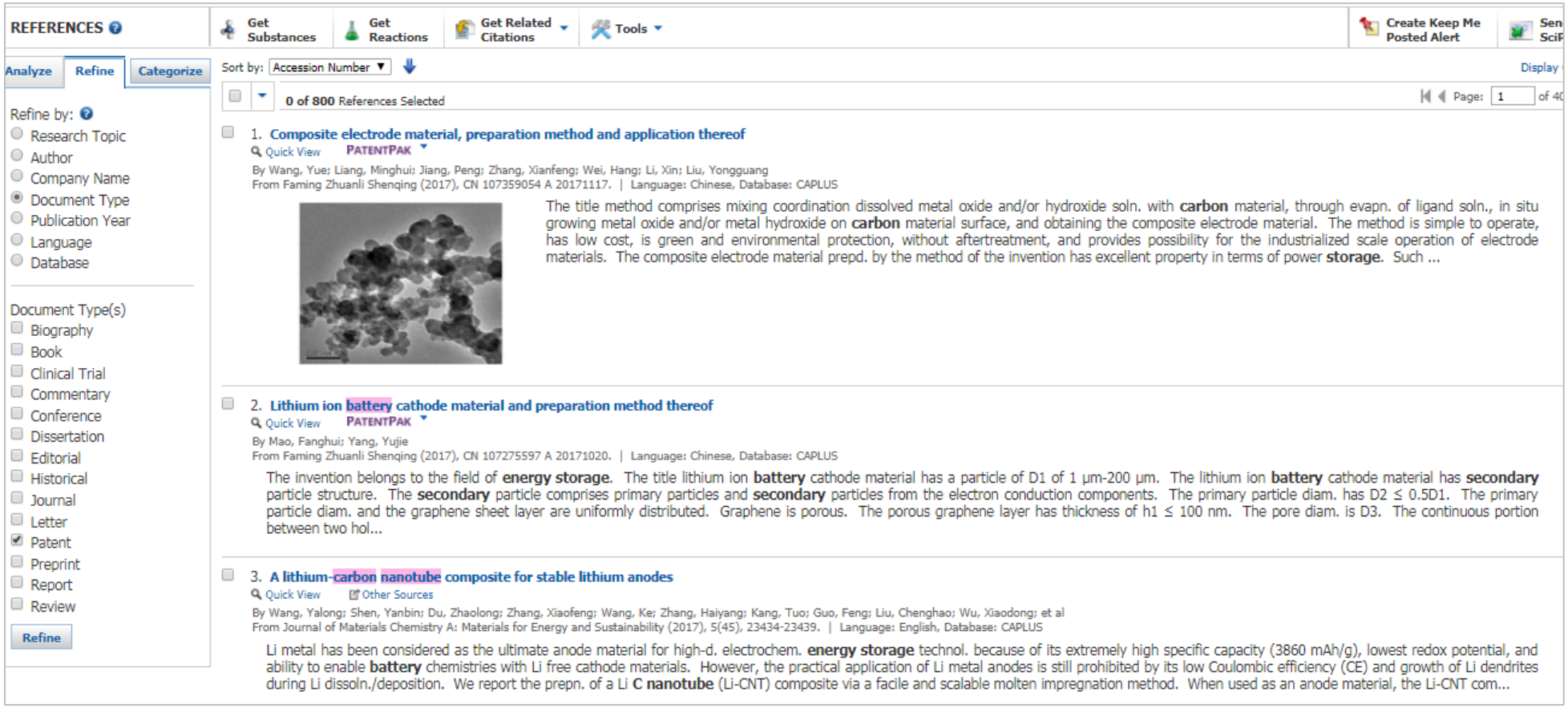
可通过Refine, 筛选专利文献



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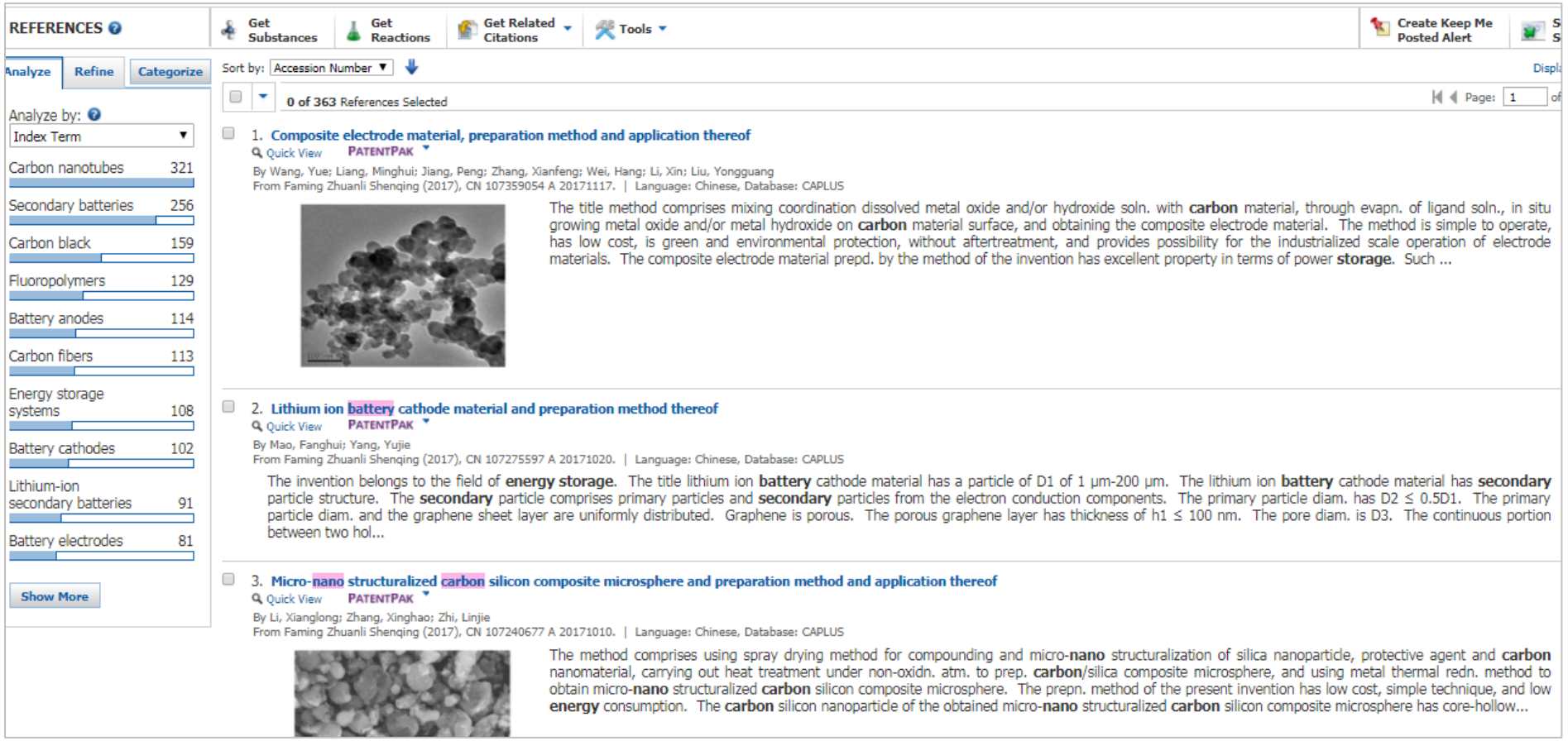
点击文献标题，可获取文献详情



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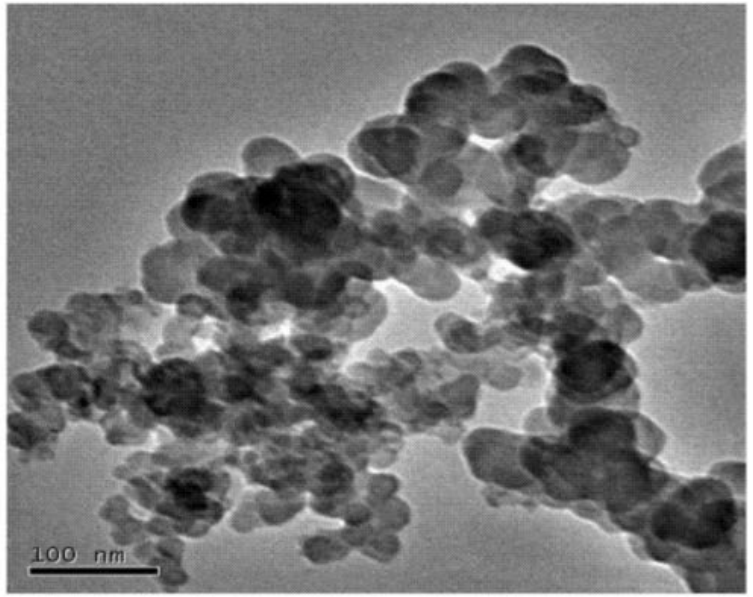
文献详情

1. Composite electrode material, preparation method and application thereof

By: Wang, Yue; Liang, Minghui; Jiang, Peng; Zhang, Xianfeng; Wei, Hang; Li, Xin; Liu, Yongguang
Assignee: National Center for Nanoscience and Technology, Peop. Rep. China

The title method comprises mixing coordination dissolved metal oxide and/or hydroxide soln. with carbon material, through evapn. of ligand soln., in situ growing metal oxide and/or metal hydroxide on carbon material surface, and obtaining the composite electrode material. The method is simple to operate, has low cost, is green and environmental protection, without aftertreatment, and provides possibility for the industrialized scale operation of electrode materials. The composite electrode material prepd. by the method of the invention has excellent property in terms of power storage. Such as the nickel hydroxide-activated carbon composite electrode material with 5% of loading amt. prepd. by the method of the invention under sweep speed of 5 mV/s, the complete electrode specific discharge capacity reaches 294 F/g, and the active substance specific capacity is up to 4917 F/g.



QUICK LINKS
0 Tags, 0 Comments

PATENT INFORMATION
Nov 17, 2017
CN 107359054
A

APPLICATION
May 9, 2016
CN 2016-10301475

PRIORITY
May 9, 2016
CN 2016-10301475

SOURCE
Faming Zhuanli Shenqing
13pp.
Patent
2017
CODEN:CNXXEV

ACCESSION NUMBER
2017:1811624
CAN168:7562
CAPLUS

LANGUAGE
Chinese

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
CN 107359054 PATENTPAK	A		Nov 17, 2017	CN 2016-10301475	May 9, 2016

Priority Application

CN 2016-10301475	May 9, 2016

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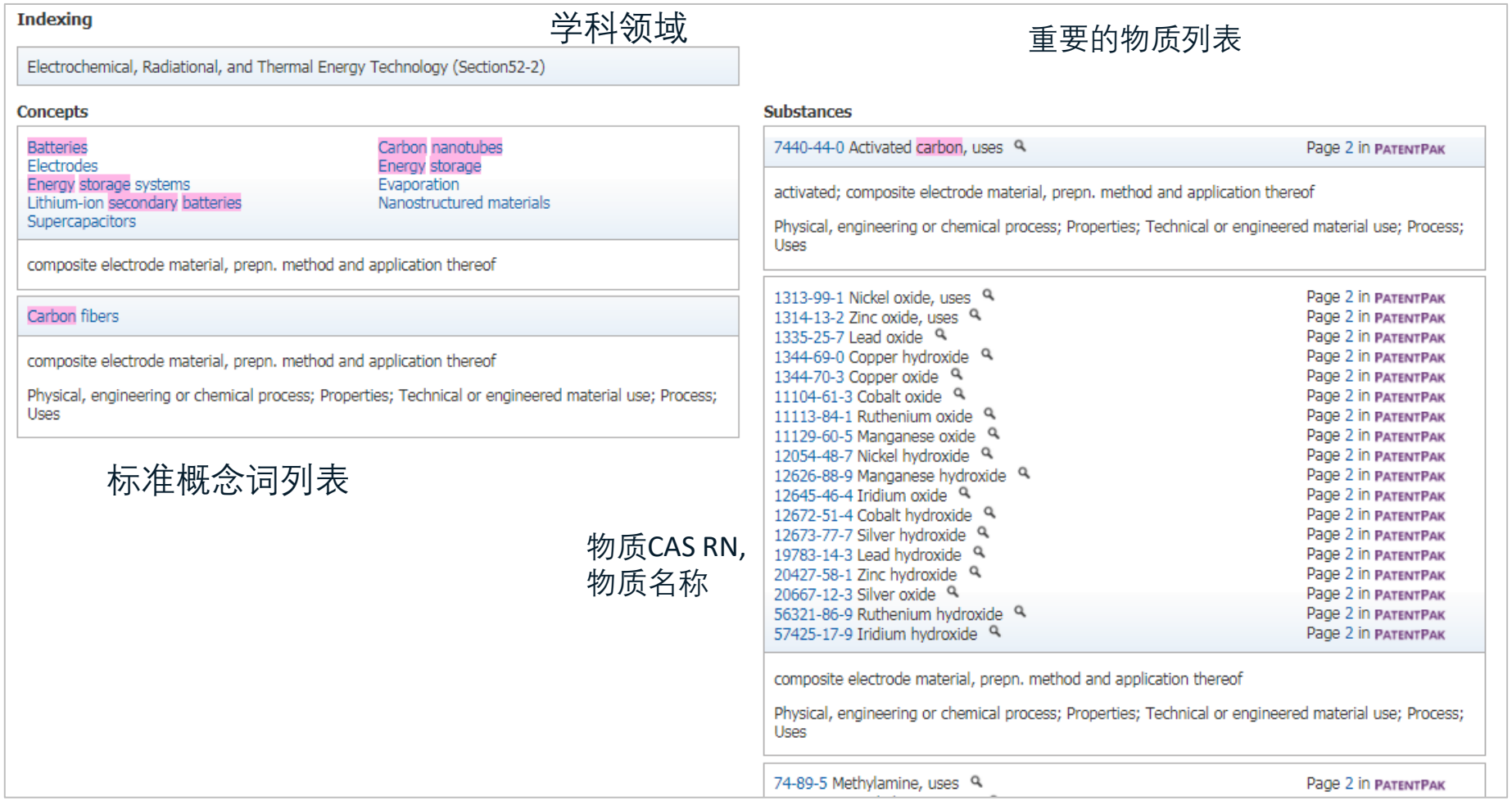
文献详情



Indexing

学科领域

Electrochemical, Radiational, and Thermal Energy Technology (Section52-2)

Concepts

Batteries
Electrodes
Energy storage systems
Lithium-ion secondary batteries
Supercapacitors
Carbon nanotubes
Energy storage
Evaporation
Nanostructured materials

composite electrode material, prepn. method and application thereof

Carbon fibers

composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

标准概念词列表

Substances

重要的物质列表

7440-44-0 Activated carbon, uses — Page 2 in PATENTPAK

activated; composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

物质功能描述

1313-99-1 Nickel oxide, uses — Page 2 in PATENTPAK
1314-13-2 Zinc oxide, uses — Page 2 in PATENTPAK
1335-25-7 Lead oxide — Page 2 in PATENTPAK
1344-69-0 Copper hydroxide — Page 2 in PATENTPAK
1344-70-3 Copper oxide — Page 2 in PATENTPAK
11104-61-3 Cobalt oxide — Page 2 in PATENTPAK
11113-84-1 Ruthenium oxide — Page 2 in PATENTPAK
11129-60-5 Manganese oxide — Page 2 in PATENTPAK
12054-48-7 Nickel hydroxide — Page 2 in PATENTPAK
12626-88-9 Manganese hydroxide — Page 2 in PATENTPAK
12645-46-4 Iridium oxide — Page 2 in PATENTPAK
12672-51-4 Cobalt hydroxide — Page 2 in PATENTPAK
12673-77-7 Silver hydroxide — Page 2 in PATENTPAK
19783-14-3 Lead hydroxide — Page 2 in PATENTPAK
20427-58-1 Zinc hydroxide — Page 2 in PATENTPAK
20667-12-3 Silver oxide — Page 2 in PATENTPAK
56321-86-9 Ruthenium hydroxide — Page 2 in PATENTPAK
57425-17-9 Iridium hydroxide — Page 2 in PATENTPAK

定位信息

物质CAS RN, 物质名称

composite electrode material, prepn. method and application thereof

Physical, engineering or chemical process; Properties; Technical or engineered material use; Process; Uses

74-89-5 Methylamine, uses — Page 2 in PATENTPAK

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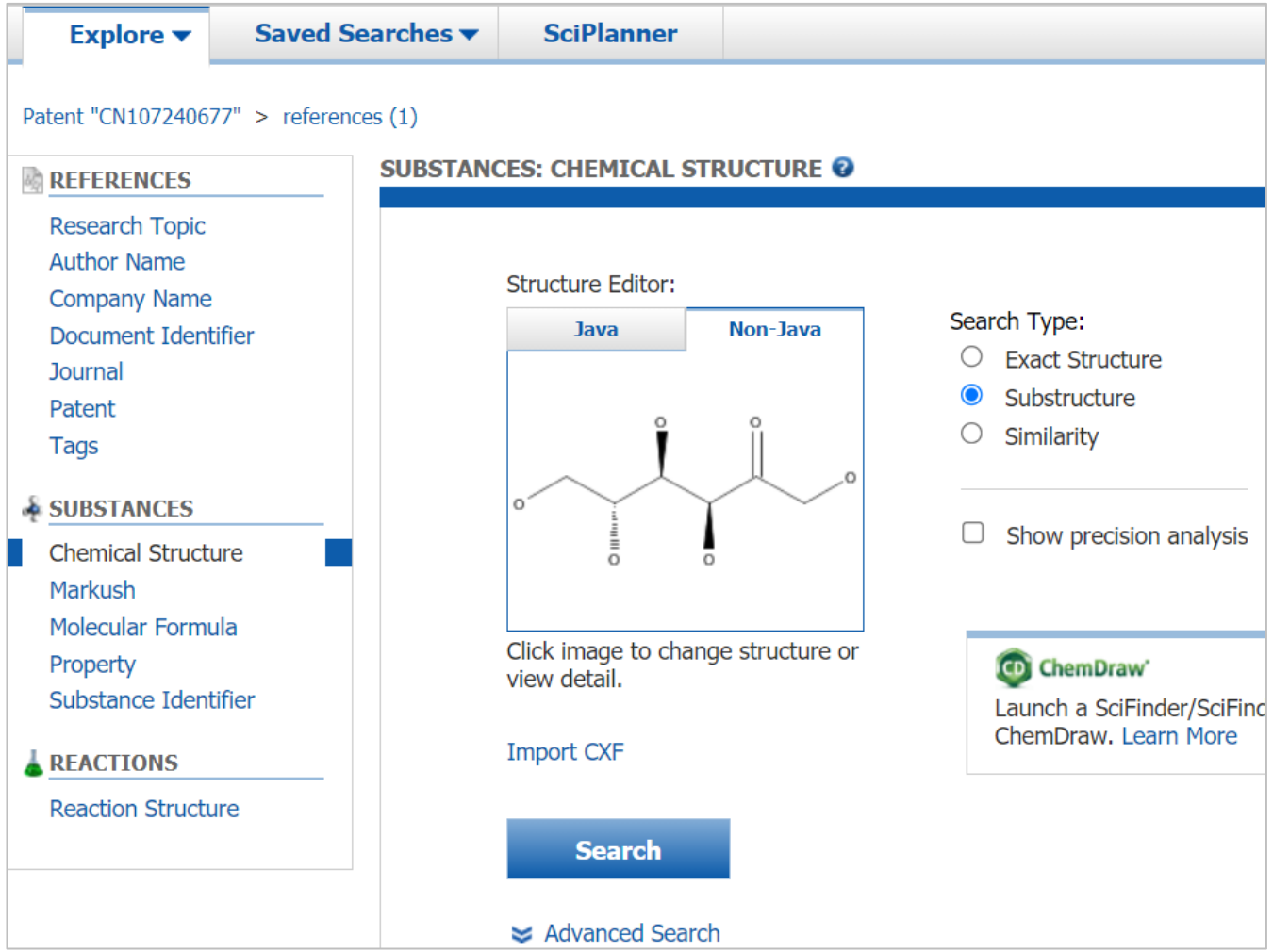
无缝连接进行新的检索



文献检索小结：

- 主题检索时，使用介词 in, with, of 等作为连接词
- 跟据检索要求选择合适的候选项
- 通过SciFinder 的Analyze/Refine功能来缩小检索的范围
- 使用Categorize可以让系统来实现自动分类
- 充分利用文献详情中增值标引信息

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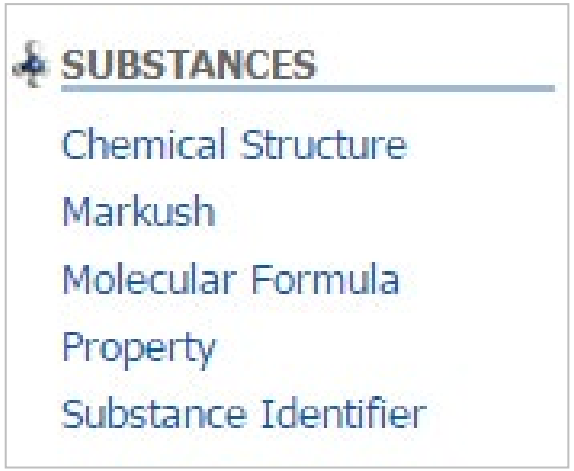
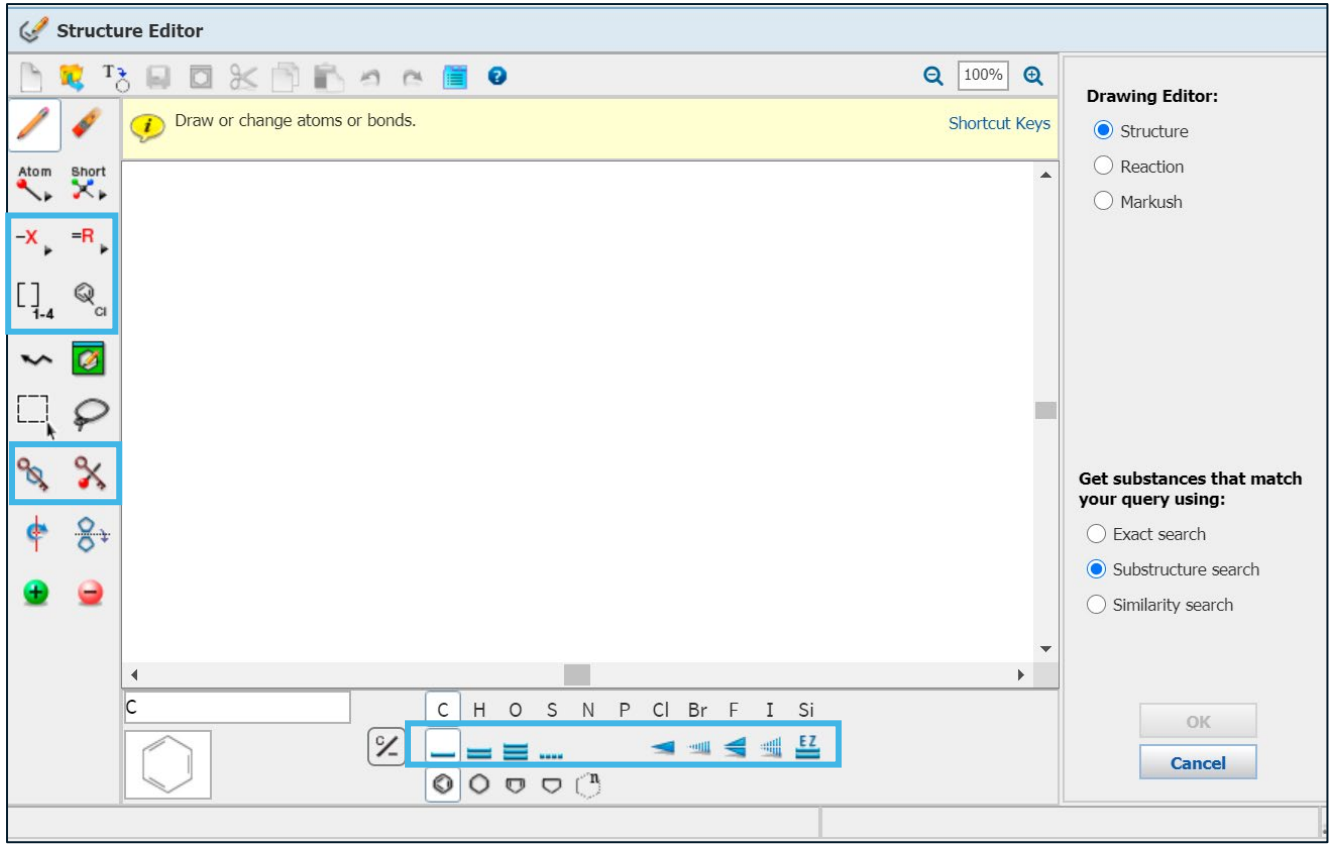
物质检索的方法

- 物质检索方法
  - —结构式检索
  - —分子式检索
  - —理化性质检索
  - —物质标识符检索：化学名称，CAS RN

- 物质检索策略推荐
  - —有机化合物，天然产物：结构检索
  - —无机物，合金：分子式检索
  - —高分子化合物：分子式检索和结构检索

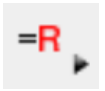


结构编辑器的使用



重要绘制工具注释

选择可变基团



自定义R基团

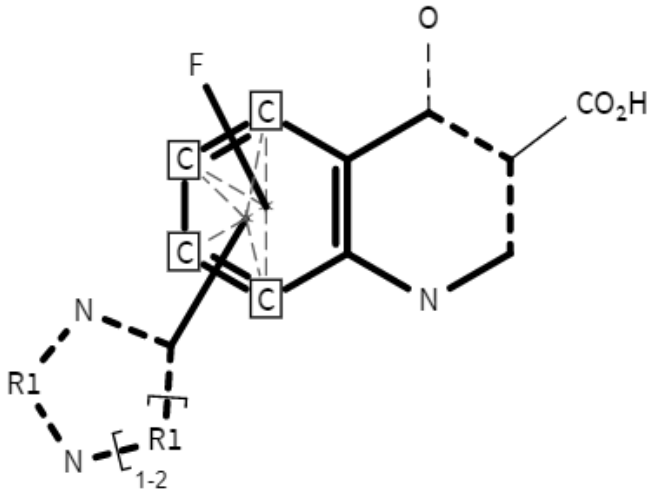
重复工具

取代位置可变

锁环工具

锁原子工具

有机化合物: 通式结构的绘制



R1 = C, O

要求:

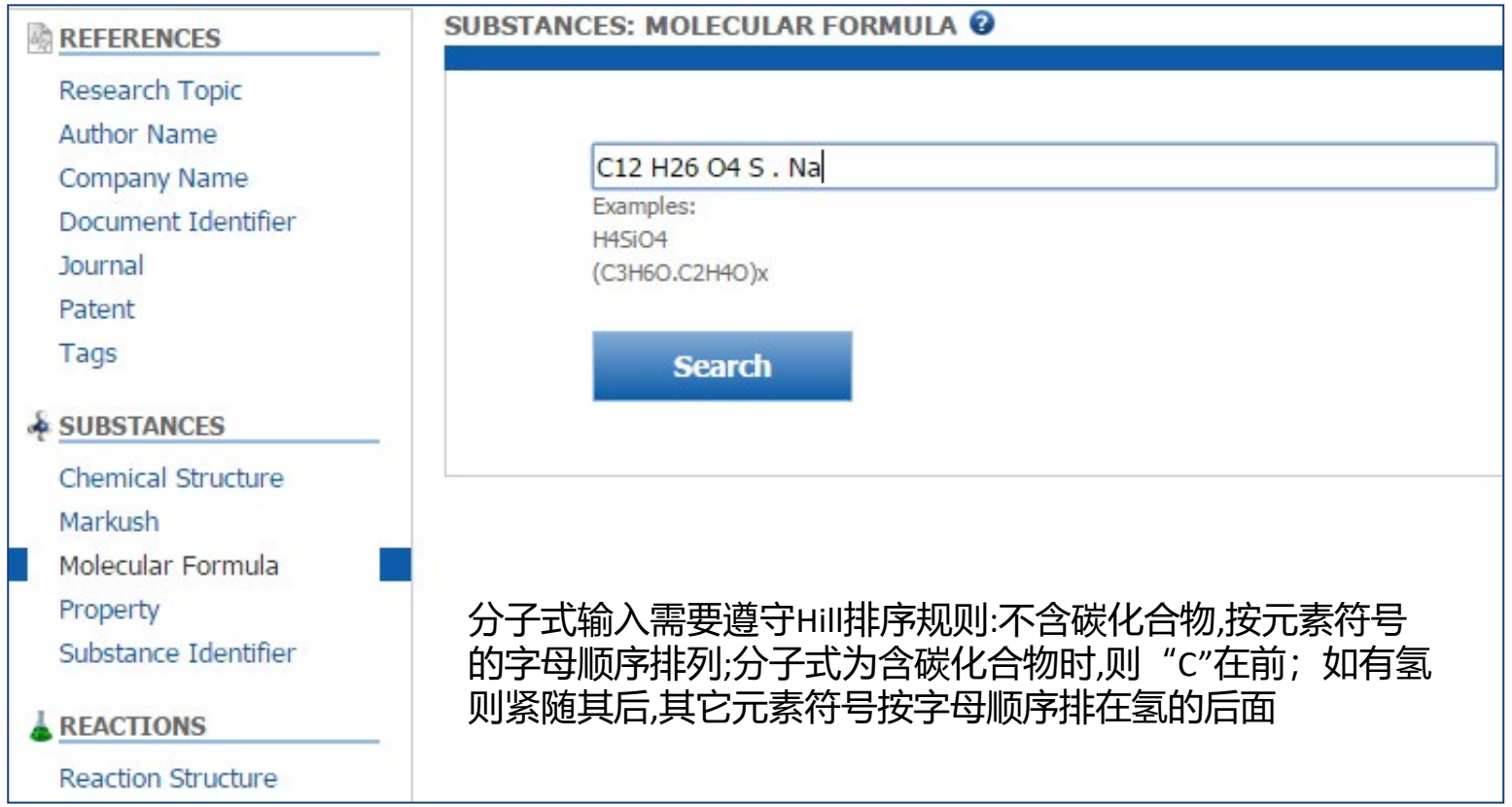
1.两个环系不能与其他环（系）形成新的稠环（系）或桥环（系）；

2. 六元含氮环上可出现互变异构，比如烯酮;

3. 六元碳环上有一个F取代和一个五至六元的饱和或非饱和杂环取代。杂环的1,3位为N原子，R1为C或O;

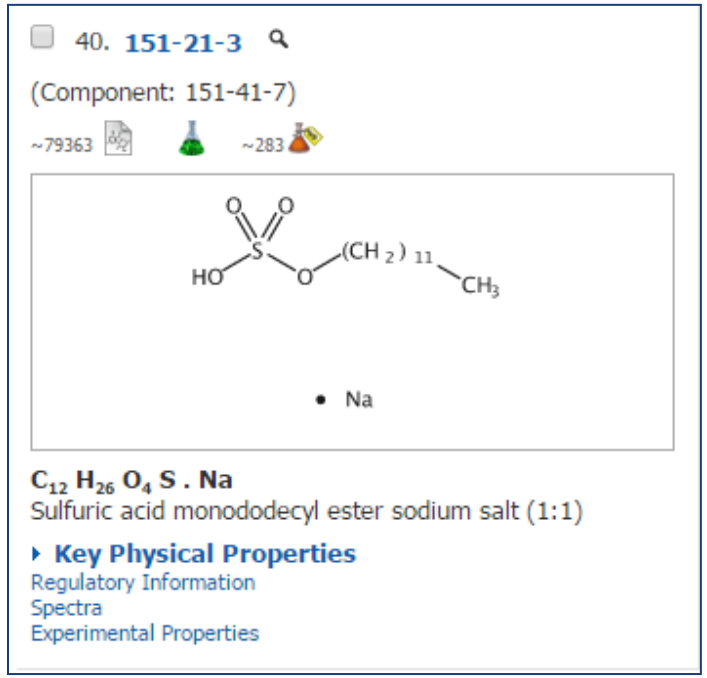
4.六元碳环上有且只有杂环和F取代，且连接位点不确定。

根据分子式检索无机化合物

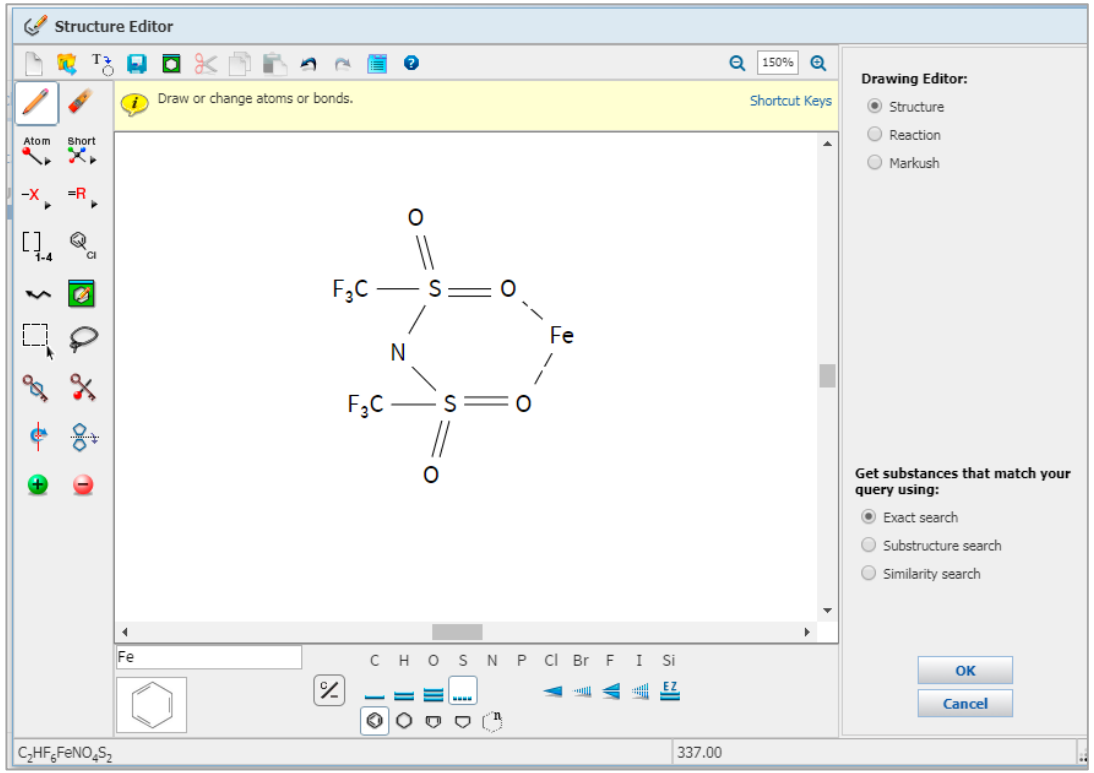


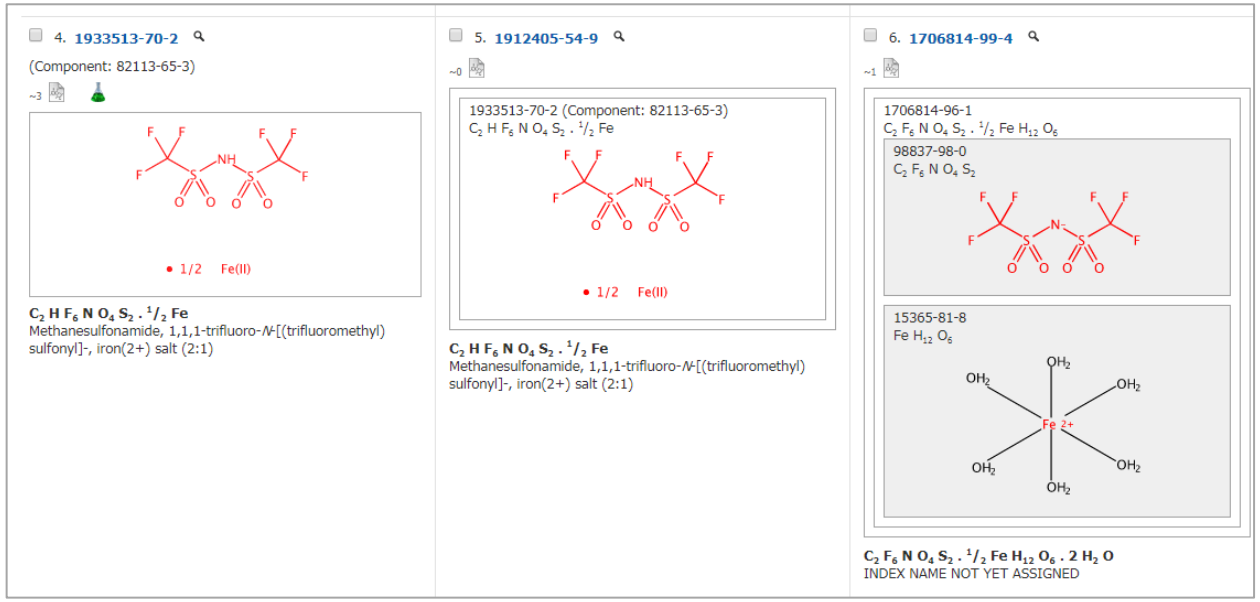
分子式输入需要遵守Hill排序规则:不含碳化合物,按元素符号的字母顺序排列;分子式为含碳化合物时,则“C”在前；如有氢则紧随其后,其它元素符号按字母顺序排在氢的后面

无机金属盐：金属离子和阴离子间用点（.）分开



根据络合物的结构来检索配位化合物





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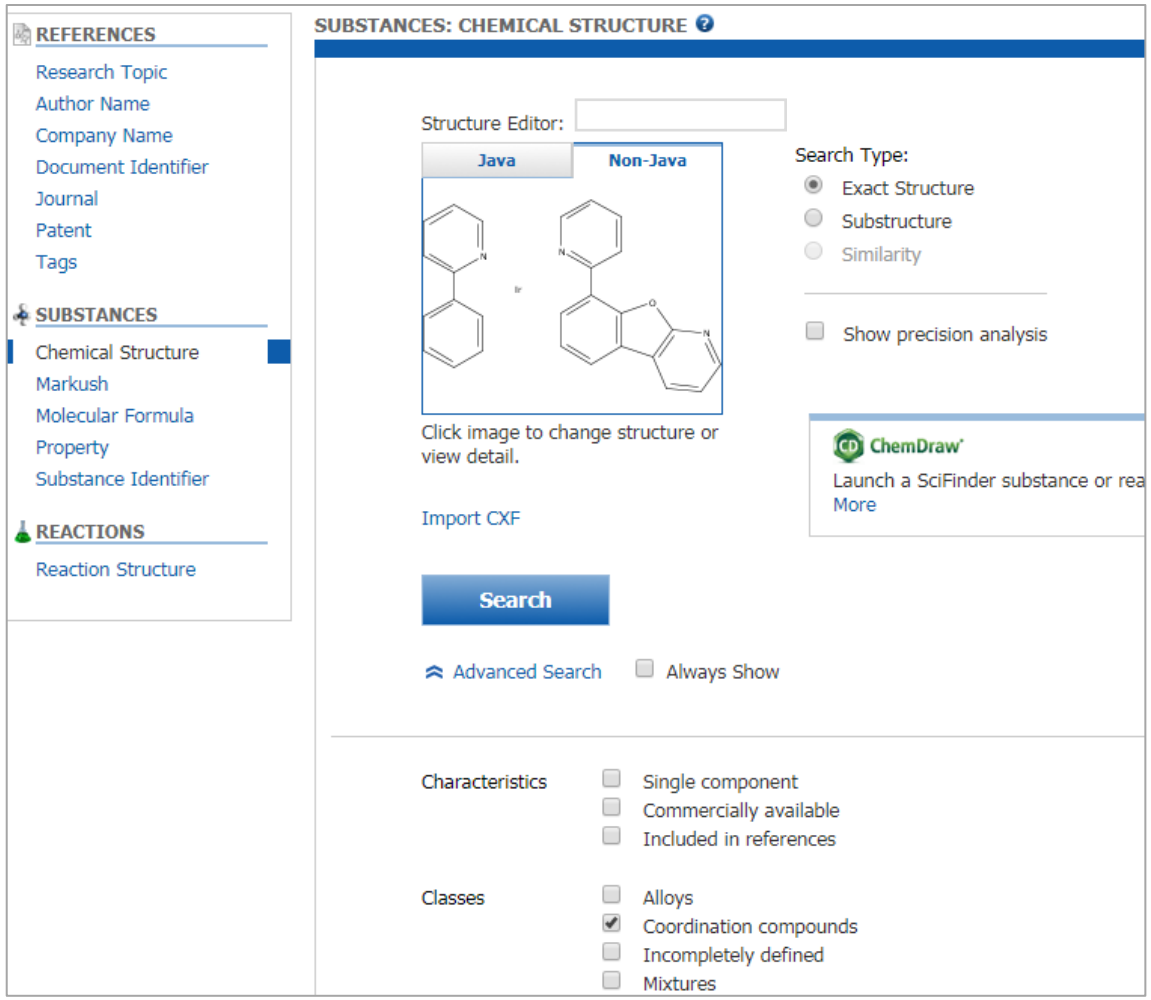
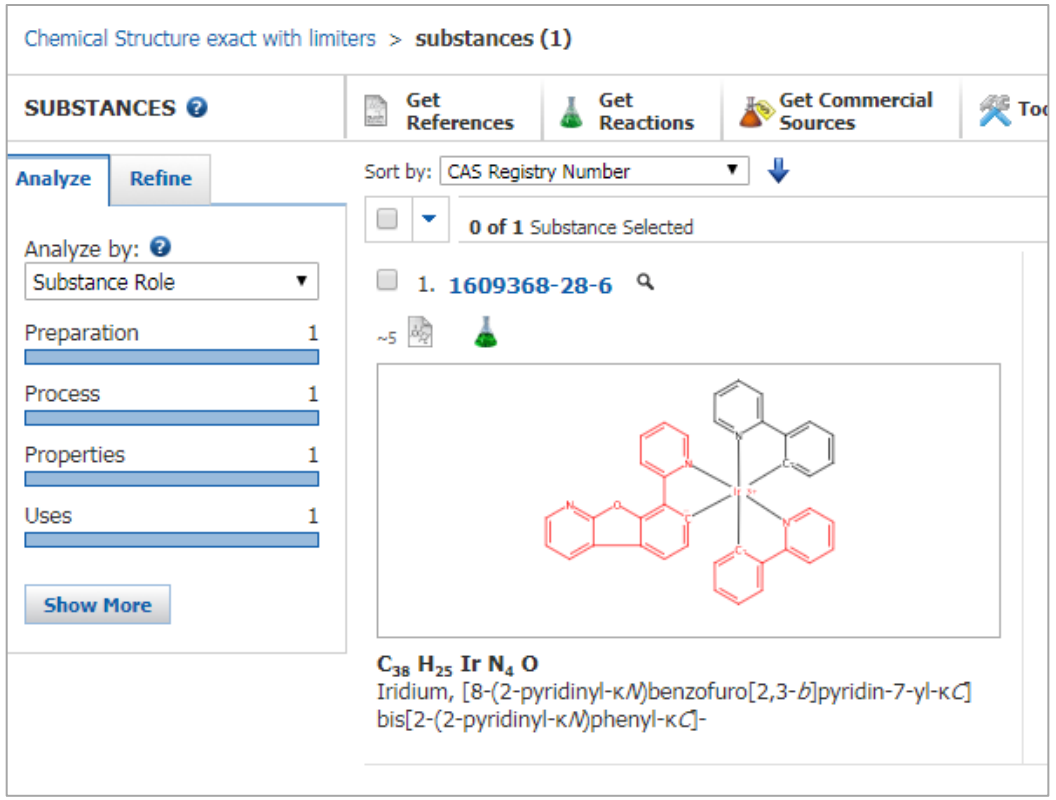
根据配体结构和中心金属原子来检索配位化合物





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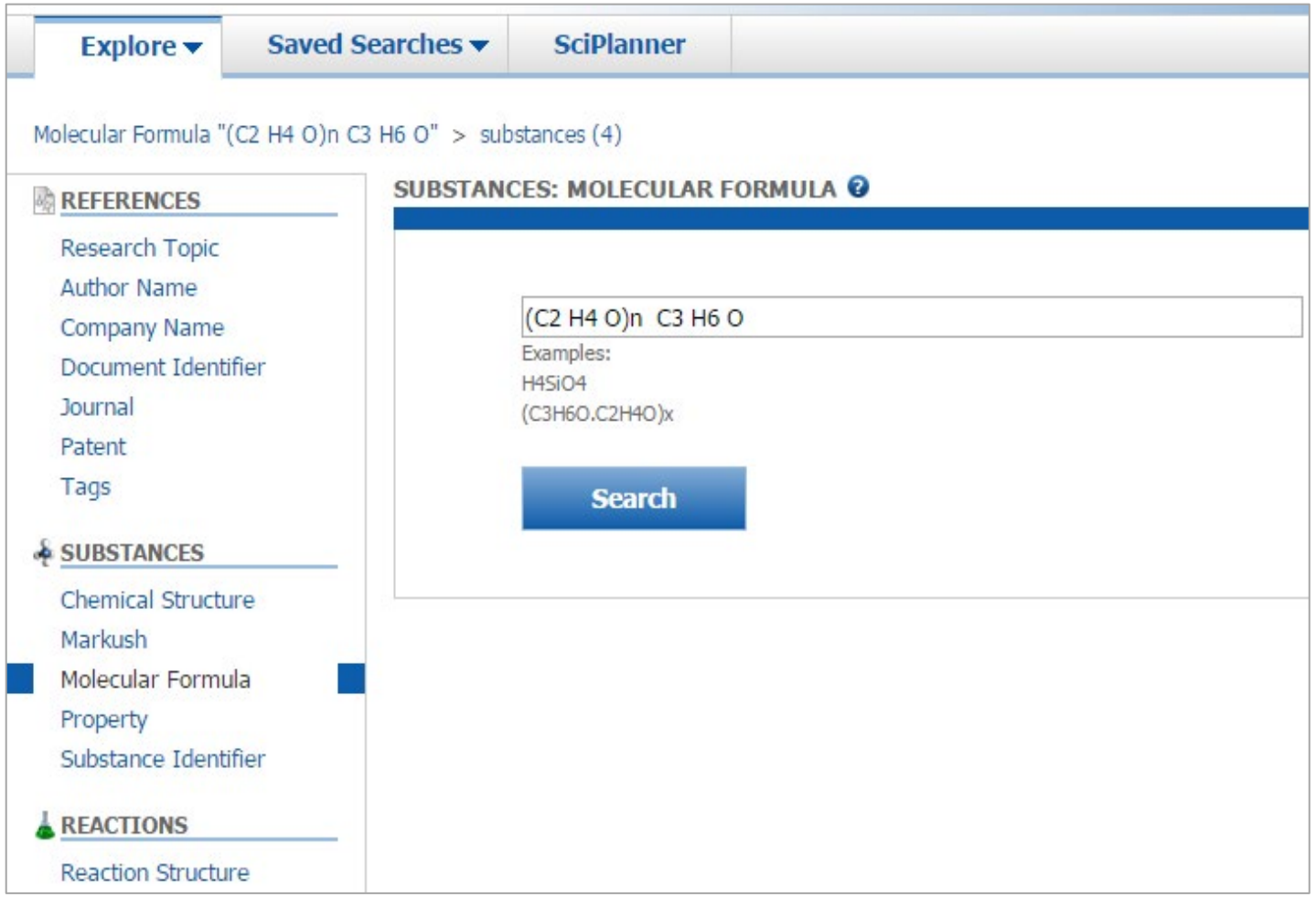
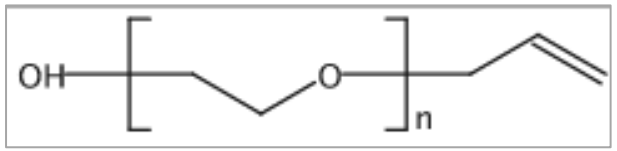
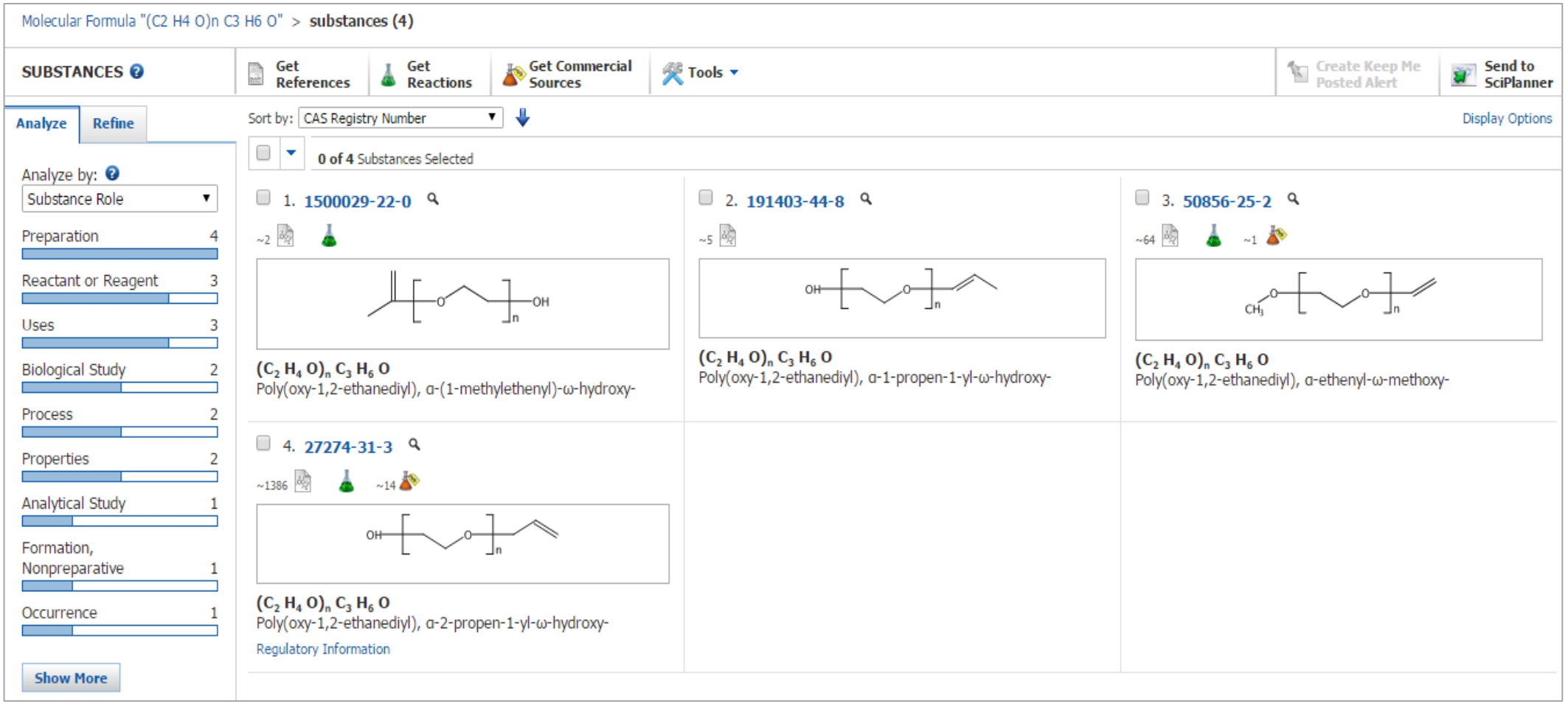
通过聚合物的重复结构单元来检索聚合物





通过聚合物的重复结构单元来检索聚合物



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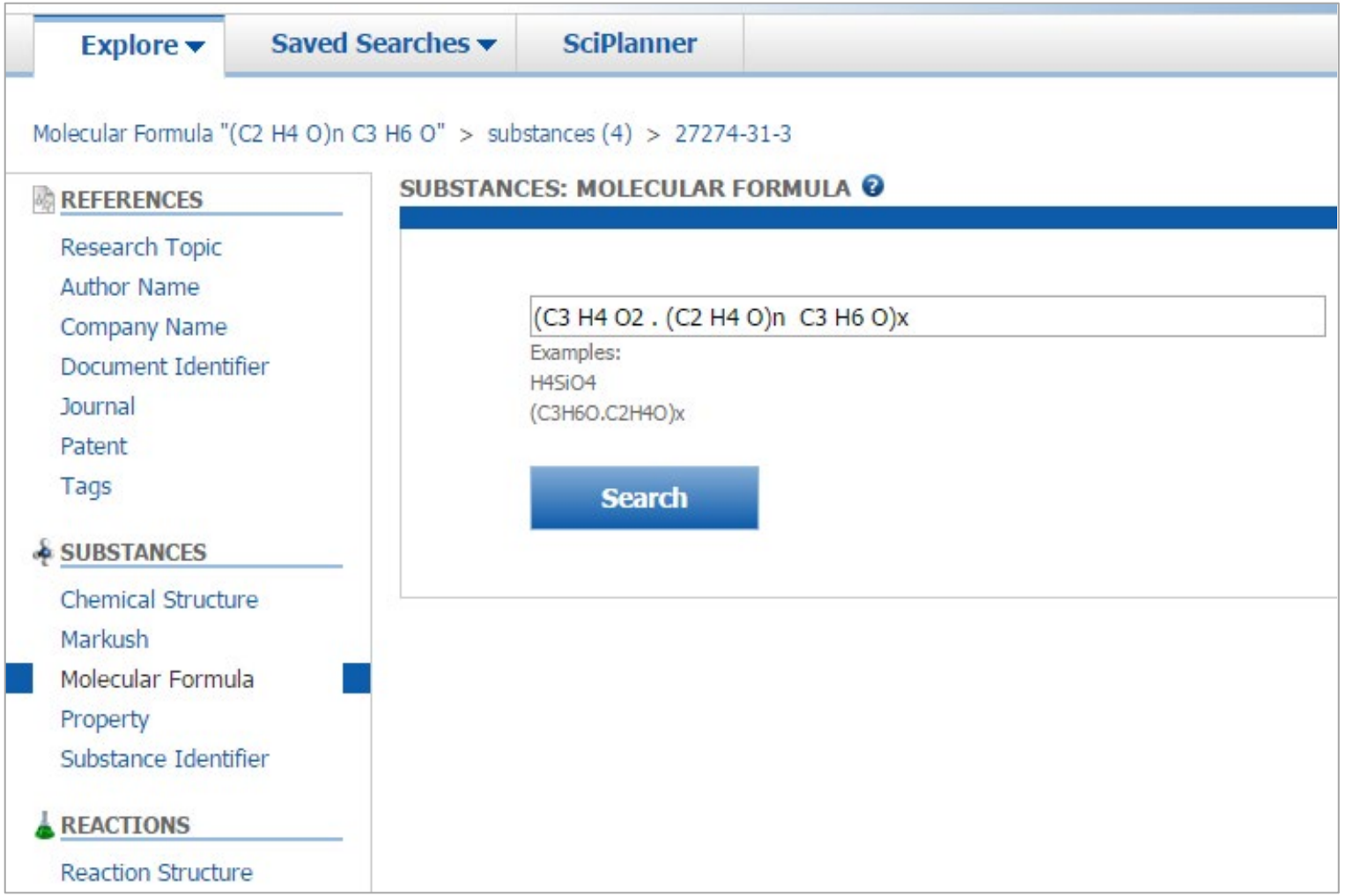
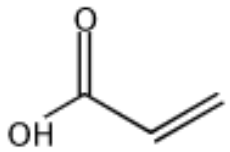
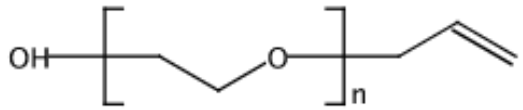
通过聚合物的重复结构单元来检索聚合物







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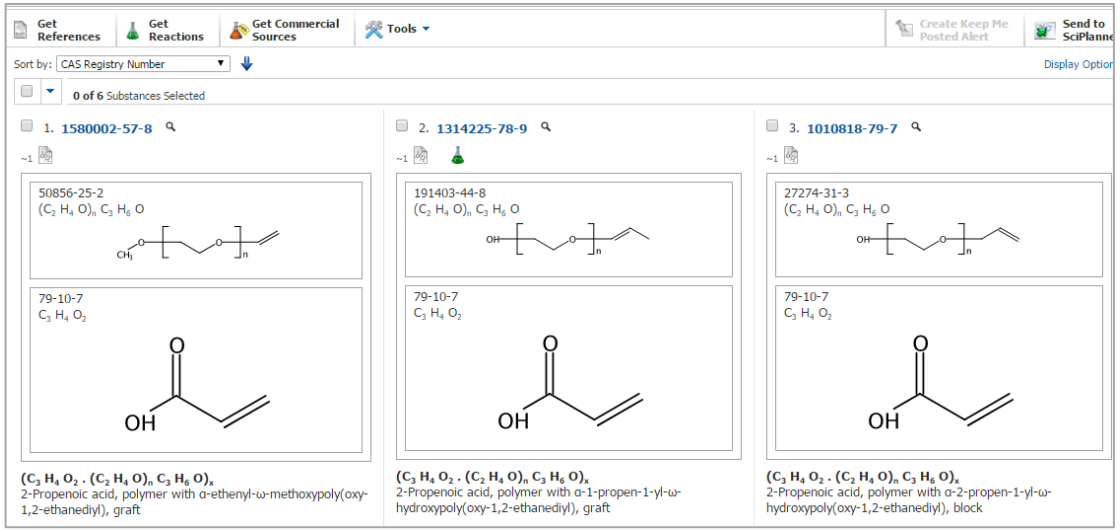

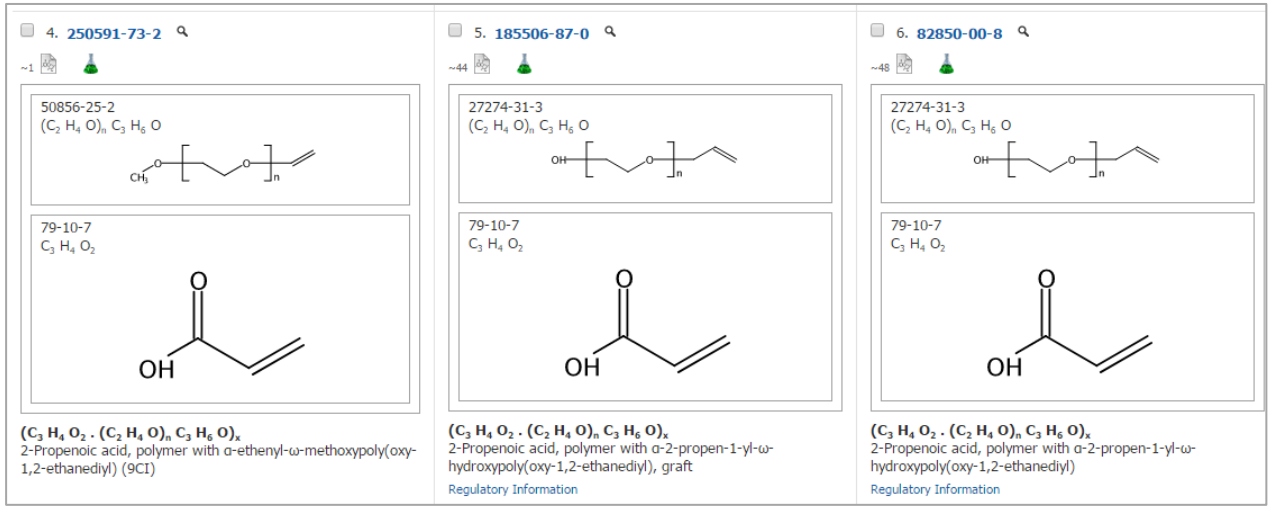

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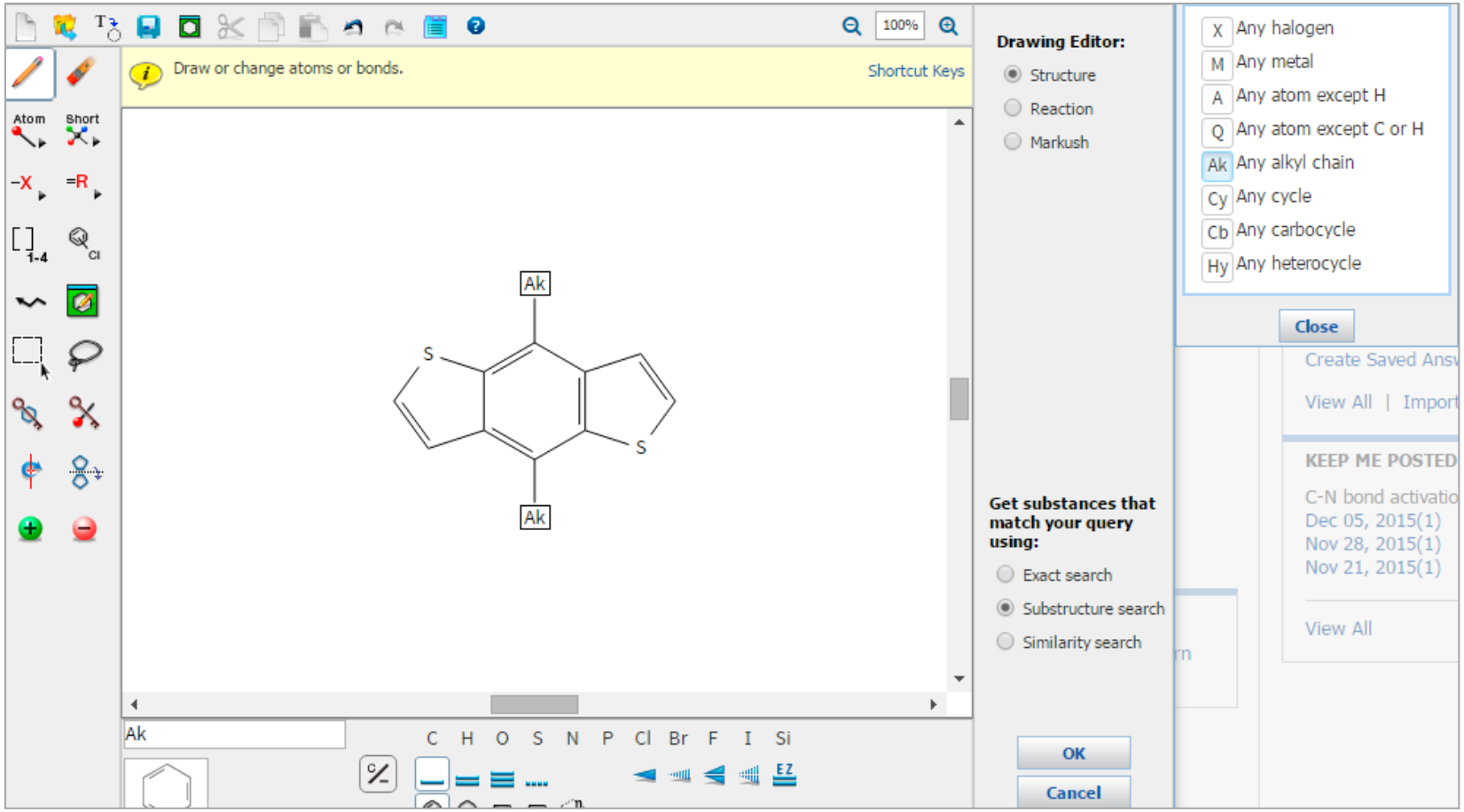
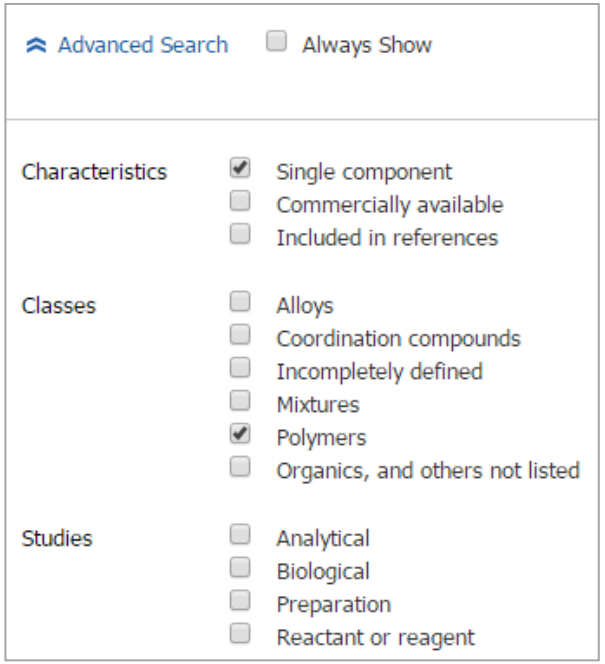
通过聚合物的重复结构单元来检索聚合物





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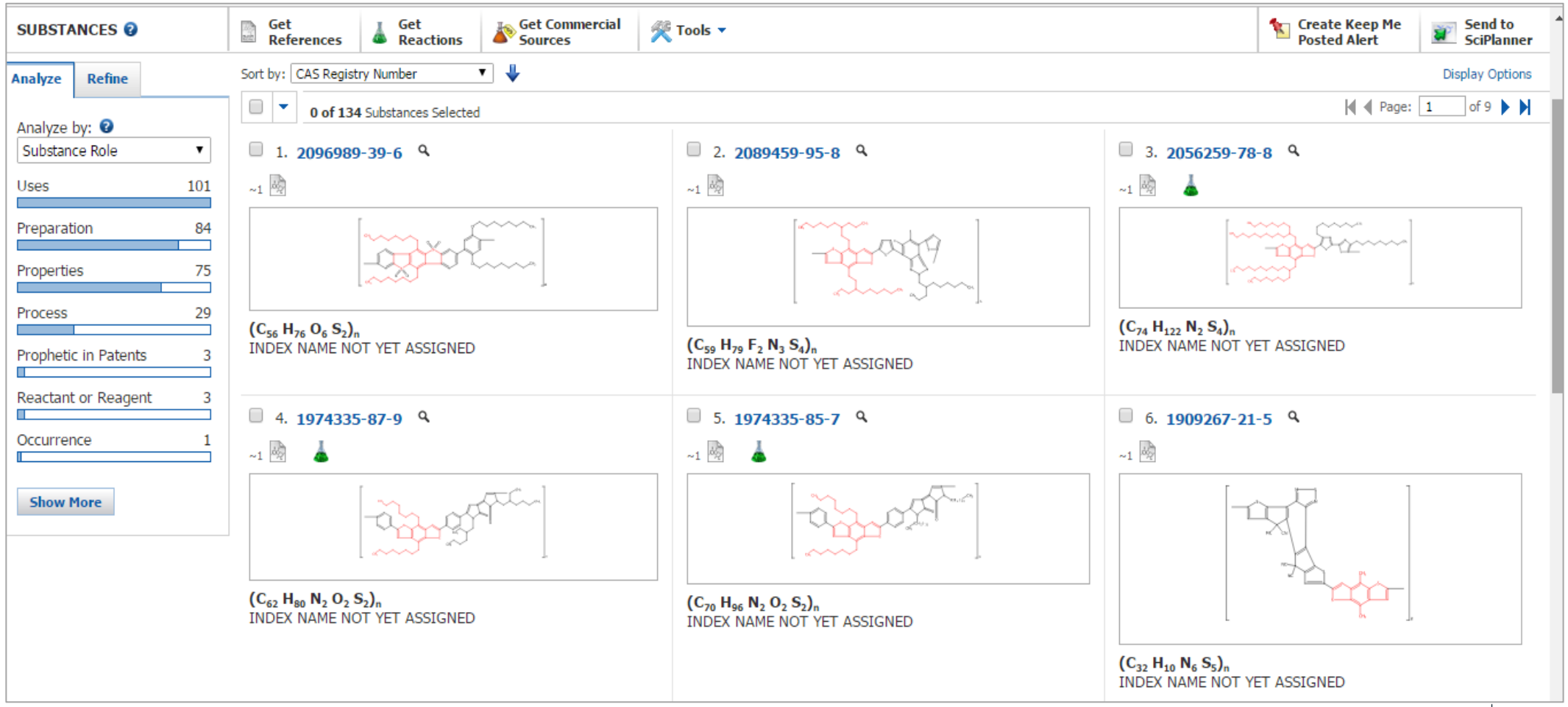

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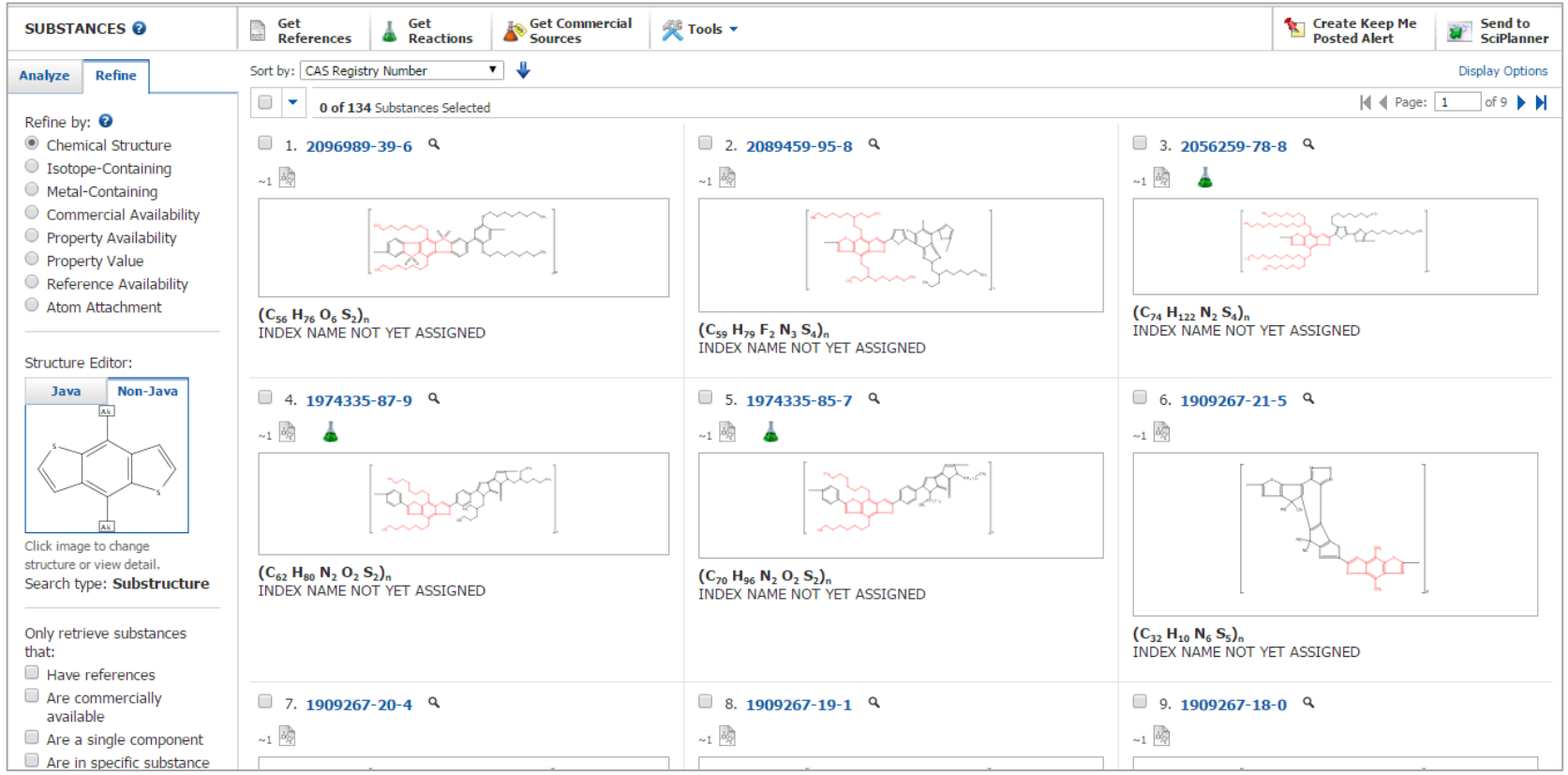
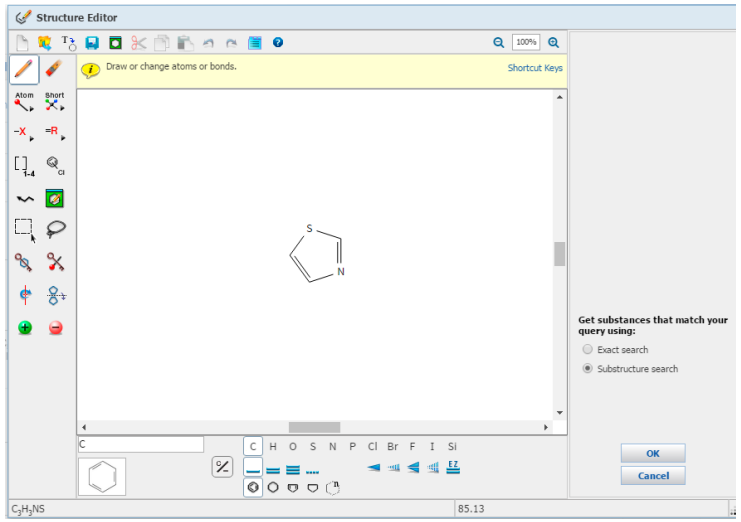
通过聚合物的重复结构单元来检索聚合物





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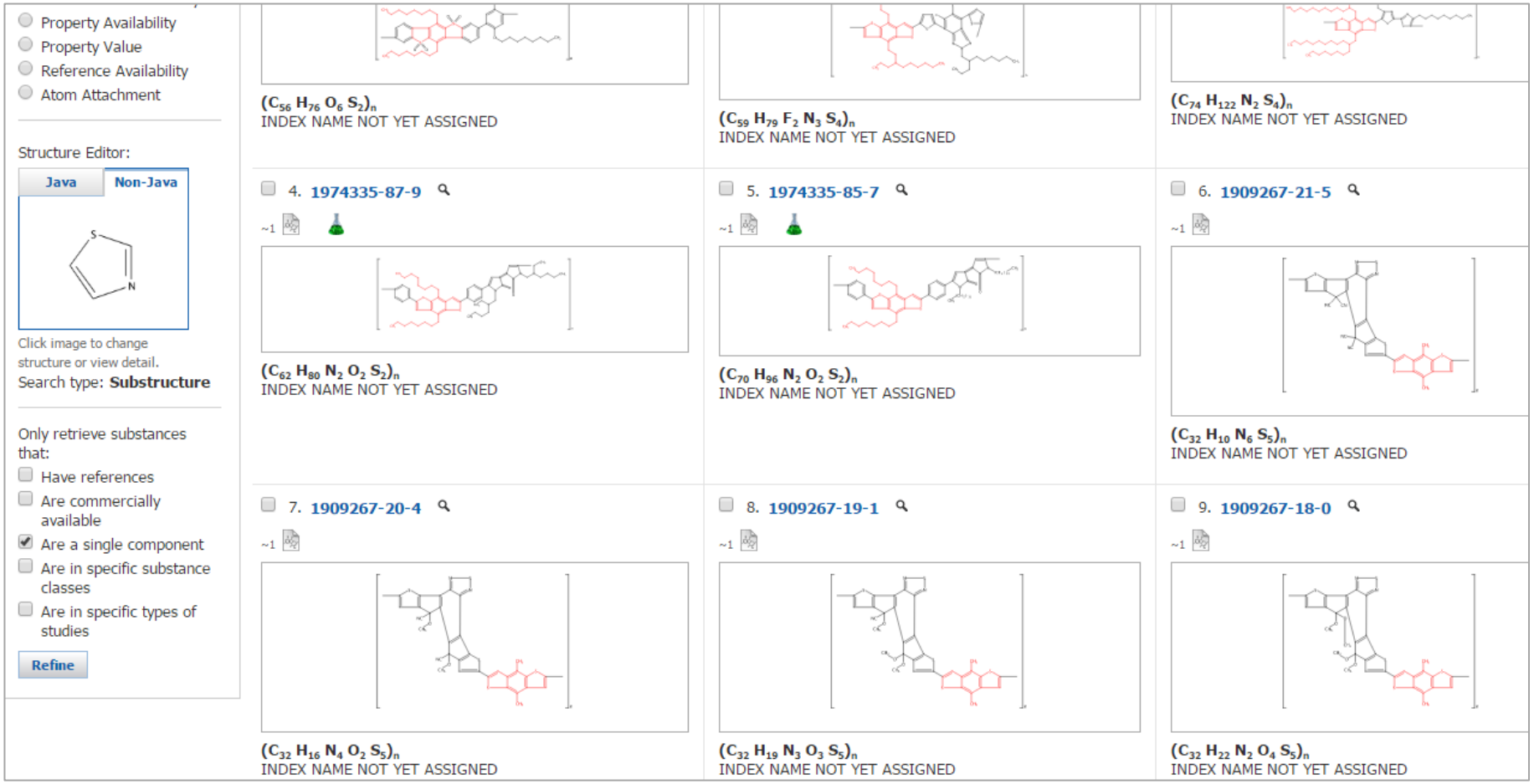

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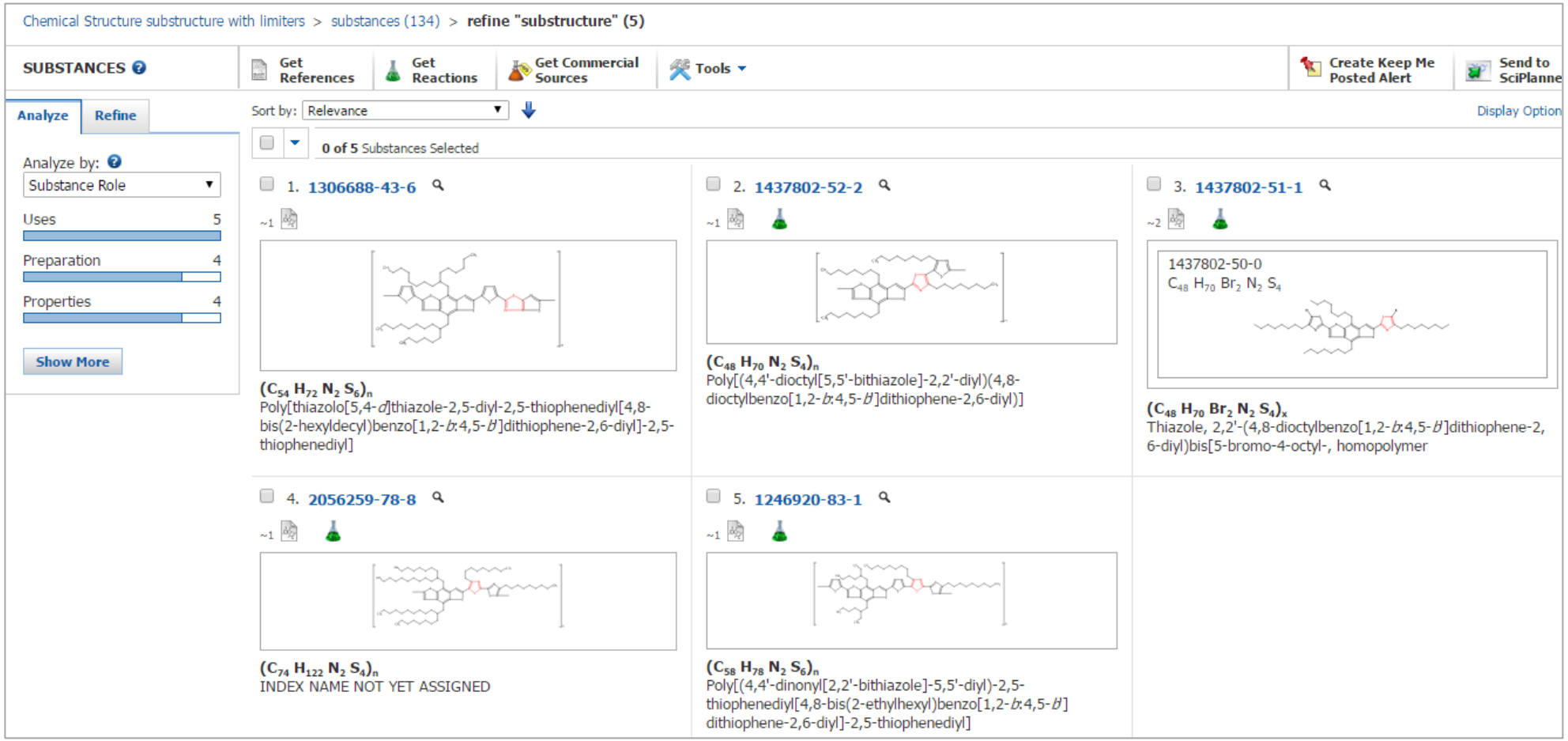

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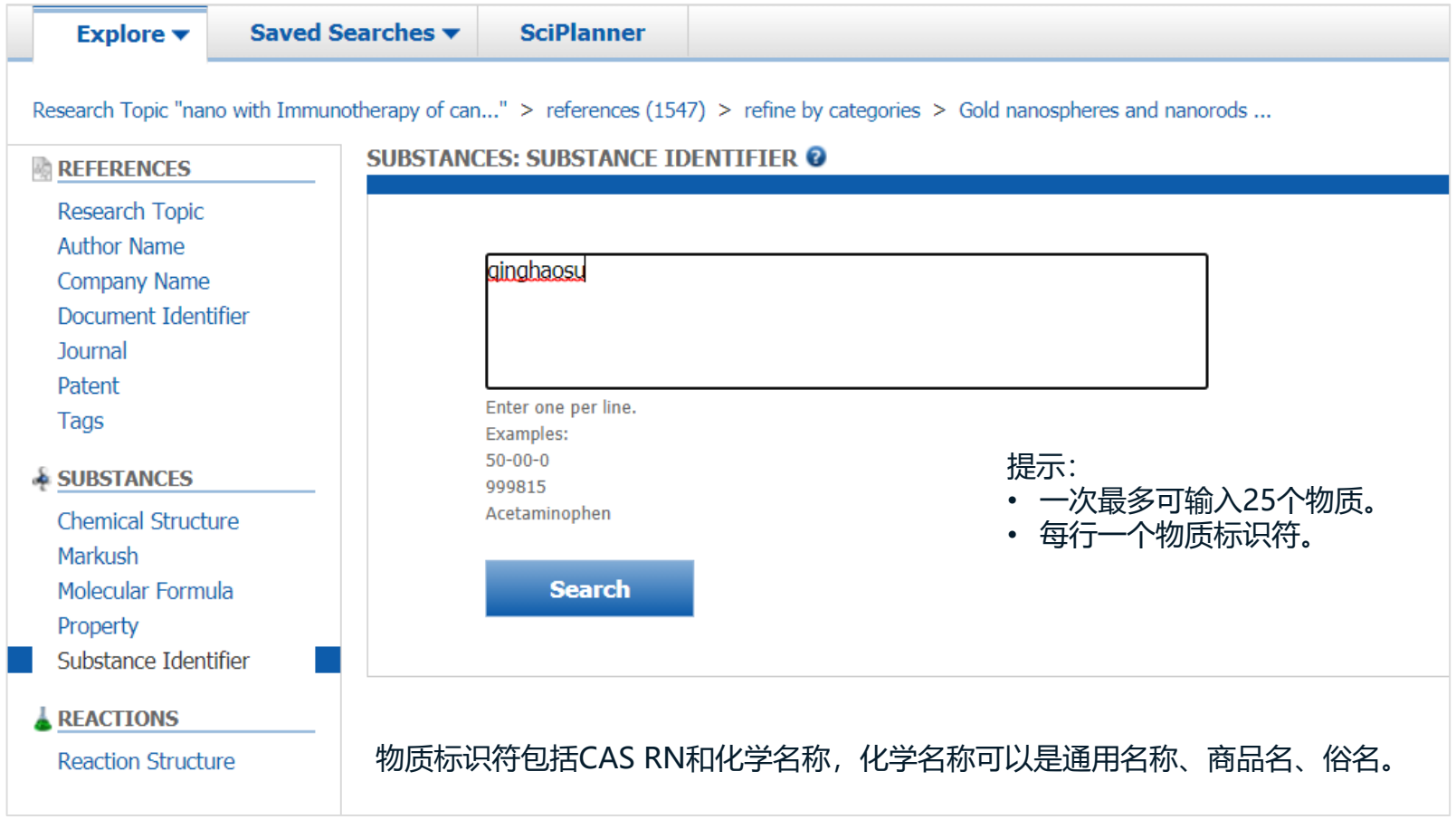
物质标识符检索



提示：
- 一次最多可输入25个物质。
- 每行一个物质标识符。

物质标识符包括CAS RN和化学名称，化学名称可以是通用名称、商品名、俗名。

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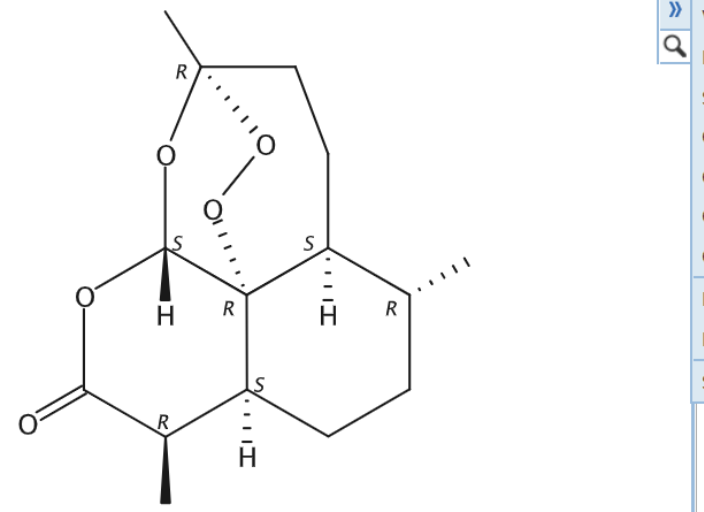
物质结果

1. 63968-64-9

~6028 ~132



Absolute stereochemistry.

CAS Registry Number: 63968-64-9

View Substance Detail

Explore by Structure

Synthesize this...

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Export as molfile

Send to SciPlanner

$C_{15}H_{22}O_5$

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

Key Physical Properties

Regulatory Information

Spectra

Experimental Properties

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点击CAS RN获取物质详情

SUBSTANCE DETAIL | Get References | Get Reactions | Get Commercial Sources

Return

CAS Registry Number 63968-64-9

~6,028 ~132

$C_{15}H_{22}O_5$

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*)-

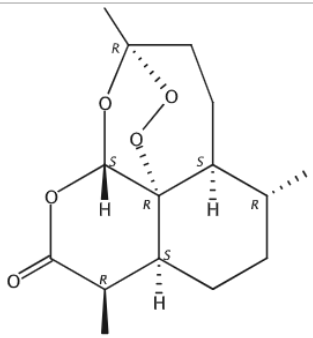
Molecular Weight
282.33

Melting Point (Experimental)
Value: 156-157 °C

Boiling Point (Predicted)
Value: 389.9±42.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.300 g/cm3

Other Names
3,12-Epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, octahydro-3,6,9-trimethyl-, [3*R*-(3α,5aβ,6β,8aβ,9α,12β,12a*R**)]-
(3*R*,5a*S*,6*R*,8a*S*,9*R*,12*S*,12a*R*)-Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one
(+)-Arteannuin
(+)-Artemisinin
(+)-Qinghaosu
View more...



Absolute stereochemistry.

▸ EXPERIMENTAL PROPERTIES

▾ EXPERIMENTAL SPECTRA

^{1}H NMR | ^{13}C NMR | Hetero NMR | IR | Mass | Raman | UV and Visible | Additional Spectra

^{13}C NMR Properties	Value	Condition	Note
Carbon-13 NMR Spectrum	See spectrum		(3)ACD
Carbon-13 NMR Spectrum	See spectrum		(4)ACD
Carbon-13 NMR Spectrum	See full text	1 of 8	(5)CAS

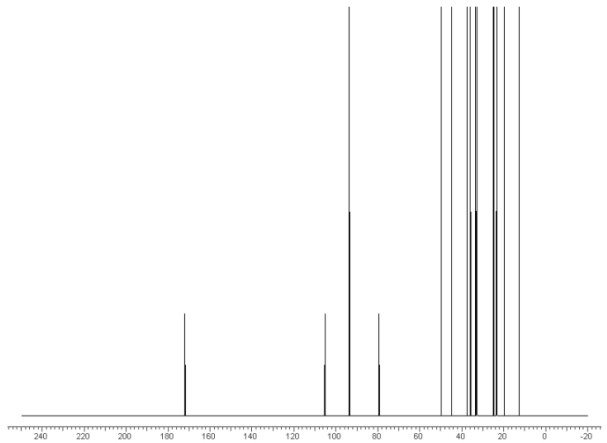
Notes

(3) ACD: Spectral data were obtained from Advanced Chemistry Development, Inc.
(4) Han, Jaehong; Journal of Natural Products 2001, V64(9), P1201-1205 CAPLUS
(5) Yadav, J. S.; Tetrahedron 2010, V66(11), P2005-2009 CAPLUS

▸ PREDICTED PROPERTIES
▸ PREDICTED SPECTRA
▸ REGULATORY INFORMATION
▸ BIOACTIVITY INDICATORS
▸ TARGET INDICATORS
▸ CAS REFERENCE ROLES
▸ ADDITIONAL DETAILS

Carbon-13 NMR Spectrum

Print



SPECTRUM ID
7MED36_38.C

CAS REGISTRY NUMBER
63968-64-9

FORMULA
$C_{15}H_{22}O_5$

CAS INDEX NAME
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*)-

NUCLEUS
13C

SOURCE
Spectral data were obtained from Advanced Chemistry Development, Inc.

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专利Markush检索的意义

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(19) World Intellectual Property Organization
International Bureau

PCT

(43) International Publication Date
15 November 2007 (15.11.2007)

(10) International Publication Number
WO 2007/129019 A1

(51) International Patent Classification:
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C07D 231/20 (2006.01) *A61P 19/02* (2006.01)
C07D 231/38 (2006.01) *A61P 31/00* (2006.01)
C07D 261/08 (2006.01) *A61P 35/00* (2006.01)
C07D 261/10 (2006.01) *A61K 31/415* (2006.01)
C07D 261/12 (2006.01) *A61K 31/42* (2006.01)
C07D 275/02 (2006.01) *A61K 31/425* (2006.01)
A61P 7/02 (2006.01)

(21) International Application Number:
PCT/GB2007/001427

(22) International Filing Date: 20 April 2007 (20.04.2007)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
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(71) Applicant (*for all designated States except US*): **ASTRAZENECA AB** [SE/SE]; S-151 85 Södertälje (SE).

(71) Applicant (*for MG only*): **ASTRAZENECA UK LIMITED** [GB/GB]; 15 Stanhope Gate, London Greater London W1K 1LN (GB).

(72) Inventors; and

(75) Inventors/Applicants (*for US only*): **GREWAL, Gurmit** [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **HENNESSY, Edward** [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **KAMHI, Victor** [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **LI, Danyang** [CN/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **OZA, Vibha** [IN/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **SAEH, Jamal, Carlos** [US/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US). **SU, Qibin** [CN/US]; AstraZeneca R & D Boston, 35 Gatehouse Drive, Waltham, Massachusetts 02451 (US).

(74) Agent: **GLOBAL INTELLECTUAL PROPERTY**; AstraZeneca AB, S-SE-151 85 Södertälje (SE).

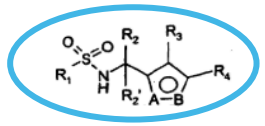
(81) Designated States (*unless otherwise indicated, for every kind of national protection available*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (*unless otherwise indicated, for every kind of regional protection available*): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: SULFONAMIDE COMPOUNDS USEFUL AS ADG RECEPTOR MODULATORS



(I)

(57) Abstract: The present invention relates to compounds of formula (I) that mediate Edg, including Edg-1, processes for their preparation, pharmaceutical compositions containing them as the active ingredient, to their use as medicaments and to their use in the manufacture of medicaments for use in the treatment in warm-blooded animals such as humans of diseases that have a significant vascularization or inflammatory component such as in tumor-related diseases. The present invention also relates to compounds that inhibit a5b1, and also that exhibit appropriate selectivity profile(s) against other integrins.

WO 2007/129019 A1

SULFONAMIDE COMPOUNDS USEFUL AS ADG RECEPTOR MODULATORS

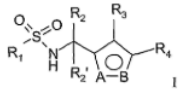
BACKGROUND OF THE INVENTION

EDG (endothelial differentiation gene) receptors belong to a family of closely related, lipid activated G-protein coupled receptors. EDG-1, EDG-3, EDG-5, EDG-6, and EDG-8 (also known as S1P1, S1P3, S1P2, S1P4, and S1P5) are identified as receptors specific for sphingosine-1-phosphate (SIP). EDG2, EDG4, and EDG7 (known also as LPA1, LPA2, and LPA3, respectively) are receptors specific for lysophosphatidic (LPA). Among the SIP receptor isotypes, EDG-1, EDG-3 and EDG-5 are widely expressed in various tissues, whereas the expression of EDG-6 is confined largely to lymphoid tissues and platelets, and that of EDG-8 to the central nervous system.

EDG receptors are responsible for signal transduction and are thought to play an important role in cell processes involving cell development, proliferation, maintenance, migration, differentiation, plasticity and apoptosis. Certain EDG receptors are associated with diseases mediated by the *de novo* or deregulated formation of vessels—for example, for diseases caused by ocular neovascularisation, especially retinopathies (diabetic retinopathy, age-related macular degeneration); psoriasis; hemangiomas such as "strawberry-marks"; various inflammatory diseases, such as arthritis, especially rheumatoid arthritis, arterial atherosclerosis and atherosclerosis occurring after transplants, endometriosis or chronic asthma; and tumor diseases; or by lymphocyte interactions, for example, in transplantation rejection, autoimmune diseases, inflammatory diseases, infectious diseases and cancer. An alteration in EDG receptor activity contributes to the pathology and/or symptomology of these diseases. Accordingly, molecules that themselves alter the activity of EDG receptors are useful as therapeutic agents in the treatment of such diseases.

SUMMARY OF THE INVENTION

These and other needs are met by the present invention which is directed to a compound of formula I



I

in free or pharmaceutically acceptable salt form, wherein:

A and B are each independently N, NR_a, O, S, or CR_b;

R_a is H, $(C_1\text{-}C_6)$alkyl, $C(O)\text{-}(C_1\text{-}C_6)$alkyl, $C(O)\text{-}NR'R''$, $CO_2(C_1\text{-}C_6)$alkyl;

R_b H, halo, $(C_1\text{-}C_6)$alkyl, cyano, $\text{-}C(O)\text{-}(C_1\text{-}C_6)$alkyl, $\text{-}CO_2(C_1\text{-}C_6)$alkyl, $C(O)\text{-}NR'R''$, wherein R' and R" are each independently at each occurrence H or $(C_1\text{-}C_6)$alkyl or X-R_c; $\text{-}CO_2H$, $\text{-}SO_2NHR$;

R_1 is aryl, heteroaryl, $(C_1\text{-}C_6)$alkyl, aralkyl, heterocycloalkyl , or heteroaralkyl;

R_2 and $R_{2'}$ are each independently H, $(C_1\text{-}C_6)$alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl, or taken together with the carbon to which they are attached form C=O;

R_3 and R_4 are each independently H, halo, $(C_1\text{-}C_6)$alkyl, $(C_3\text{-}C_6)$cycloalkyl, $(C_3\text{-}C_6)$cycloalkyl$(C_1\text{-}C_6)$alkyl, heterocycloalkyl, aralkyl, aryl, $(C_2\text{-}C_6)$alkenyl, $(C_2\text{-}C_6)$alkynyl, or heteroaralkyl, or X-R_c;

X is S, O, or NR_d;

R_c is H or $(C_1\text{-}C_6)$alkyl;

R_d is H, $(C_1\text{-}C_6)$alkyl, aryl, heteroaryl, heterocyclo, $(C_2\text{-}C_6)$alkenyl, $(C_2\text{-}C_6)$alkynyl, aralkyl, heteroaralkyl, $(C_3\text{-}C_6)$cycloalkyl$(C_1\text{-}C_6)$alkyl, heterocycloalkyl$(C_1\text{-}C_6)$alkyl, acyl, acyloxy, acylamino, or $(C_1\text{-}C_6)$alkoxycarbonyl$(C_1\text{-}C_6)$alkyl, or cyano; and

each R_1, R_2, $R_{2'}$, R_3, R_a, R_b, R_c, and R_d may be optionally substituted on carbon by azido, halo, nitro, cyano, hydroxy, trifluoromethoxy, NR'R", $\text{-}CO_2H$, $C(O)\text{-}(C_1\text{-}C_6)$alkyl, $\text{-}CO_2(C_1\text{-}C_6)$alkyl, $\text{-}C(O)\text{-}NR'R''$, $S(C_1\text{-}C_6)$, $SO_p(C_1\text{-}C_6)$alkyl, $SO_pNH(C_1\text{-}C_6)$alkyl, $SO_pNR'R''$ $(C_2\text{-}C_6)$alkenyl, $(C_2\text{-}C_6)$alkynyl, or $(C_1\text{-}C_6)$alkoxy, wherein R' and R" are each independently hydrogen, $(C_1\text{-}C_6)$alkyl, $(C_3\text{-}C_6)$cycloalkyl, $(C_3\text{-}C_6)$cycloalkyl$(C_1\text{-}C_6)$alkyl, or aryl.

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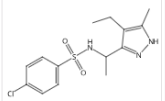
专利中的物质表达

PATENTPAK A CAS SOLUTION | PAGE 28 /72 | ZOOM | DOWNLOAD PDF PDF+

Key Substances in Patent

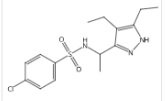
CAS RN 957128-74-4



Analyst Markup Locations (1)

Page 28

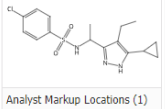
CAS RN 957128-75-5



Analyst Markup Locations (1)

Page 28

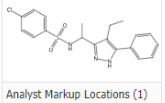
CAS RN 957128-76-6



Analyst Markup Locations (1)

Page 28

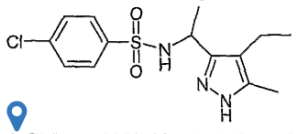
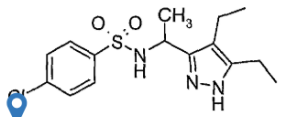
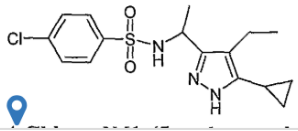
CAS RN 957128-77-7



Analyst Markup Locations (1)

Page 29

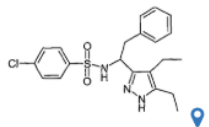
Table 1

Ex	Compound	^{1}H NMR	M/Z	Int
1	 **4-Chloro-*N*-[1-(4-ethyl-5-methyl-1*H*-pyrazol-3-yl)ethyl]benzenesulfonamide**	(400 MHz, DMSO-D6) δ ppm 0.82 - 0.92 (m, 3 H) 1.23 (d, 3 H) 1.99 (s, 3 H) 2.10 - 2.21 (m, 2 H) 4.30 - 4.39 (m, 1 H) 7.53 (m, 2 H) 7.61 - 7.70 (m, 2 H) 7.99 (d, 1 H) 11.99 (s, 1 H)		1
2	 **4-Chloro-*N*-[1-(4,5-diethyl-1*H*-pyrazol-3-yl)ethyl]benzenesulfonamide**	(400 MHz, DMSO-D6) δ ppm 0.89 (t, *J*=7.58 Hz, 3 H) 1.06 (t, *J*=7.58 Hz, 3 H) 1.24 (d, *J*=7.07 Hz, 3 H) 2.11 - 2.22 (m, 2 H) 2.38 (q, *J*=7.58 Hz, 2 H) 4.33 - 4.44 (m, 1 H) 7.49 - 7.59 (m, 2 H) 7.63 – 7.65 (m, 2 H) 8.02 (m, 1 H), 12.01 (broad s, 1 H).	341	1
3		(400 MHz, DMSO-D6) δ ppm 0.54 - 0.65 (m, 2 H) 0.75 - 0.85 (m, 2 H) 0.93 (t, 3 H) 1.24 (d, 3		1

0.81 mmol) is then added in one portion, and the mixture is allowed to stir at 0 °C for 2 min and is allowed to warm to room temperature over 3 min. Glacial HOAc (0.50 mL) is added to quench the reaction, followed by absolute EtOH (2 mL). Hydrazine monohydrate (150 µL, 3.1 mmol) is added, and the mixture is allowed to stir at room temperature. After 45 min, the reaction is partitioned between EtOAc and H_2O. The aqueous layer is extracted with EtOAc, and the combined organics are washed with brine, dried ($MgSO_4$), filtered, and concentrated. The crude material is purified by silica gel chromatography (gradient elution; R_f in 50:50 hexanes:EtOAc ≈ 0.23) to give a viscous oil that is lyophilized to give a colorless solid (54 mg, 28%).

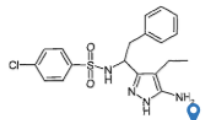
Example 5 may be prepared in two steps from intermediate 2a as outlined below:

4-Chloro-*N*-[1-(4,5-diethyl-1*H*-pyrazol-3-yl)-2-phenylethyl]benzenesulfonamide: (Example 5):



A 25 mL round bottom flask is charged with *N*-(1-benzyl-3-ethyl-2,4-dioxohexyl)-4-chlorobenzenesulfonamide (**Intermediate 2a**, 104 mg, 0.25 mmol) and MeOH (4.0 mL). Hydrazine monohydrate (50 µL, 1.03 mmol) is added, and the solution is allowed to stir at room temperature for 1 h. The volatile components are removed under reduced pressure, and the crude material is purified by silica gel chromatography (EtOAc as eluent) to give a colorless oil. Lyophilization affords a solid material (16 mg, 15%).

***N*-[1-(5-Amino-4-ethyl-1*H*-pyrazol-3-yl)-2-phenylethyl]-4-chlorobenzenesulfonamide (Example 6):**



A 50 mL round bottom flask is charged with *N*-(1-{5-amino-1-[(4-chlorophenyl)sulfonyl]-4-ethyl-1*H*-pyrazol-3-yl}-2-phenylethyl)-4-

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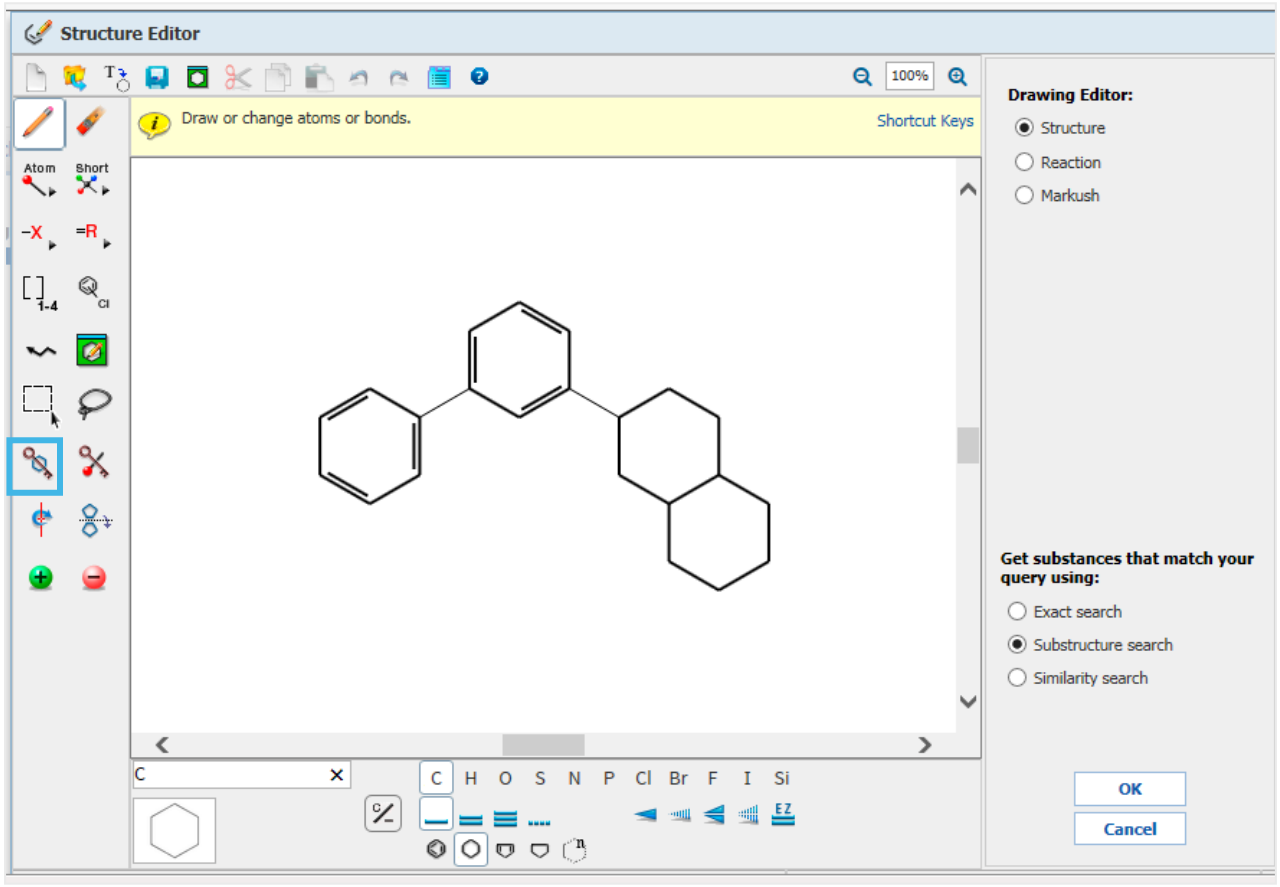
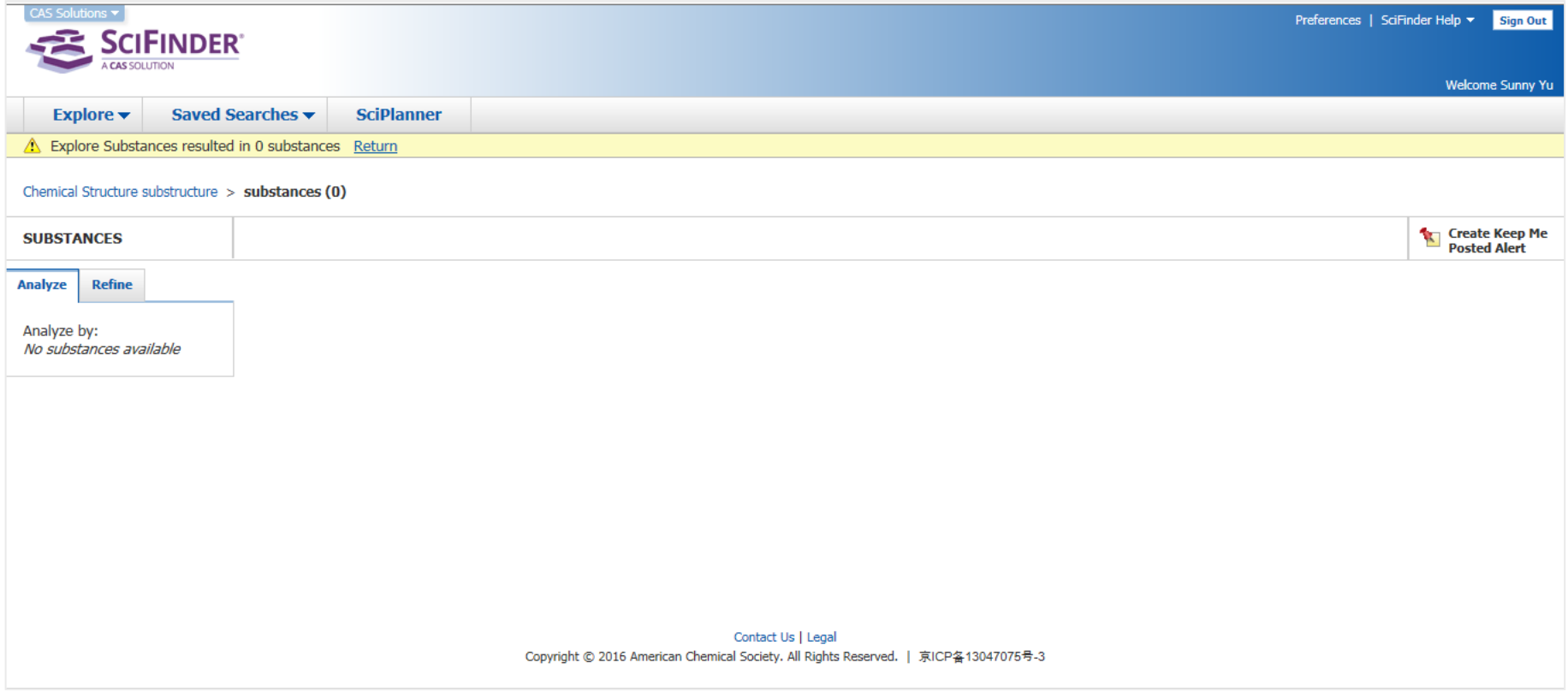
专利中的物质表达方式

- 确定物质[Specific Substance]：
  - 具有表征数据的物质（一般为实施例中的物质，会被CAS Registry收录）
  - 专利中其他确定物质 （只有有充分的证据证明此物质存在，才会被CAS Registry收录）
- 预测性物质[Prophetic Substance]：
  - 使用通式结构（CAS Markush)表示的预测物质，一个通式结构可以表示上百或上千个化学物质 （会被CAS Markush数据库收录）
  - 通常，实施例中只表征Markush结构中的部分物质，更大量的结构则被隐藏在Markush结构中，受到保护

绘制结构，并检索文献中报道的确定结构的物质



物质亚结构检索结果为零



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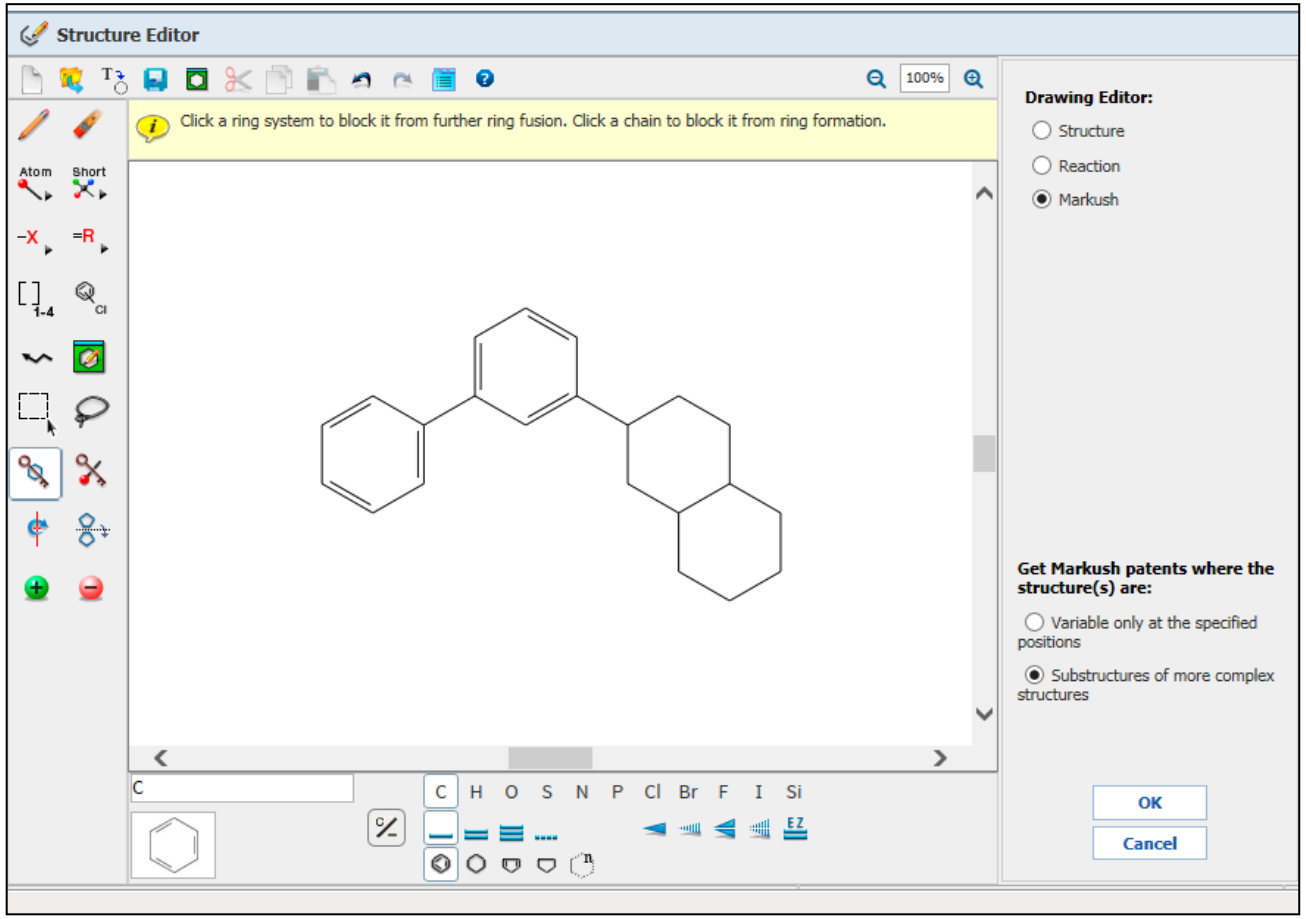
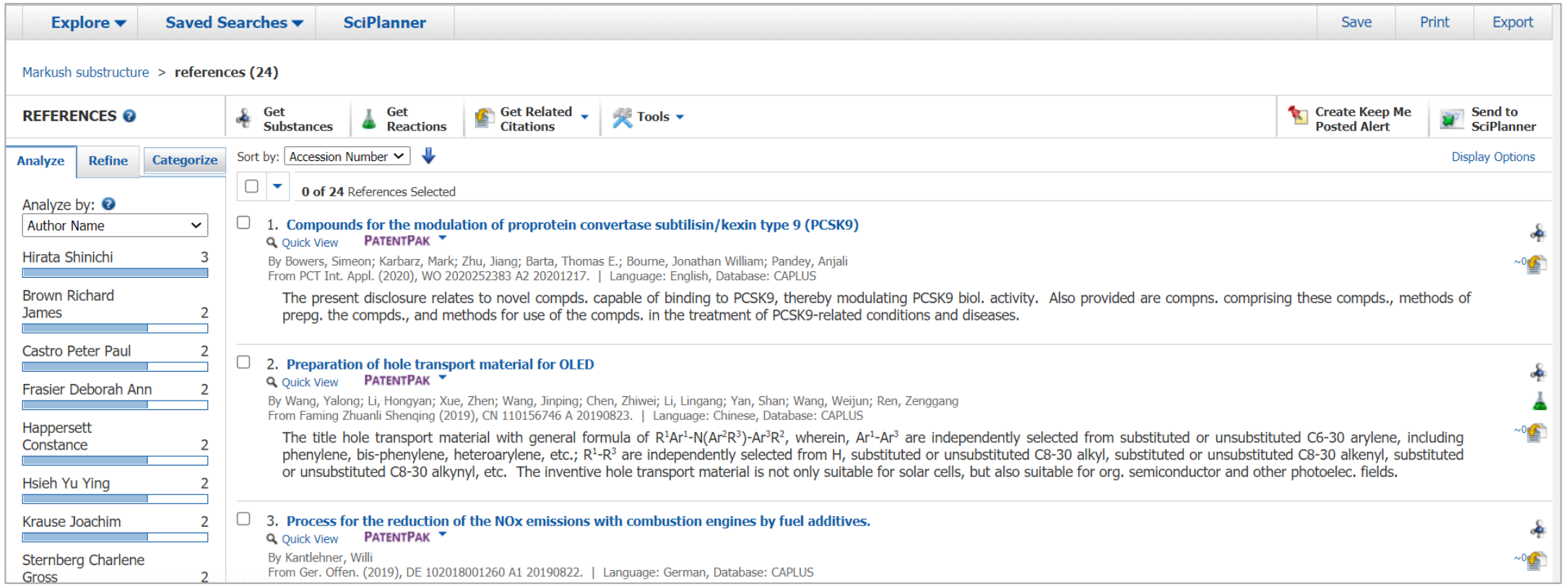
物质Markush结构检索



在SciFinder中进行Markush检索（系统在进行Markush检索时，将自动进行环锁定）

第一种是指除了所设置的可变基团外，其他位位点默认锁定。
第二种是开放位点允许有取代

Markush检索结果集：24项专利文献



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物质检索小结：

- 物质的检索方法汇总和适用性；
- 充分使用结构编辑器中的绘图工具，灵活绘制结构；
- 有机物、无机物、配位化合物和聚合物等物质的检索方法；
- 物质Markush结构检索，规避专利风险

大纲

- CAS SciFinder介绍
- 文献相关信息的获取策略
  - 文献检索方法
  - 文献结果分析、精炼和详情
- 物质相关信息的获取策略
  - 物质检索方法
  - 如何检索无机化合物、配位化合物和聚合物
  - 物质结果分析、精炼和详情
- **反应相关信息的获取策略**
  - 反应的获取方法
  - 反应结果分析、精炼及详情

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化合物制备信息的获取方法

方法1：基于物质名称和主题词获取到合成制备信息；

方法2：基于物质的CAS号检索合成制备信息；

方法3：在CAS REACT中获取到该结构的精确合成信息；

方法4：在CAS REACT中获取到该结构的精确反应信息、该结构的盐、同位素、立体构型等合成信息。

反应的检索方法

方法1：在文献检索Research Topic中输入preparation of 50-78-2或者synthesis of aspirin进行检索

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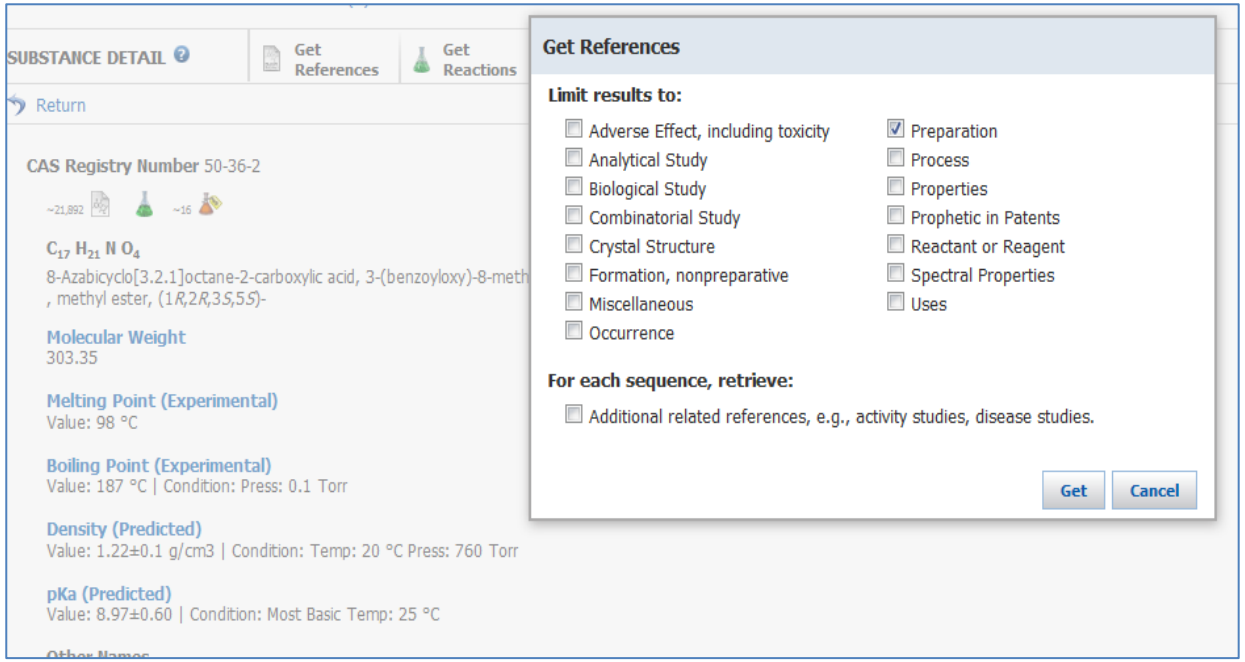
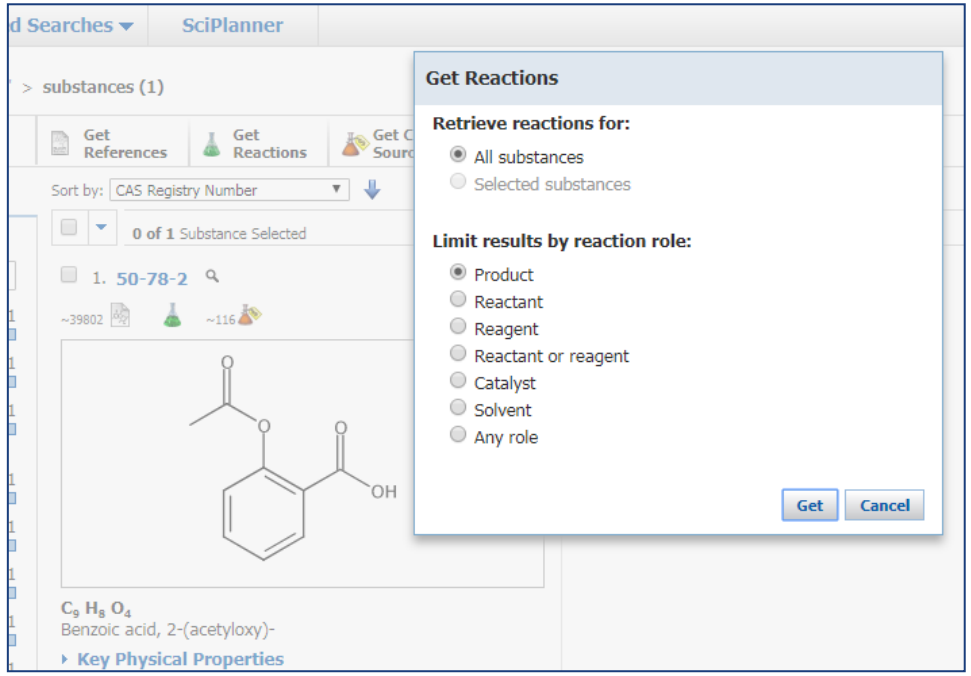
反应的检索方法

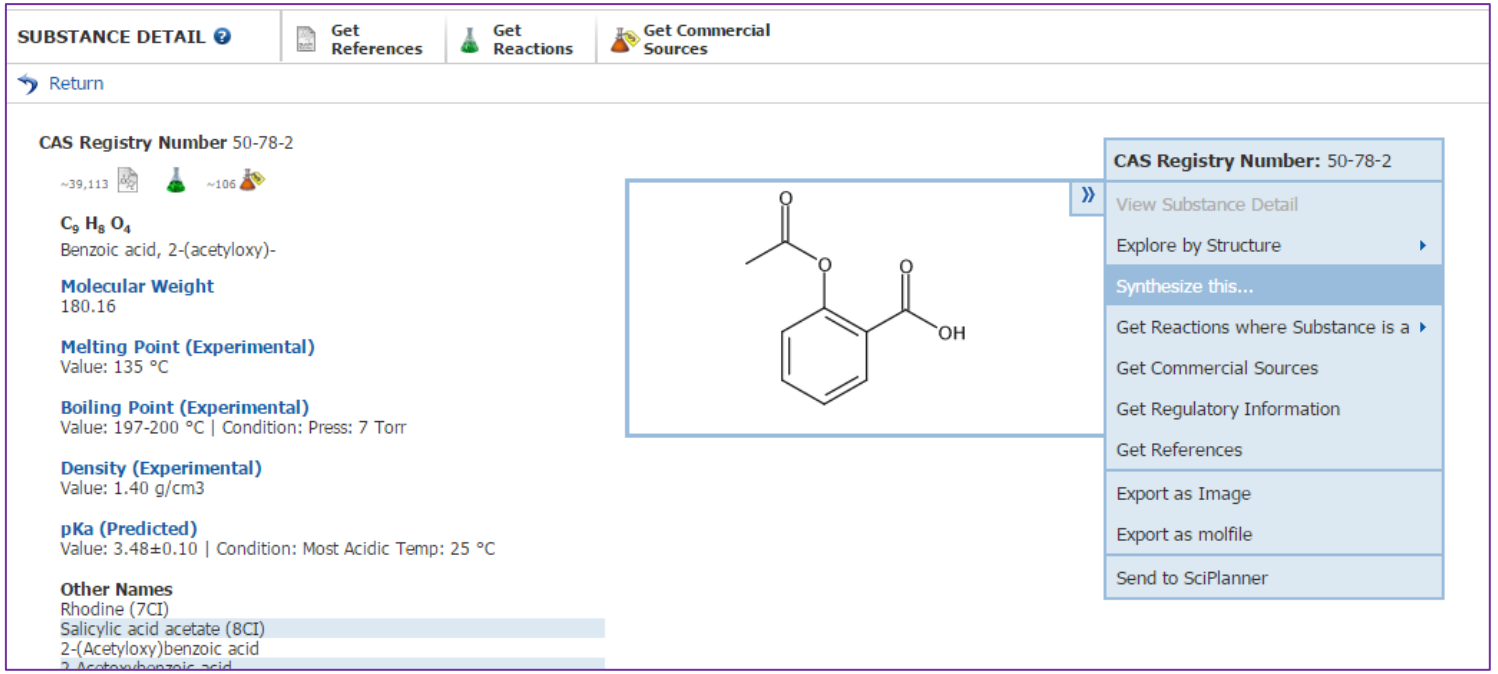
方法2：检索物质后，在物质信息详情页面，可以由此物质获得制备(preparation)相关文献或者产物为此物质的反应。





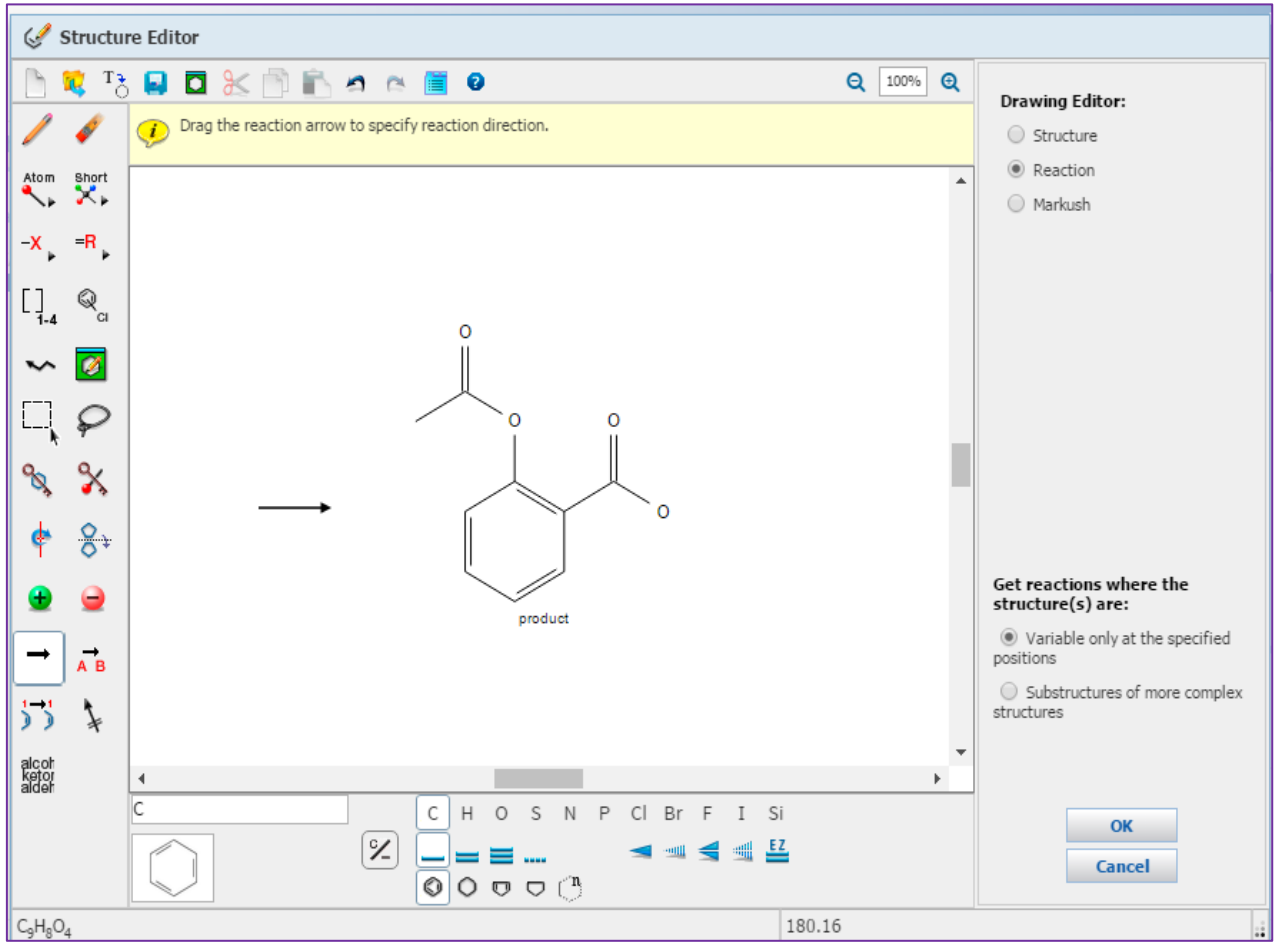
反应的检索方法

方法3：也可以点击物质结构右上角的蓝色双箭头，点击Synthesis this，获得相关反应

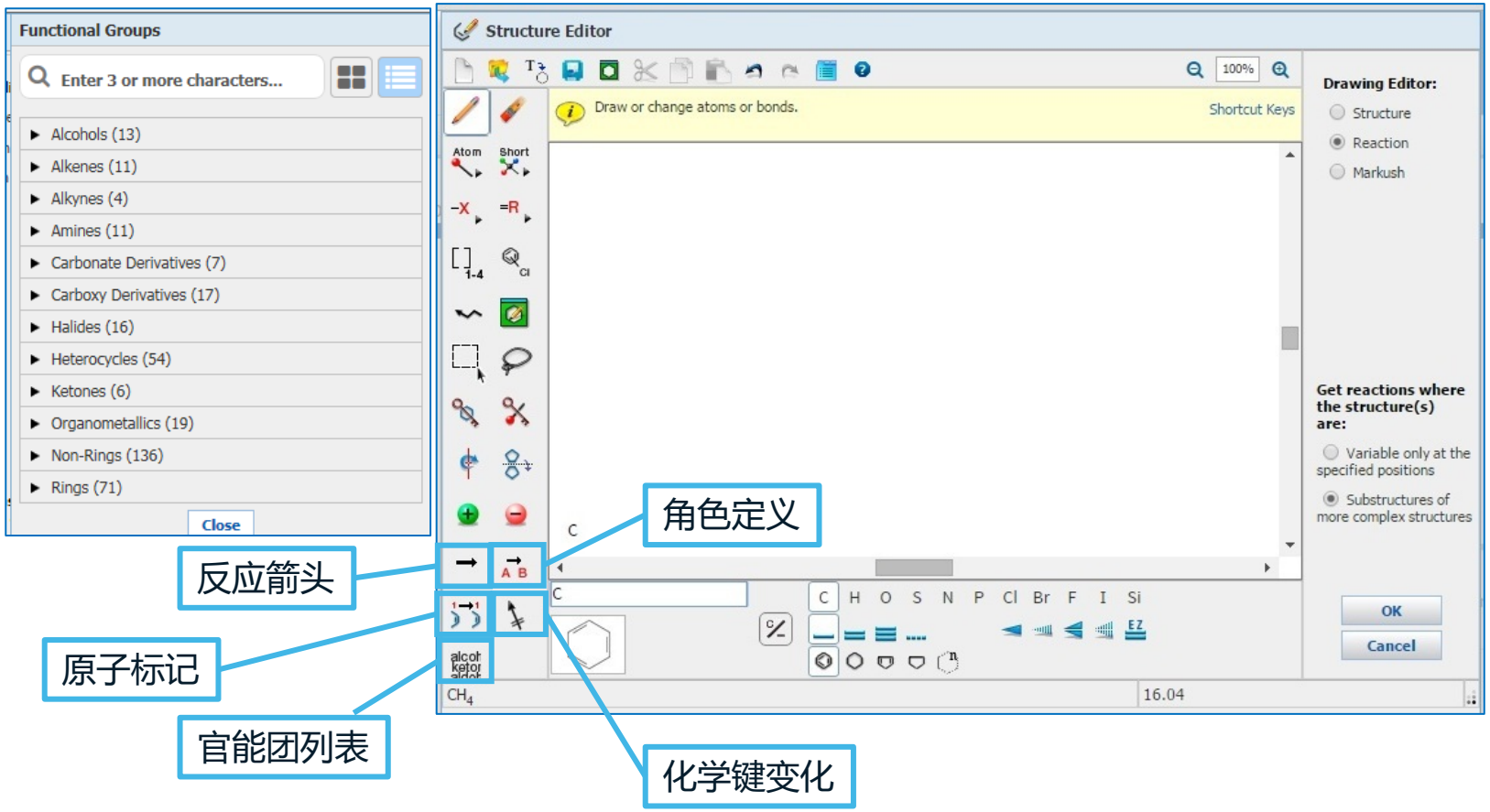


反应的检索方法

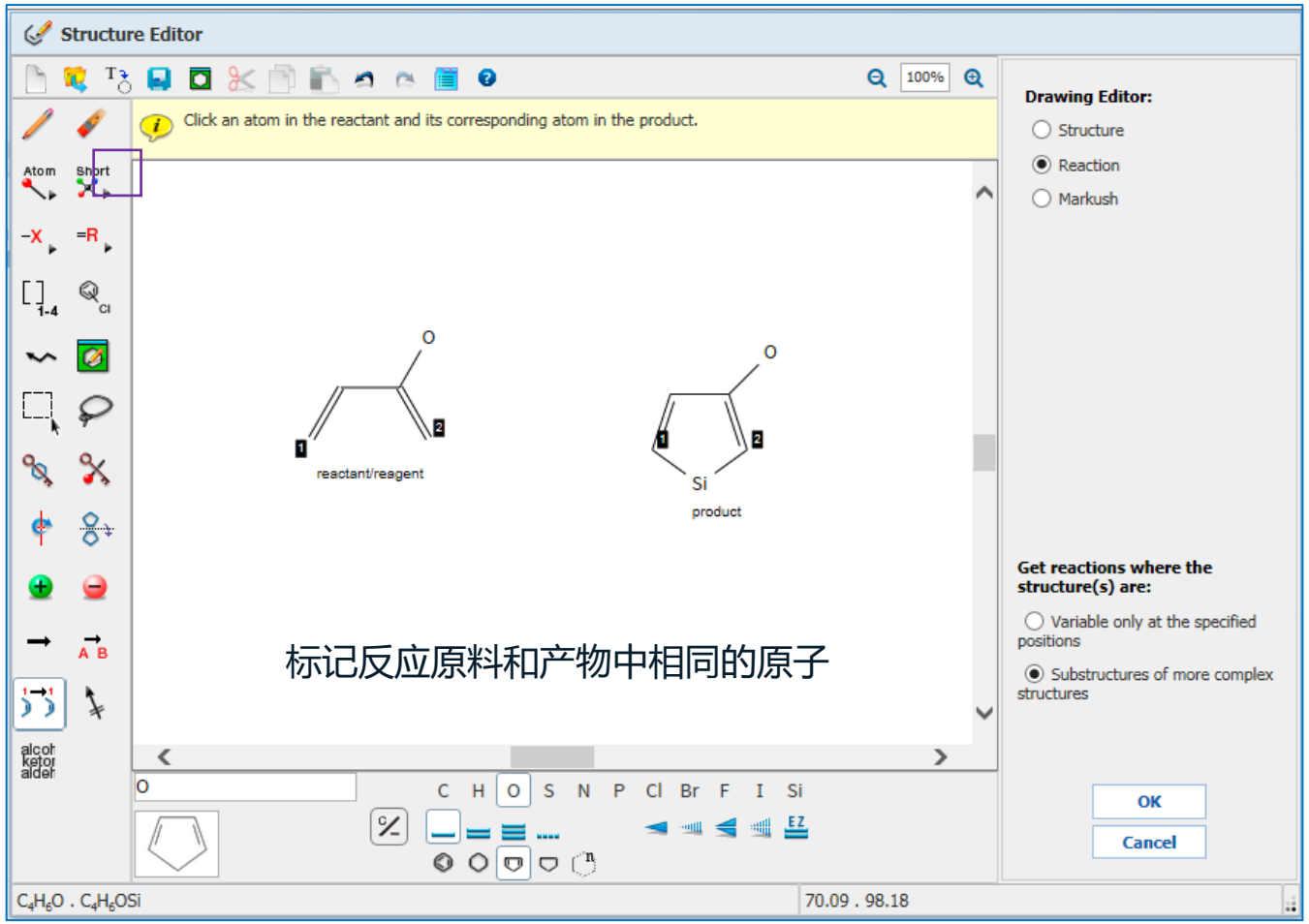
方法4：在SciFinder反应检索编辑器中绘制结构，获得反应。



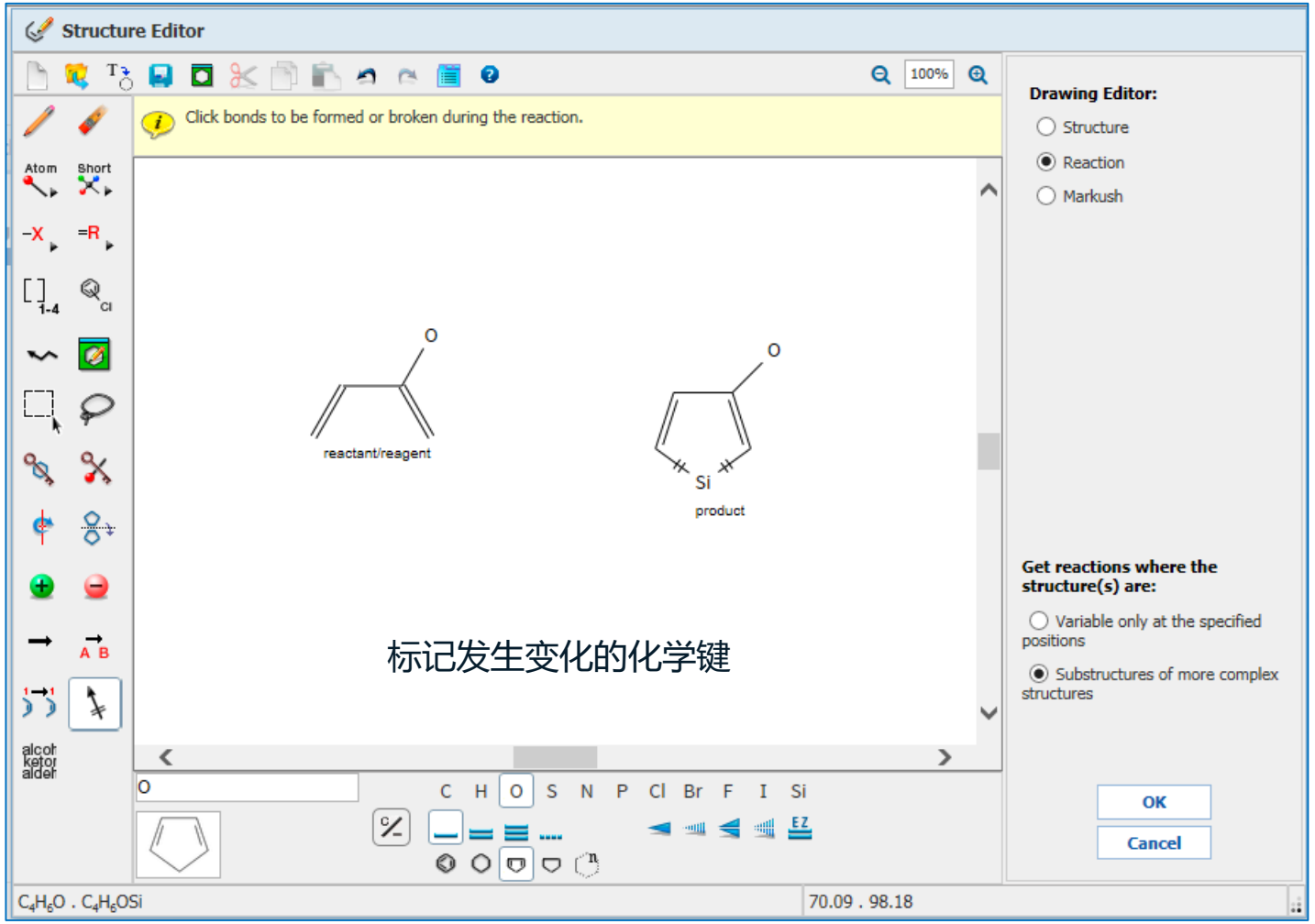
结构编辑器：绘制反应工具



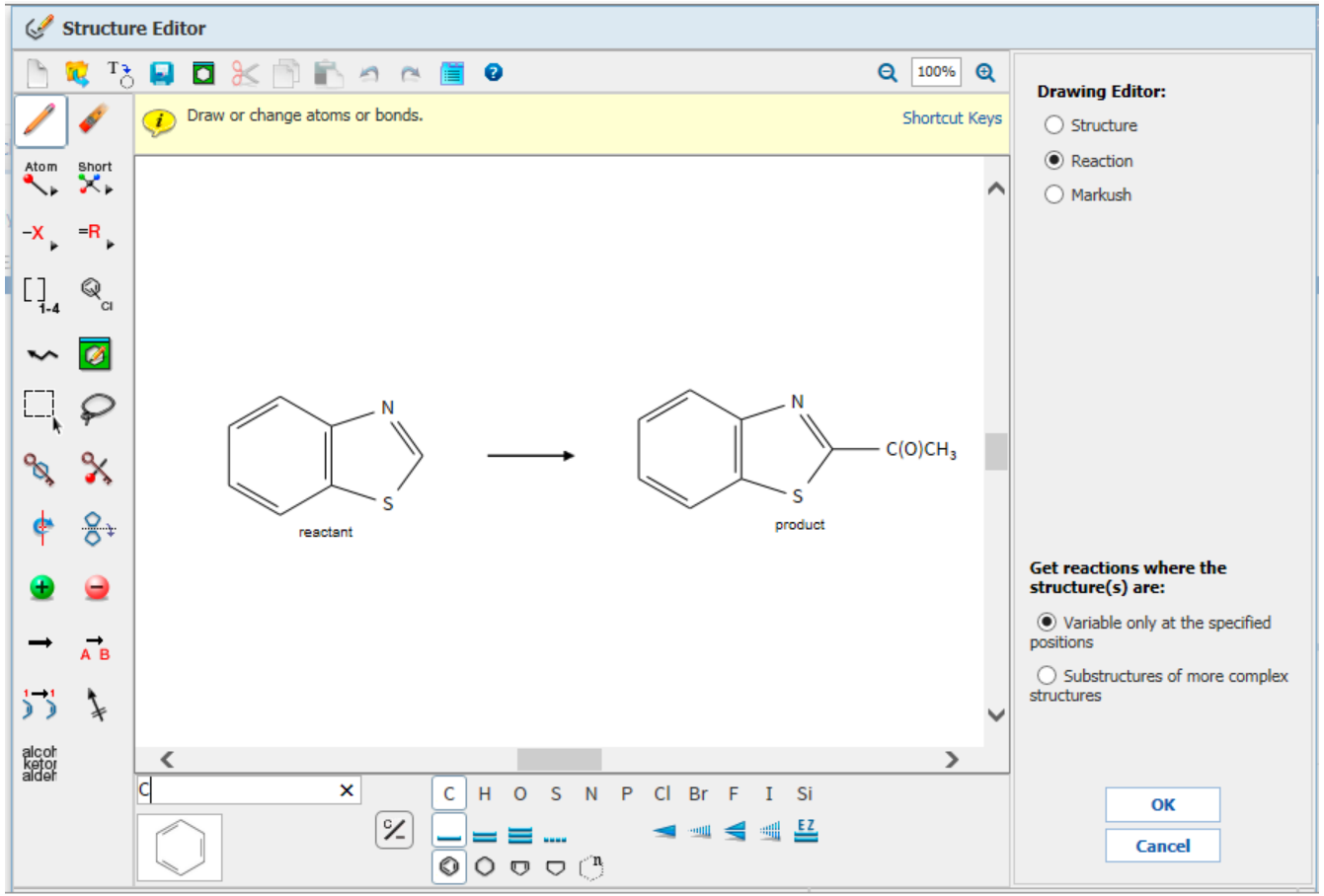
反应前后物质中的原子标记



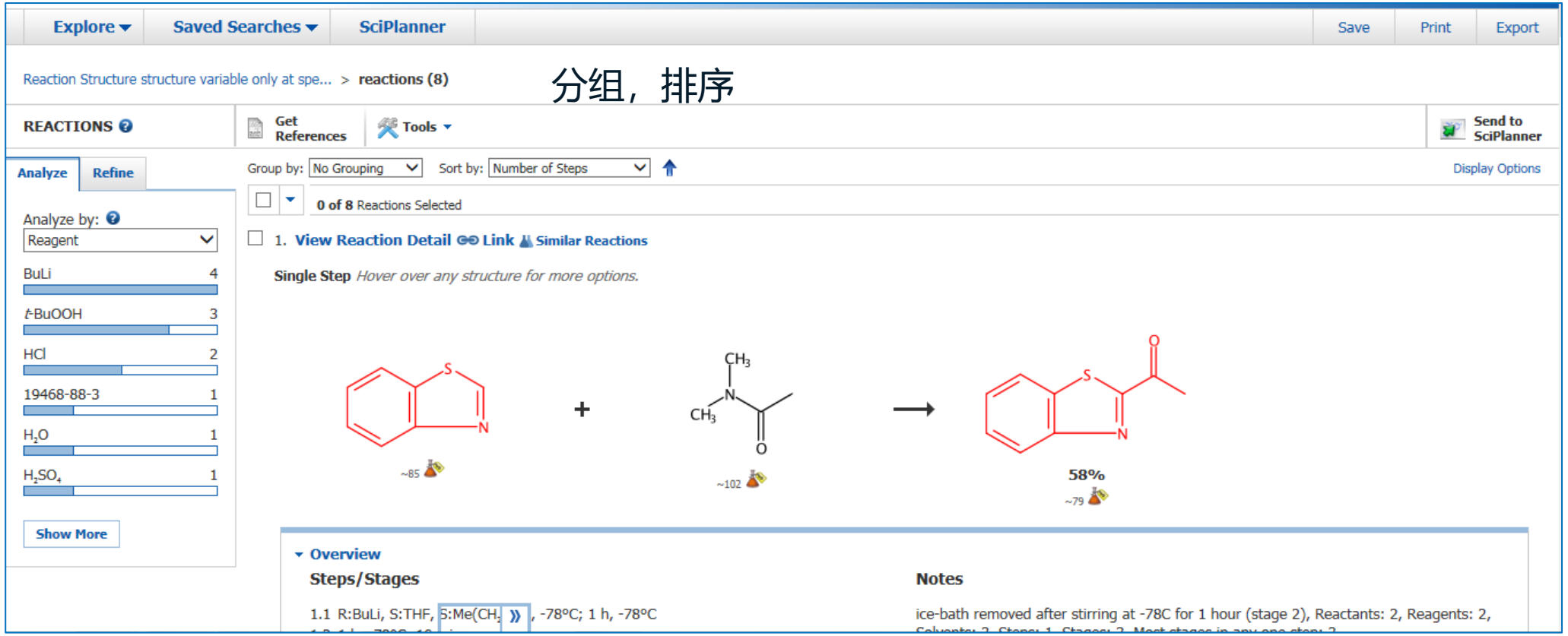
发生变化的化学键标记



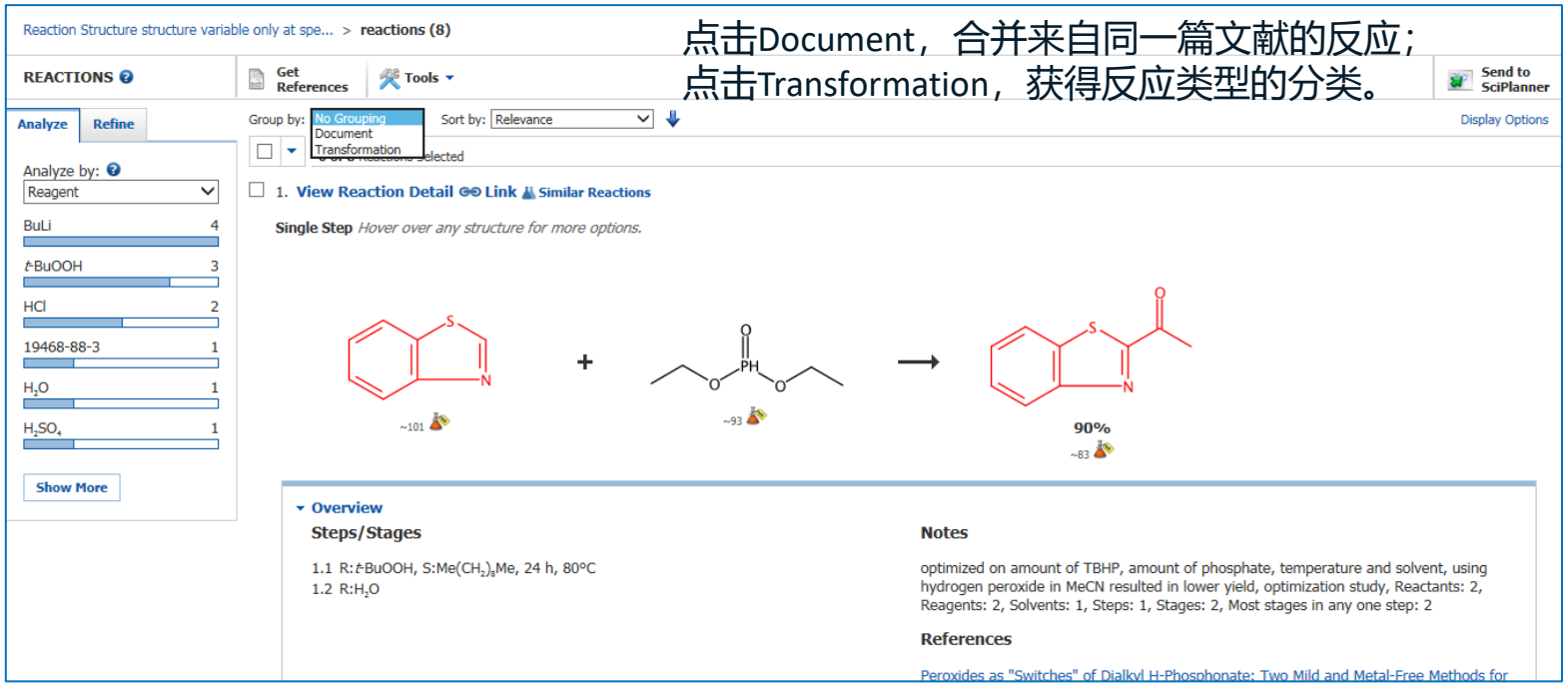
精确结构反应检索：绘制反应式



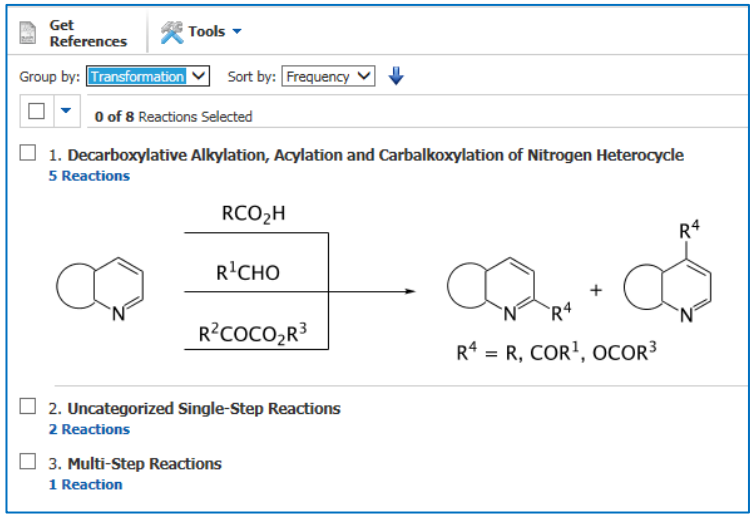
精确结构反应检索：查看反应结果集



精确结构反应检索：查看反应结果集



点击Document，合并来自同一篇文献的反应；
点击Transformation，获得反应类型的分类。



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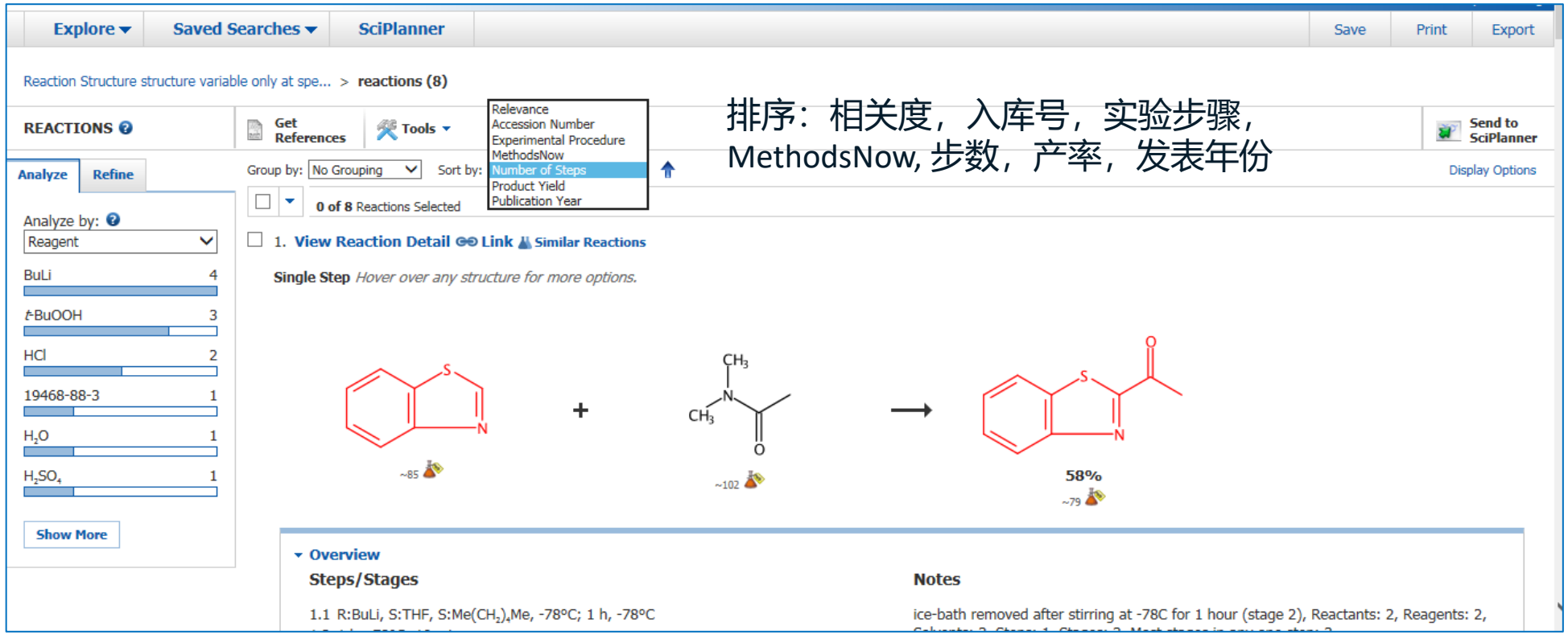
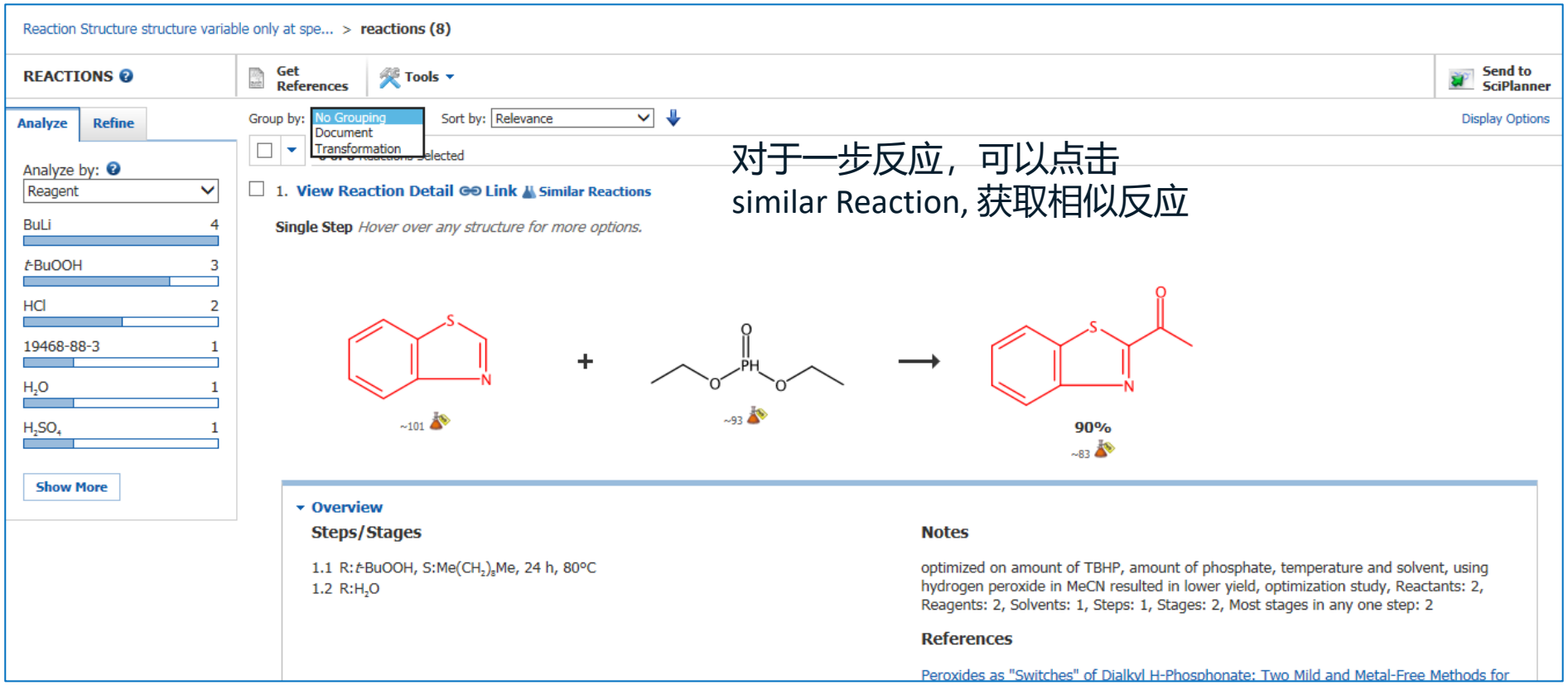
精确结构反应检索：查看反应结果集



排序：相关度，入库号，实验步骤，MethodsNow, 步数，产率，发表年份

精确结构反应检索：查看反应结果集



对于一步反应，可以点击
similar Reaction, 获取相似反应

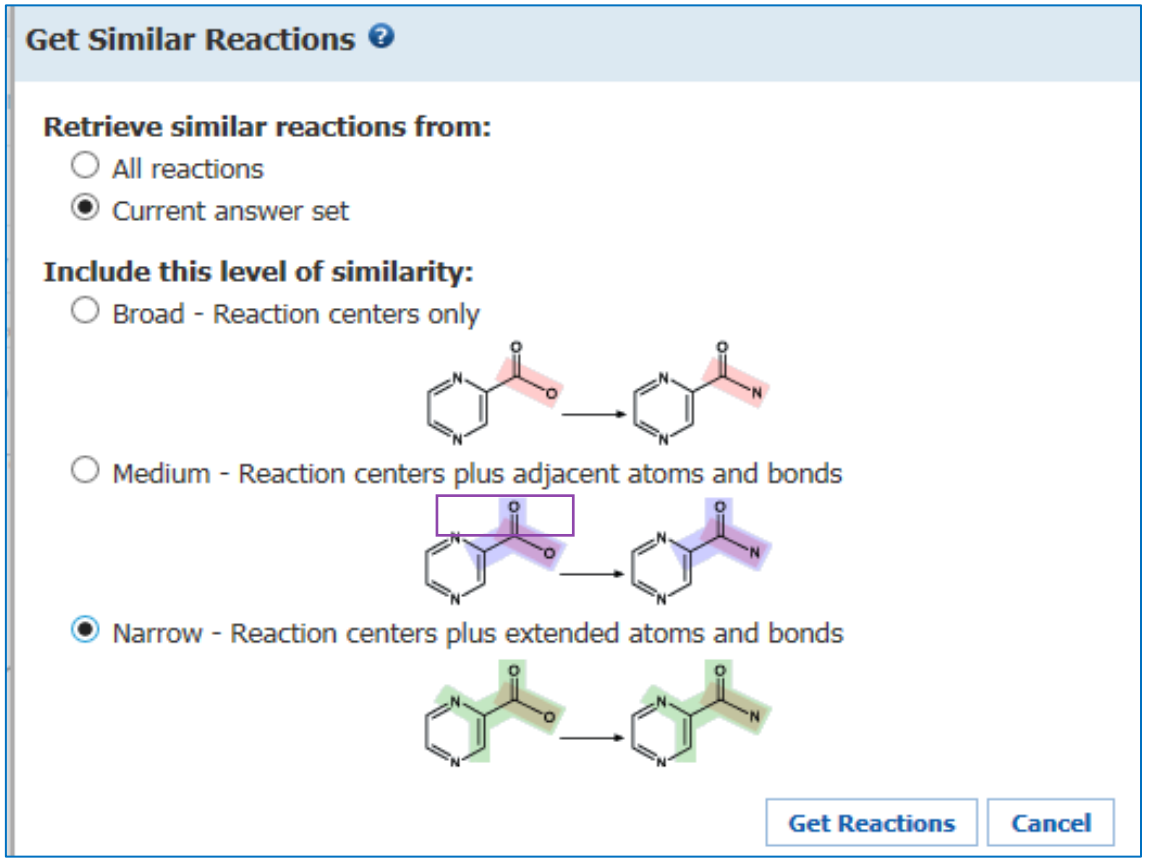
精确结构反应检索：获取相似反应

相似度限制：

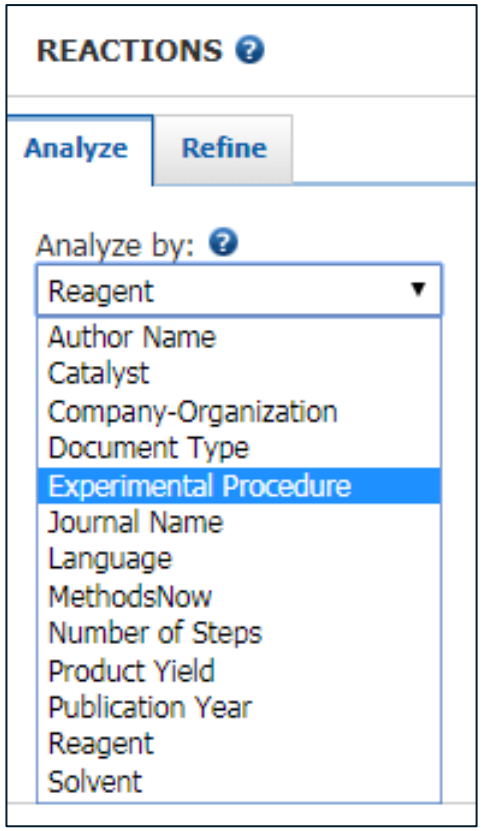
Broad：仅反应中心相似

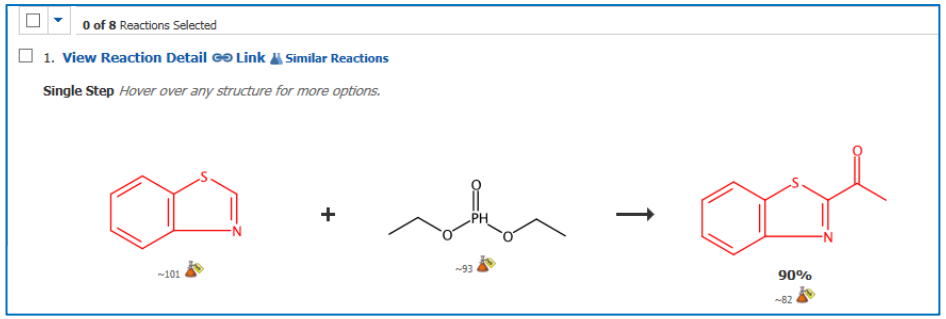
Medium：反应中心及附属原子和键

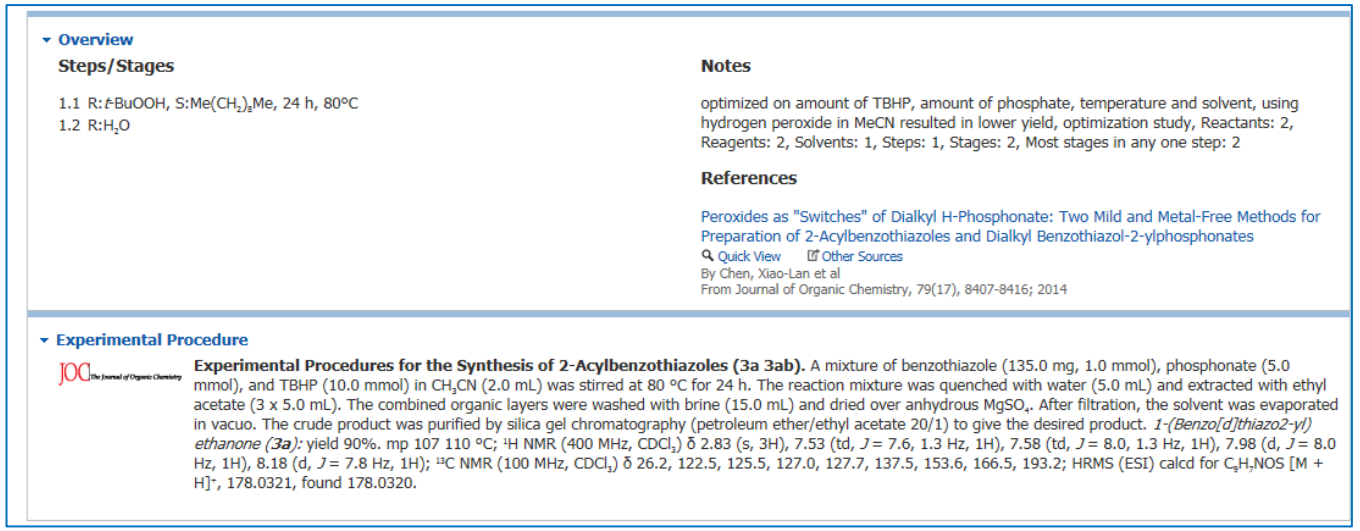
Narrow：反应中心及扩展的原子和键



精确结构反应检索：查看感兴趣的反应信息

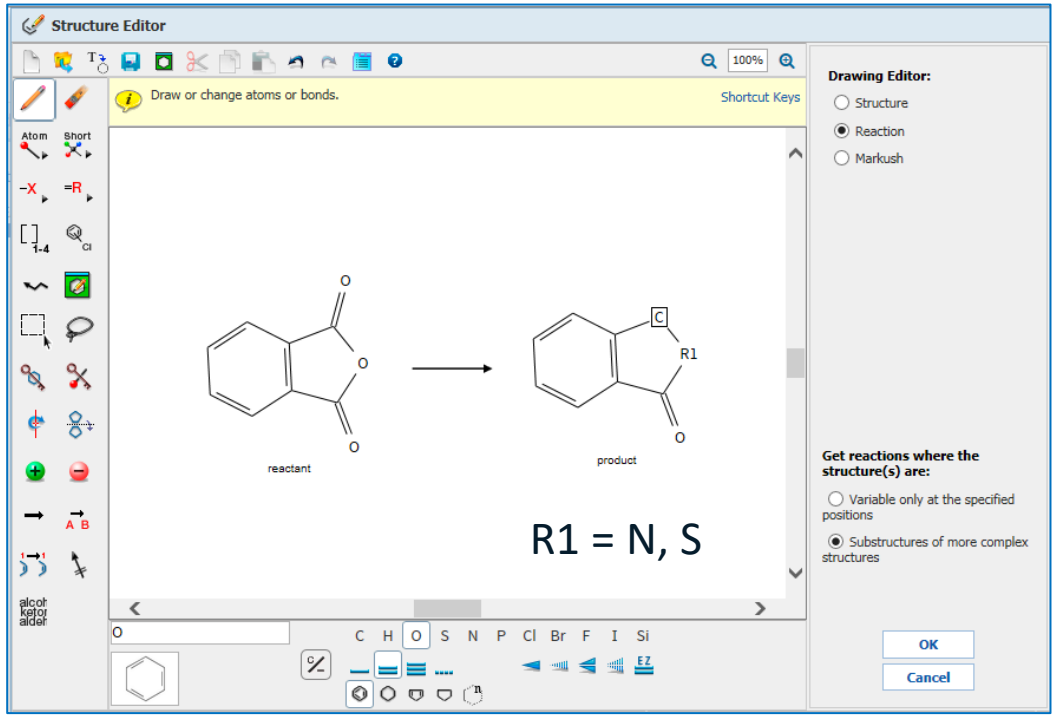






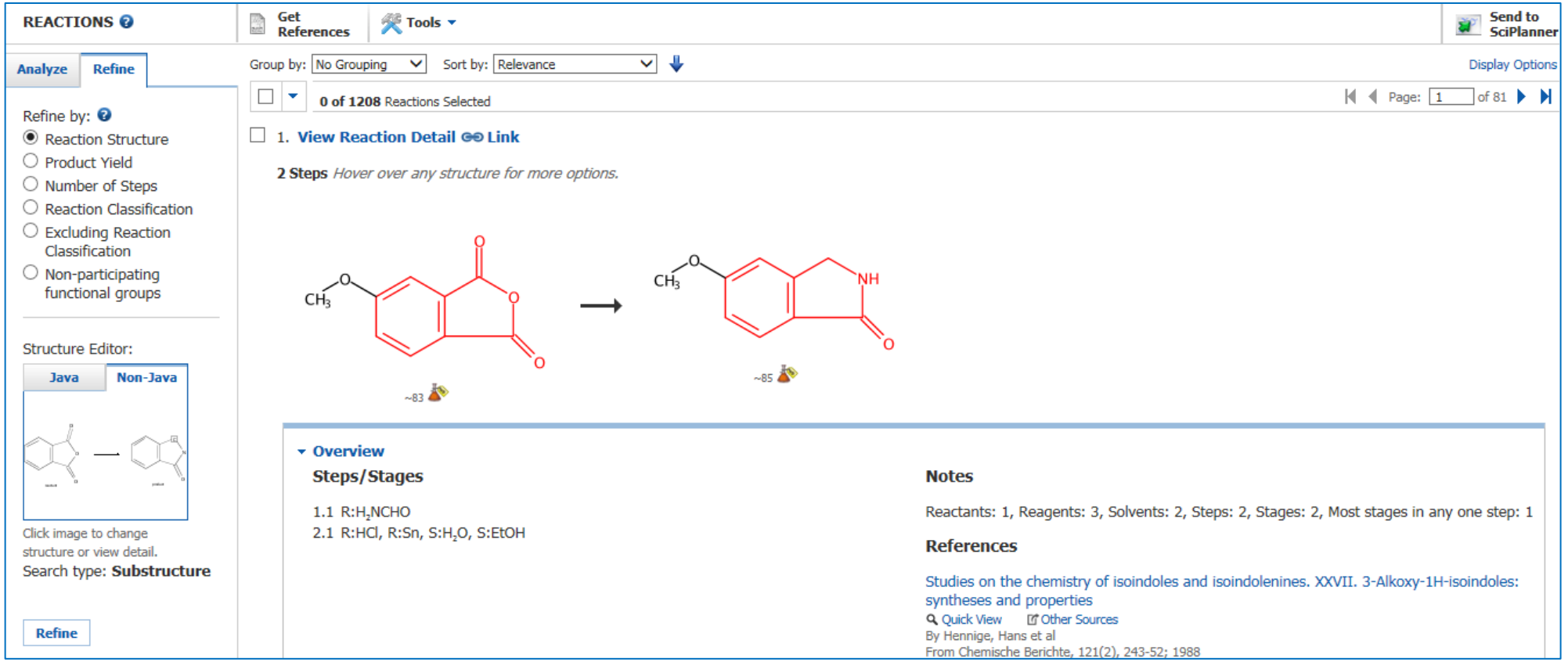
实验步骤

亚结构反应检索: 绘制反应式

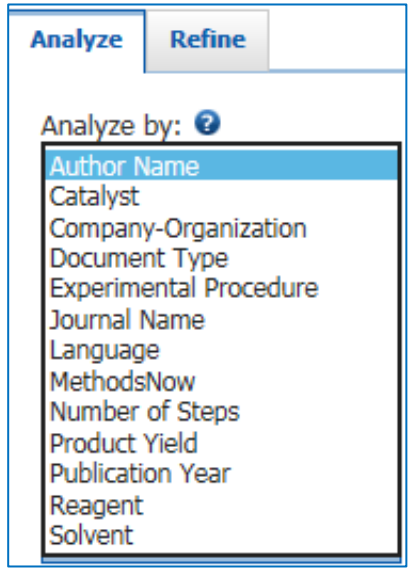


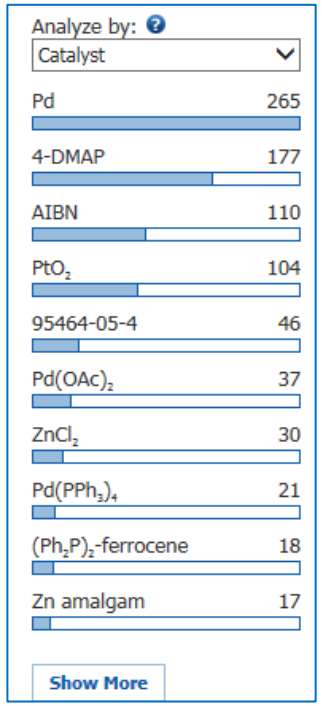
输入的反应物和产物结构可以被修饰，但母体结构不变

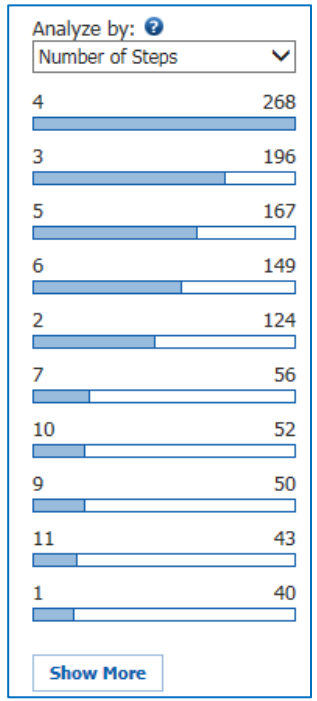
亚结构反应检索：获得反应结果集

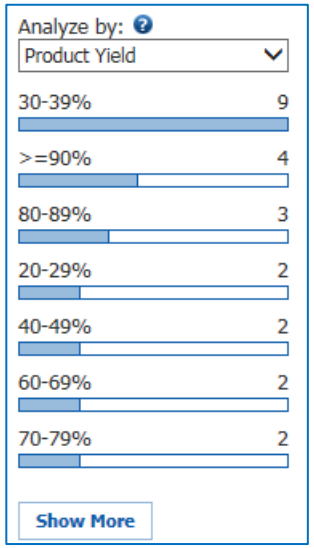


亚结构反应检索：分析处理









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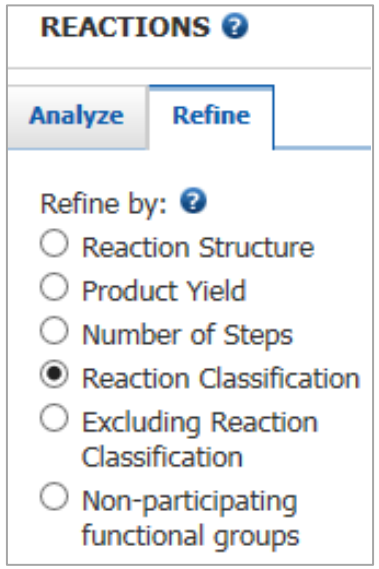
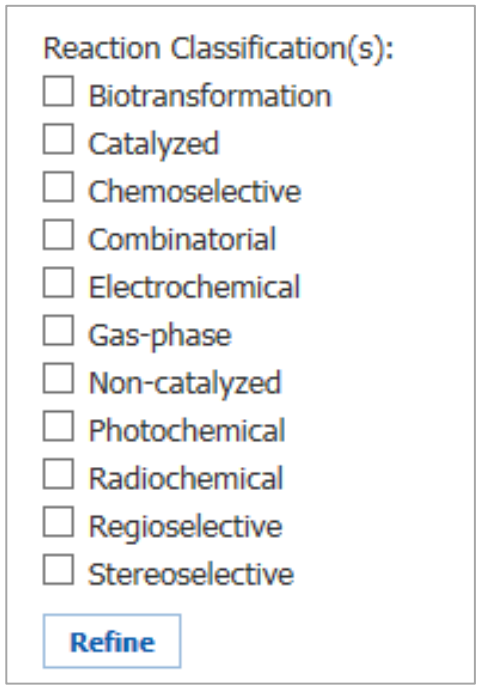
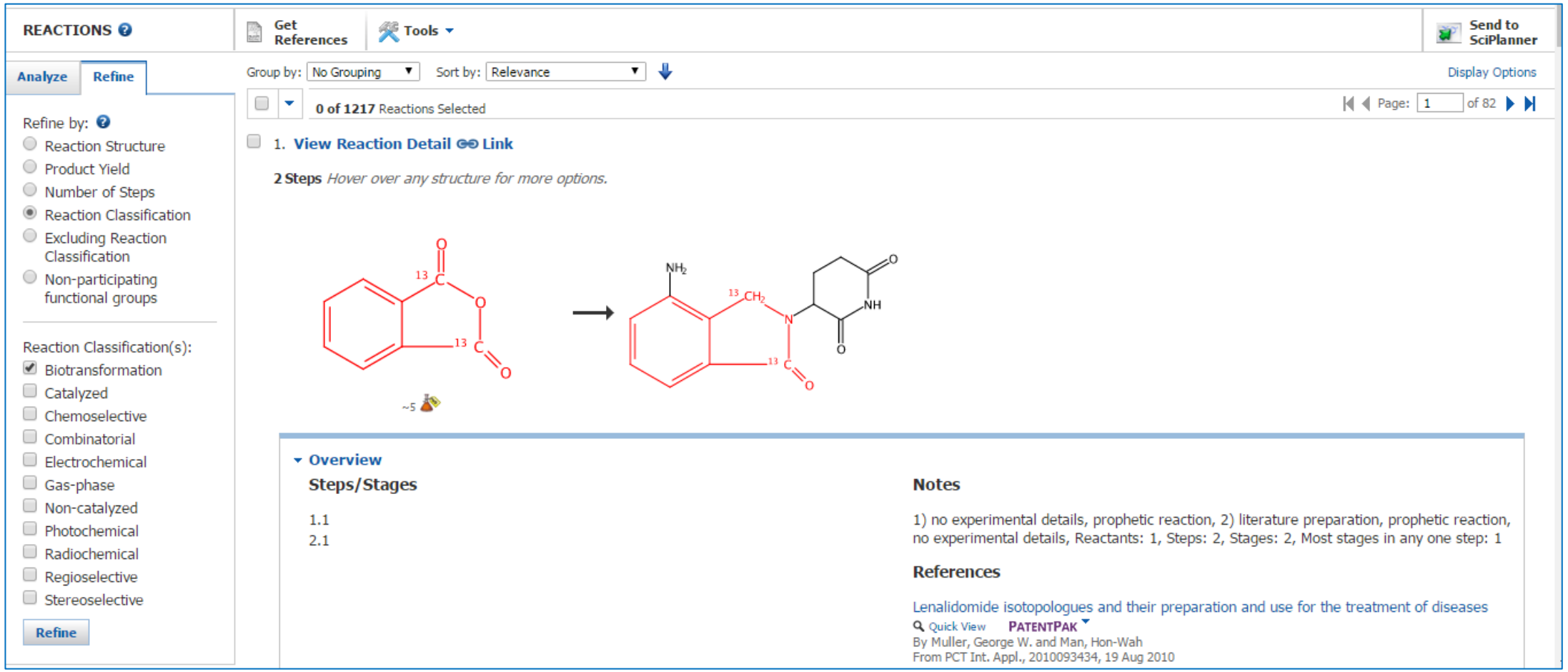
亚结构反应检索：筛选处理





生物转化
催化反应
化学选择性
组合化学
电子化学
气相反应
非催化反应
光化学
放射化学
区域选择反应
立体选择反应

亚结构反应检索：勾选反应类型



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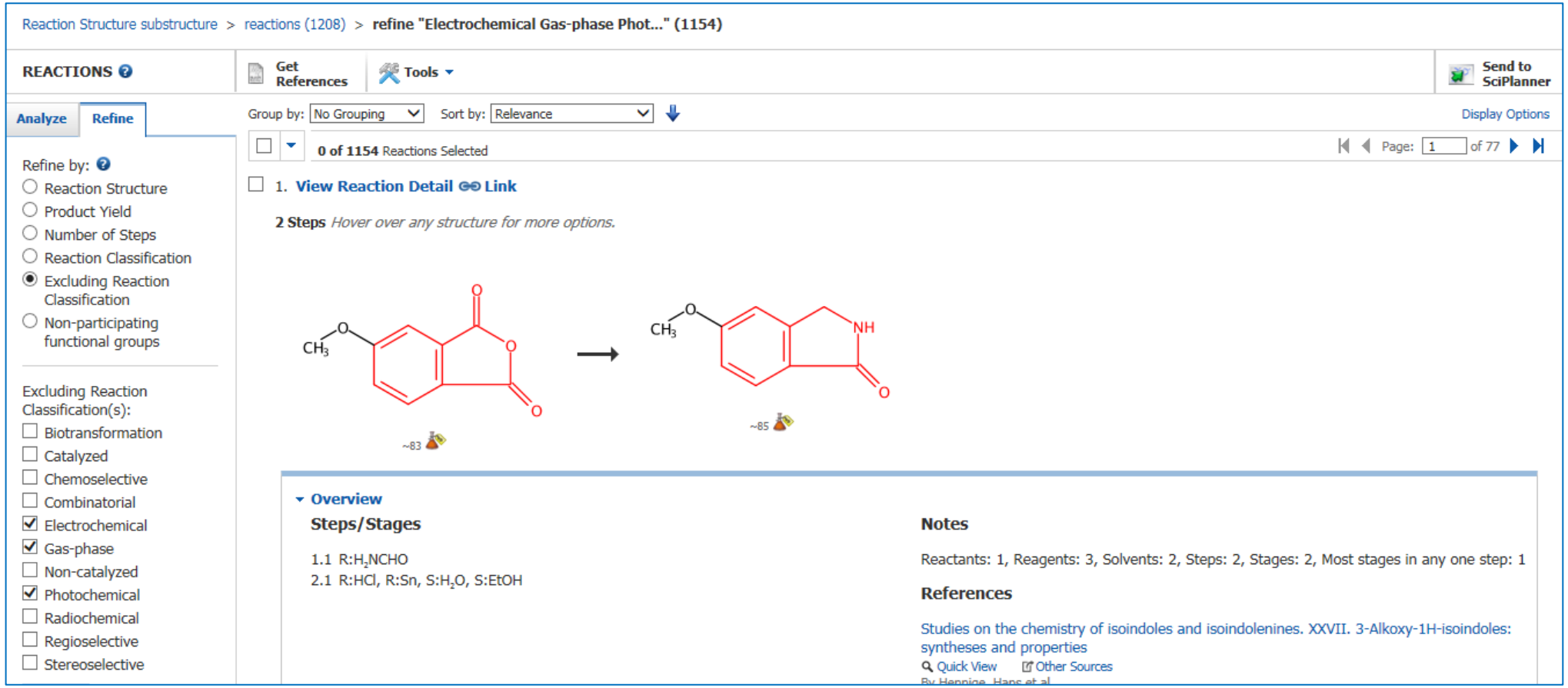
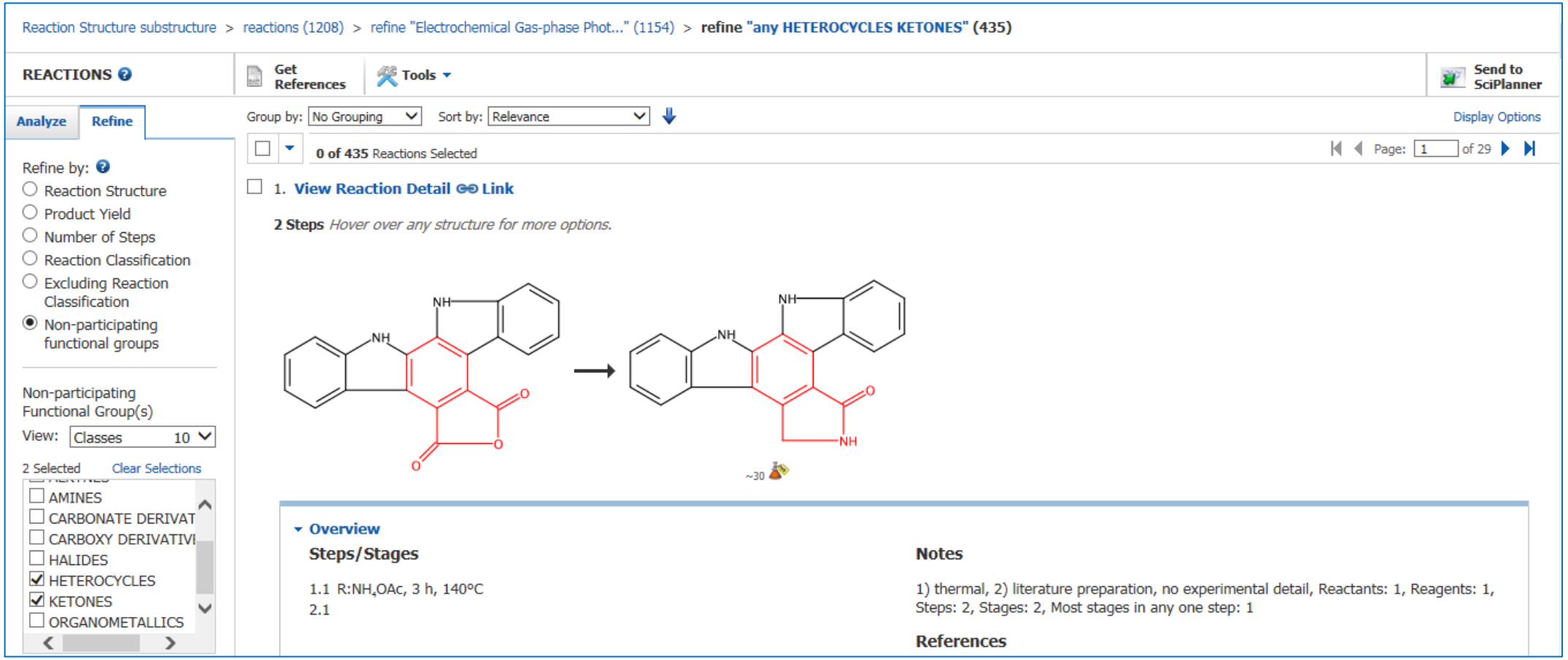
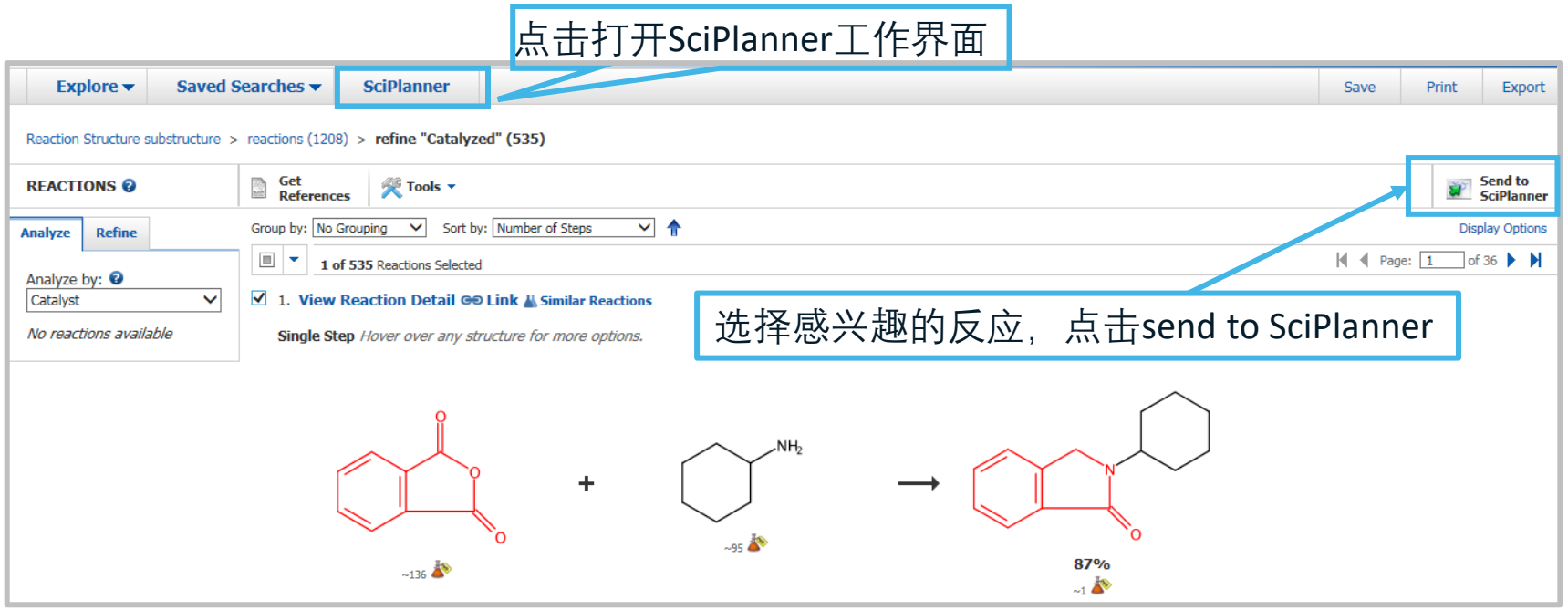
亚结构反应检索：排除反应类型



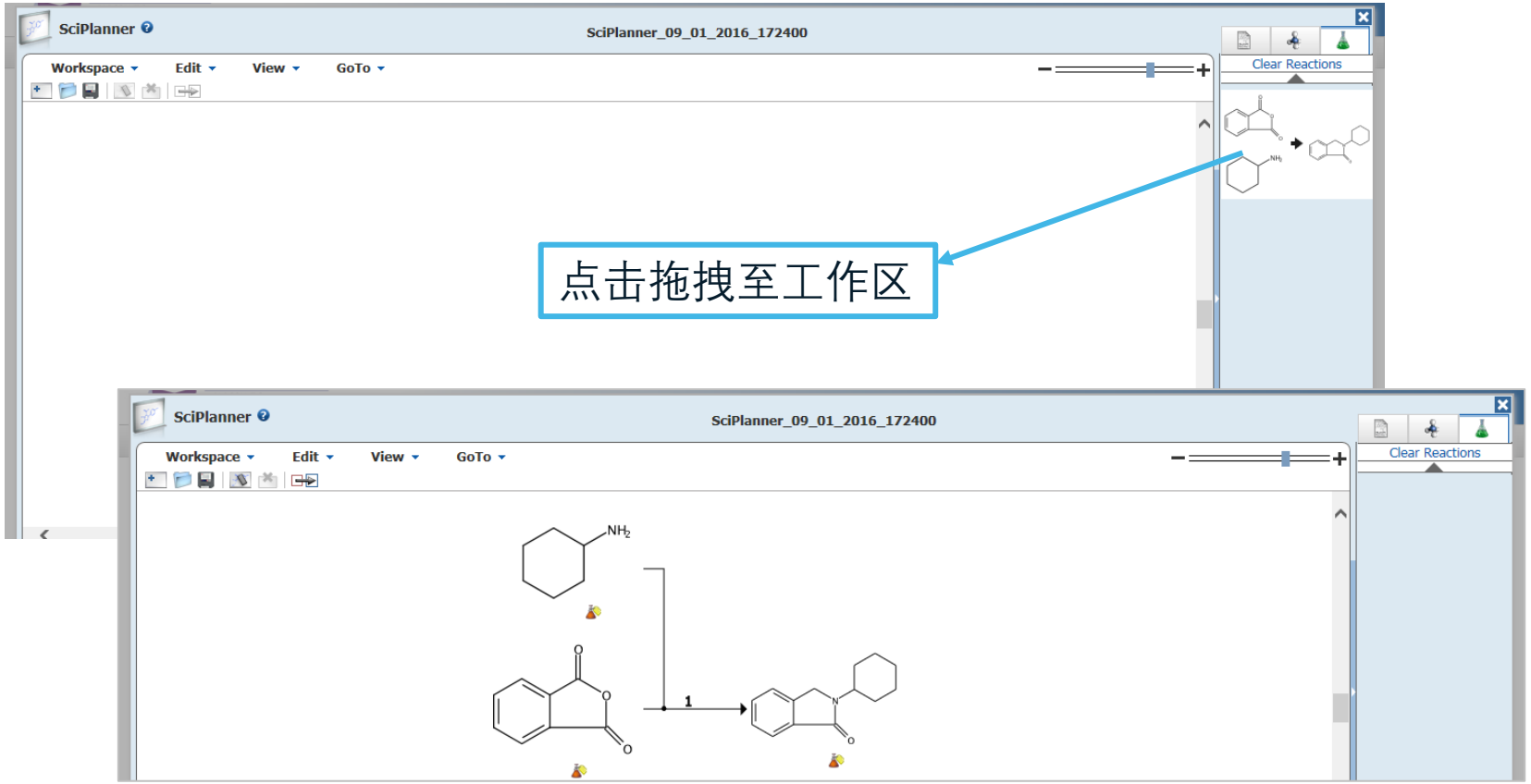
亚结构反应检索：筛选官能团



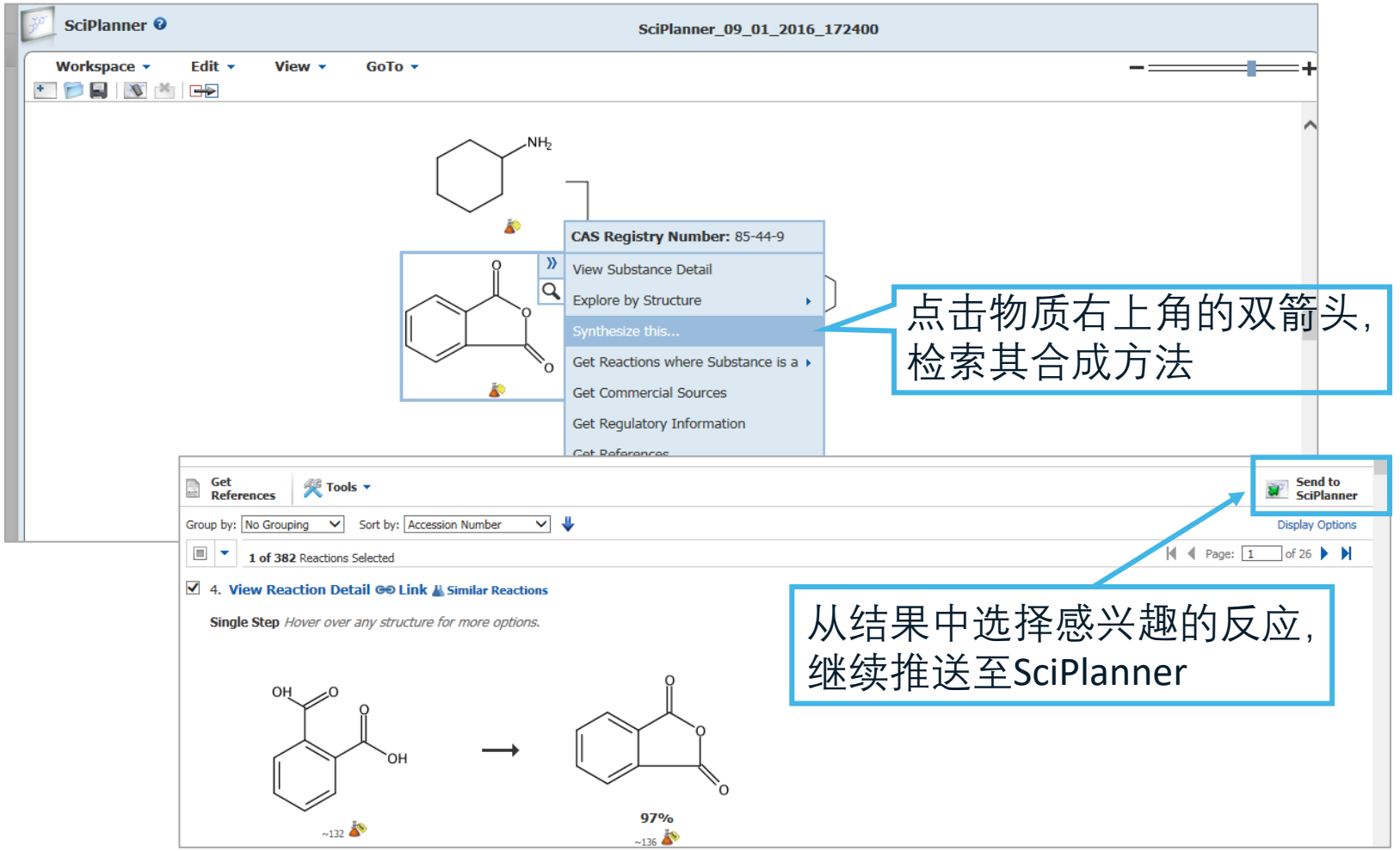
利用SciPlanner设计拟合成反应路线



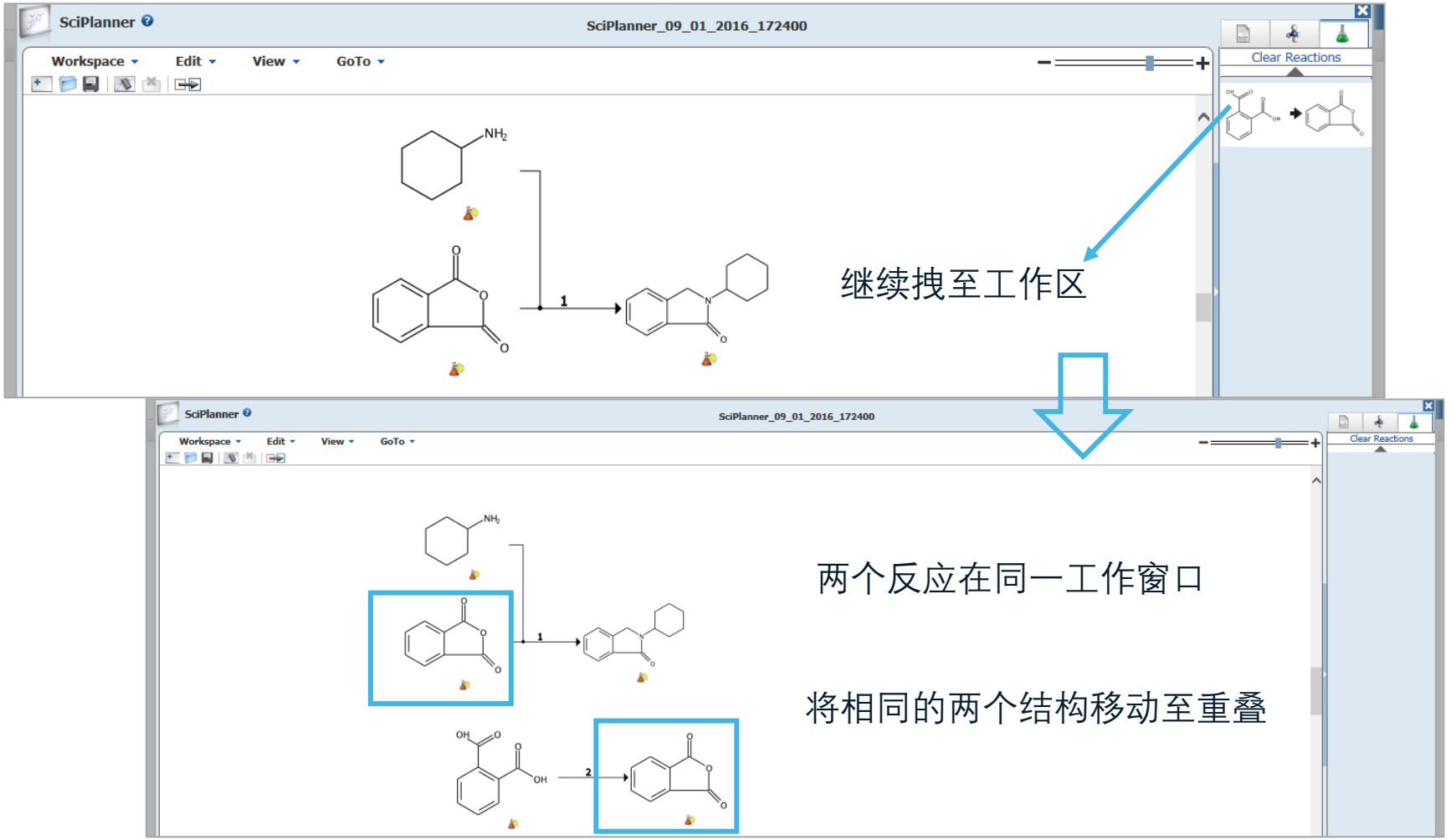
SciPlanner工作界面



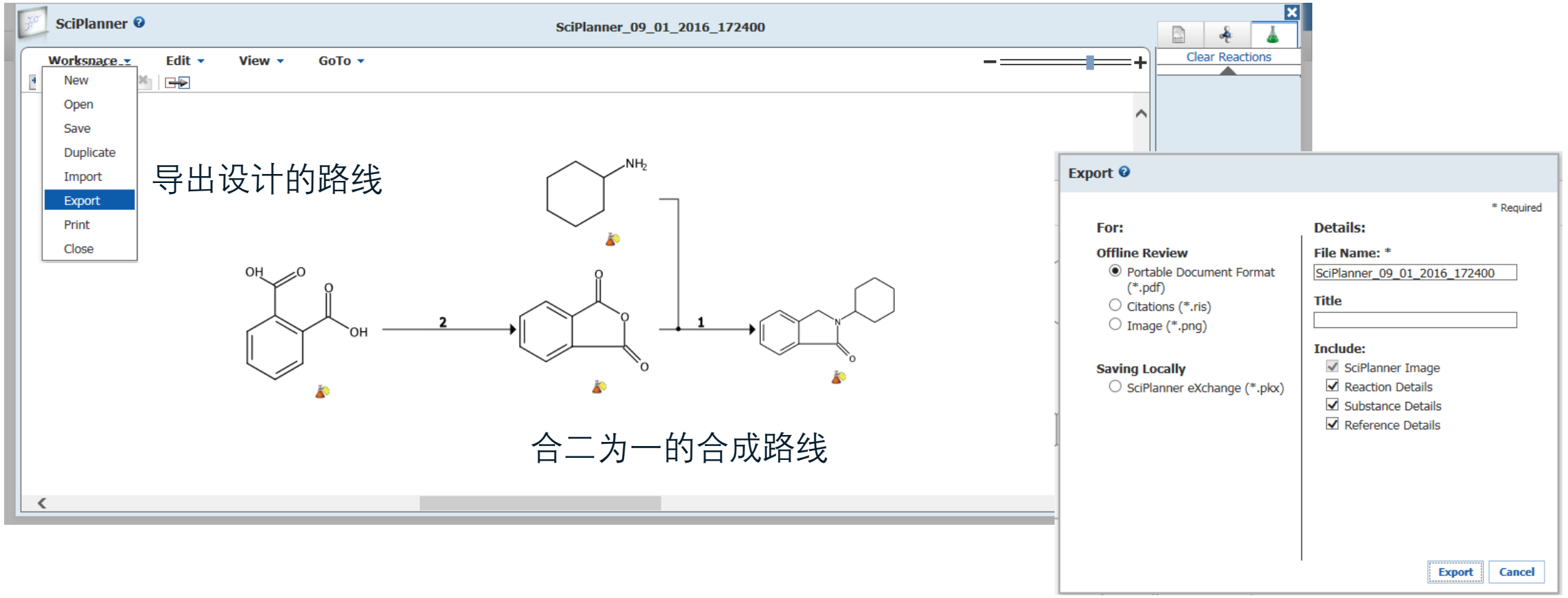
SciPlanner工作界面



SciPlanner工作界面



SciPlanner——设计拟合成的反应路线



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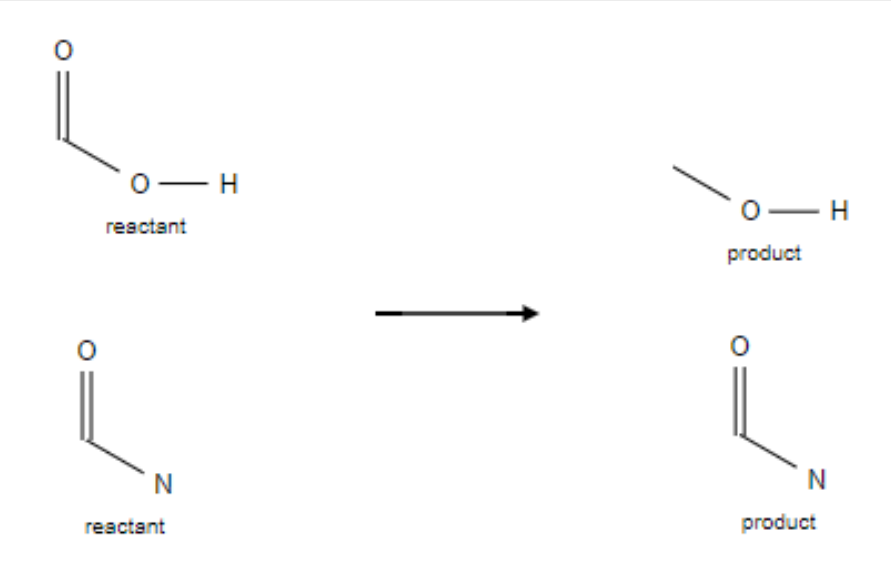
片段结构的化学选择性反应

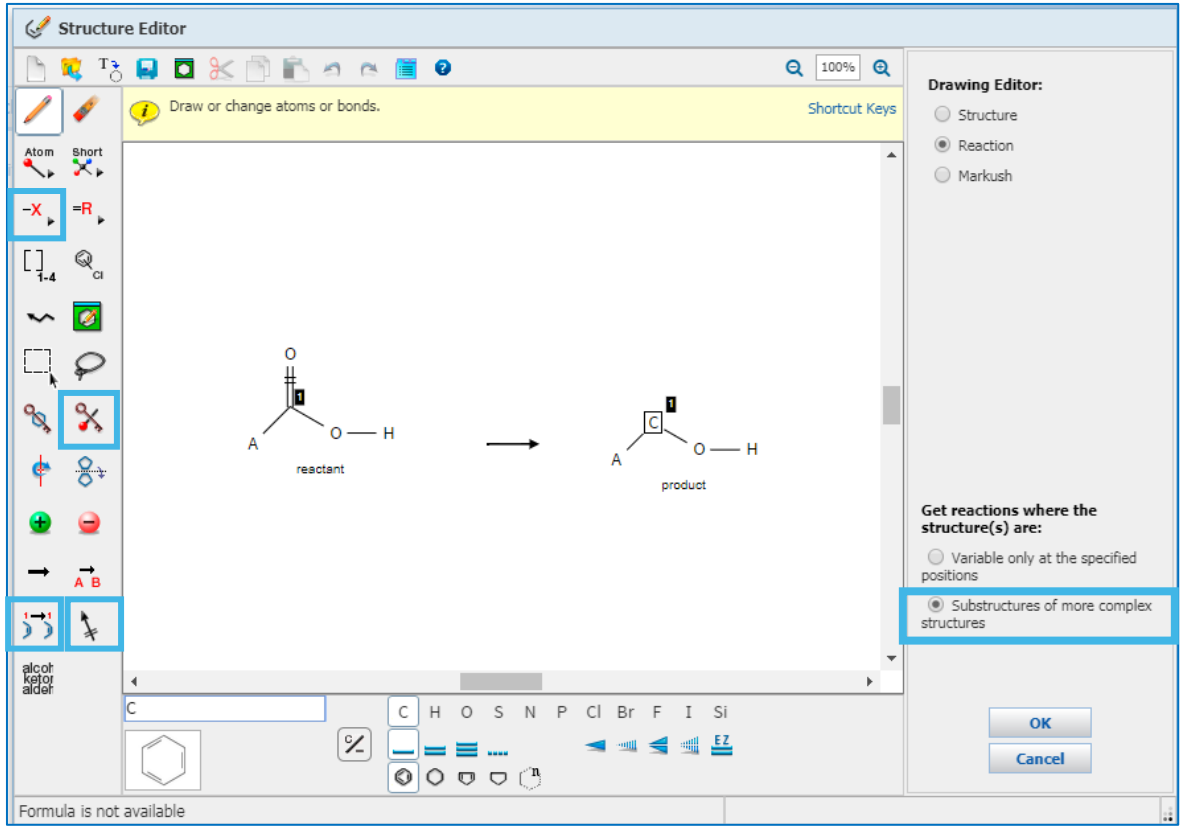


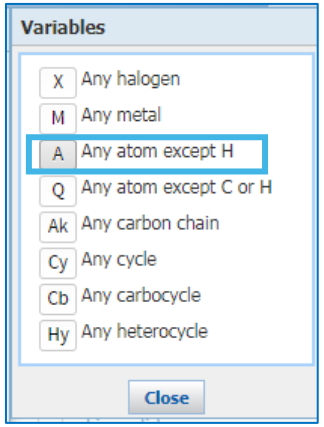
检索要求：

1. 反应物中含有羧基和酰胺基团；
2. 反应物种的羧基被还原为产物中的羟基；
3. 反应物中的酰胺基在反应后没有发生变化。

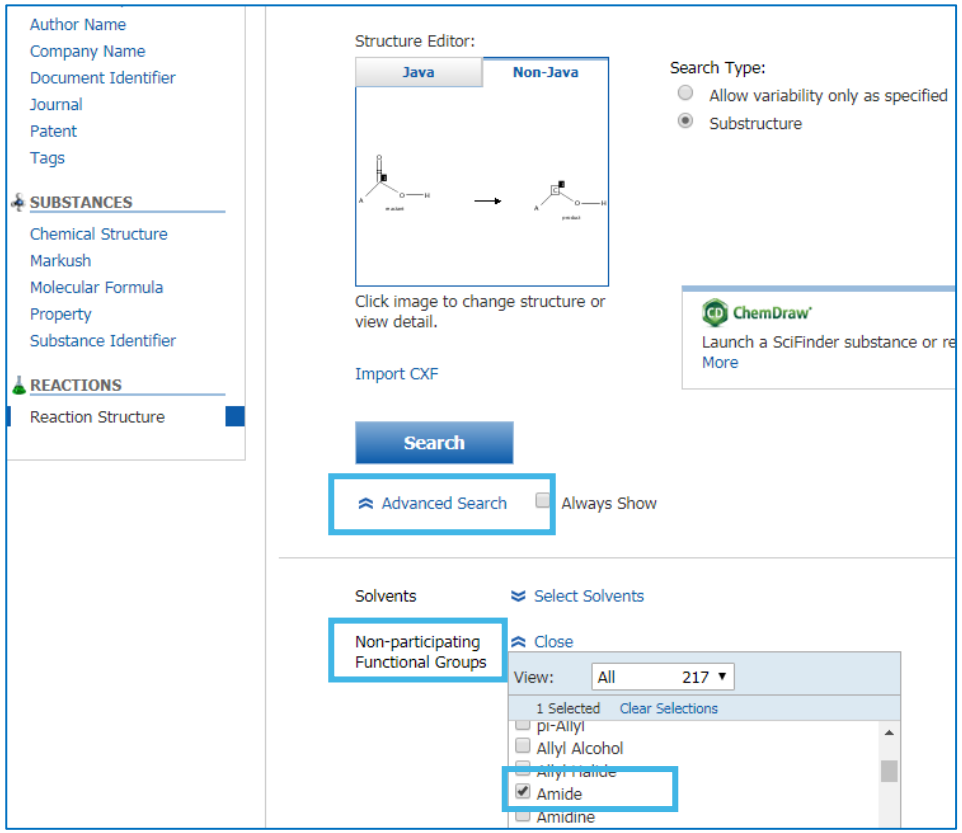
分析：
化学选择性反应可以使用non-participating functional groups来限定不参与反应的官能团。

绘制反应式





可提前选择不参与反应的官能团



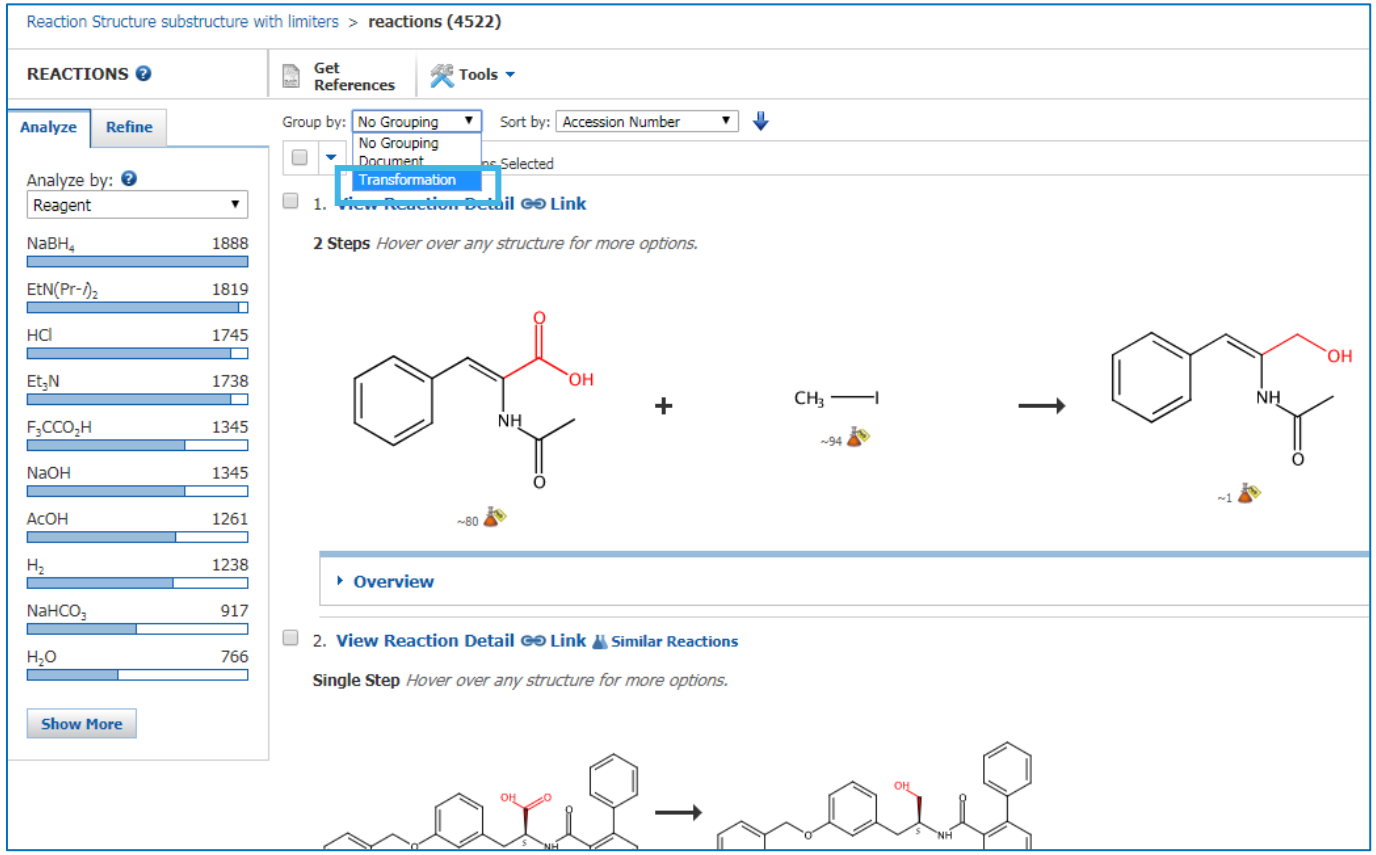
1. 点击高级检索；

2. 点击不参与反应官能团；

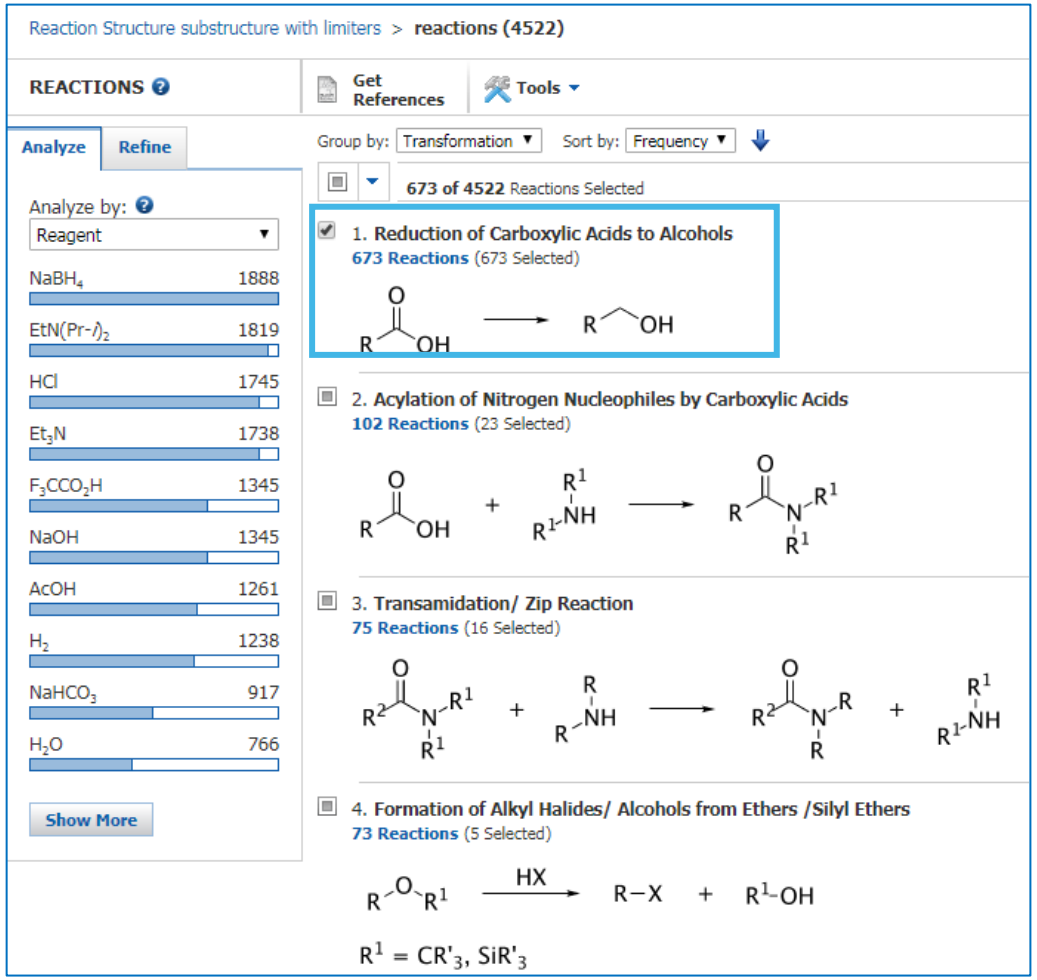
3. 选择酰胺amide。

反应结果分组

点击Group by中的Transformation，显示反应类型



Group by Transformation根据反应转化类型分组



选择羧酸还原为醇的这类反应

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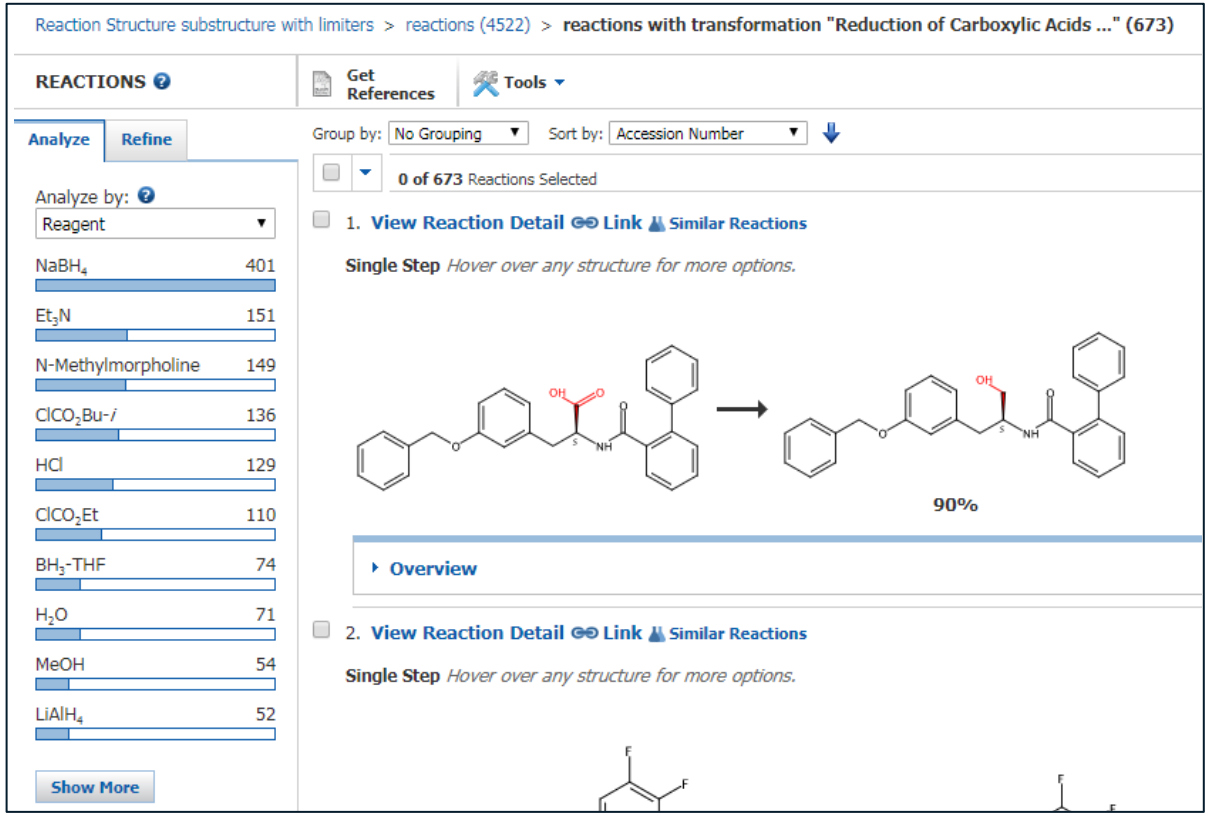
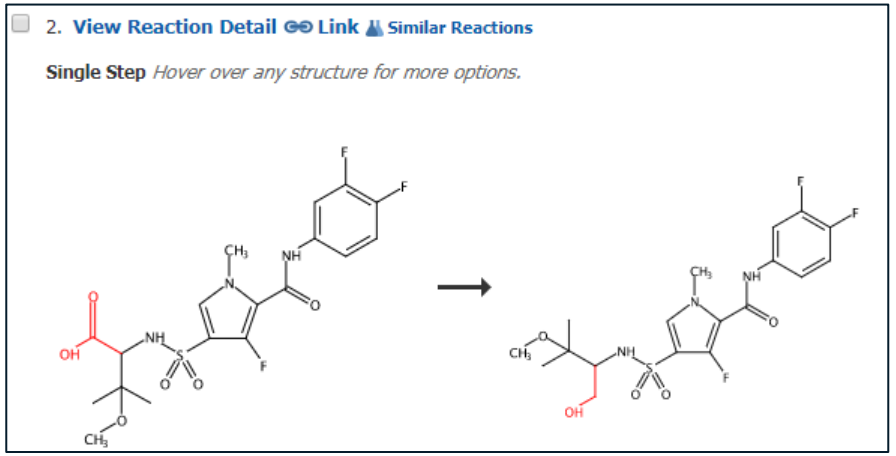
获得反应结果





反应检索小结：

- 反应检索方法汇总与区分；
- 反应绘制工具的灵活使用；
- 反应结果的快速纵览及筛选，例如non-participating functional group；
- 反应结果分组：Group by Transformation/Document
- 相似反应的获取获得更多启发
- SciPlanner工具助于自定义设计拟合成反应路线

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谢 谢 关 注!

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