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如何在SciFinder中检索物质信息

2017.3.2

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A CAS SOLUTION

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提纲

- 合金的检索
- 无机复合物的检索
- 聚合物的检索
- 检索具有相同结构特征物质
- Markush检索
- 如何判断物质的新颖性
- 如何检索有同位素标记的物质

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SciFinder检索选项——物质检索

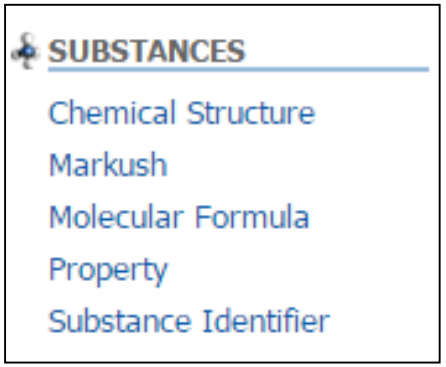
- 物质检索方法

  —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

分子式书写规则—Hill 规则

- 单一组分物质：
  - 对于不含C的物质，按照字母顺序排序
  - 对于含C的物质，C、H写在前面，其他的按照字母顺序排列
  - 相邻的两个元素之间必须有区分号，即数字或者空格，倘若数字为1，那么可以用空格来区分
  - 区分大小写

- 多组分物质：
  - 每一组分必须遵照单一组分物质的分子式来书写。
  - 不同组分之间的排序按照各组分的首元素的字母顺序排序，但是含C组分的一定排在不含C的组分前面。用点将不同的组分分开
  - 倘若不同组分的首元素相同，则看元素数量多少，数量多的排在前面，若元素数量一样，则按次元素的顺序排列。

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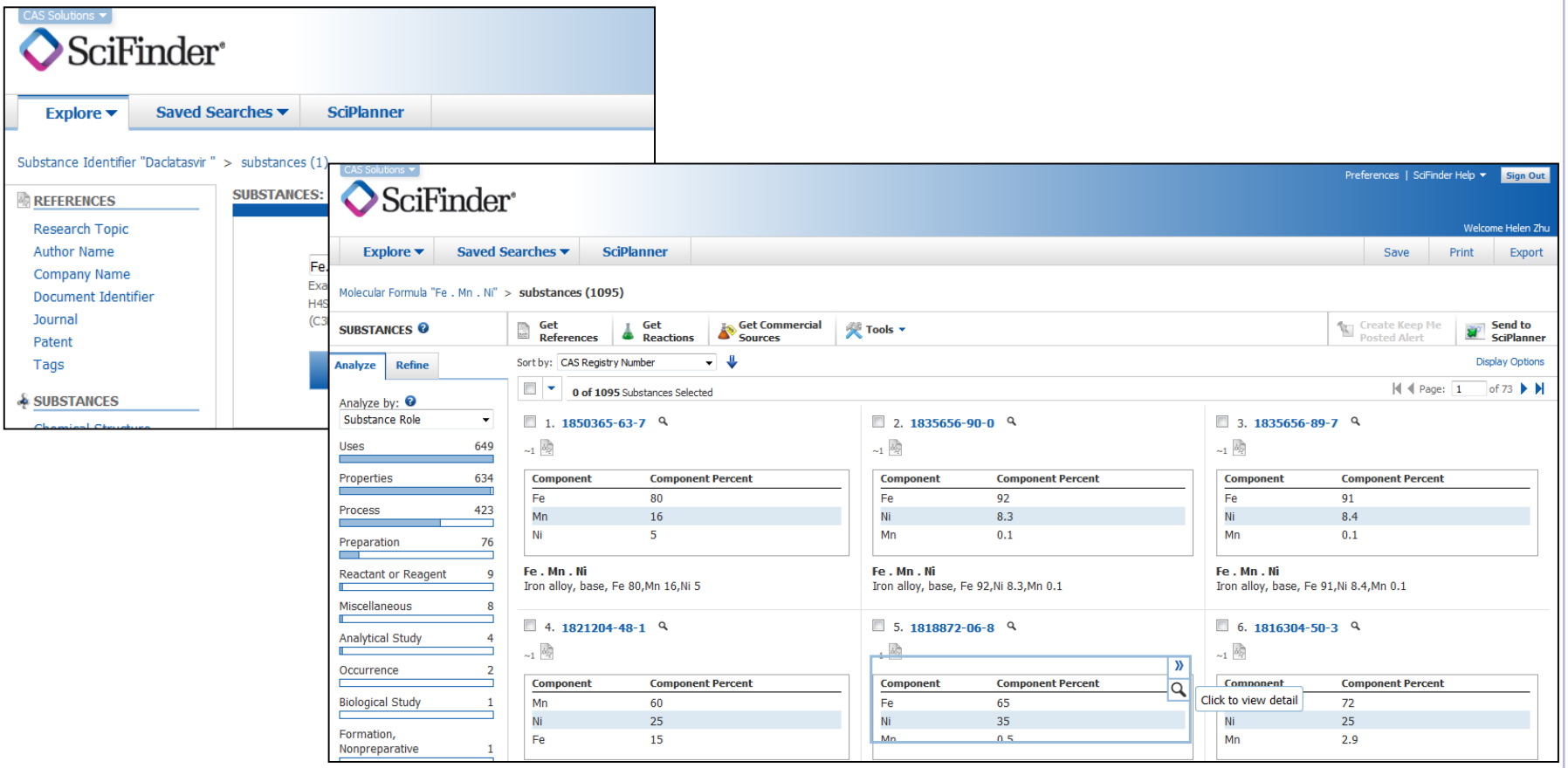
合金的检索

检索铁、锰、镍合金



合金物质以列表形式呈现

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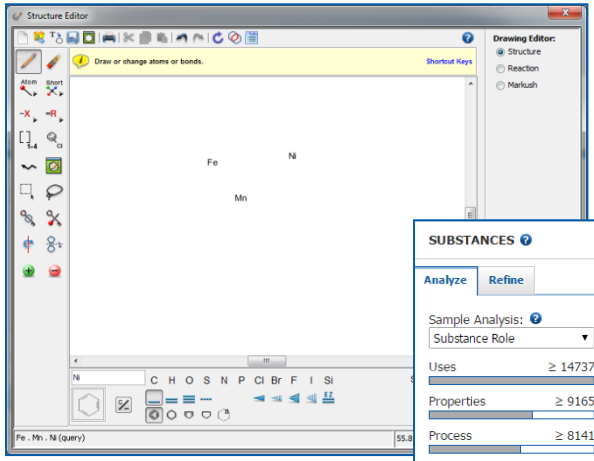
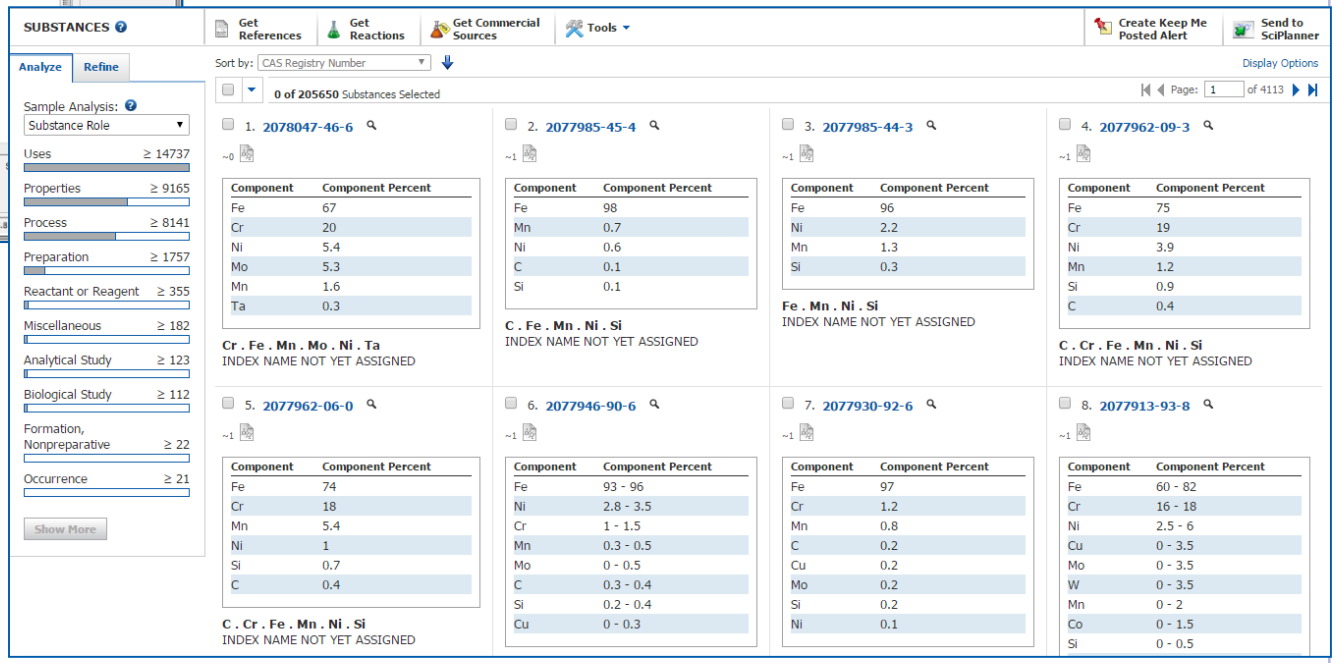
合金的检索

检索参杂铁、锰、镍原子的合金





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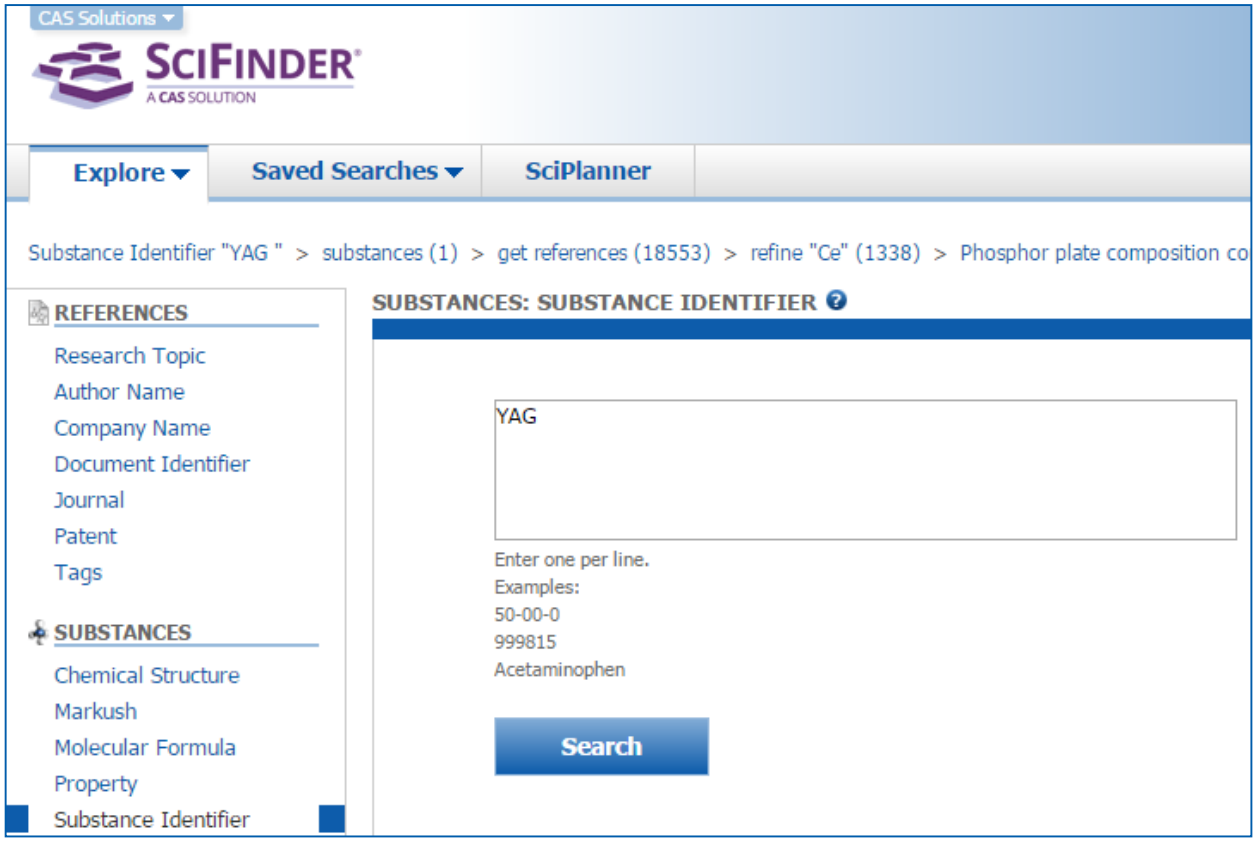
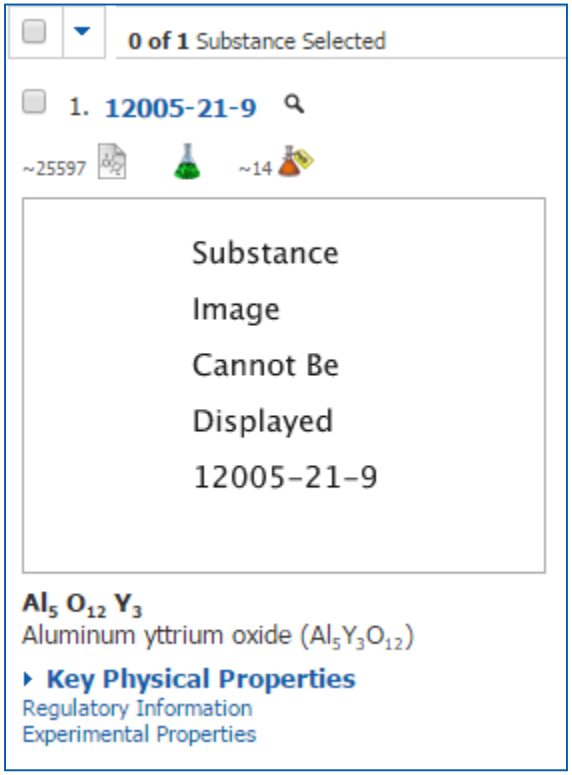
无机复合物的检索

检索YAG: Ce3+复合物及相关文献



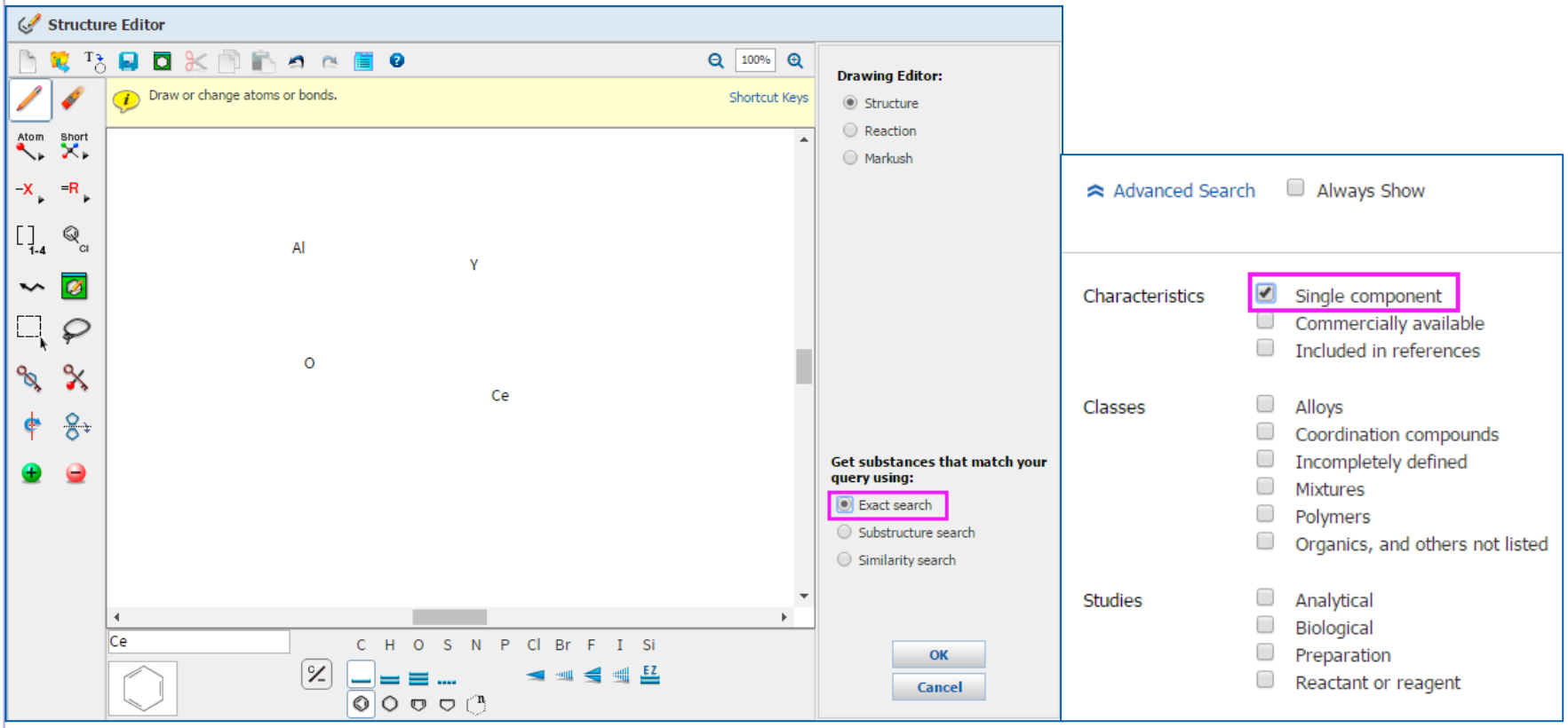
先通过物质标识符检索底物YAG

无机复合物的检索



了解YAG的分子式，
主要是元素组成 Al、O、 Y

无机复合物的检索



画入所有原子，选择精确结构检索，
随后选择单一组份

无机复合物的检索

Sort by: CAS Registry Number ▼ Display Options

0 of 111 Substances Selected Page: 1 of 3

1. 2055033-00-4

Component	Component Ratio
O	12
Y	1.5
Ce	1.5
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{1.5}Y_{1.5}O_{12}$)

2. 1947312-57-3

Component	Component Ratio
O	12
Y	3
Ce	0.1
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.1}Y_3O_{12}$)

3. 1879158-42-5

Component	Component Ratio
O	2
Y	0.1
Ce	0.8
Al	0.1

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{0.1}Ce_{0.8}Y_{0.1}O_2$)

4. 1877290-93-1

Component	Component Ratio
O	12
Y	2.65
Ce	0.35
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.35}Y_{2.65}O_{12}$)

5. 1821155-37-6

Component	Component Ratio
O	11.7
Y	2.98
Ce	0.02
Al	4.8

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{4.8}Ce_{0.02}Y_{2.98}O_{11.7}$)

6. 1821155-35-4

Component	Component Ratio
O	12.3
Y	2.98
Ce	0.02
Al	5.2

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_{5.2}Ce_{0.02}Y_{2.98}O_{12.3}$)

7. 1693710-50-7

Component	Component Ratio
O	12
Y	2.1
Ce	0.9
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.9}Y_{2.1}O_{12}$)

8. 1693710-49-4

Component	Component Ratio
O	12
Y	2.25
Ce	0.75
Al	5

Al . Ce . O . Y
Aluminum cerium yttrium oxide
($Al_5Ce_{0.75}Y_{2.25}O_{12}$)

9. 1693710-48-3 10. 1639807-13-8 11. 1639807-12-7 12. 1639807-11-6

人工通过列表上的比例判断目标物质，然后获取相关文献。

文献全吗？

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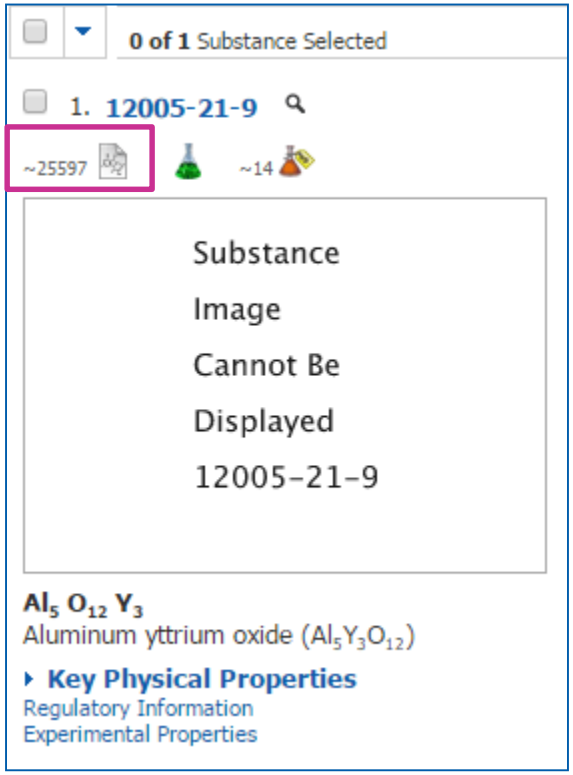
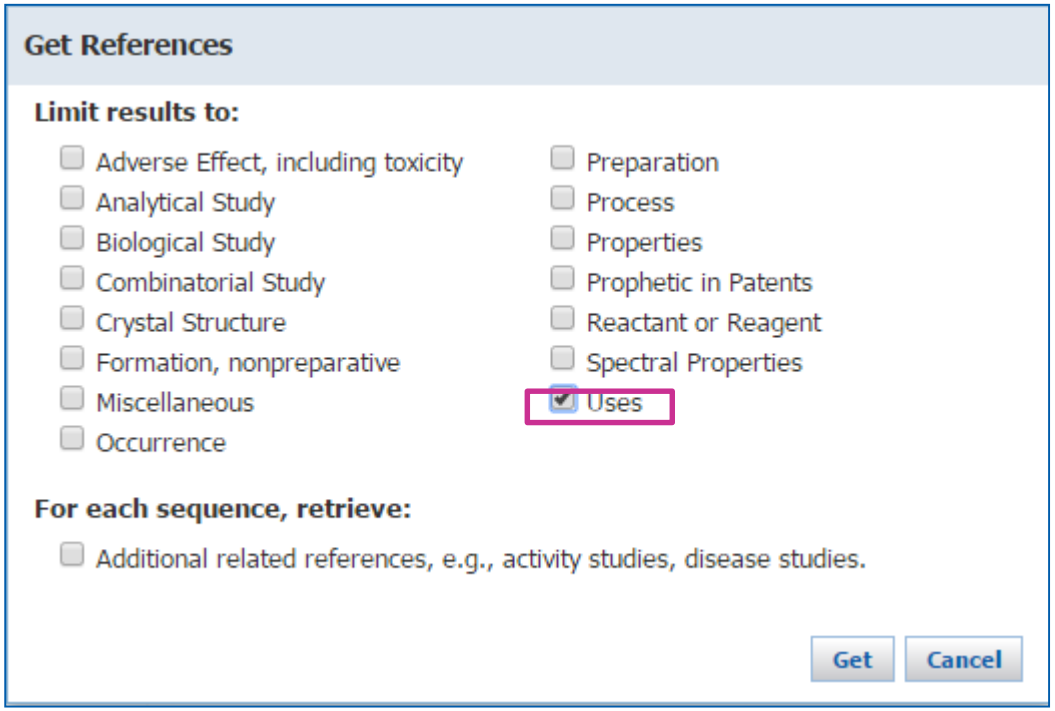
无机复合物的检索





通过底物获得应用相关的文献

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无机复合物的检索

Substance Identifier "YAG " > substances (1) > **get references (18553)** > refine "Ce" (1338) > Phosphor plate composition com...

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | **Refine** | Categorize

Refine by:
- Research Topic
- Author
- Company Name
- Document Type
- Publication Year
- Language
- Database

Research Topic
Ce

Examples:

The effect of antibiotic residues on dairy products

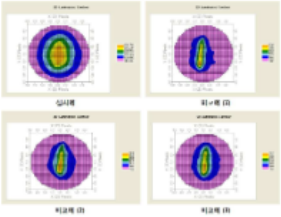
Photocyanation of aromatic compounds

Refine

Sort by: Accession Number ▼ | Display Options

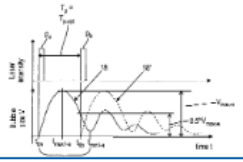
0 of 18553 References Selected | Page: 1 of 928

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**
   Quick View | PATENTPAK
   By Won, Ju Yeon; Kim, Won Jin
   From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS



An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (Ce), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel ($MgAl_2O_4$).

2. **Cleaning system and method for operating the cleaning system**
   Quick View | PATENTPAK
   By Lukac, Nejc; Lukac, Matjaz; Jezersek, Matija; Gregorcic, Peter
   From Eur. Pat. Appl. (2017), EP 3127502 A1 20170208. | Language: English, Database: CAPLUS



The invention relates to a cleaning system being configured for cleaning, including fragmentation, debridement, material removal, irrigation, disinfection and decontamination, of cavities filled with a liq.. The cleaning system comprises an electromagnetic radiation system and the liq. A treatment handpiece and its exit component are configured to irradiate the liq. within the cavity with the radiation beam, wherein a wavelength of the radiation beam is chosen for significant absorption of the radiation beam in the liq.. The electromagnetic radiation system is adapted to generate a first va...

用Ce限定文献

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无机复合物的检索

Substance Identifier "YAG " > substances (1) > get references (18553) > **refine "Ce" (1338)** > Phosphor plate composition com...

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine | Categorize

Analyze by: Author Name

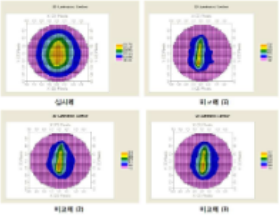
Hirosaki Naoto	18
Takeda Takashi	14
Nikl M	12
Liang Xiaojuan	11
Xiang Weidong	11
Do Young Rag	10
Fujita Shunsuke	8
Funahashi Shiro	8
Mares J A	8
Nikl Martin	8

Show More

Sort by: Accession Number | Display Options

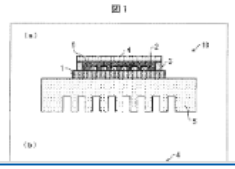
0 of 1338 References Selected | Page: 1 of 67

1. **Phosphor plate composition comprising phosphor powder and sintering agent for vehicle headlamp**
Quick View | PATENTPAK
By Won, Ju Yeon; Kim, Won Jin
From Repub. Korean Kongkae Taeho Kongbo (2017), KR 2017014153 A 20170208. | Language: Korean, Database: CAPLUS



An embodiment of the present invention relates to a phosphor plate compn. having wide luminescent region while improving brightness, comprising yttrium aluminum garnet (YAG) or gadolinium yttrium aluminum garnet (GdYAG) phosphor powders doped with at least one dopant selected from cesium (**Ce**), gadolinium (Gd) and neodymium (Nd); and at least one sintering agent selected from any one of lithium fluoride (LiF), magnesium oxide (MgO) and spinel ($MgAl_2O_4$).

2. **Light emitting device improves heat dissipation efficiency of heat generated in wavelength converting member and illuminating device including light emitting device**
Quick View | PATENTPAK
By Harada, Masamichi; Yoshimura, Kenichi; Onuma, Hiroaki
From Jpn. Kokai Tokkyo Koho (2017), JP 2017028097 A 20170202. | Language: Japanese, Database: CAPLUS



The present invention relates to a light emitting device and illuminating device including the light emitting device. Light emitting device comprises of multiple light emitting elements, substrate on which multiple light emitting elements are mounted, wavelength converting member for converting a wavelength of light emitted from multiple light emitting elements. The wavelength conversion member includes phosphor sealed with a sealing material for converting the wavelength of the light and a holding material for holding the phosphor. The holding material is characterized in that it contains ...

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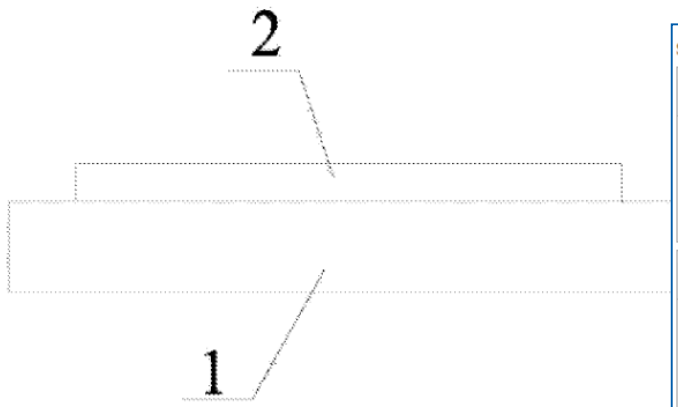
无机复合物的检索

5. Microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their production method

By: Cao, Dun-Hua; Dong, Yong-Jun; Liang, Yue-Shan
Assignee: Peop. Rep. China

The present invention relates to a Ce:YAG wafer-based composite structure comprising a Ce:YAG wafer and a red light emitting layer fixed on the Ce:YAG wafer. The present invention also relates to a method for the prepn. of the Ce:YAG wafer-based composite structure. The optical composite structure realizes a wide waveband luminescence from green light to red light, and can be widely used in the fields of detection equipment and illumination devices.



Substances

7440-45-1 Cerium, properties — Page 7 in PATENTPAK

YAG doped with; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Modifier or additive use; Properties; Technical or engineered material use; Uses

12005-21-9 YAG — Page 7 in PATENTPAK

cerium-doped, europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

7440-53-1 Europium, properties — Page 6 in PATENTPAK

dopant; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Modifier or additive use; Properties; Technical or engineered material use; Uses

1314-36-9 Yttrium oxide (Y2O3), properties — Page 6 in PATENTPAK

europium-doped; microchip composite luminescent structures based on Ce:YAG and having a wide luminescence spectrum, and their prodn. method

Properties; Technical or engineered material use; Uses

该文中没有标引物质1947312-57-3，
却是我们需要的文献

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无机复合物的检索

PATENTPAK A CAS SOLUTION

PAGE 7 /7 ZOOM DOWNLOAD PDF

Key Substances in Patent

CAS RN 7440-53-1

Eu

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 6

CAS RN 1314-36-9

Yttrium oxide (Y_2O_3)

Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 6

CAS RN 7440-45-1

Ce

US 2016/0341832 A1 Nov. 24, 2016
3

nm~700 nm, and thus achieving a wide waveband luminescence from green light to red light.

[0042] The purpose, technical solutions and beneficial effects of the present invention are described with reference to the above particular examples. Nevertheless, it will be understood that the above examples are not provided to limit the present invention. The invention is intended to cover various modifications and equivalent arrangements included within the spirit and scope of the claims.

1. A Ce:YAG wafer-based composite structure, wherein said composite structure comprises:

a Ce:YAG wafer; and

a red light emitting layer fixed on said Ce:YAG wafer.

2. The Ce:YAG wafer-based composite structure according to claim **1**, wherein the main emission peak of said red light emitting layer is at 580 nm~660 nm.

3. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a deposited film capable of emitting red light.

4. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a transparent colloid layer doped with red fluorescent powder.

5. The Ce:YAG wafer-based composite structure according to claim **2**, wherein said red light emitting layer is a crystalline, a ceramic or a glass doped with red light

6. A method for the preparation of a Ce:YAG wafer-based composite structure, comprising:

(1) producing a Ce:YAG wafer by Czochralski process, temperature gradient process or Kyropoulos process;

(2) grinding and polishing the Ce:YAG wafer produced in step (1) to obtain a fluorescent wafer having desired size; and

(3) adding a red light emitting layer on the fluorescent wafer obtained in step (2).

7. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a red light emitting film deposited by physical or chemical vapor deposition.

8. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a transparent colloid layer doped with red fluorescent powder.

9. The method for the preparation of a Ce:YAG wafer-based composite structure according to claim **6**, wherein the red light emitting layer added in step (3) is a crystalline, a ceramic or a glass doped with red light luminescence center of rare earth or transition metal and fixed on the fluorescent wafer.

专利中仅仅以文字方式提到此物质

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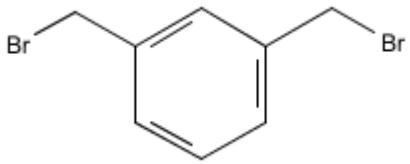
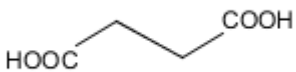
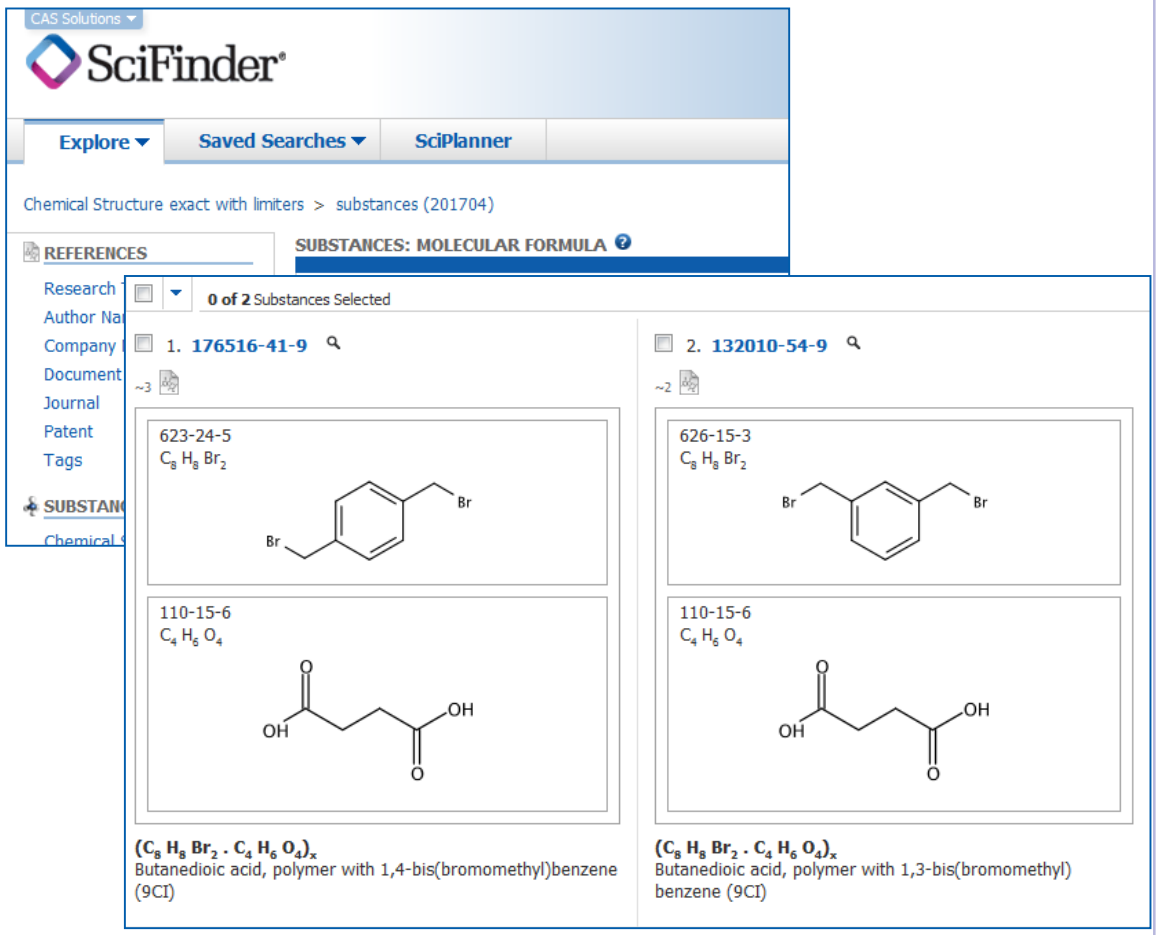
聚合物的检索

已知起始原料的聚合物





（C8 H8 Br2 . C4 H6 O4）x



分子式检索后会得到同分异构体

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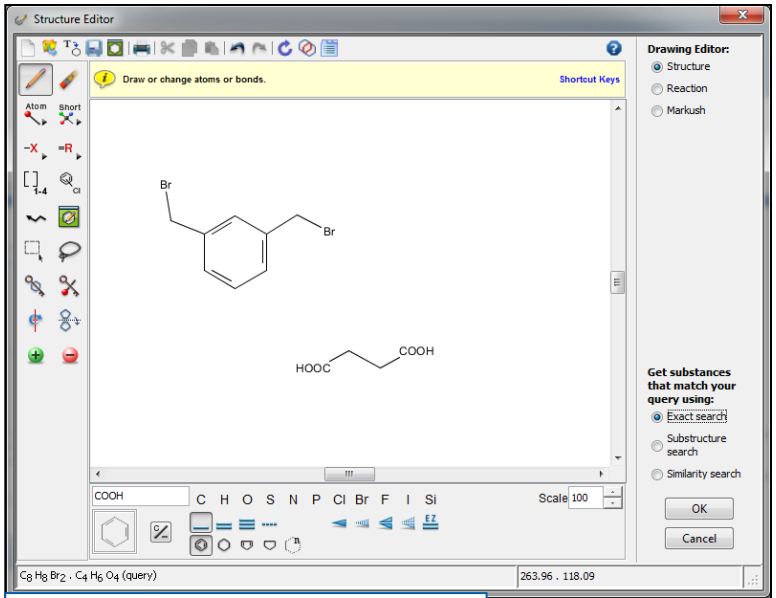
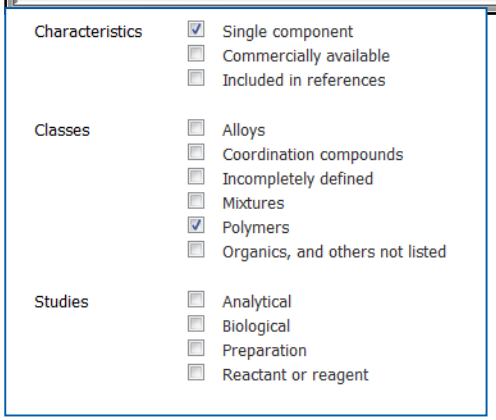
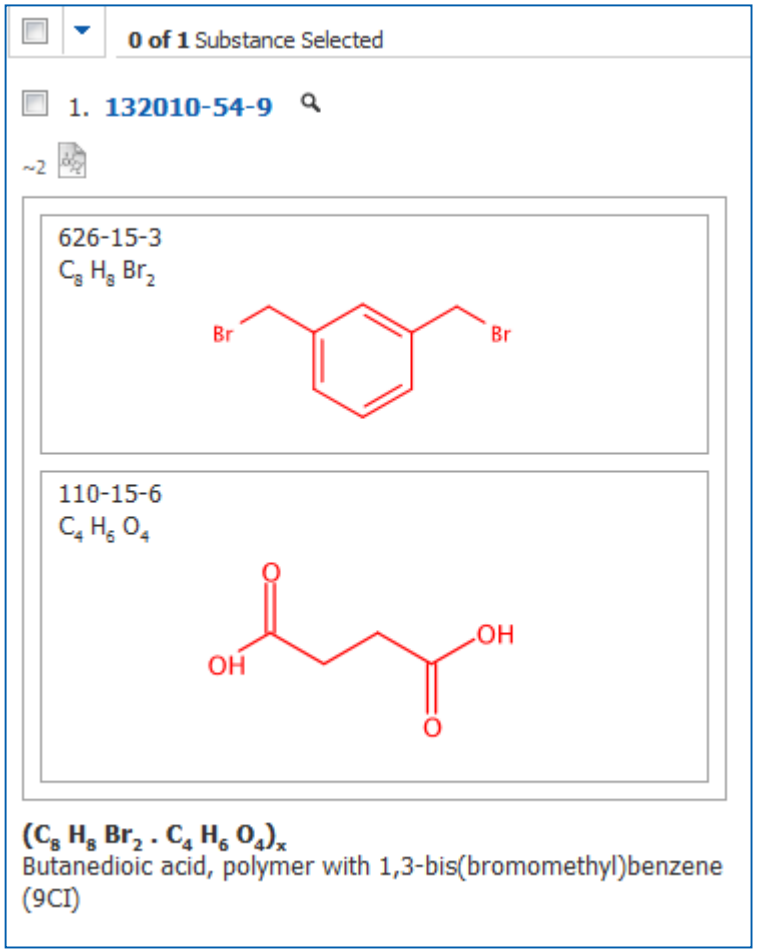
聚合物的检索





单一组分

聚合物



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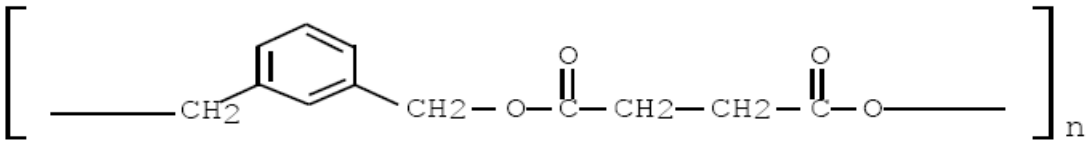
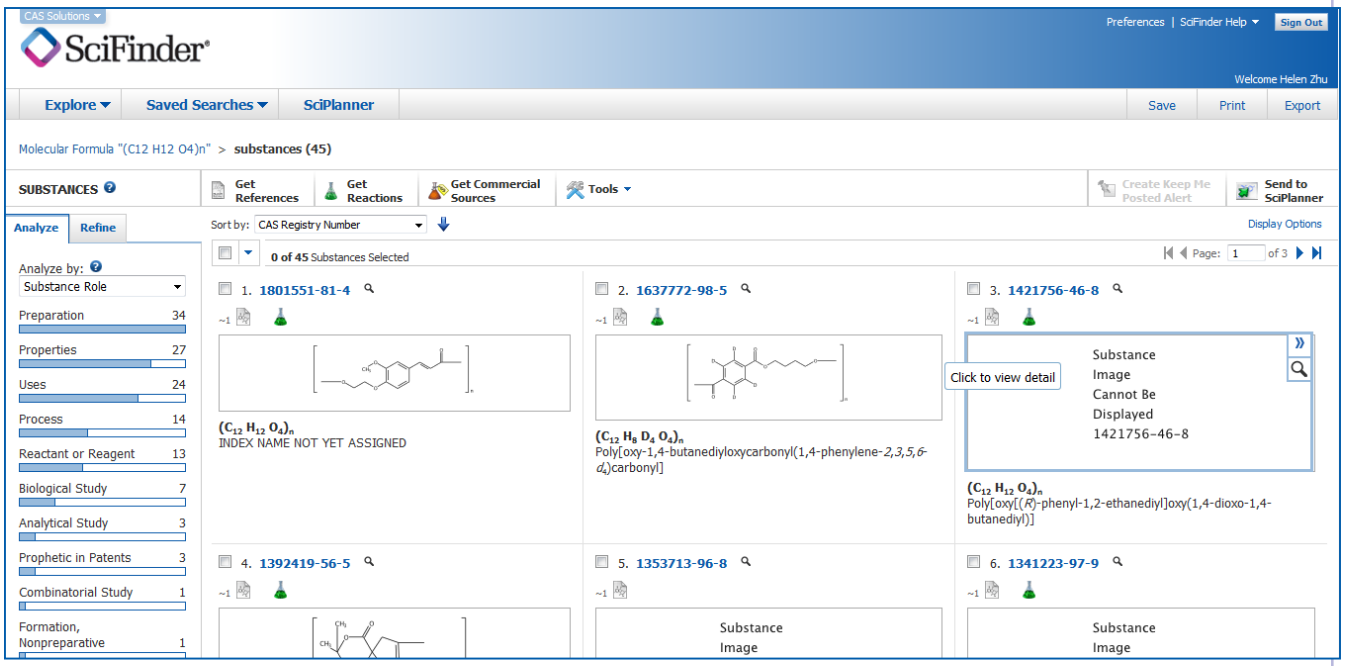
聚合物的检索

已知重复单元的聚合物

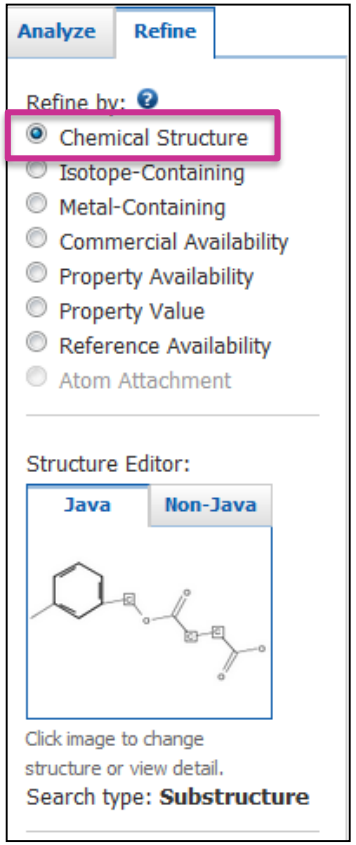


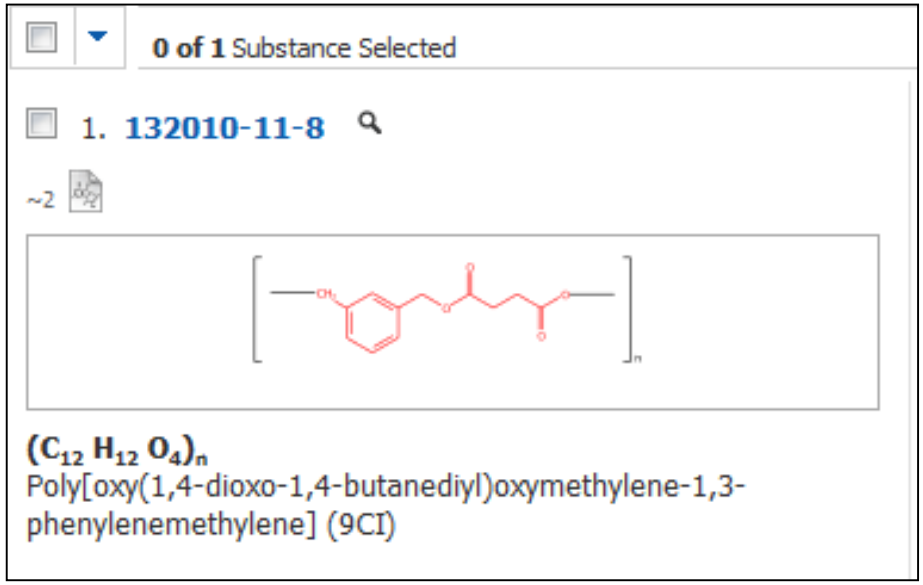
(C12 H12 O4)n



SciFinder®
A CAS SOLUTION

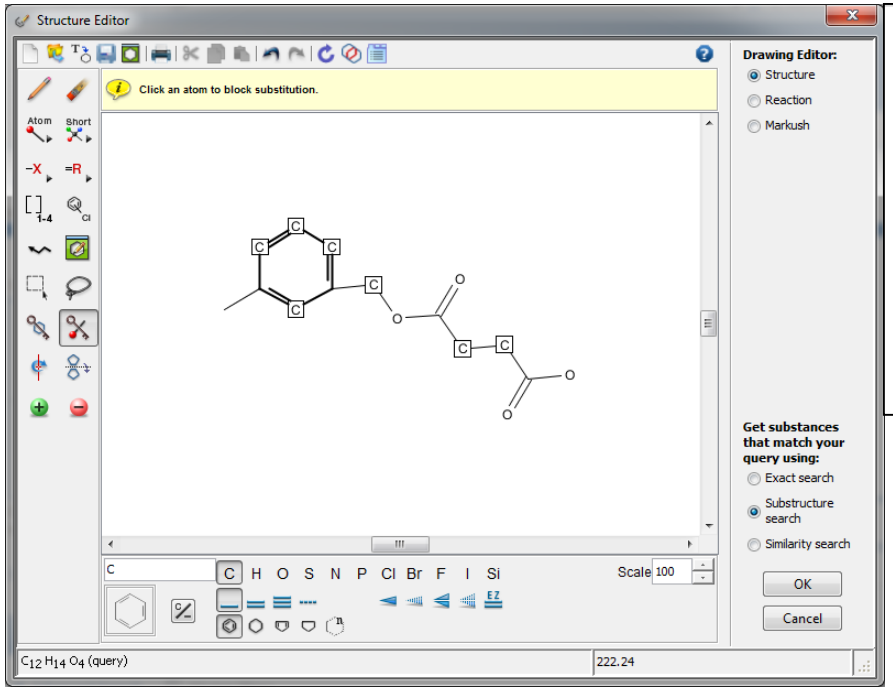
聚合物的检索





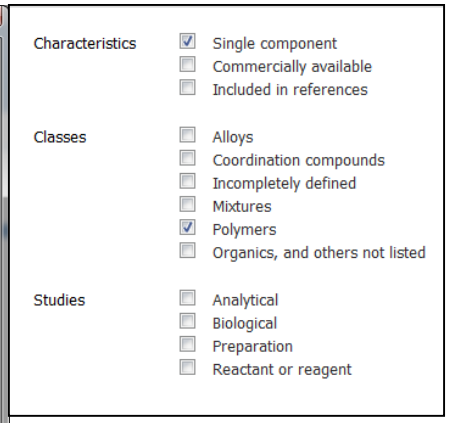
利用结构特征进行Refine，迅速查找需要的物质

聚合物检索



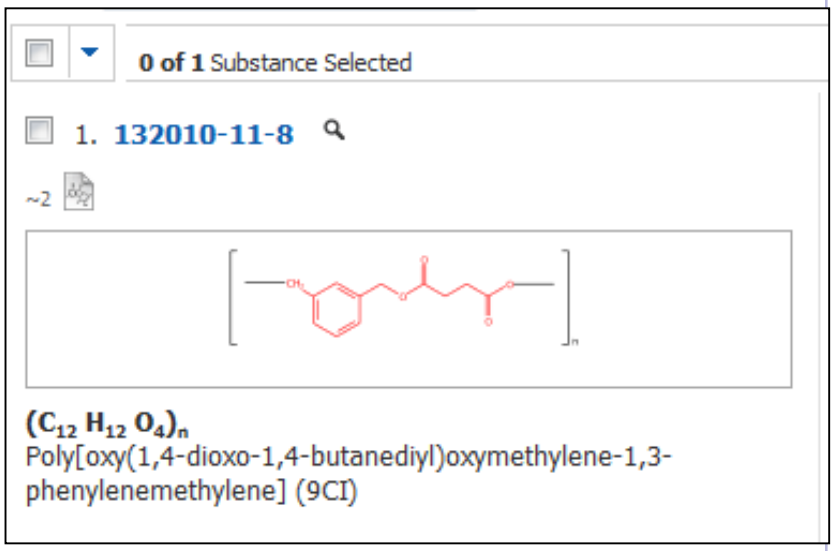
绘制好SRU后用亚结构检索

因为两段为开放状态



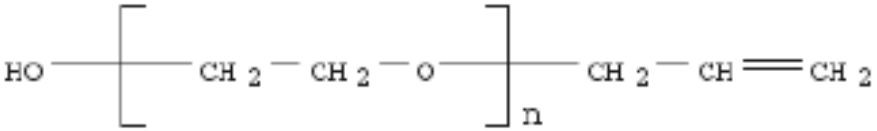
单一组分

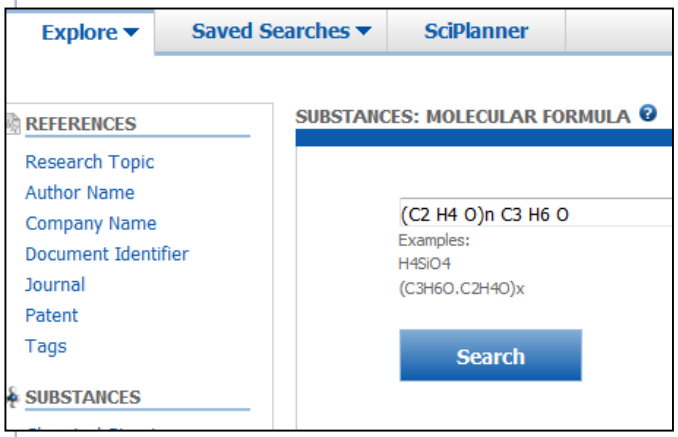
聚合物



聚合物的检索

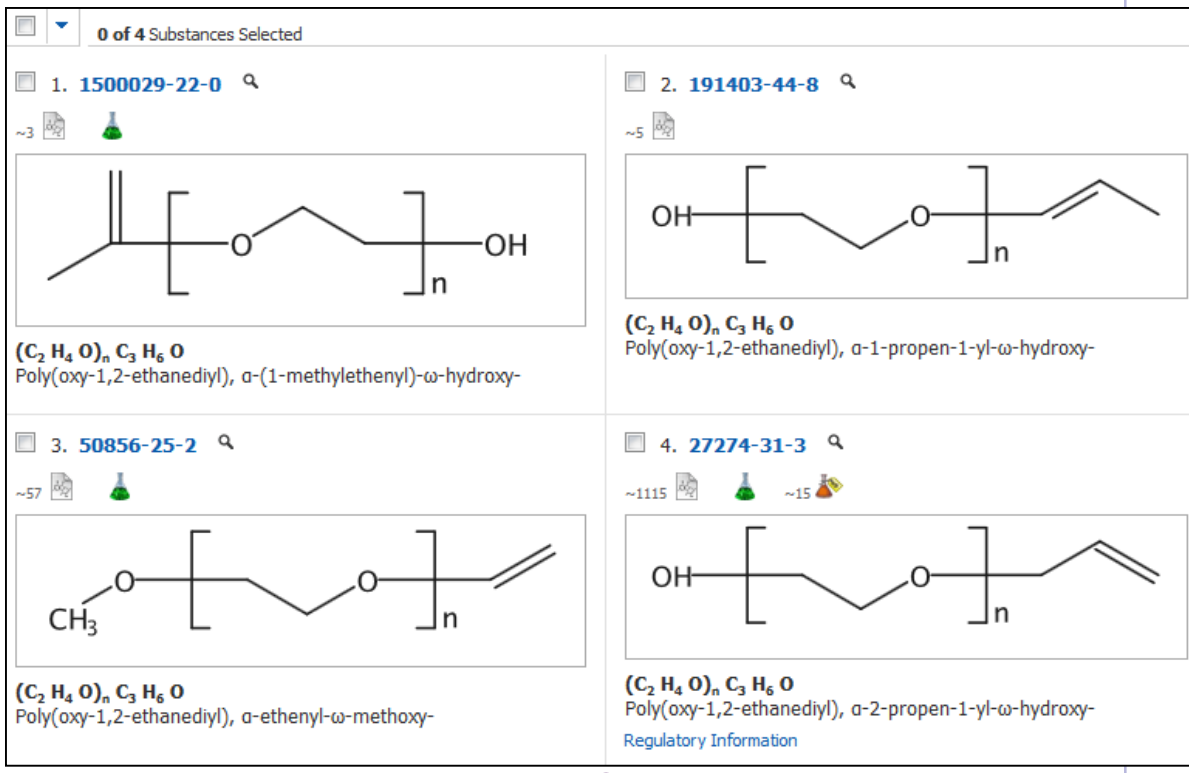
含端基和SRUs的聚合物





(C2 H4 O)n C3 H6 O

SRU部分　　两端部分



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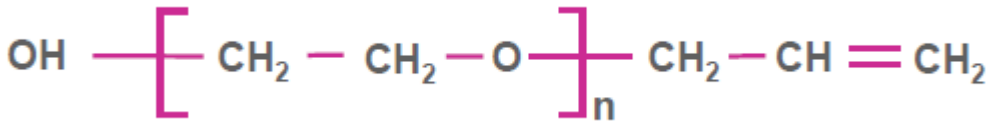
聚合物的检索

杂化聚合物的检索：

检索由以下聚合物和2-丙烯酸（C3H4O2）聚合生成的聚合物

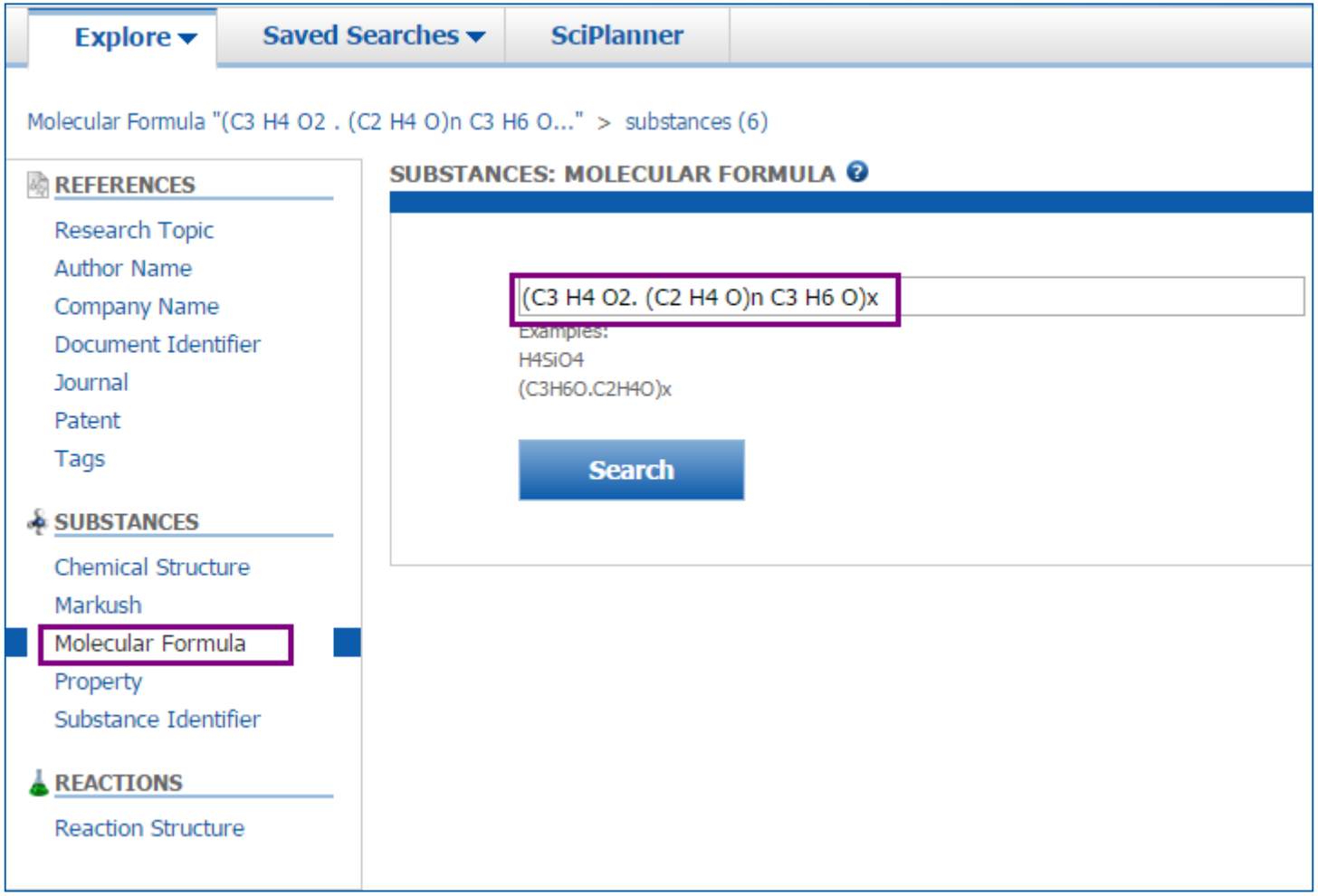


检索策略：分子式检索

(C3 H4 O2. (C2 H4 O)n C3 H6 O)x

丙烯酸部分　SRU部分　两端部分

聚合物的检索



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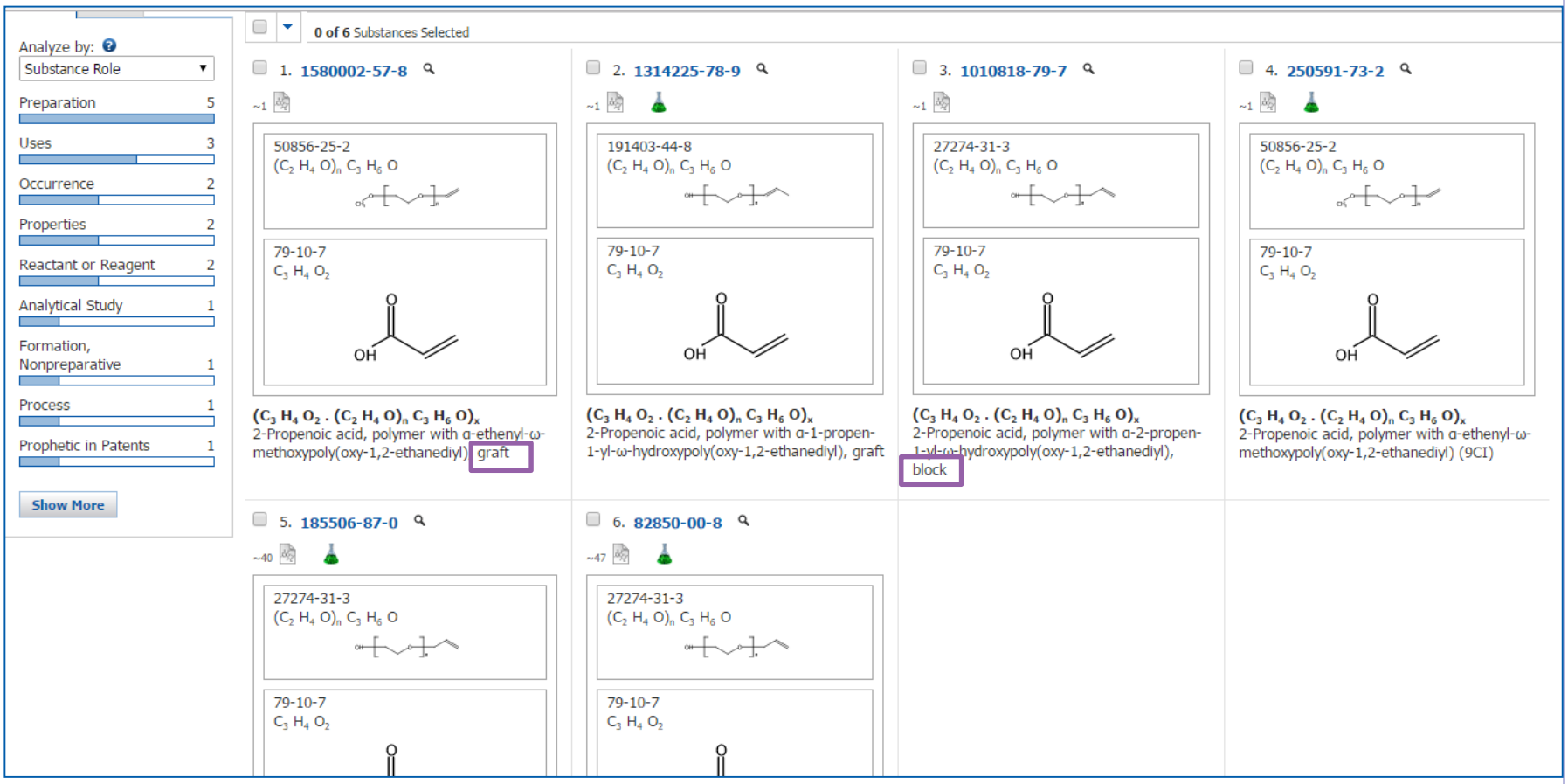
聚合物的检索



Block：嵌段聚合物

Graft：接枝聚合物

聚合物的检索

后处理聚合物的检索：

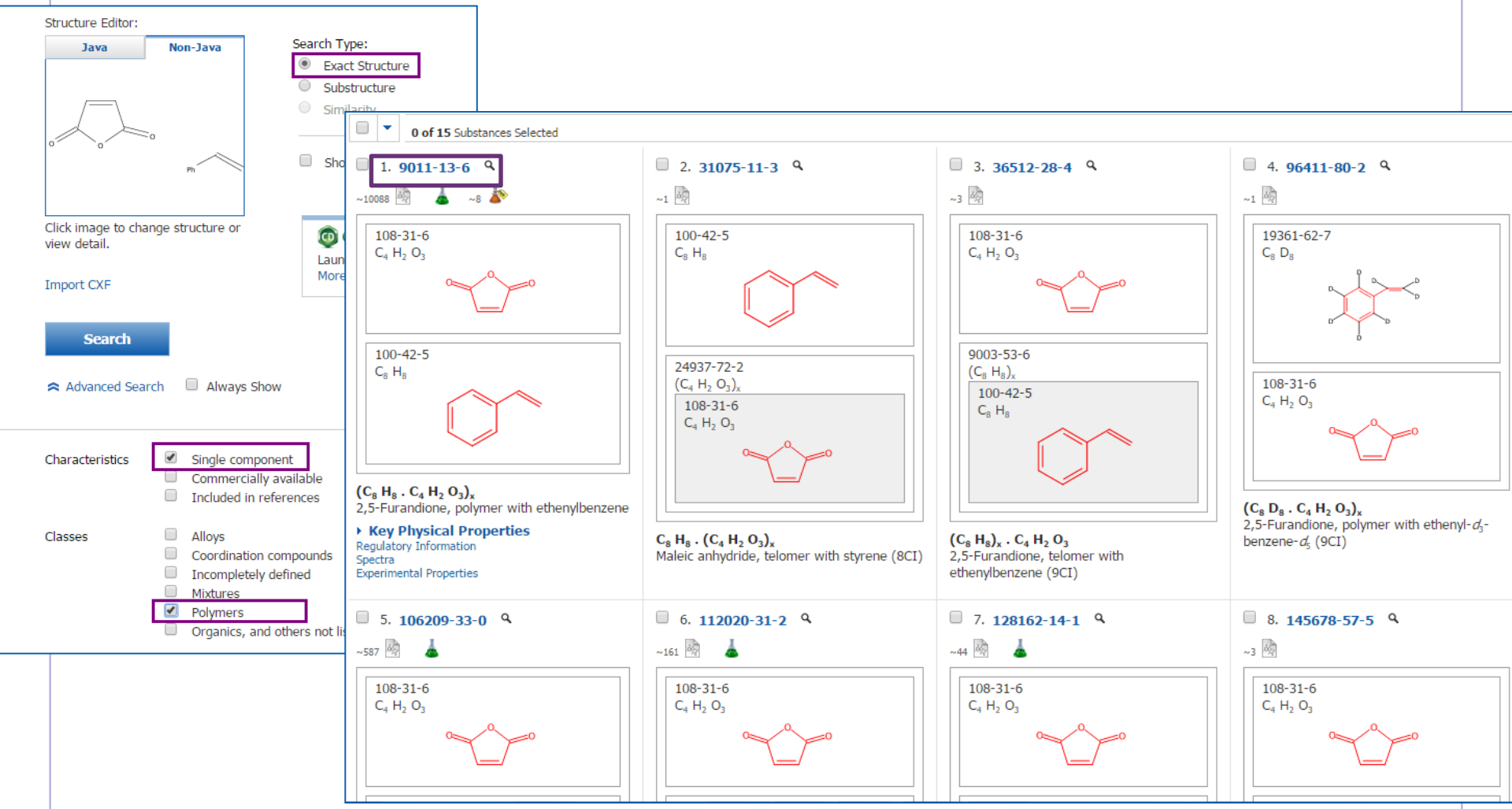
检索对由2, 5-呋喃二酮和苯乙烯聚合而成的物质进行结构修饰的聚合物

检索策略：

1. 先检索由2, 5-呋喃二酮和苯乙烯聚合而成的物质，获得CAS登记号
2. 主题检索相应的CAS登记号加D
3. 如果有具体的修饰要求，可在topic中直接加入相应的词，

   如：sulfonated xxxx-xx-xd，ester xxxx-xx-xd

聚合物的检索



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聚合物的检索

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Chemical Structure exact with limiters > substances (15)

REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush

REFERENCES: RESEARCH TOPIC

9011-13-6D

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

REFERENCES | Get Substances | Get Reactions | Get Related Citations | Tools | Create Keep Me Posted Alert | Send to SciPlanner

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Analyze by: Author Name

Konishi Kunihiko	24
Maeda Hiroshi	20
Yagi Norio	20
Chiba Takashi	19
Kitsunai Tomoyuki	18
Tong Wei	17
Kurokawa Kinya	16
Cao Min	15
Niimura Tetsuya	15
Sun Donghai	15

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0 of 2013 References Selected | Page: 1 of 101

1. **Lubricant composition comprising branched diesters and viscosity index improver**
   Quick View | PATENTPAK
   By Sanson, Julien; Champagne, Nicolas; Benard, Francois
   From PCT Int. Appl. (2017), WO 2017021332 A1 20170209. | Language: English, Database: CAPLUS
   The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

2. **Thermosetting adhesive sheet with excellent dimensional stability, adhesion, heat resistance, flexibility, electrical insulation, dielectric constant and dielectric loss tangent for protecting printed wiring board**
   Quick View | PATENTPAK
   By Sakaguchi, Takeshi; Ogiwara, Naoto; Tosaki, Koichi; Kishi, Hiromasa; Kobayashi, Hidenobu
   From Jpn. Tokkyo Koho (2017), JP 6074698 B1 20170208. | Language: Japanese, Database: CAPLUS
   Title sheet is formed from a thermosetting compn. comprising a resin A1, an organometallic compd. and a tri or more functional epoxy group-contg. compd., wherein the resin A1 does not have an epoxy group and has a reactive functional group capable of reacting with at least one of the organometallic compd. or epoxy group-contg. compd., a functional group except a reactive functional group and a functional group with a hetero atom except halogen, a resin A2 does not have a reactive functional group and has a functional group with a hetero atom except halogen, a resin A3 has neither a reactive fu...

3. **Lubricant composition comprising branched diesters and viscosity index improver**
   Quick View | PATENTPAK
   By Sanson, Julien; Champagne, Nicolas; Benard, Francois
   From Eur. Pat. Appl. (2017), EP 3124579 A1 20170201. | Language: English, Database: CAPLUS
   The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

4. **Thermosetting resin composition with excellent metal foil adhesiveness and dielectric and heat resistance properties for forming prepreg, laminated board and printed wiring board**
   Quick View | PATENTPAK
   By Yoshino, Hiroaki; Yanagida, Makoto
   From Jpn. Kokai Tokkyo Koho (2017), JP 2017019906 A 20170126. | Language: Japanese, Database: CAPLUS
   Title compn. comprises (A) a polyimide curing agent which is a polyimide compd. obtd. by reacting (a) a maleimide compd. having at least two N-substituted maleimide groups in one mol., (b) an aniline compd. having two arom. amino groups in one mol. and (c) an aminophenol compd. having one arom. amino group and at least one arom. hydroxyl group in one mol. in a mole ratio of [(a): (b) : (c)] 4.0: 0.1-1.0: 0.1-1.0, and having bonding degree of 7 calcd. from the formula: bonding degree = wt. av. mol. wt./charged av. mol.

聚合物的检索

1. Lubricant composition comprising branched diesters and viscosity index improver

By: Sanson, Julien; Champagne, Nicolas; Benard, Francois
Assignee: Total Marketing Services, Fr.

The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver. The invention refers to lubricant compns. comprising a specific diester together with a viscosity index improver.

Patent Information

Patent No.		Kind	Language	Date	Application No.	Date
WO 2017021332	PATENTPAK	A1		Feb 9, 2017	WO 2016-EP68229	Jul 29, 2016
EP 3124579	PATENTPAK	A1	English	Feb 1, 2017	EP 2015-179371	Jul 31, 2015

Priority Application

EP 2015-179371	A	Jul 31, 2015

Indexing

Fossil Fuels, Derivatives, and Related Products (Section51-8)

Concepts

Base oils
Lubricating oil additives
Crankcase oil
Transesterification

lubricant compn. comprising branched diesters and viscosity index improver

Polyolefins

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

Lubricating oil additives

viscosity improvers; lubricant compn. comprising branched diesters and viscosity index

Substances

78-79-5D Isoprene, polymers
106-99-0D Butadiene, polymers
9003-31-0D Polyisoprene, hydrogenated
9011-13-6D Styrene-maleic anhydride copolymer, esters
25038-32-8D Isoprene-styrene copolymer, hydrogenated

lubricant compn. comprising branched diesters and viscosity index improver

Modifier or additive use; Uses

64-18-6 Formic acid
124-07-2 Octanoic acid
143-07-7 Dodecanoic acid
157336-71-5
1627922-75-4

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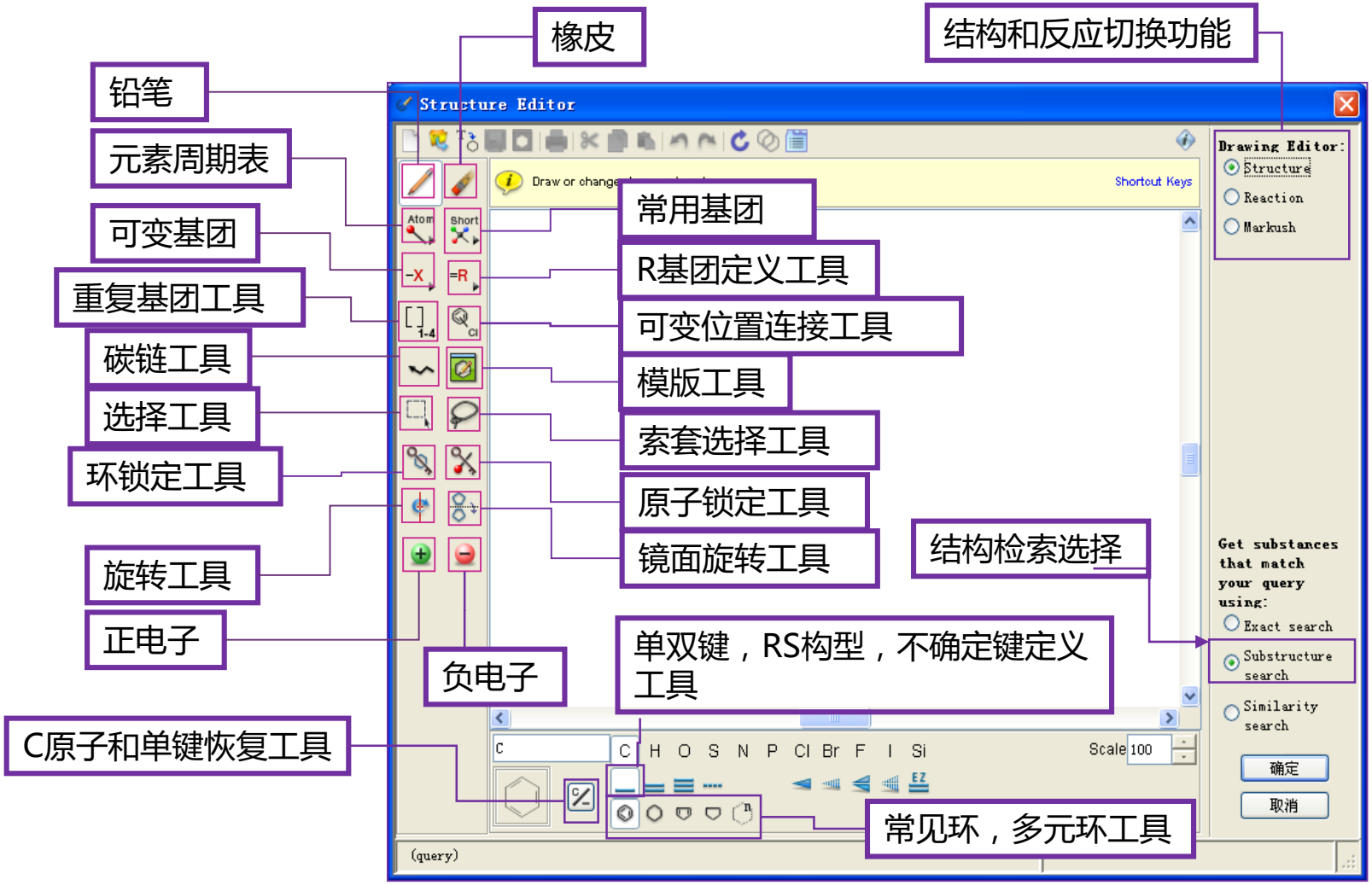
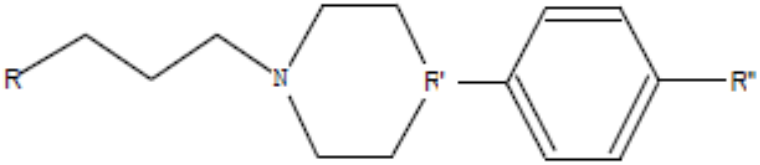
绘图面板


橡皮
结构和反应切换功能
铅笔
元素周期表
可变基团
重复基团工具
碳链工具
选择工具
环锁定工具
旋转工具
正电子
C原子和单键恢复工具
负电子
常用基团
R基团定义工具
可变位置连接工具
模版工具
索套选择工具
原子锁定工具
镜面旋转工具
结构检索选择
单双键，RS构型，不确定键定义工具
常见环，多元环工具
Structure Editor
Drawing Editor:
Structure
Reaction
Markush
Shortcut Keys
Get substances that match your query using:
Exact search
Substructure search
Similarity search
确定
取消
Scale 100
(query)

检索具有相同结构特征的物质

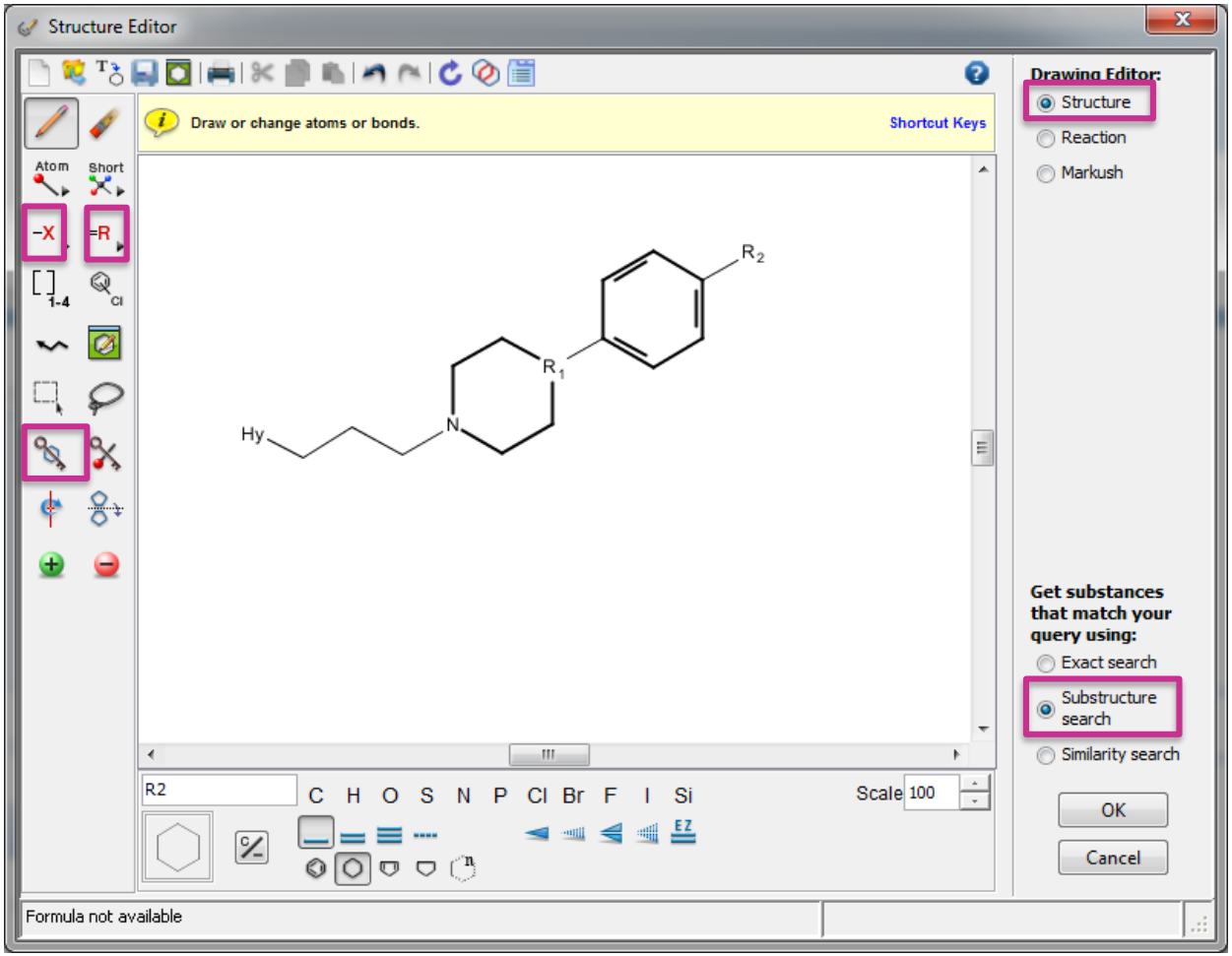
查询报道具有如下结构特征专利文献:



要求:

- R = 任意杂环
- R' = C, N, P
- R" = C,N
- 6 圆环均为单环
- 价键不饱和的地方均允许有取代

检索具有相同结构特征的物质



检索具有相同结构特征的物质

CAS Solutions

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Chemical Structure substructure > substances (3048)

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0 of 3048 Substances Selected | Page: 1 of 204

Analyze by: Substance Role

Preparation	1682
Biological Study	1523
Uses	1288
Reactant or Reagent	201
Analytical Study	86
Properties	70
Prophetic in Patents	41
Combinatorial Study	22
Process	3

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1. 1873376-11-4

$C_{27}H_{38}N_4O$

INDEX NAME NOT YET ASSIGNED

2. 1868051-25-5

Click to view detail

Absolute stereochemistry.

$C_{26}H_{26}FN_5O_4$

Benzamide, 4-[4-[(1*S*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

3. 1868051-24-4

Absolute stereochemistry.

$C_{26}H_{26}FN_5O_4$

Benzamide, 4-[4-[(1*R*)-3-(7-fluoro-1,2-dihydro-5-nitro-1-oxo-3-isoquinolinyl)-2-cyclopenten-1-yl]-1-piperazinyl]-*N*-methyl-

Key Physical Properties

4. 1868051-23-3

5. 1868051-22-2

6. 1868051-02-8

Markush检索

- 具体物质[Specific Substance]：

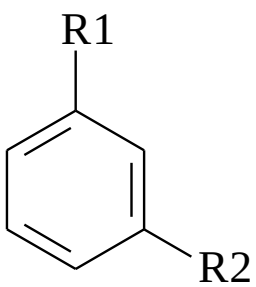
  — 以具体化学结构陈述的特定物质，会被分配CAS RN

- 预测性物质[Prophetic Substance]：

  — 使用Markush结构陈述的预测物质，一个Markush可以陈述上百或上千个化学物质

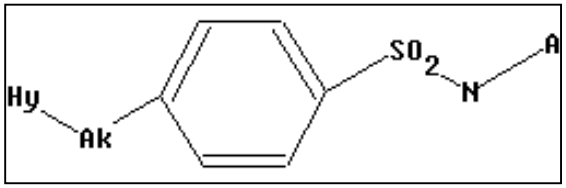
  — 专利中所陈述的预测物质，不会被分配CAS RN

  — Markush检索，能检索到通过结构检索检不到的专利

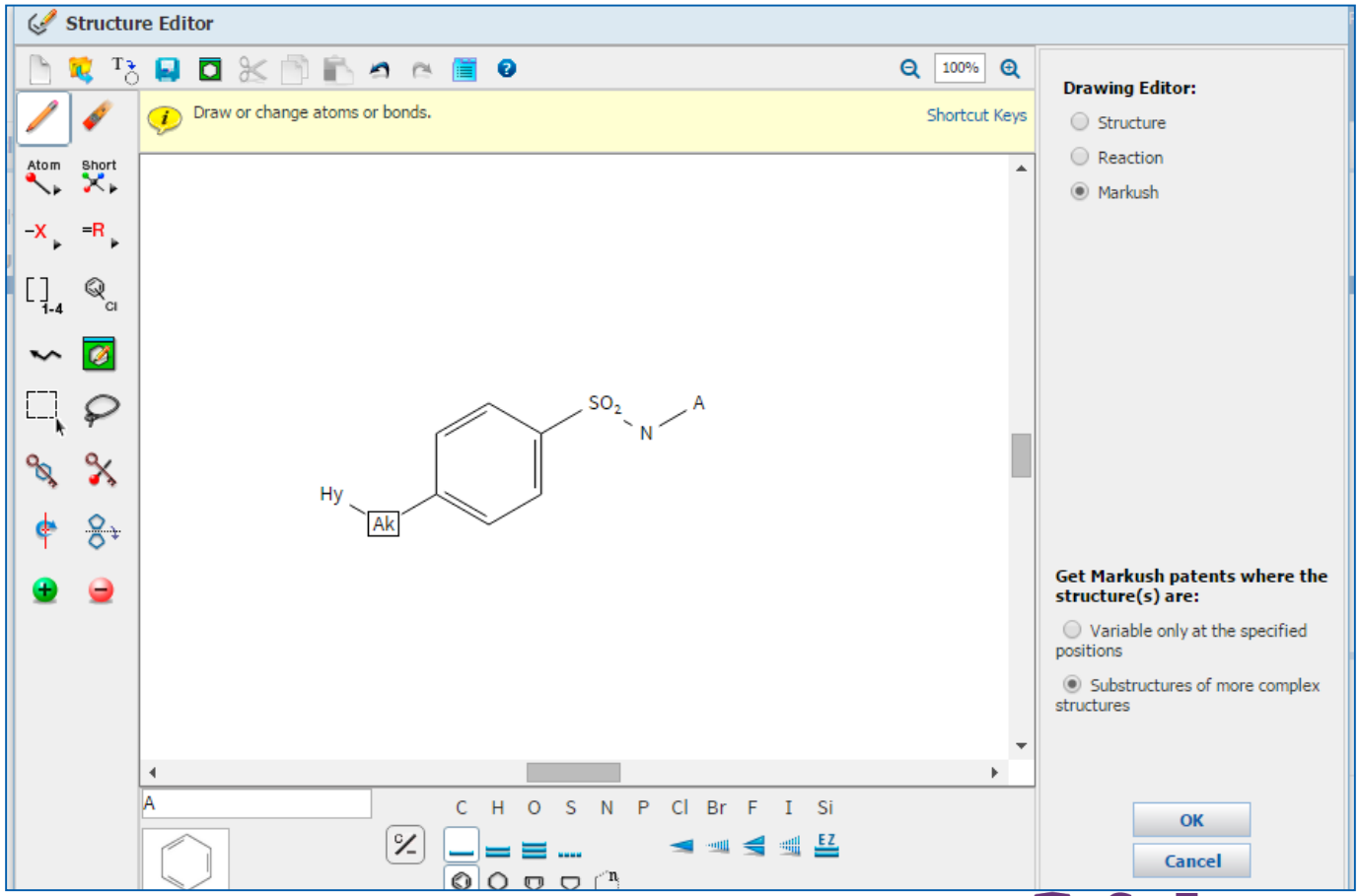


R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH_2–halogen, —CH(–CH_3)–halogen,



可用SciFinder中的Markush检索查看专利中化合物结构保护范围。



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Markush检索

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Markush substructure > **references (1969)** > Compounds and methods for anti...

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Analyze by:
Document Type ▾

Patent 1969

Journal 1

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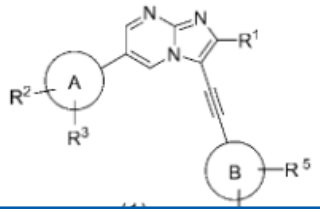
0 of 1969 References Selected | Page: 1 of 99

1. **Compounds and methods for anticoagulation therapy**
Quick View | PATENTPAK
By Allende Rodriguez, Mikel; Hermida Santos, Jose; Montes Diaz, Ramon; Oyarzabal Santamarina, Julen
From PCT Int. Appl. (2016), WO 2016120432 A1 20160804. | Language: English, Database: CAPLUS

The invention relates to certain compds. that are inducers of Heat shock 70 kDa protein 1A/1B (HSPA1A/B) and their use for anticoagulation therapy; and to a method for anticoagulation therapy that comprises the administration of one of these inducer compds. It has been here proved that induction of Heat shock 70 kDa protein 1A/1B by administration of one of these inducer compds. has antithrombotic effects without accelerating or altering bleeding time.

2. **Preparation of new imidazopyrimidine derivatives as negative allosteric modulators of metabotropic glutamate receptor subtype 2 (mGlu2 receptor)**
Quick View | PATENTPAK
By Urashima, Kuniko; Tojo, Kengo; Koike, Shoko; Masumoto, Shuji
From Jpn. Kokai Tokkyo Koho (2016), JP 2016132660 A 20160725. | Language: Japanese, Database: CAPLUS



The title imidazo[1,2-a]pyrimidine derivs. I [R^1 = H or halogen; ring A Ph or pyridyl; R^2, R^3 (same or different) = hydrogen, halogen, C_{1-4} alkyl or C_{1-4} alkoxy each optionally substituted with 1-5 halogen atoms; or in case where R^2 and R^3 are at the adjacent substitution position, R^2 and R^3 together with ring A form C_{5-8} carbocyclic ring (optionally substituted with 1-5 halogen or 1-2 hydroxy group) or 5- or 6-membered satd. heterocyclic ring; ring B = Ph or pyridyl; R^4, R^5 (same or different) = H, halogen, hydroxy, amino, $-C(O)OR^a$, $-C(O)NR^aR^b$, SO_3H, $SO_2NR^aR^b$, SO_2R^b, or $NR^aSO_2R^b$; R^a, R^b (same...

全部是专利

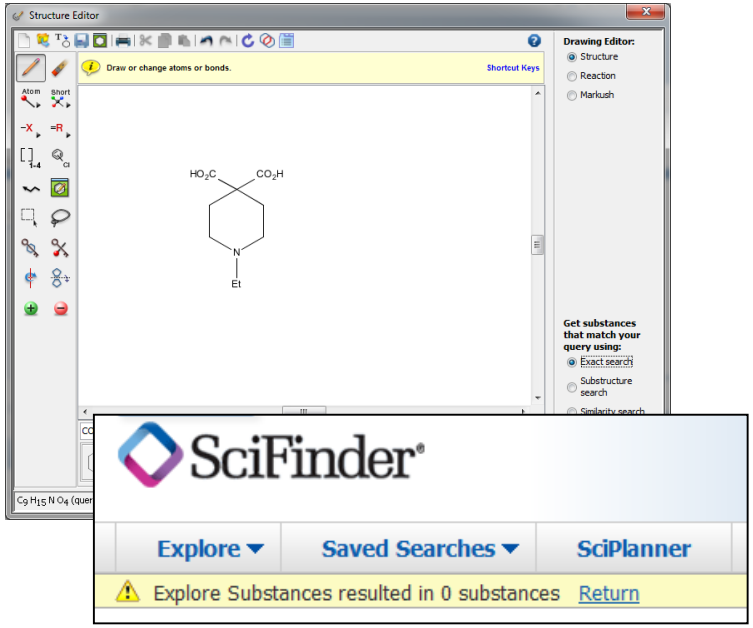
SciFinder A CAS SOLUTION

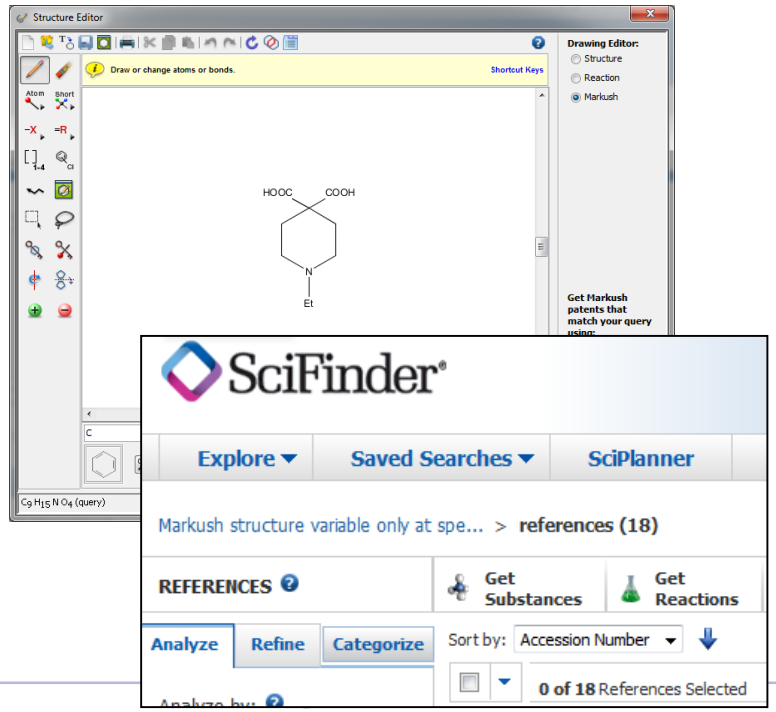
如何判断结构的新颖型

新颖性：是否存在？是否能申请专利？

SciFinder相关物质库：Registry和Marpat

检索方法：物质检索？Markush检索？





如何判断结构的新颖型

- SciFinder中的Markush检索仅仅只做初步的专利评估
- 尽量不要画具体结构进行检索
- 如果Markush检索结果为零，请对结构进行适当的扩展后再检索。
- 检索结果仍然为零，不代表一定没有被其他专利保护

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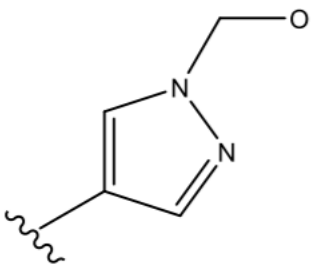
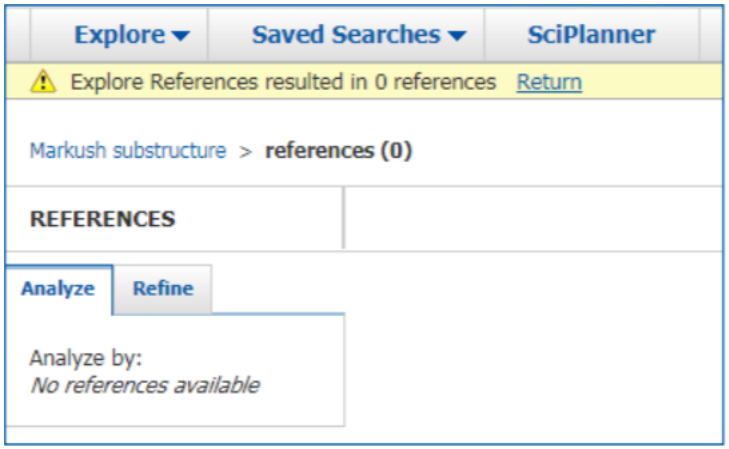
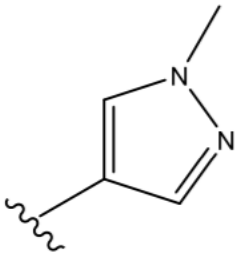
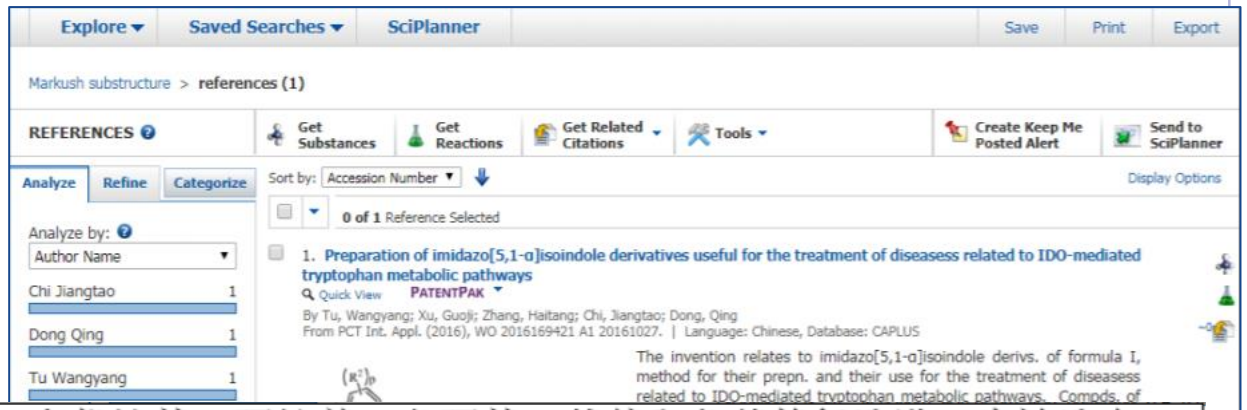
如何判断结构的新颖型









其中所述的烷基、卤代烷基、环烷基、杂环基、芳基和杂芳基任选进一步被选自烷基、卤代烷基、卤素、氨基、硝基、氰基、羟基、烷氧基、卤代烷氧基、羟烷基、环烷基、杂环基、芳基、杂芳基、$-R^a$、$-OR^7$、$-C(O)R^7$、$-C(O)OR^7$、$-S(O)_mR^7$、

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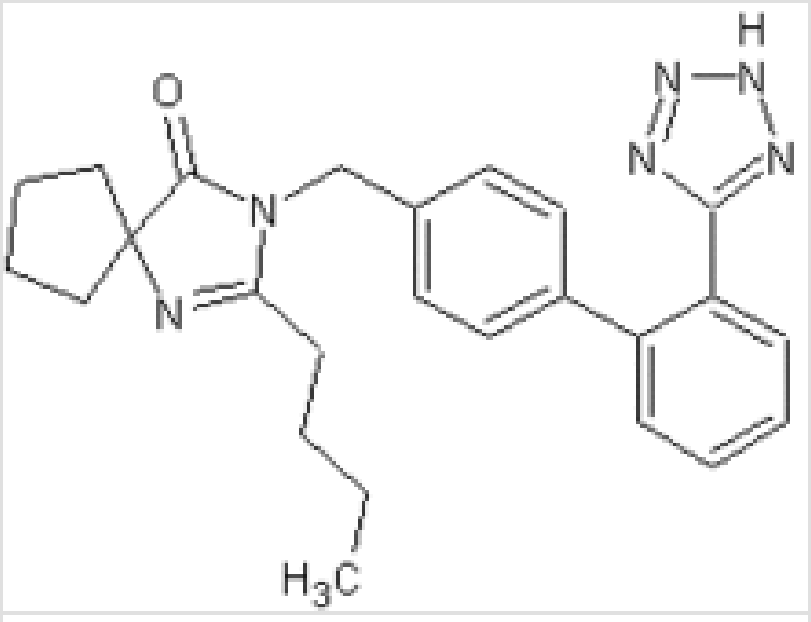
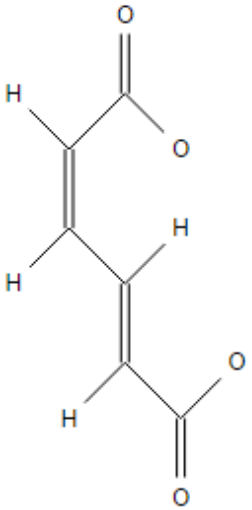
检索有同位素标记的物质



检索厄贝沙坦的氘代化合物

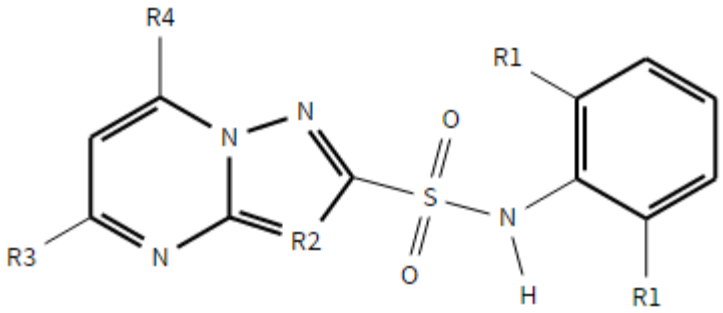
物质检索练习

- 检索Na2HPO4
- 检索由乙烯、1,3-丁二烯和第三个物质组成的聚合物
- 检索环上有以下结构特征的天然化合物



物质检索练习

- 找到包含如下物质的**所有**相关文献:



要求:

- R1 = X, H, -NO2, -CF3
- R2 = C 或 N
- R3 = 任意非氢原子
- R4 = 2-5个碳的碳链
- 结构中的环不发生稠环

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