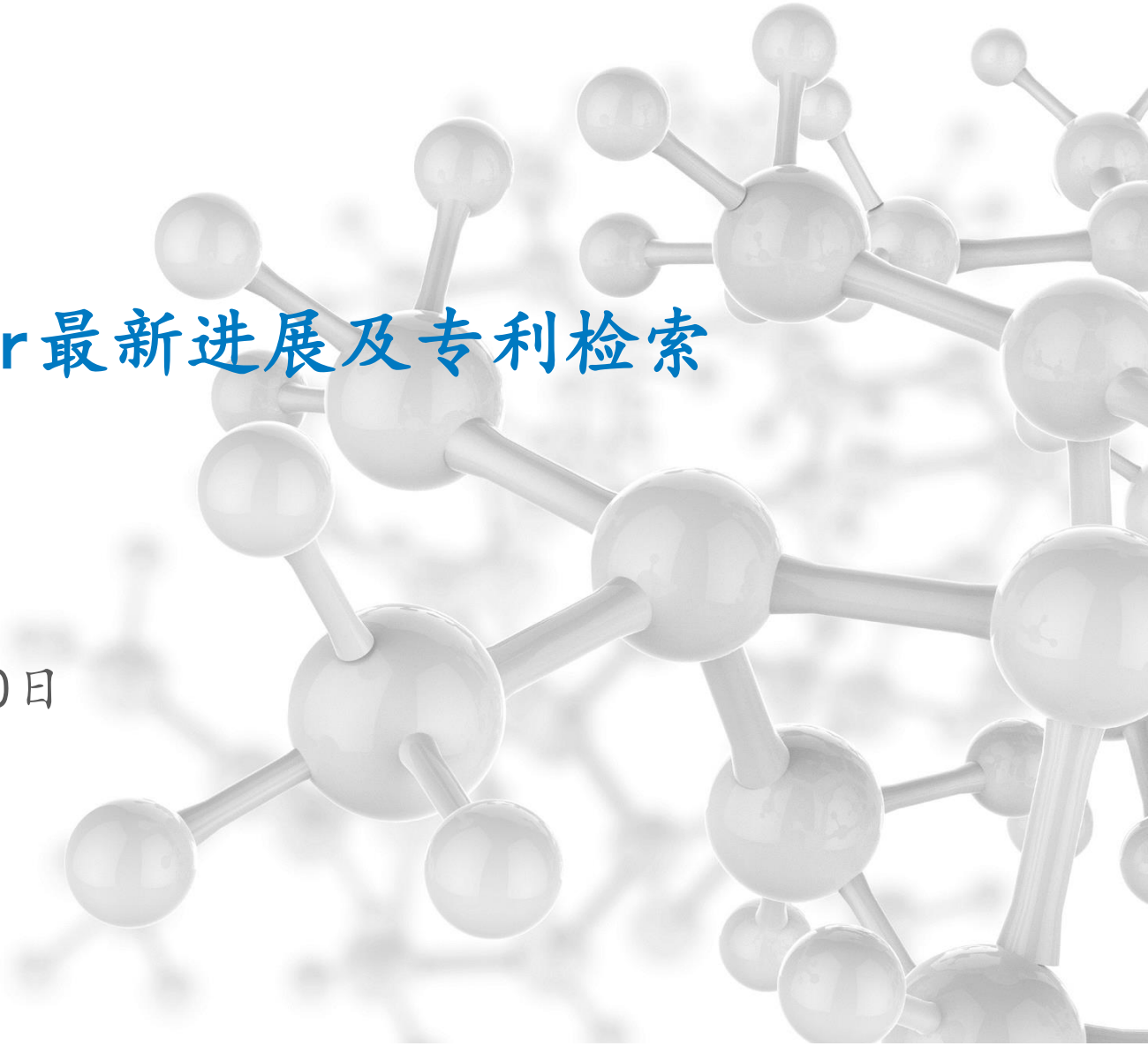

SciFinder最新进展及专利检索

2015年8月20日

议程

- SciFinder 2014-2015最新进展
- 专利检索举例

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- PatentPak – 专利工作流解决方案。即时获取专利中难以发现的化学信息及熟识语言专利族成员

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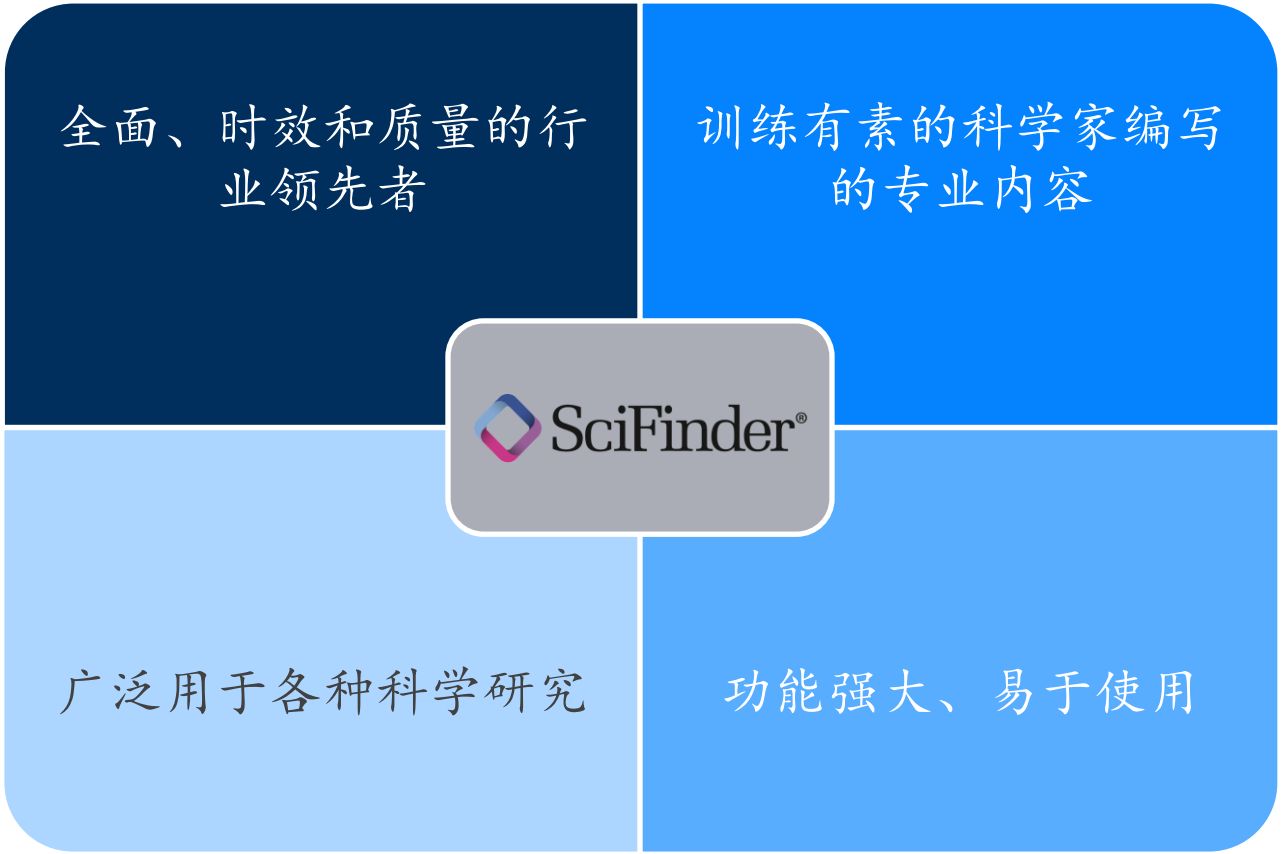

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- 可阅读性和用户体验都得到了改进

为用户提供最有价值的资源：时间

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    - 来自11个主要专利局的PDF专利全文
    - 多语言专利族PDF文件
    - 定位标引的重要化学物质所在专利页码
  - 在SciFinder中可直接使用

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  - 从ChemDraw的结构或反应无缝传输到SciFinder

- Analyze功能的改进
  - 对文献分析不再限制数量。互动分析条和Show More功能现在能分析任意多的文献量
  - 默认分析数量已经从1000条增加到20000条

PatentPak为用户检索和获取专利中关键化学信息节省时间

- 来自11个主要专利局的PDF专利全文
- 多语言的专利族PDF文件
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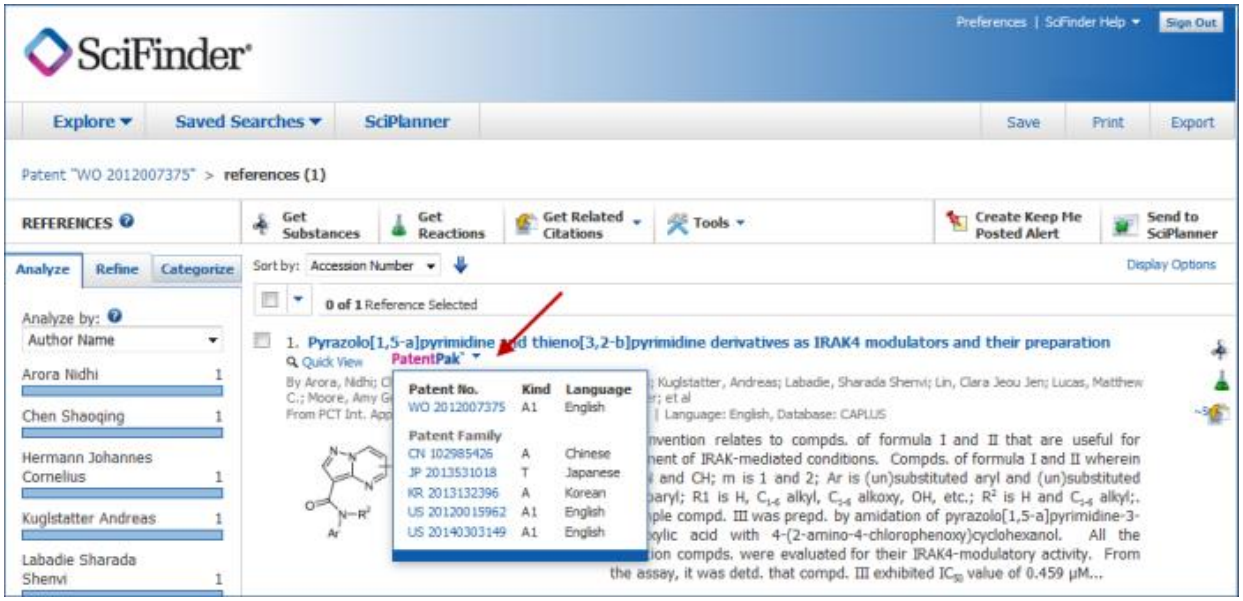

SciFinder 和 ChemDraw 整合

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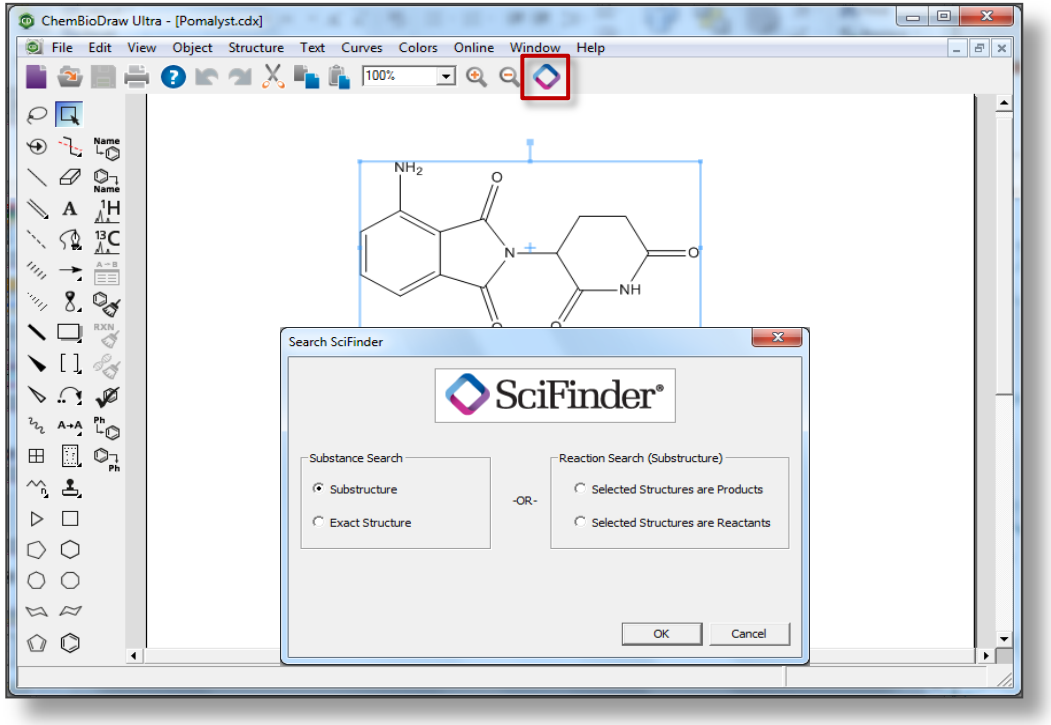
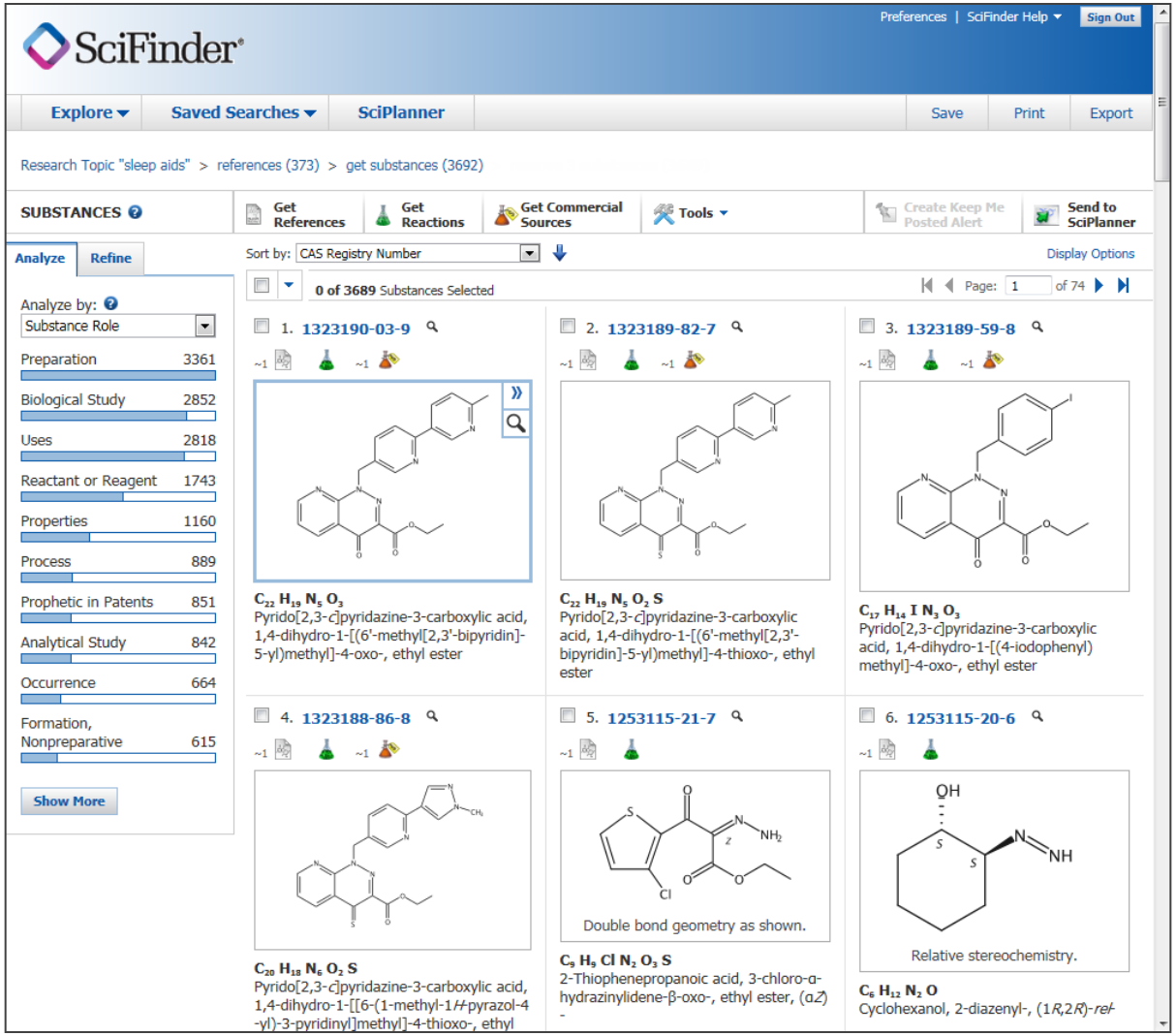


改进—Analyze功能

- 分析的文献数量不再有限制
  - 互动分析条和Show More功能可以分析任意数量的文献
- 默认分析数量也已经从1000条提高到了20000条



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- 经常被查询的商业信息会被置于答案集的前端
  - 供应商信息
  - 纯度
  - 规格
  - 库存状态
  - 运输信息
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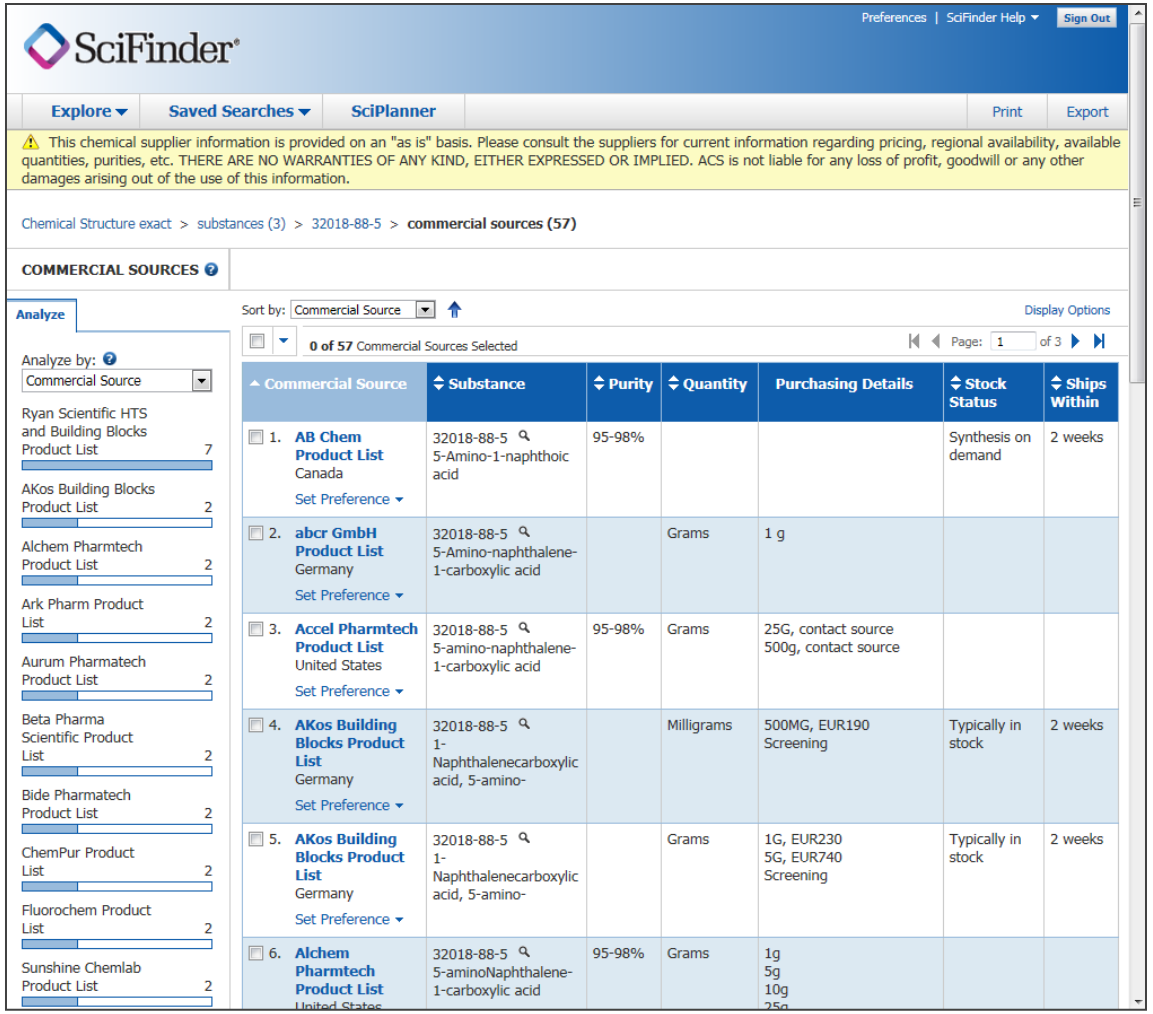
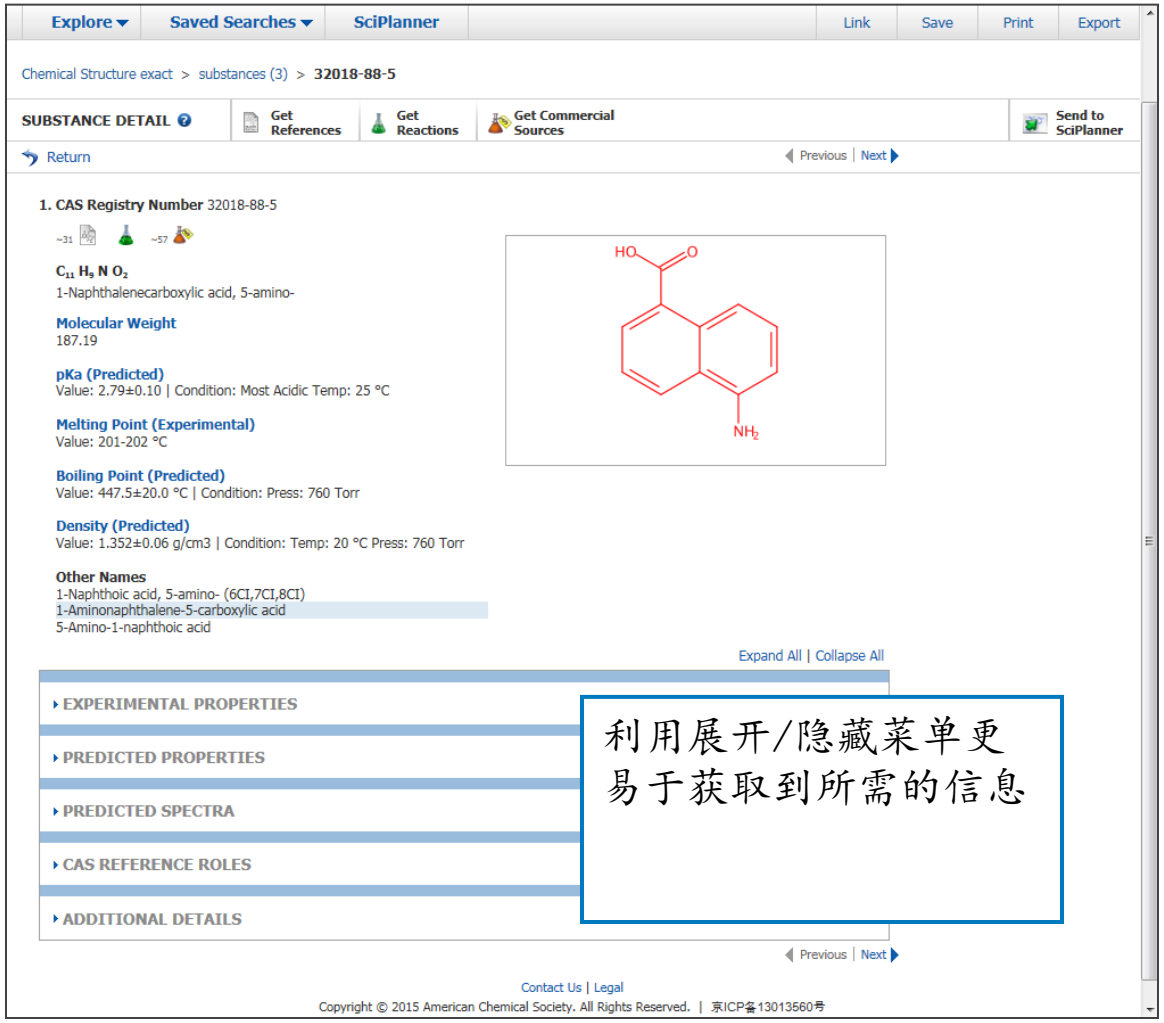


可阅读性和用户体验的改进

- 物质详情查看
  - 物理性质被置于显示页的顶端，便于快捷获取需要的物理性质数据
  - 展开/隐藏菜单便于快捷查找到自己需要的内容
  - 可自行勾选所需要的打印或导出的内容
- 更易于阅读的格式显示管制品信息，可快速定位感兴趣的内容
- 物质答案集展示
  - 管制信息、实验理化性质和图谱信息都以链接形式呈现
  - 在商业来源图标旁显示了供应商数量

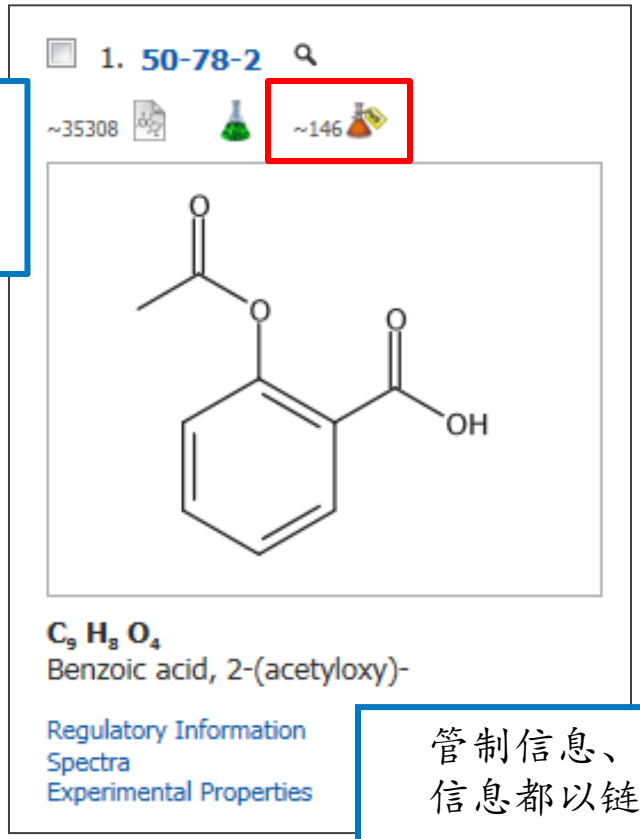
物质详情显示页排列的改进提高了结果可读性

- 常用的物理性质被置于显示页的顶端，用户更易于获取所需的信息
- 可勾选需要打印或导出的内容



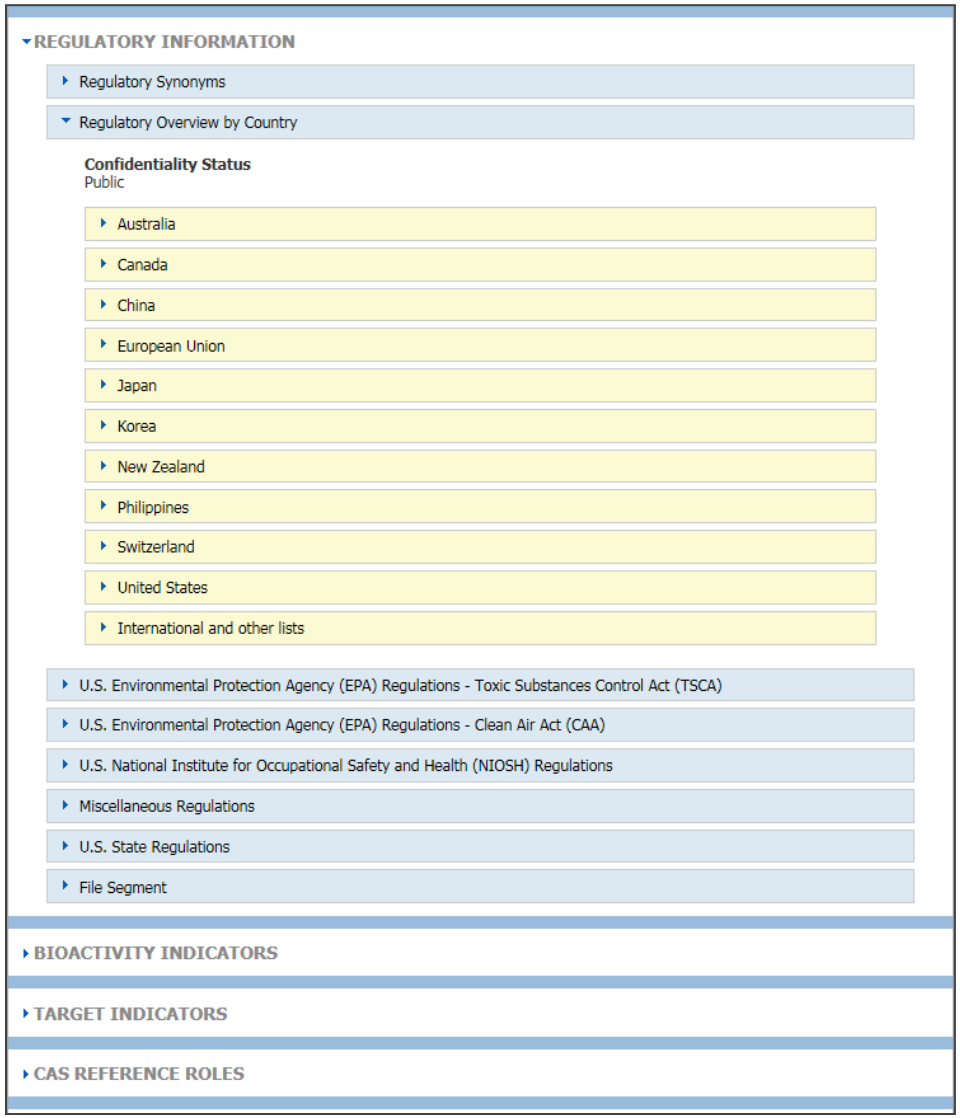
显示物质

商业来源图标包括了供应商数量



管制信息、实验理化性质和图谱信息都以链接形式呈现

管制信息显示格式的改进，更便于用户快速获取所需信息，甚至可以直接按照国家进行获取



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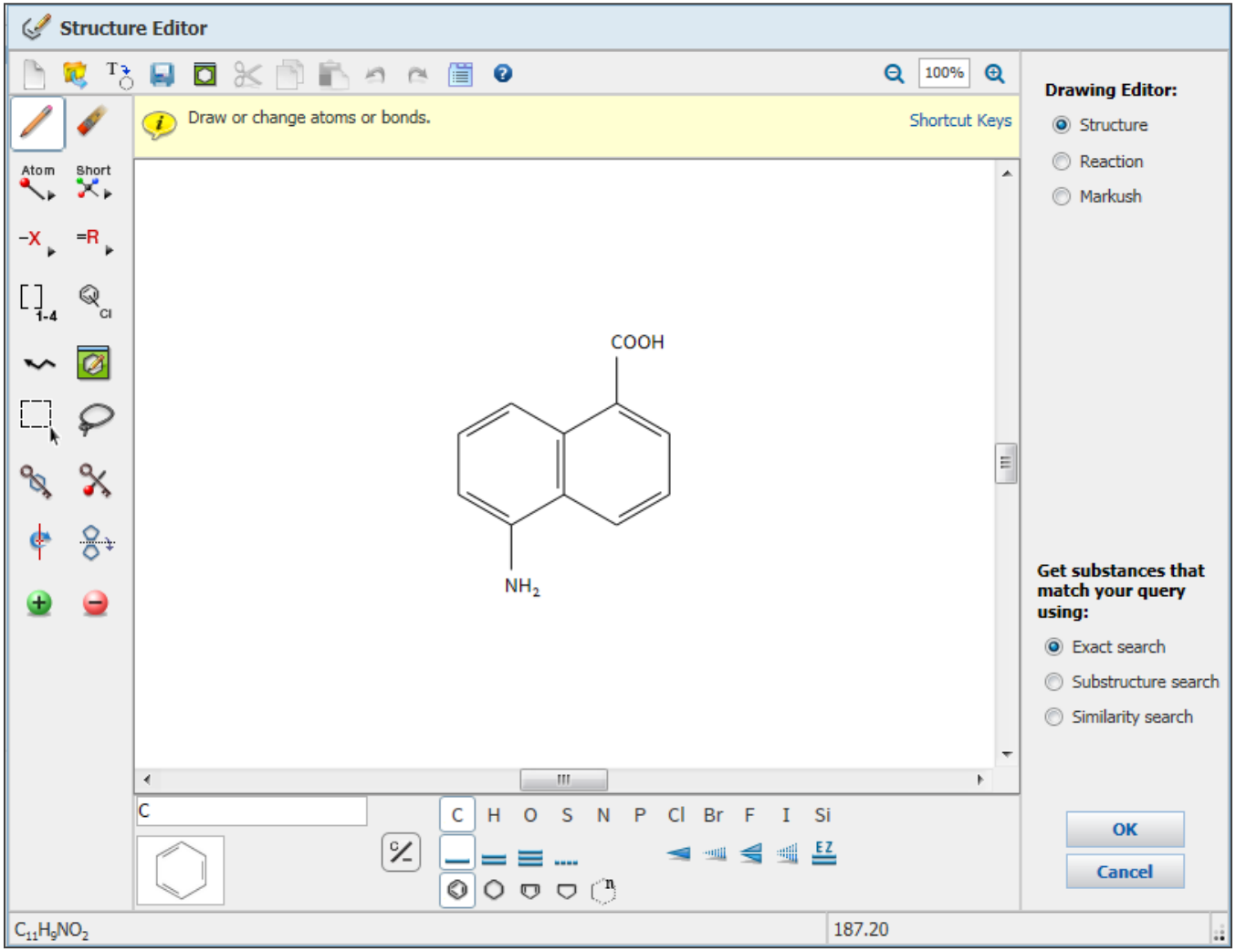

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CAS科学家理解并人工标引文献，使化学信息更易被发现

Source Selection

Title

Process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)$_3$P as a ligand as an electroluminescence source for display devices

Bibliographic Information

Inventor: Nakashima, Harue; Kawakami, Sachiko
Patent Assignee: Semiconductor Energy Laboratory Co., Ltd., Japan (JP)
Source: PCT Int. Appl. pp. 21 *In English*
CODEN: PIXXD2

Abstract

A process for the synthesis of secondary amines is presented via condensation of aniline with an aryl halide using palladium as a catalyst and (t-Bu)$_3$P as a ligand in the key step. Thus, N-(4-diphenylamino)phenylaniline is synthesized in 42% yield by condensation of N,N-diphenyl-N-(4-bromophenyl)amine with aniline. The process avoids protecting groups though the use of a palladium catalyst and (t-Bu)$_3$P as a ligand. N-(4-diphenylamino)phenylaniline can be used as an electroluminescence source for display devices including a light-emitting diodes, flat panel displays, liq. crystal display devices (no data).

Indexing

Index Terms:

19606-98-5P
Device Component Use (DEV) Industrial Manufacture (IMF) Preparation (PREP) Synthetic Preparation (SPN) Uses (USES)
(process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)$_3$P as a ligand to be used as an electroluminescence source for display devices)

29344-72-7P
36809-26-4P
Industrial Manufacture (IMF) Preparation (PREP) Reactant (RCT) Reactant or Reagent (RACT) Synthetic Preparation (SPN)
(process for synthesis of substituted secondary amines via condensation of aniline with aryl halides with a palladium catalyst and (t-Bu)$_3$P as a ligand to be used as an electroluminescence source for display devices)

Authority Processing

(54) Title: METHOD FOR

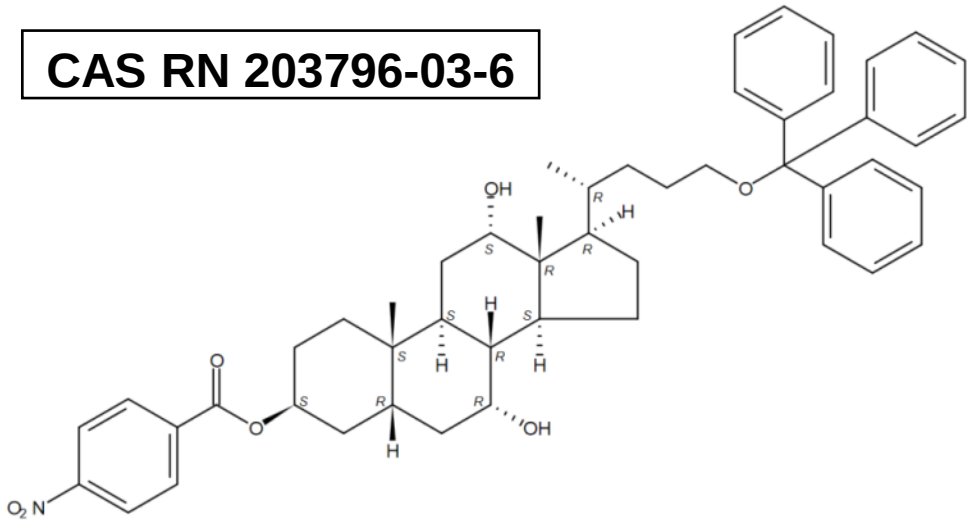
(57) Abstract: One embo... reaction of aniline with aryl...

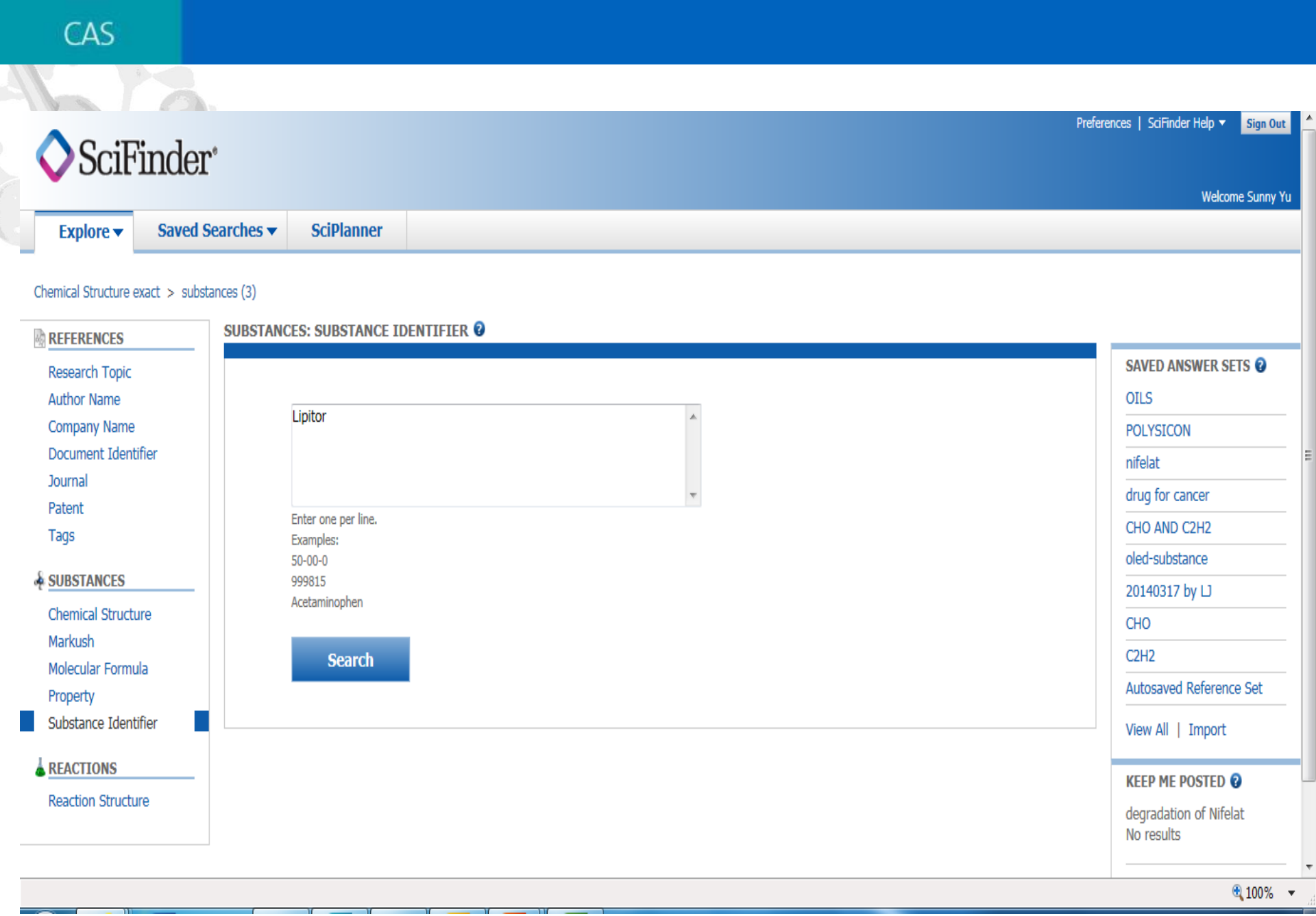
...e by the

该处披露了详细的标引过程，如文中容易被遗漏的结构信息

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste. Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding $NaHCO_3$ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na_2SO_4. The desired product (2.72 g, 85% yield) was obtained as white powder after SiO_2 chromatography (Et2 O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529,1489, 1448, 1345 cm^{-1} ; ^{1}H
8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H
(bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2
Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multip
(d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); ^{13}C NMR ($CDCl_3$, 75 M
144.70, 136.79, 130.77, 128.88, 127.86, 126.98, 123.70,
64.22, 47.79, 46.79, 42.15, 39.76, 37.47, 35.52, 35.34, 3
28.74, 27.71, 26.85, 26.30, 25.16, 23.41, 17.98, 12.77; H
(thioglycerol+Na^+ matrix) m/e: ([M+Na]$^+$) 808.4203 (53

CAS RN 203796-03-6

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(Component: 134523-00-5)

~1,626 ~154

$C_{33}H_{35}FN_2O_5 \cdot {}^1/_2Ca$

1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), (β*R*,δ*R*)-

Other Names

1*H*-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1), [*R*-(*R**,*R**)]-

Atocor

Atoraz

Atorvastatin calcium

Atorvastatin hemicalcium

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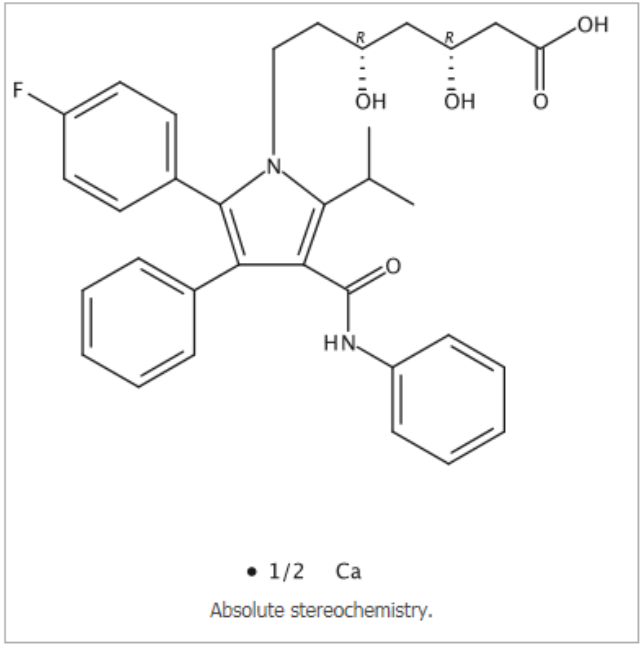

Absolute stereochemistry.

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▸ EXPERIMENTAL SPECTRA

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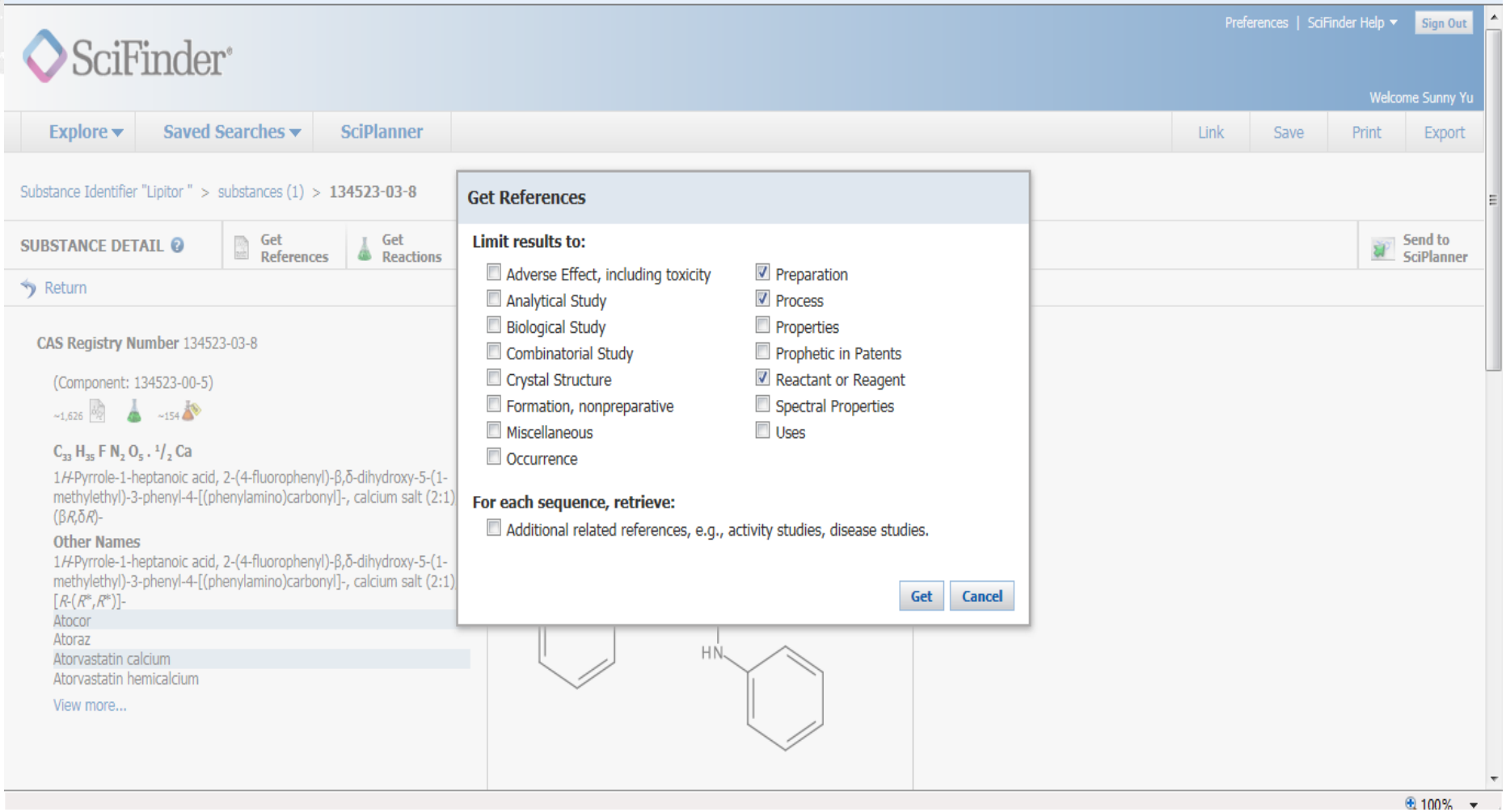
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CAS Registry Number 134523-03-8
(Component: 134523-00-5)
~1,626
~154
C33 H35 F N2 O5 . 1/2 Ca
1H-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1) (βR,δR)-
Other Names
1H-Pyrrole-1-heptanoic acid, 2-(4-fluorophenyl)-β,δ-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-, calcium salt (2:1) [R-(R*,R*)]-
Atocor
Atoraz
Atorvastatin calcium
Atorvastatin hemicalcium
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Analytical Study
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- [x] Patent
- [ ] Preprint
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- [ ] Review

Refine

1. **Oral pharmaceutical compositions for use in dyslipidemias**
Quick View | PatentPak

By Barranco Hernandez, Gustavo; Senosiain Pelaez, Juan Pablo; Garcia-Salgado Lopez, Enrique Raul; Luna Guiza, Maria del Coral
From Mex. Pat. Appl. (2014), MX 2013006332 A 20141219. | Language: Spanish, Database: CAPLUS

The invention relates to a solid oral pharmaceutical compn. contg. a statin and another antilipidemic agent, to a method for the prodn. of said compn., and to the use of said combination for producing a pharmaceutical formulation that can be used to treat metabolic syndrome, type II diabetes, or other diseases. The invention further relates to the use of a pharmaceutical combination formed by atorvastatin and fenofibrate, for producing a medicament that can be used to increase the levels of HDL2a and HDL2b, and to reduce the levels of HDL3a, HDL3b and HDL3c.

2. **Simple and rapid method for preparation of atorvastatin hemi-calcium**
Quick View | PatentPak

By Duan, Yuqiang; Wang, Liye; Jia, Yuxiang; Luo, Ming
From Faming Zhuanli Shenqing (2015), CN 104447487 A 20150325. | Language: Chinese, Database: CAPLUS

The present invention discloses a method of atorvastatin hemi-calcium prepn., which consists of six steps to obtain atorvastatin hemi-calcium pure product. The special thing is that on the one hand the hydrolysis of atorvastatin ester and transformation into calcium salt are simultaneously carried out in one step in one-pot, on another aspect obtained crude atorvastatin hemi-calcium can be purified by heat refluxing in Et acetate, Pr acetate, or Bu acetate, cooling, and crystn. The present invention simplifies the process steps, shortens the reaction time, makes the reaction more thorough, c...

3. **An improved kilogram-scale preparation of atorvastatin calcium**
Quick View | Other Sources

By Novozhilov, Yuri V.; Dorogov, Mikhail V.; Blumina, Maria V.; Smirnov, Alexey V.; Krasavin, Mikhail
From Chemistry Central Journal (2015), 9, 7. | Language: English, Database: CAPLUS

A high-yielding synthesis of atorvastatin calcium salt on 7 kg scale is developed, that affords >99.5% product purities by introducing the following key improvements: i. isolating the pure product of the ketal deprotection step as cryst. solid, and ii. using a convenient Et acetate extn. procedure to isolate the pure atorvastatin calcium at the ester hydrolysis and counter-ion exchange step.

4. **Preparation of atorvastatin derivatives**
Quick View | PatentPak

By Wu, Fanhong; Wang, Zhonghua; Li, Bing; Yu, Xiaodong; Wu, Fulong; Zhu, Yanghin; Li, Yuanmei

100%

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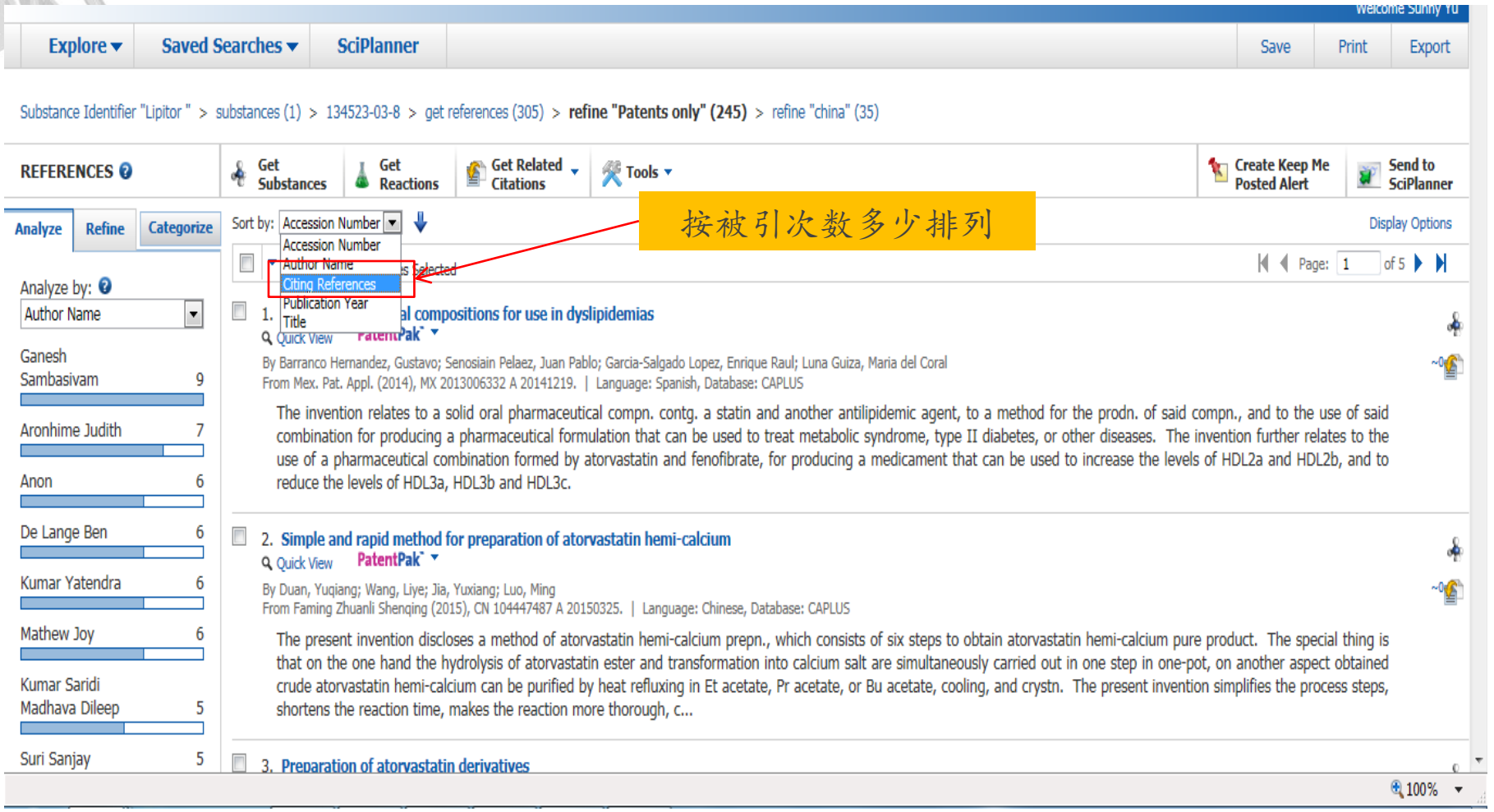
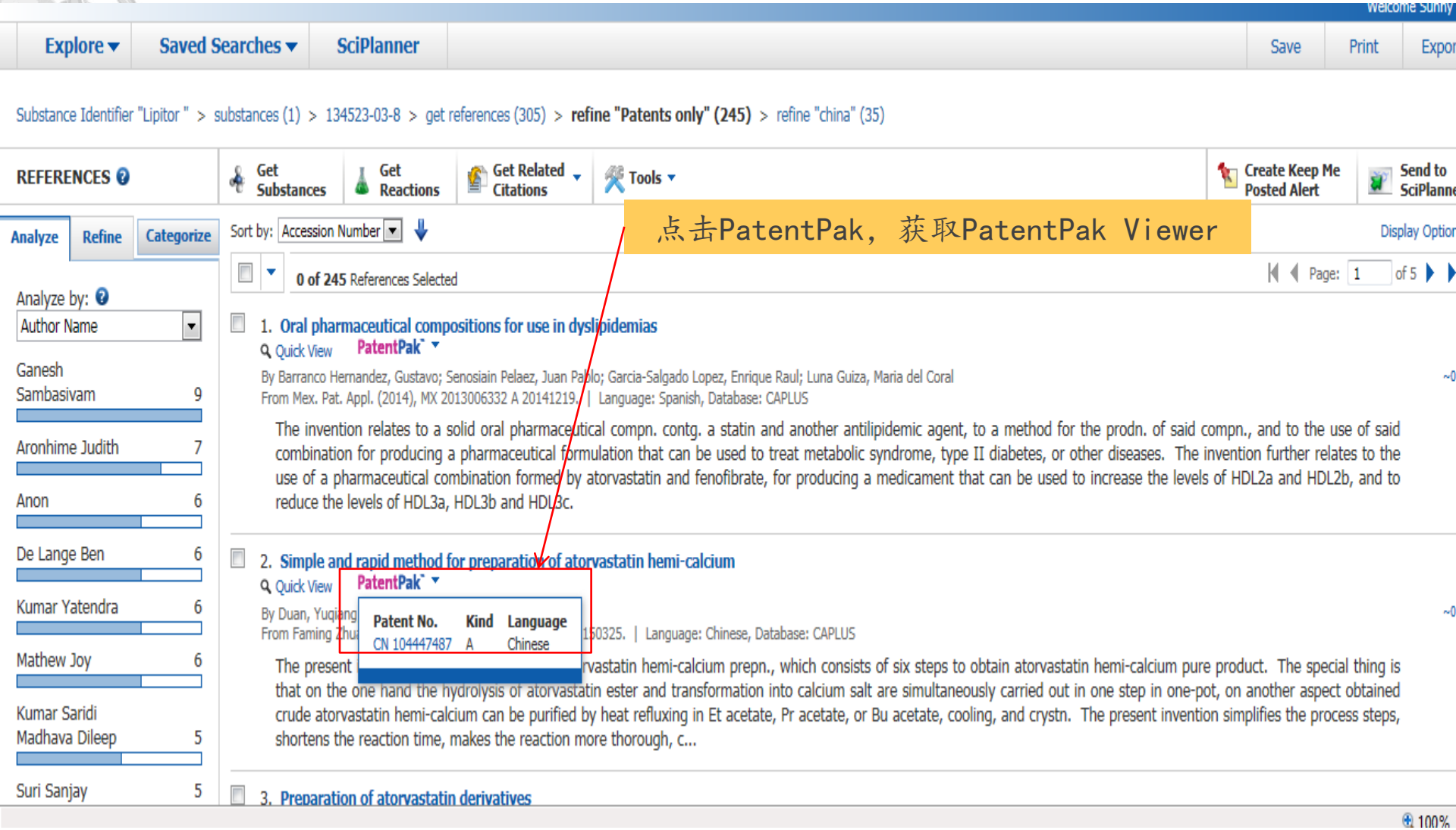


CAS

PatentPak—专利工作流程解决方案



PatentPak—专利工作流程解决方案

PatentPak—专利工作流程解决方案

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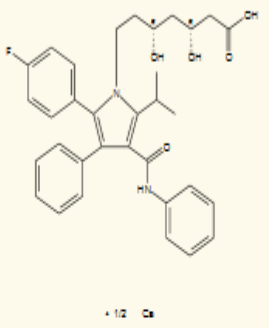
Key Substances in Patent

CAS RN 134523-03-8



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Analyst Markup Location

page 4

CAS RN 1305-62-0

HO—Ca—OH

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Analyst Markup Location

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CAS RN 134395-00-9

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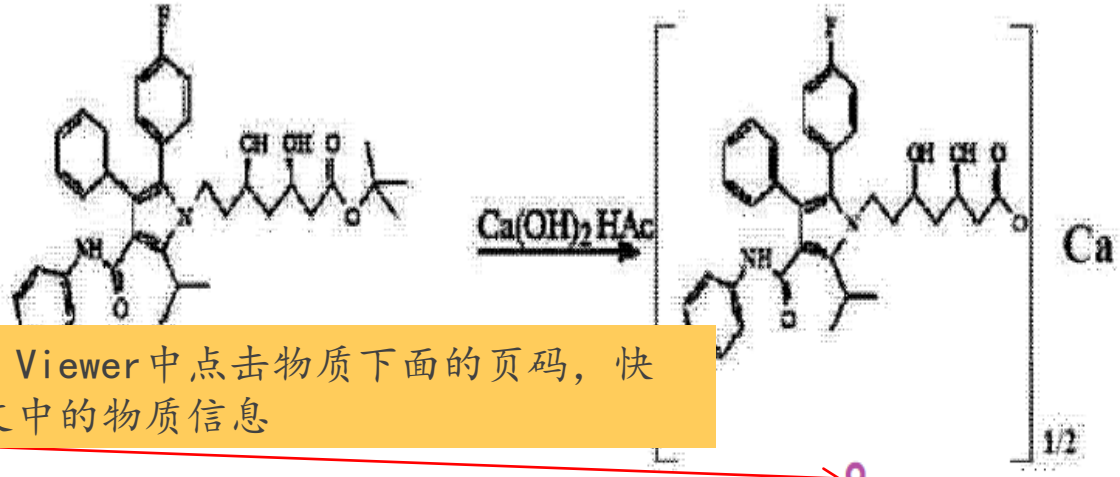
[0015] 下面结合实施例对本发明做详细说明，而不是限定本发明的保护范围。

[0016] 本发明的合成路线如下：



实施例 1

向反应瓶中加入 100 ml 水、15ml 乙醇、20 g R-(R*,R*)-2-(4-氟基苯)-β，δ-二羟基-5-(1-异丙基)-3-苯基-4-〔(苯胺)羰基〕-1H-吡咯-1-庚酸叔丁酯(0.03mol)以及 4 g 氢氧化钙(0.10mol)，将混合物搅拌并加热混合物至 45℃，然后继续搅拌并向混合物中滴加 5g(0.08mol)醋酸，用 HPLC 跟踪反应，7 小时左右反应即可进行完毕。反应结束后，

njay 5

3. Preparation of atorvastatin derivatives

PatentPak—专利工作流程解决方案

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Key Substances in Patent

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page 4

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HO—Ca—OH

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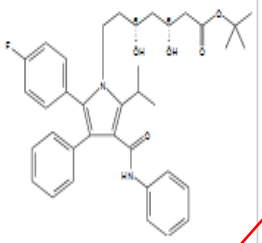

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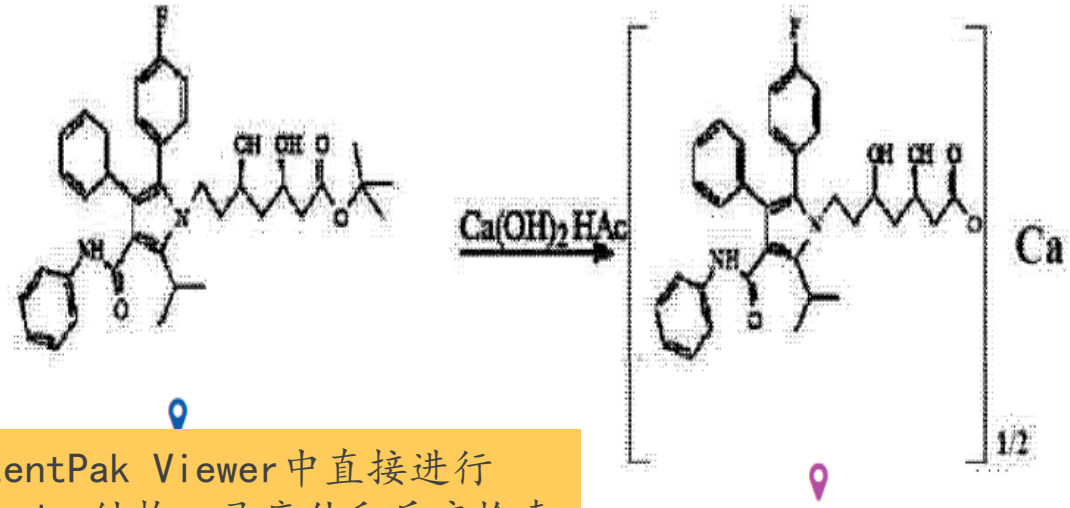
Structure
Markush
Reactions

[0015] 下面结合实施例对本发明做详细说明，而不是限定本发明的保护范围。

[0016] 本发明的合成路线如下：



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实施例 1

向反应瓶中加入 100 ml 水、15ml 乙醇、20 g R-(R*,R*)-2-(4-氟基苯)-β，δ-二羟基-5-(1-异丙基)-3-苯基-4-〔(苯胺)羰基〕-1H-吡咯-1-庚酸叔丁酯(0.03mol)以及 4 g 氢氧化钙(0.10mol)，将混合物搅拌并加热混合物至 45℃，然后继续搅拌并向混合物中滴加 5g(0.08mol)醋酸，用 HPLC 跟踪反应，7 小时左右反应即可进行完毕。反应结束后，

3. Preparation of atorvastatin derivatives

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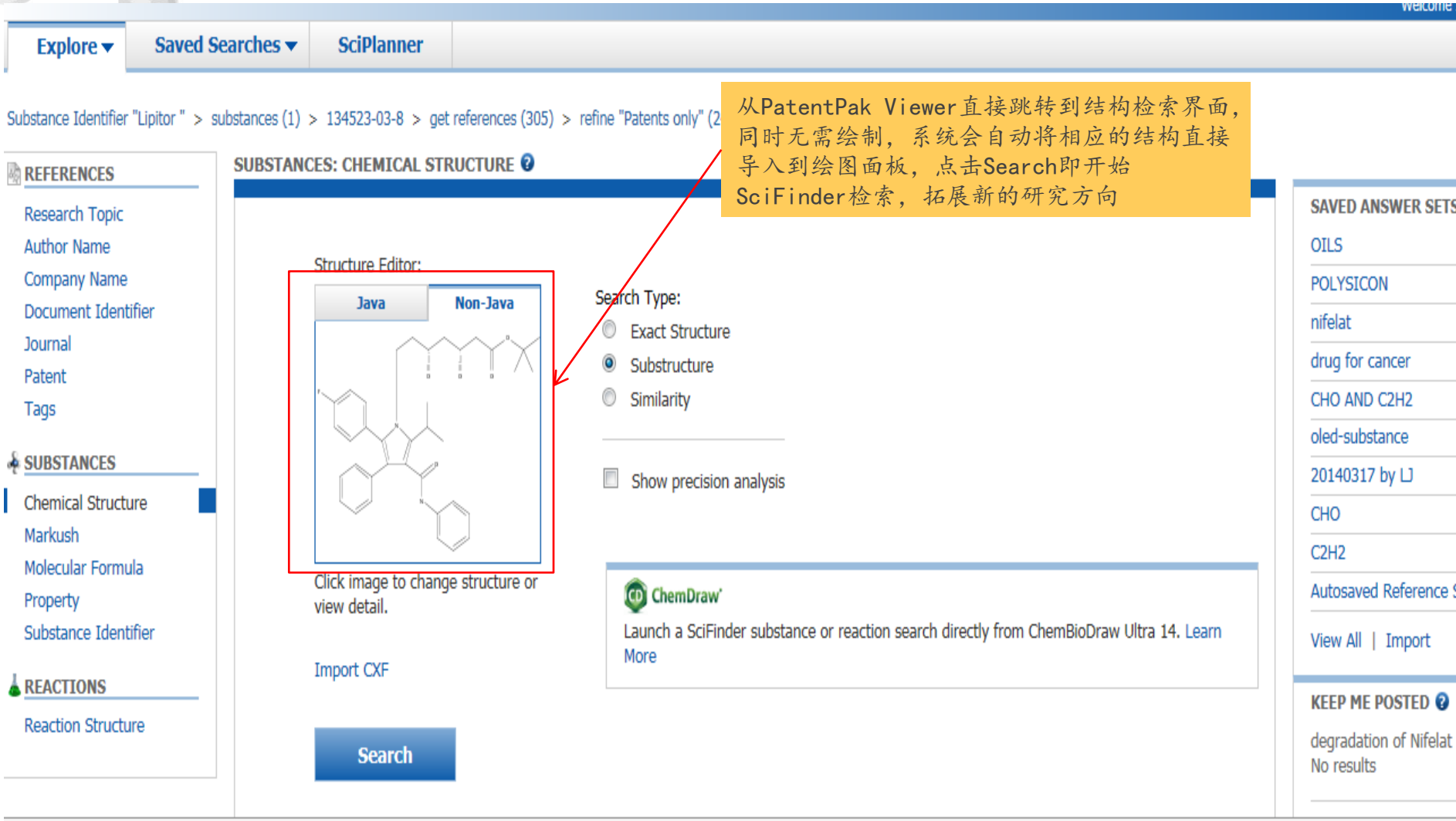
PatentPak—专利工作流程解决方案



议程

- SciFinder® 2014-2015最新进展
- 专利检索举例

--获取立普妥合成、制备最具影响力的专利文献

--如何从结构式出发获取完整的专利文献

在专利中表示物质的方式

- 确定物质[Specific Substance]:
  - 以确定的化学结构所表示的物质
- 预测性物质[Prophetic Substance]:
  - 使用Markush结构表示的预测物质，一个Markush可以表示上百或上千个化学物质

专利中的确定物质[Specific Substance]

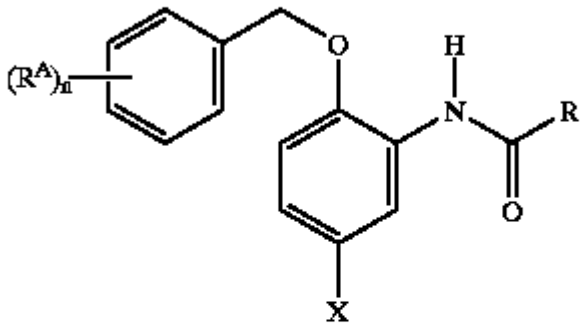
- 在专利权利要求书(claim)中所描述的确定化学物质会被Registry数据库收录
- 对于专利中其他确定物质，只有有充分的证据证明此物质存在，（有详尽的实验数据，一般为实施例中的物质），才会被Registry收录

专利中所收录的预测性物质1

(57) **ABSTRACT**

Disclosed is a compound comprising a 2-benzyloxy-5-haloacylanilide having the structural formula I:

Formula I



wherein

R is hydrogen or an alkyl group,

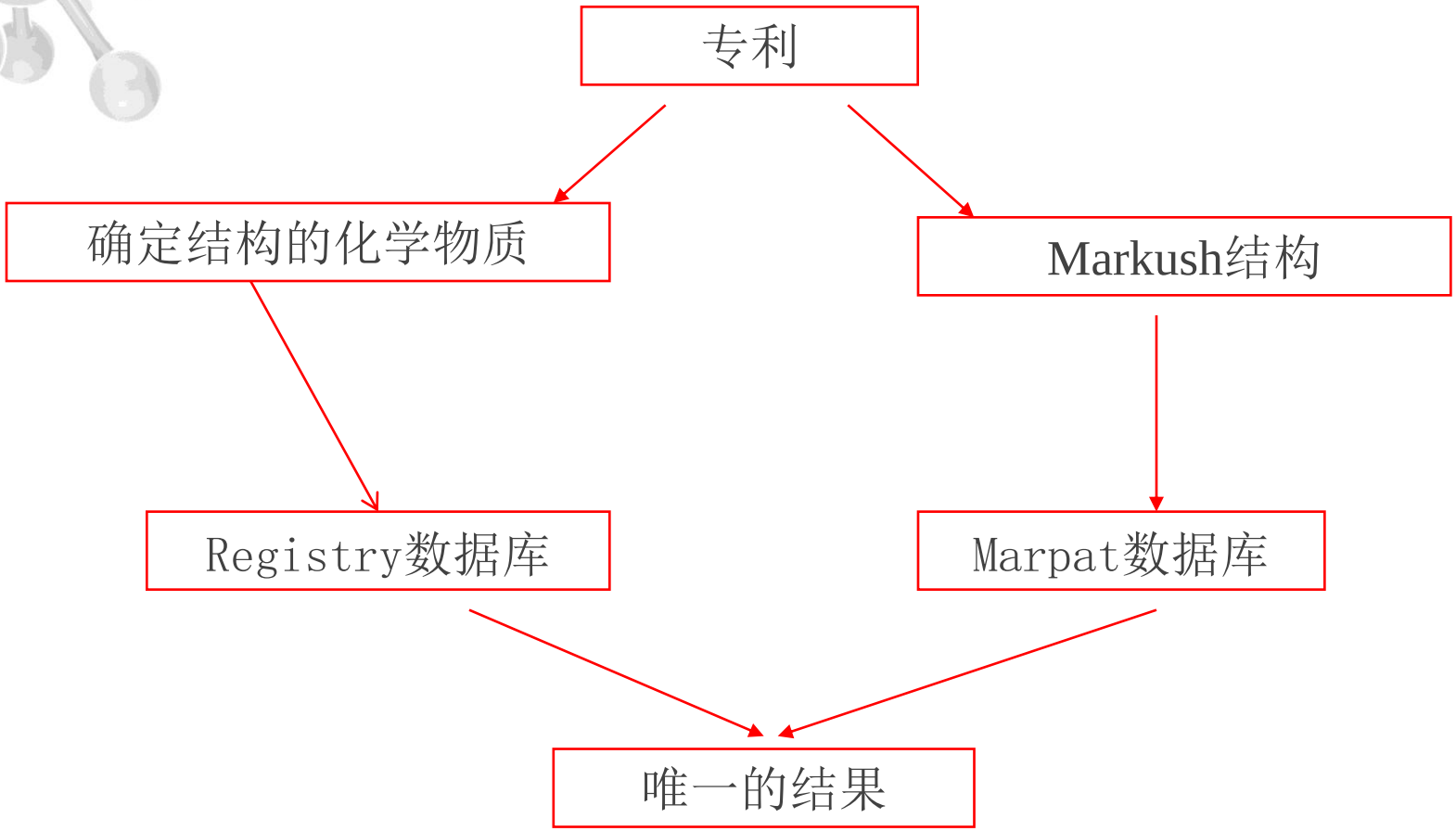
R^A is a substituent and n is 0–5; and

X is a halogen.

Also disclosed is a method for preparing a coupler using the compound. The compound and method simplify the preparation of photographic couplers.

5 Claims, No Drawings

获取完整化合物文献信息途径



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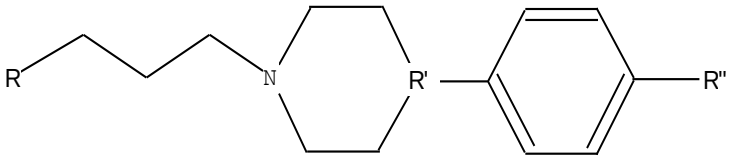
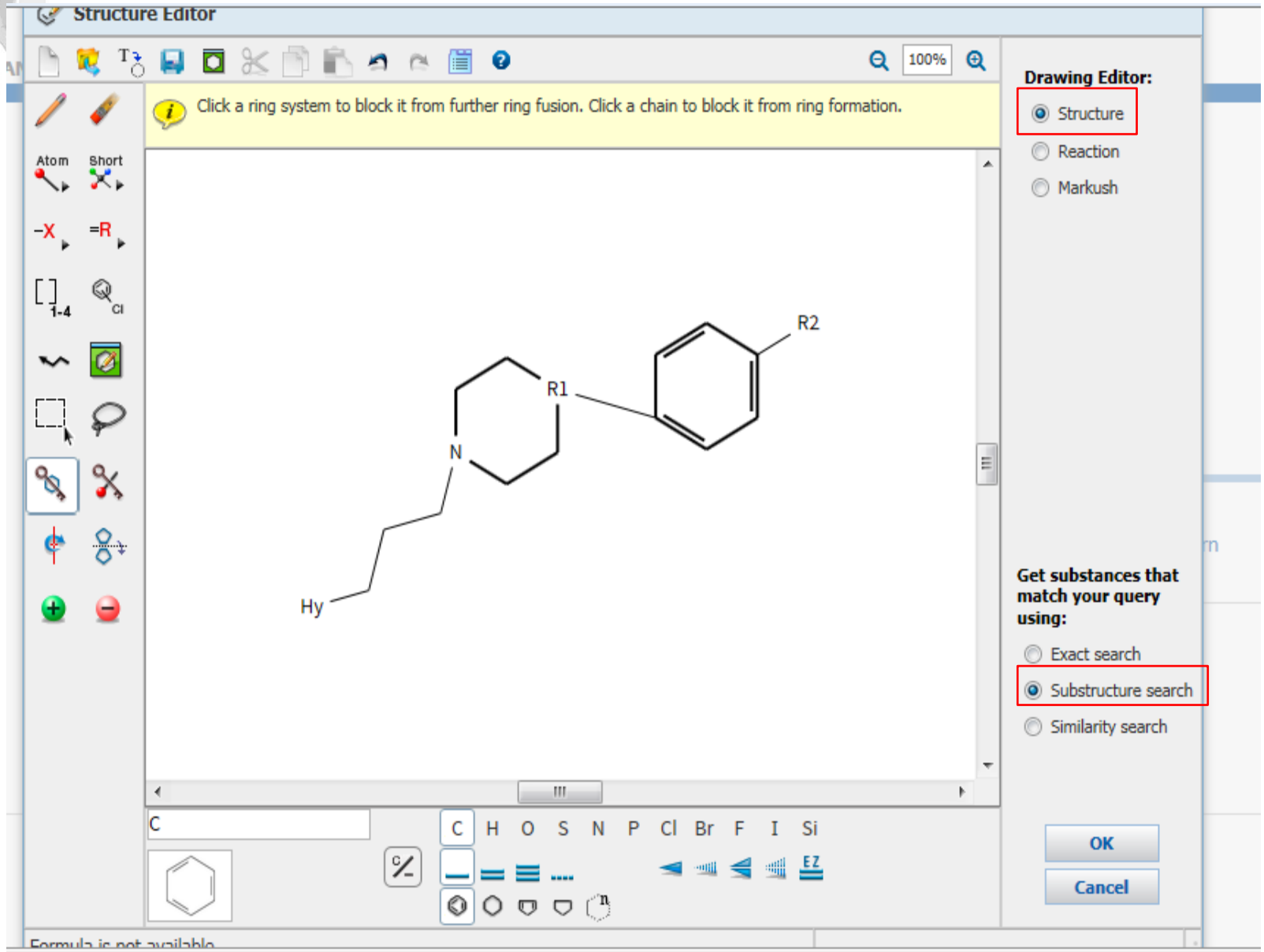


要求:

- 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

绘制结构，并检索文献中报道的确定结构的物质



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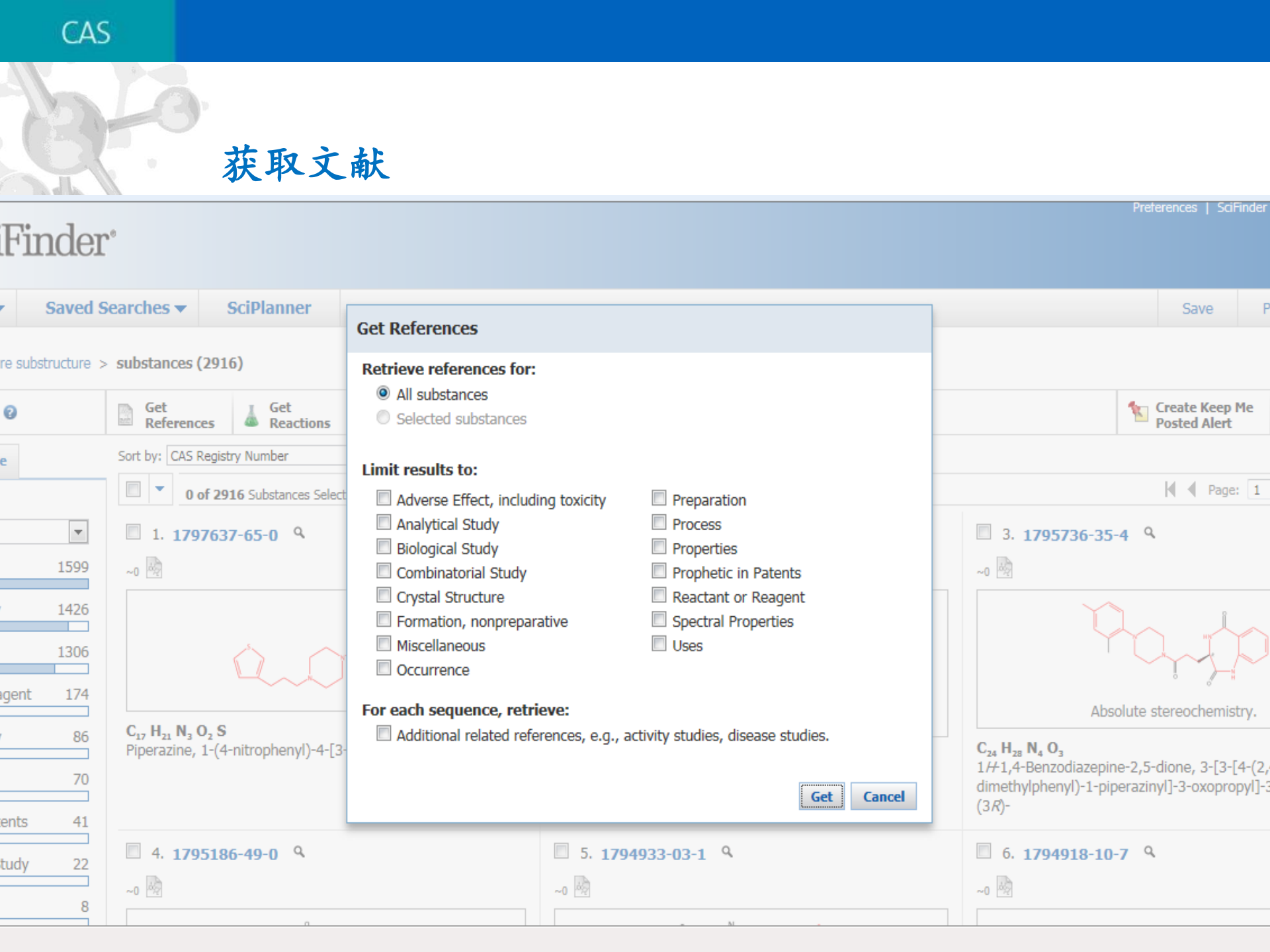
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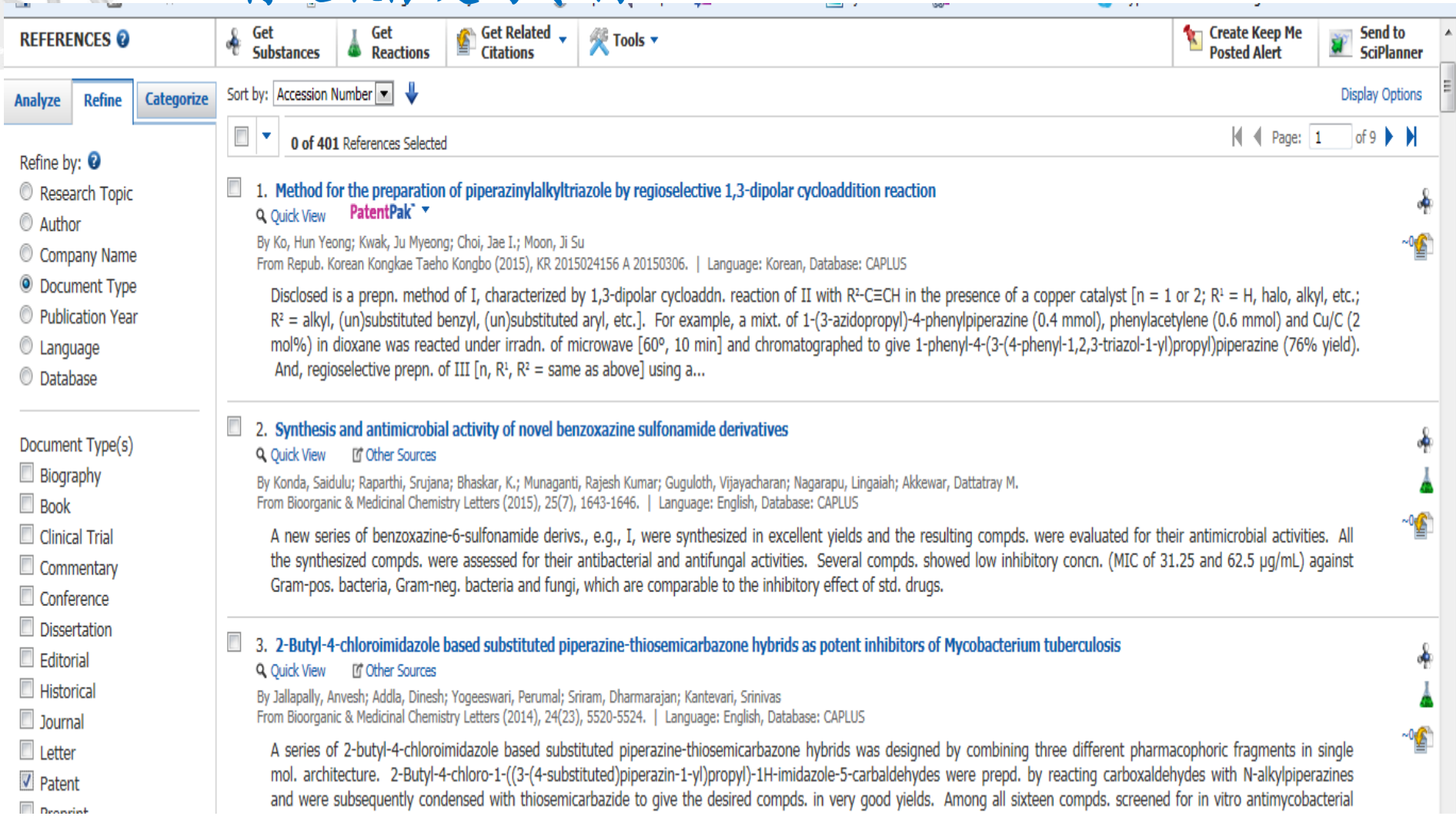
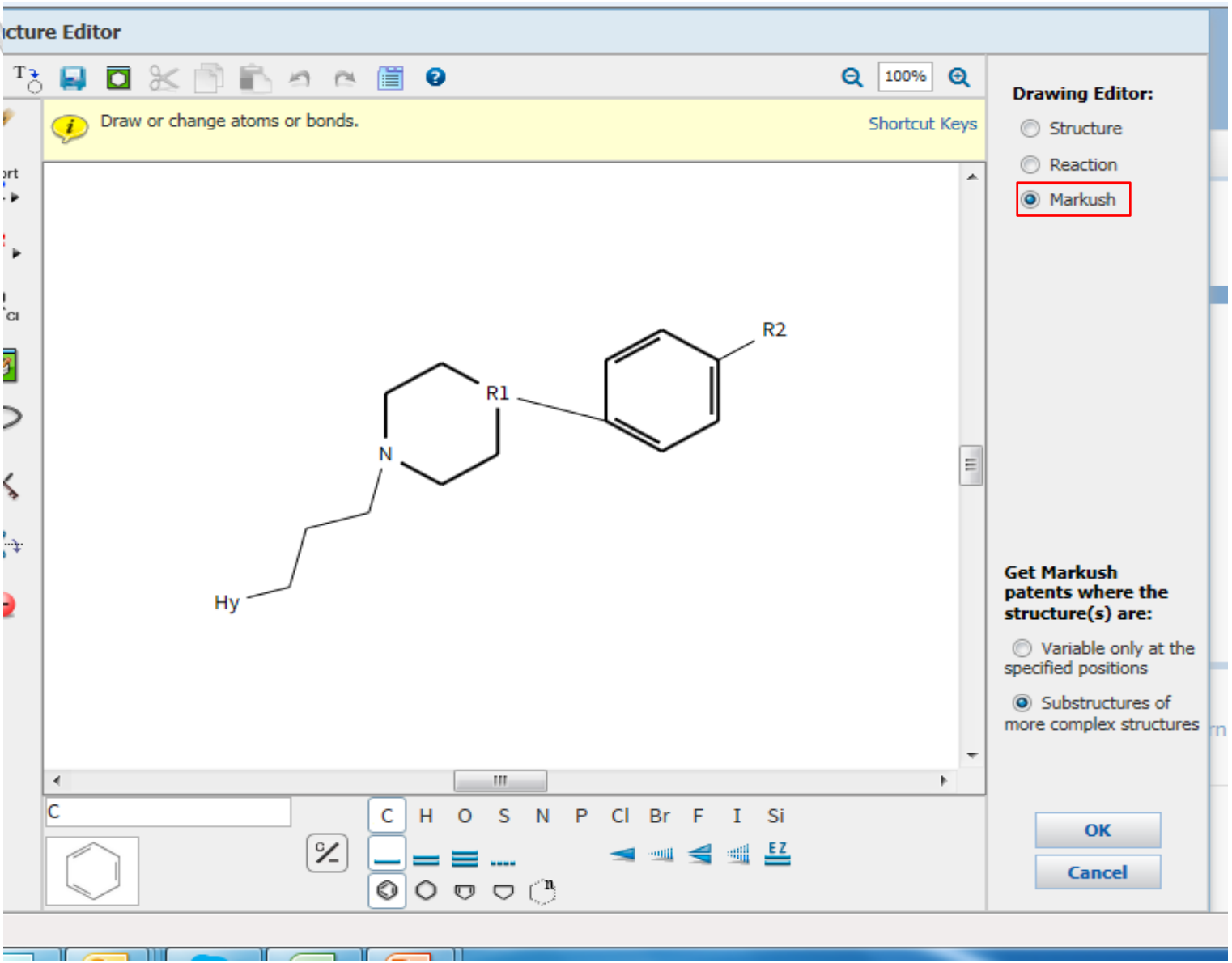


绘制结构，并用Markush检索，获取报道Markush结构的专利



获得报道Markush结构的专利，并将结果与报道确定结构的文献进行合并、去重

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- Emonds Alt Xavier 10
- Proietto Vincenzo 10
- Saxena Anil Kumar 10

1. Preparation of functionalized and substituted indoles as anticancer agents

Quick View | PatentPak

By James, Ian; Dixon, Ian; Bu, Xian

From PCT Int. Appl. (2015), WO 2015074124 A1 20150528. | Language: English, Database: CAPLUS

The invention relates substituted indoles as tropomyosin inhibitors; processes for their prepn., and methods for treating or preventing proliferative diseases, preferably cancer, using compds. of the invention. Compds. of formula I wherein R^1 is substituted Ph, substituted piperazinyl, substituted pyrazolyl, etc.; R^2 is Me, substituted Ph, substituted pyridyl, etc.; R^3 is NH_2 and derivs., piperazinyl, morpholinyl, etc.; R^4 is H and methyl; R^7 is H, alkyl, alkoxy; X^1 is $(CH_2)_{0-5}$; X^2 = X^3 = O, NH, CO, etc.; X^4 is O, NH and derivs.; and pharmaceutically acceptable drugs and prodrugs thereof, are...

2. Novel compositions useful for inhibiting HIV-1 infection and methods using same

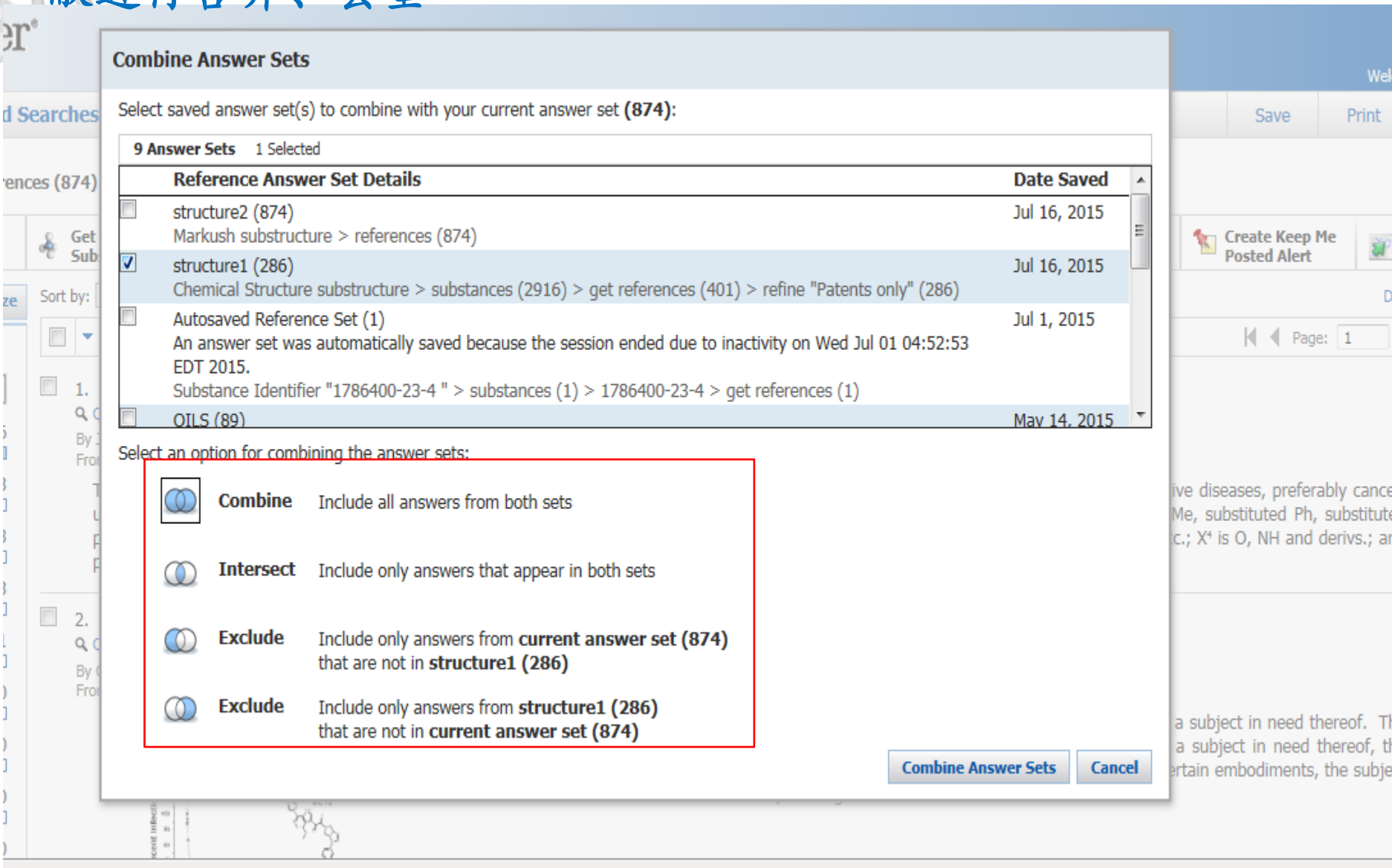
Quick View | PatentPak

By Cocklin, Simon

From PCT Int. Appl. (2015), WO 2015051230 A1 20150409. | Language: English, Database: CAPLUS

The present invention includes novel compns. useful for preventing or treating an HIV-1 infection in a subject in need thereof. The present invention further includes a novel method of preventing or treating an HIV-1 infection in a subject in need thereof, the method comprising administering to the subject an effective amt. of a compd. of the invention. In certain embodiments, the subject is further administered at least one addnl. therapeutic agent.

获得报道Markush结构的专利，并将结果与报道确定结构的文献进行合并、去重



获得完整的报道Markush结构、确定结构的专利文献

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1. **Preparation of functionalized and substituted indoles as anticancer agents**

Quick View | PatentPak

By James, Ian; Dixon, Ian; Bu, Xian

From PCT Int. Appl. (2015), WO 2015074124 A1 20150528. | Language: English, Database: CAPLUS

The invention relates substituted indoles as tropomyosin inhibitors; processes for their prepn., and methods for treating or preventing proliferative diseases, preferably cancer, using compds. of the invention. Compds. of formula I wherein R^1 is substituted Ph, substituted piperazinyl, substituted pyrazolyl, etc.; R^2 is Me, substituted Ph, substituted pyridyl, etc.; R^3 is NH_2 and derivs., piperazinyl, morpholinyl, etc.; R^4 is H and methyl; R^7 is H, alkyl, alkoxy; X^1 is $(CH_2)_{0-5}$; X^2 = X^3 = O, NH, CO, etc.; X^4 is O, NH and derivs.; and pharmaceutically acceptable drugs and prodrugs thereof, are...

2. **Novel compositions useful for inhibiting HIV-1 infection and methods using same**

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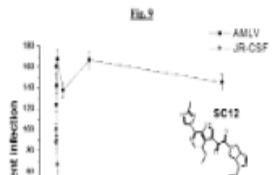
By Cocklin, Simon

From PCT Int. Appl. (2015), WO 2015051230 A1 20150409. | Language: English, Database: CAPLUS



The present invention includes novel compns. useful for preventing or treating an HIV-1 infection in a subject in need thereof. The present invention further includes a novel method of preventing or treating an HIV-1 infection in a subject in need thereof, the method comprising administering to the subject an effective amt. of a compd. of the invention. In certain embodiments, the subject is further administered at least one addnl. therapeutic agent.

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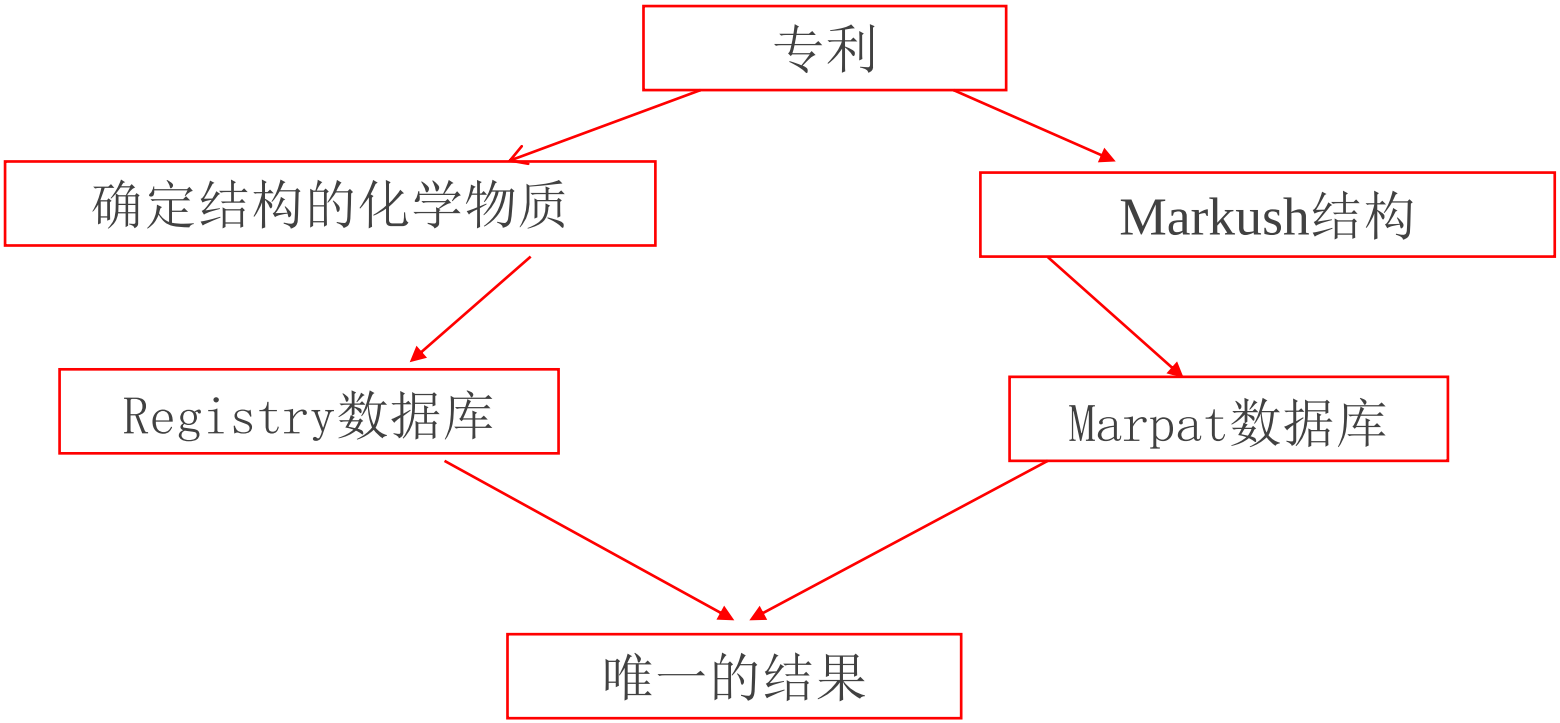

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