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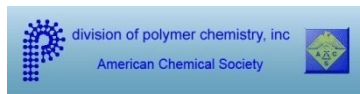
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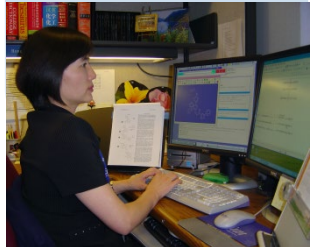
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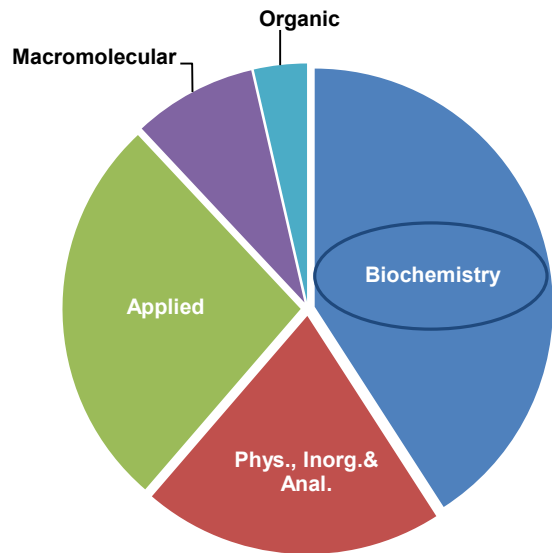
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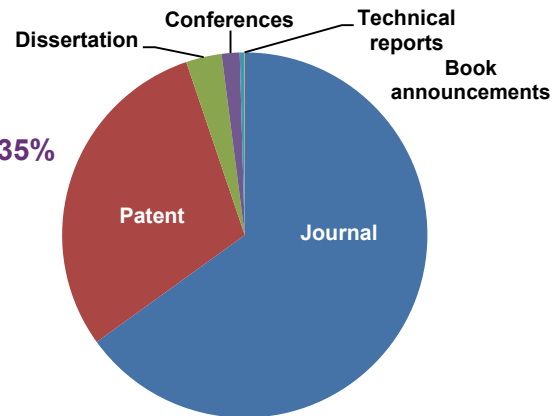
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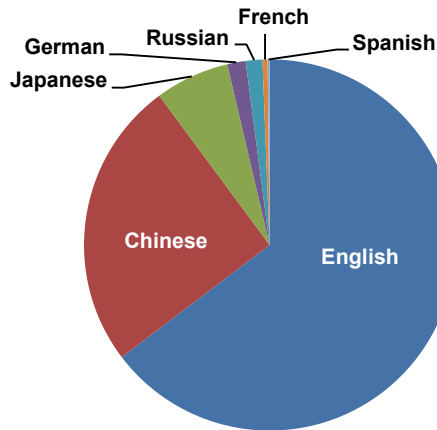
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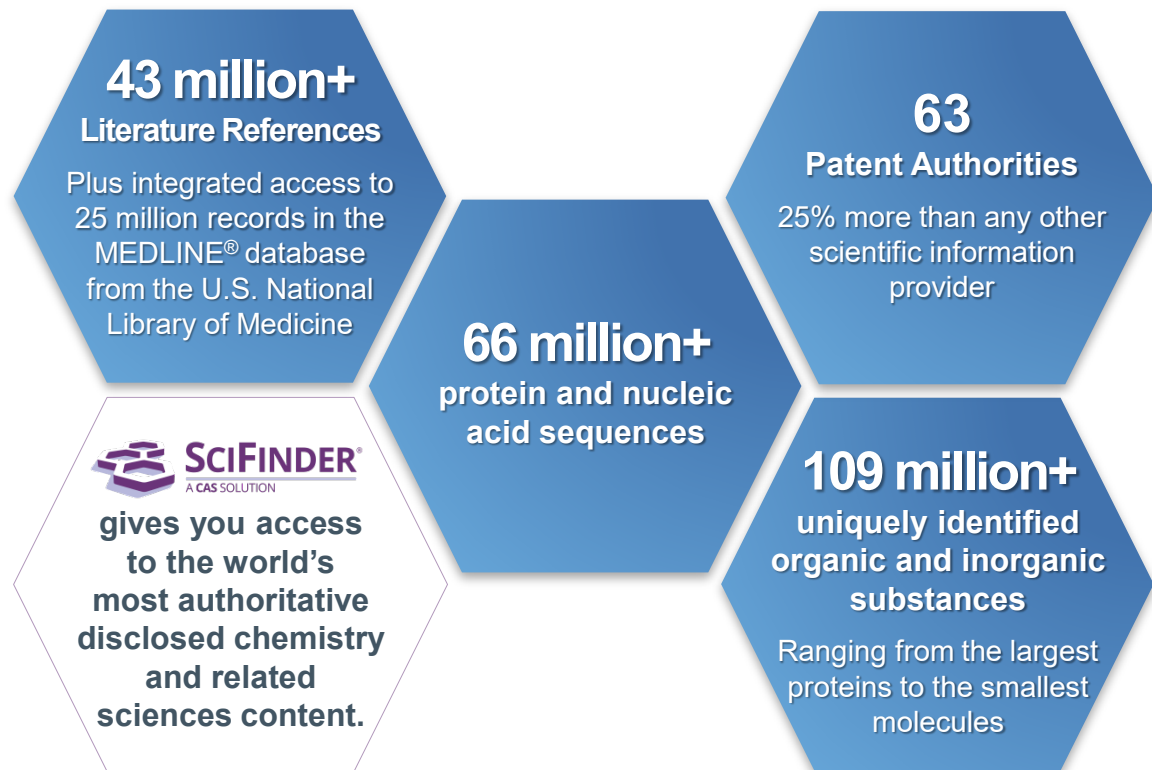
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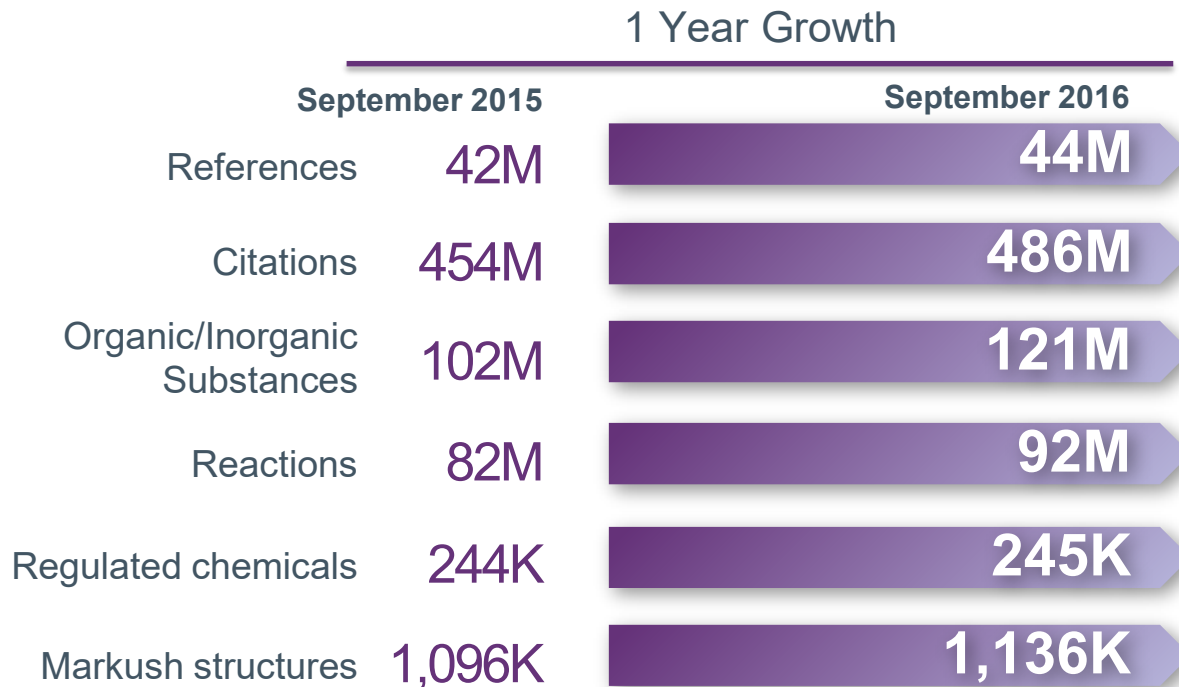


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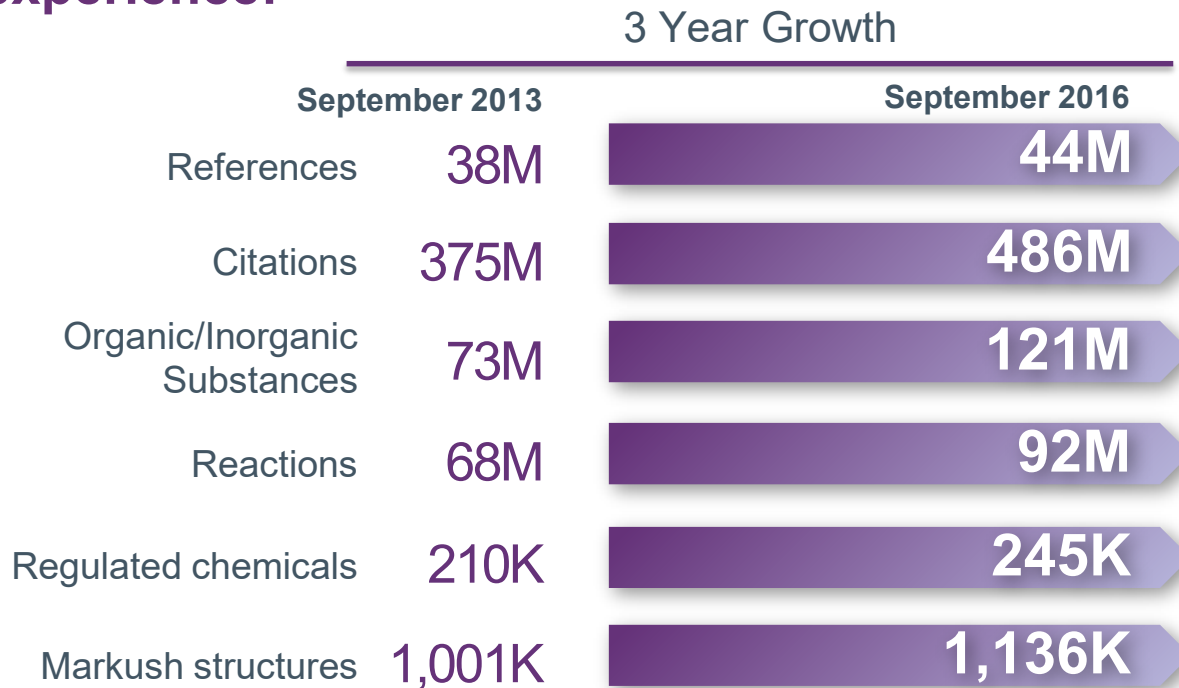


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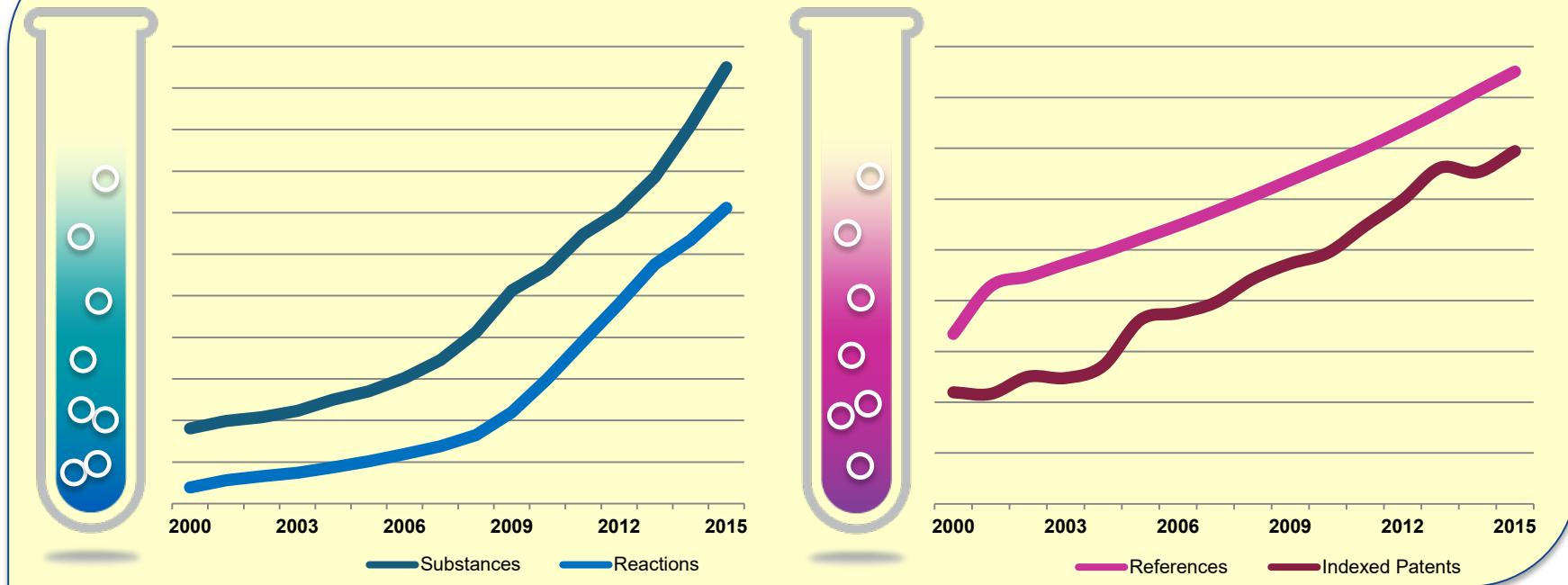


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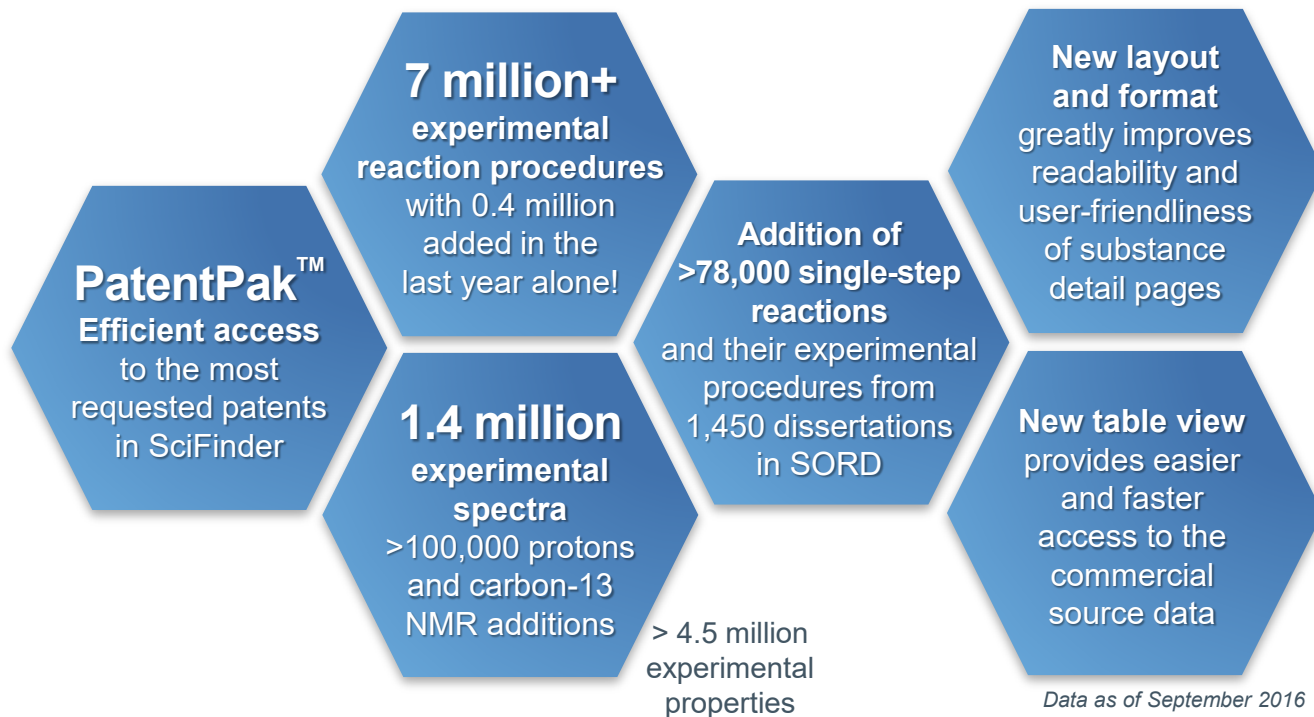
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48. CAS Registry Number 50-23-7

~55,285 ~305

C₂₁ H₃₀ O₅
Pregn-4-ene-3,20-dione, 11,17,21-trihydroxy-, (11β)-

Molecular Weight
362.46

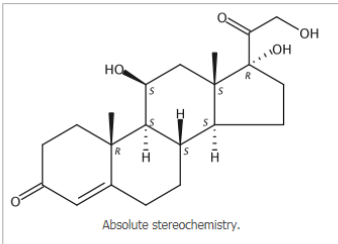
pKa (Predicted)
Value: 12.47±0.70 | Condition: Most Acidic Temp: 25 °C

Melting Point (Experimental)
Value: 217-220 °C (decomp)

Boiling Point (Predicted)
Value: 566.4±50.0 °C | Condition: Press: 760 Torr

Density (Experimental)
Value: 1.4 g/cm³

Other Names
Cortisol (8CI)
11β,17,21-Trihydroxypregn-4-ene-3,20-dione
11β,17,21-Trihydroxyprogesterone
11β,17α,21-Trihydroxypregn-4-ene-3,20-dione
11β-Hydroxycortisone
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Absolute stereochemistry.

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Indicators	References
Anti-infective agents (all) > > > Antibacterial agents	220
Anti-infective agents (all) > > > Antibiotics	338
Anti-infective agents (all) > > > Antimicrobial agents	122
Anti-infective agents (all) > > > Antiviral agents	179
Anti-infective agents (all) > > > Fungicides	226
Anti-inflammatory agents (all) > Antiarthritics	64
Anti-inflammatory agents (all) > Anti-inflammatory agents	871
Anti-inflammatory agents (all) > Antirheumatic agents	98
Anti-inflammatory agents (all) > Nonsteroidal anti-inflammatory drugs	265
Antitumor agents (all) > Antiangiogenic agents	60
Antitumor agents (all) > Antitumor agents	404
Dermatological agents (all) > Dermatological agents	73
Immune agents (pharmaceutical) > Allergy inhibitors	83
Immune agents (pharmaceutical) > > Immunomodulators	117
Immune agents (pharmaceutical) > > Immunosuppressants	213
Natural products, pharmaceutical	89
Nervous system agents (all) > > > Analgesics	216
Nervous system agents (all) > > > Anesthetics	209
Receptor antagonists (all) > > Antihistamines	124
Respiratory system agents (all) > Antiasthmatics	104
Wound healing promoters	55

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1. Select a heading and category.

Category Heading	Category
All	Substances in biology (221)
General chemistry	Animal pathology (69)
Biotechnology	Immunology (72)
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Genetics & protein chemistry	Endocrinology (48)
Physical chemistry	Anatomy (27)
Polymer chemistry	Substances in adverse effects (16)
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Technology	
Analytical chemistry	
Environmental chemistry	

Biology > Immunology

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<input type="checkbox"/> Interferons, α	5
<input type="checkbox"/> Vaccines	5
<input type="checkbox"/> Interleukin 2	3
<input type="checkbox"/> Interleukin 4	3
<input type="checkbox"/> Leukotriene B4	3
<input type="checkbox"/> RANTES (chemokine)	3
<input type="checkbox"/> Spleen	3
<input type="checkbox"/> Tumor necrosis factor α	3
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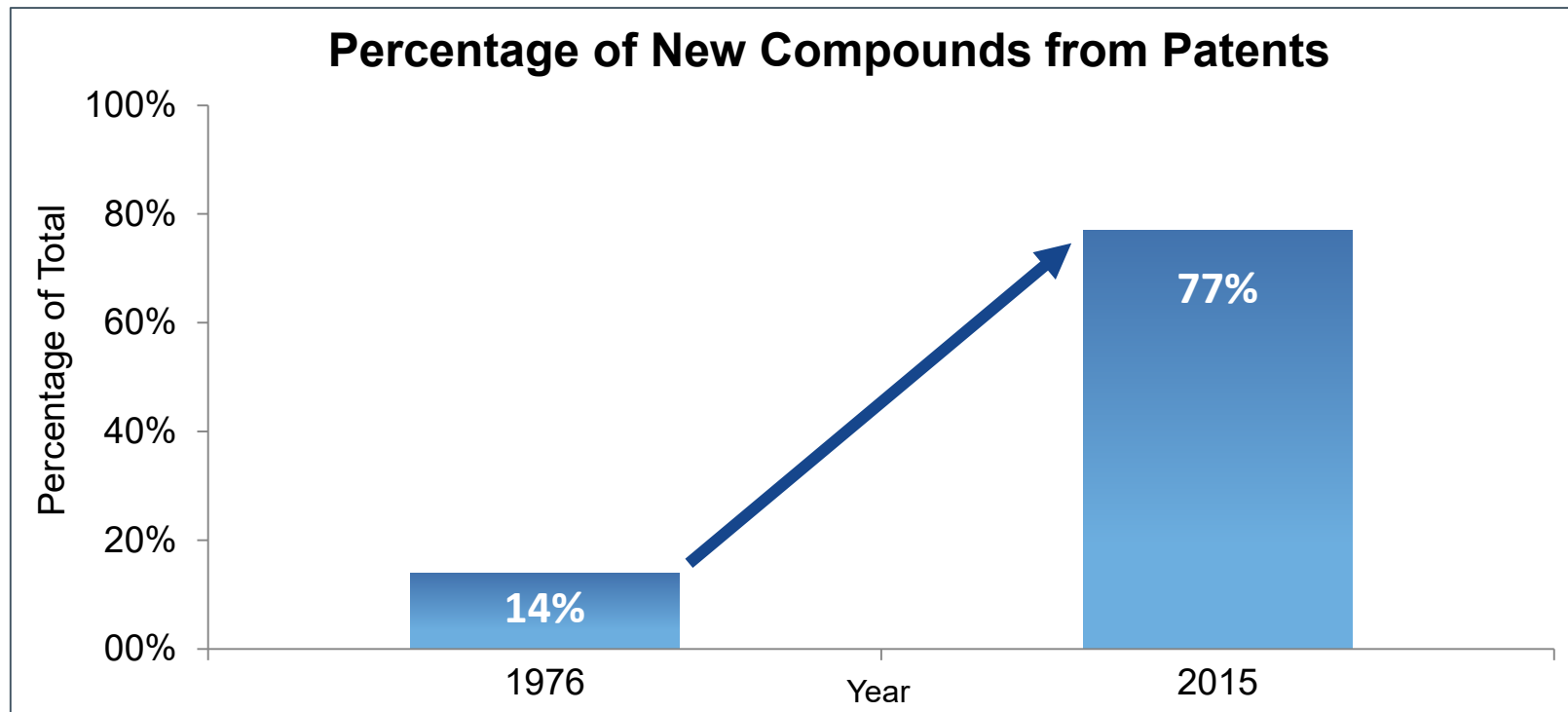
1. **28911-01-5**

~2061 ~34

C₁₇ H₁₂ Cl₂ N₄
 4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine, 8-chloro-6-(2-chlorophenyl)-1-methyl-

Regulatory Information
 Spectra
 Experimental Properties

Increasingly, new compounds in the literature are first disclosed in patents



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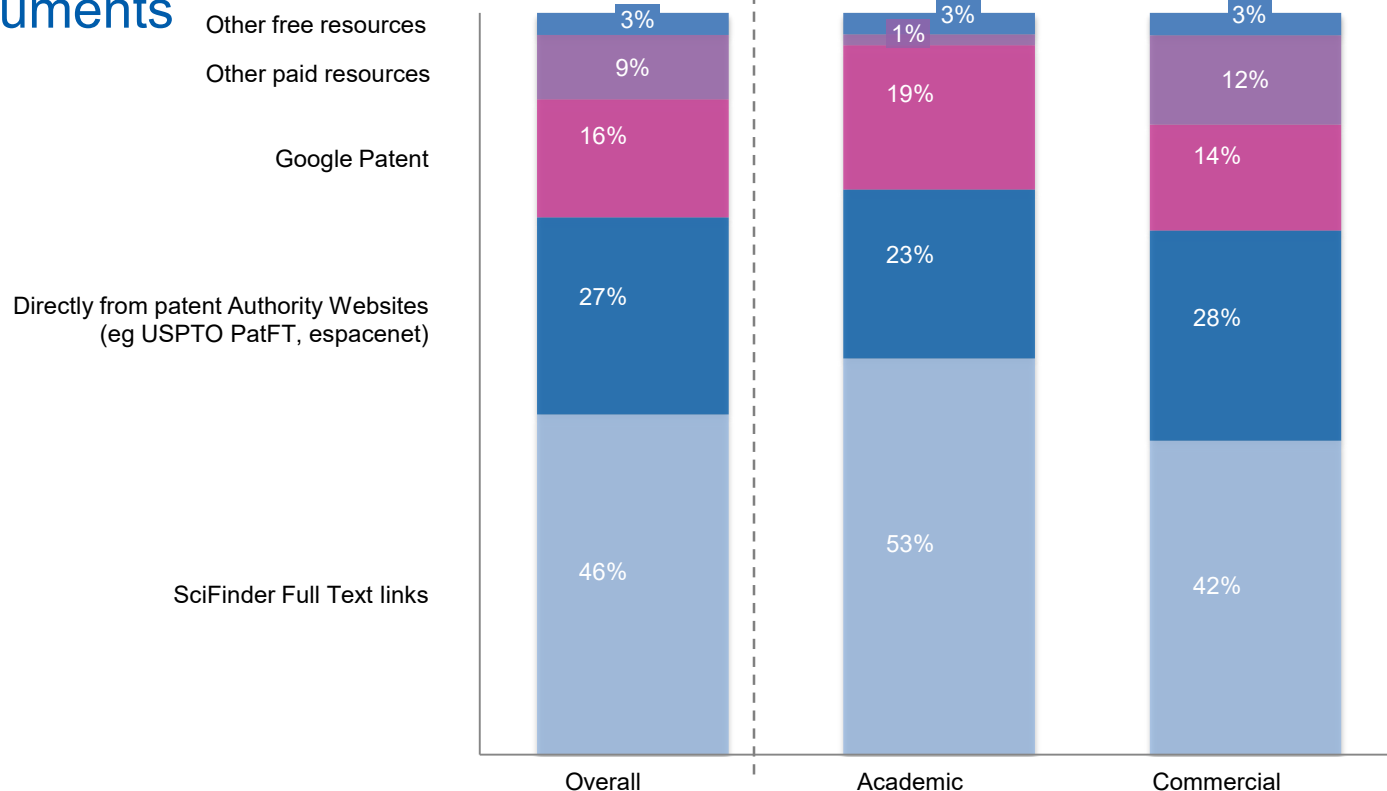


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9. Process for the preparation of favipiravir

Quick View

PATENTPAK

By Bao, Jinyuan; H
From Faming Zhua

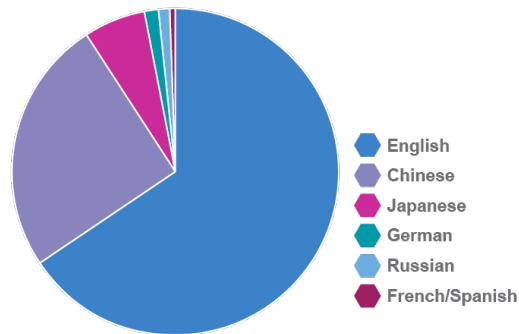
Patent No.	Kind	Language
CN 104496917	A	Chinese

qing

A 20150408. | Language: Chinese, Database: CAPLUS

The invention relates to process for the prepn. of favipiravir. For example, favipiravir was prepd. from 3-bromopyrazine-2-carboxylic acid to afford Me 3-amino-6-bromopyrazine-2-carboxylate, which underwent diazotization and fluorination to afford Me 3-(benzyloxy)-6-fluoropyrazine-2-carboxylate, which underwent debenzoylation and

Original publication
languages not
in English **35%**



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(12) 发明专利申请



(10) 申请公布号 CN 104496917 A

(43) 申请公布日 2015.04.08

(21) 申请号 201410769599.5

(22) 申请日 2014.12.15

(71) 申请人 南京华威医药科技开发有限公司

地址 210012 江苏省南京市仙林大学城纬地
路9号

(72) 发明人 包全运 黄辉 梅玉伟 张孝前

(51) Int. Cl.

C07D 241/24(2006.01)

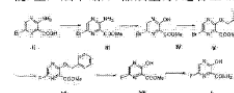
权利要求书2页 说明书6页

(54) 发明名称

一种法匹拉韦的合成方法

(57) 摘要

本发明属于药物化学领域,具体涉及一种法匹拉韦的合成方法。该方法是:以式(II)为原料,经过羧基保护生成化合物(III),在浓硫酸和亚硝酸的作用下经重氮水解反应生成化合物(IV),然后经苄基保护反应生成化合物(V),然后在氯化钾和四丁基溴化铵的作用下生成化合物(VI),脱苄基保护基生成化合物(VII),然后加入氯化氢进行氯化反应生成法匹拉韦(式I)。本发明提供的方法反应周期短,操作简便,生产成本低,产品质量好,适合工业化生产。



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Quick View

PATENTPAK

By Bao, Jinyuan; H
From Faming Zhua

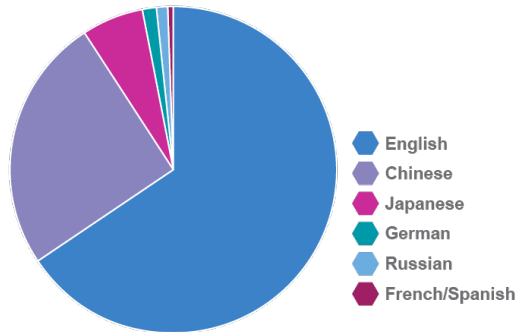
Patent No.	Kind	Language
CN 104496917	A	Chinese

qing

A 20150408. | Language: Chinese, Database: CAPLUS

The invention relates to process for the prepn. of favipiravir. For example, favipiravir was prepd. from 3-bromopyrazine-2-carboxylic acid to afford Me 3-amino-6-bromopyrazine-2-carboxylate, which underwent diazotization and fluorination to afford Me 3-(benzyloxy)-6-fluoropyrazine-2-carboxylate, which underwent debenzoylation and

Original publication
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(71) 申请人 南京华威医药科技开发有限公司

地址 210012 江苏省南京市仙林大学城纬地
路9号

(72) 发明人 包全运 黄辉 梅玉伟 张孝前

(51) Int. Cl.

C07D 241/24(2006.01)

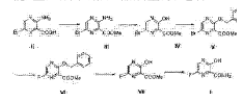
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(54) 发明名称

一种法匹拉韦的合成方法

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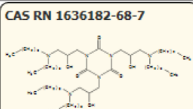
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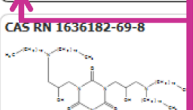
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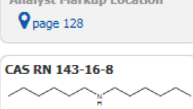
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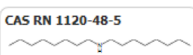
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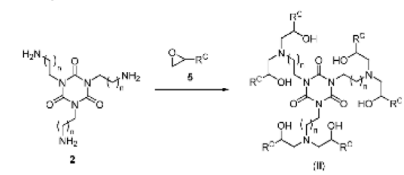
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Compound 1-8: ^1H NMR (500 MHz, CDCl_3) δ 4.08–4.12 (m, 3H), 3.92–3.94 (m, 3H), 3.80–3.83 (m, 3H), 2.35–2.52 (m, 18H), 1.26–1.42 (m, 96H), 0.88 (t, $J = 7.0$ Hz, 9H). HRMS (ESI) calcd for $\text{C}_{77}\text{H}_{144}\text{N}_6\text{O}_6$ $[\text{M}+\text{H}]^+$ 1190.1220, found 1190.1140.

Compound 1-9: ^1H NMR (500 MHz, CDCl_3) δ 4.08–4.12 (m, 3H), 3.90–3.94 (m, 3H), 3.80–3.84 (m, 3H), 2.35–2.52 (m, 18H), 1.25–1.42 (m, 132H), 0.88 (t, $J = 7.0$ Hz, 9H). HRMS (ESI) calcd for $\text{C}_{92}\text{H}_{168}\text{N}_6\text{O}_6$ $[\text{M}+\text{H}]^+$ 1442.4037, found 1442.4077.

Example 2. Preparation of the Compounds of Formula (II)

[00279] Compounds of Formula (II), and salts thereof, may be prepared by the synthetic sequence outlined below in Scheme 2. Alternatively, compounds of Formula (II) may be synthesized by other methods described herein or known in the art.



Scheme 2. Exemplary synthesis of compounds of Formula (II), wherein R^C and n are as described herein.

000 126/11

WO 2014/179562 PCT/US2014/036355

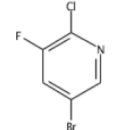
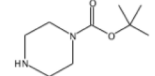
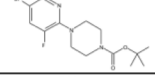
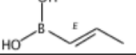
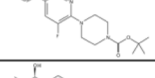
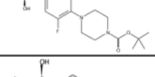
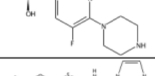
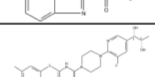
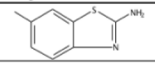

[00280] In one set of experiments, a mixture of compounds 2 and 5 in EtOH was irradiated in the microwave oven at 150°C for 5 h. The reaction mixture was purified by flash column chromatography to yield a compound of Formula (II).

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Key Substances in Patent

Mark	Page #	CAS RN	Name	Structure
101	p.151	831203-13-5	Pyridine, 5-bromo-2-chloro-3-fluoro-	
102	p.151	57260-71-6	1-Piperazinecarboxylic acid, 1,1-dimethylethyl ester	
103	p.151	1289048-68-5	1-Piperazinecarboxylic acid, 4-(5-bromo-3-fluoro-2-pyridinyl)-, 1,1-dimethylethyl ester	
104	p.151	7547-97-9	Boronic acid, B-(1E)-1-propen-1-yl-	
105	p.151	1416788-07-2	1-Piperazinecarboxylic acid, 4-[3-fluoro-5-(1E)-1-propen-1-yl-2-pyridinyl]-, 1,1-dimethylethyl ester	
106	p.151	1416788-08-3	1-Piperazinecarboxylic acid, 4-[5-[(1S,2S)-1,2-dihydroxypropyl]-3-fluoro-2-pyridinyl]-, 1,1-dimethylethyl ester	
107	p.151	1416788-09-4	1,2-Propanediol, 1-[5-fluoro-6-(1-piperazinyl)-3-pyridinyl]-, (1S,2S)-	
108	p.151	833491-50-2	1H-Imidazole-1-carboxamide, N-(6-methyl-2-benzothiazolyl)-	
121	p.151	1416788-16-3	1-Piperazinecarboxamide, 4-[5-[(1S,2S)-1,2-dihydroxypropyl]-3-fluoro-2-pyridinyl]-N-(6-methyl-2-benzothiazolyl)-	
109	p.153	2536-91-6	2-Benzothiazolamine, 6-methyl-	

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Advanced Search

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

利用化合物結構、Markush結構、分子式、化合物性質(沸點、玻璃轉化溫度、折射率、抗拉強度、旋光性...)、化合物名、貨號、CAS 號碼 進行文獻搜索

REACTIONS

- Reaction Structure

利用化合物結構尋找相關反應條件文獻

SAVED ANSWER SETS

PU DEMO

gentex company

VIOLOGEN

OCCURRENCE

Autosaved Substance Set

View All | Import

KEEP ME POSTED

notrogen contain
No results

risperidone
Aug 27, 2016(43)
Aug 20, 2016(22)

View All

Reference :Research Topic



主題搜索範例(Aqueous Pigment):

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

REFERENCES: RESEARCH TOPIC ?

輸入研究主題

Examples:

The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Search

Advanced Search

主題搜索範例(Aqueous Pigment):

Research Topic "aqueous pigment" > references (673) > 搜索到673篇文獻 主題為 Aqueous Pigment

REFERENCES



Get Substances



Get Reactions



Get Related Citations



View Only
CHEMZENT



Tools



Create Keep Me
Posted Alert



Send to
SciPlanner

Analyze

Refine

Categorize

Analyze by:

Document Type

Patent 626

Journal 47

General Review 4

Article 3

JOURNAL ARTICLE 3

RESEARCH

SUPPORT NONUS

GOVT 1

搜索到673篇文獻 中
專利626篇 期刊 47篇

Sort by: Accession Number



Display Options

0 of 673 References Selected

Page: 1 of 34

1. Aqueous pigment dispersion and aqueous ink [Machine Translation].

Quick View

Other Sources

By Kawaharada, Yukihiro

From Jpn. Kokai Tokkyo Koho (2016), JP 2016169286 A 20160923. | Language: Japanese, Database: CAPLUS

[Machine Translation of Descriptors]. To provide an aq. **pigment** dispersion having excellent dispersion stability of fine particle size, and excellent optical d. of the resulting image, and aq. ink. The aq. **pigment** dispersion comprises at least, a **pigment** (A), anionic group-contg. org. polymer compd. (B), copolymer (C) of (meth)acrylic acid, (meth)acrylate and acrylate having a polyoxyethylene group contg. linear or branched alkyl group with 18-22 carbon at the end, and the mass ratio of component (C) and **pigment** (A) is in the range of 1/1000-7/100, and the aq. ink using the same.

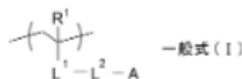
2. Aqueous pigment dispersions with good dispersibility and stability, and aqueous ink compositions using them

Quick View

PATENTPAK

By Kato, Takahiro

From Jpn. Kokai Tokkyo Koho (2016), JP 2016160331 A 20160905. | Language: Japanese, Database: CAPLUS



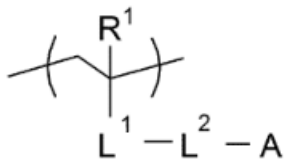
The **pigment** dispersions contain (A) aq. media, (B) pigments, and (C) polymer dispersants having (c1) constitutional units of $\text{CH}_2\text{CR}^1(\text{L}^1\text{L}^2\text{A})$ ($\text{R}^1 = \text{H, Me; L}^1 = \text{CO}_2, \text{O}_2\text{C, CONR}^2, \text{phenylene; R}^2 = \text{H, C}_{1-6} \text{ alkyl; L}^2 = \text{single bond, C}_{1-12} \text{ alkylene, C}_{2-12} \text{ alkenylene, CO, NR}^6, \text{O, S, SO, SO}_2, \text{these combined divalent group; R}^6 = \text{H, C}_{1-6} \text{ alkyl; A} = \text{C}_{6-10} \text{ polycyclic structure}$) (c2) constitutional units having ionic groups, and (c3)

主題搜索範例(Aqueous Pigment): 專利檢索

2. Aqueous pigment dispersions with good dispersibility and stability, and aqueous ink compositions using them

By: Kato, Takahiro
Assignee: Fujifilm Corp., Japan

The **pigment** dispersions contain (A) aq. media, (B) pigments, and (C) polymer dispersants having (c1) constitutional units of $\text{CH}_2\text{CR}^1(\text{L}^1\text{L}^2\text{A})$ ($\text{R}^1 = \text{H, Me; L}^1 = \text{CO}_2, \text{O}_2\text{C, CONR}^2, \text{phenylene; R}^2 = \text{H, C}_{1-4} \text{ alkyl; L}^2 = \text{single bond, C}_{1-12} \text{ alkylene, C}_{2-12} \text{ alkenylene, CO, NR}^3, \text{O, S, SO, SO}_2, \text{these combined divalent group; R}^3 = \text{H, C}_{1-4} \text{ alkyl; A} = \text{C}_{22} \text{ polycyclic structure}$), (c2) constitutional units having ionic groups, and (c3) SR^4 or $\text{SR}^4\text{CO}_2\text{R}^5$ ($\text{R}^4 = \text{alkyl, aryl; R}^5 = \text{alkylene; R}^5 = \text{H, alkyl}$). Thus, an aq. dispersion contg. **Pigment Yellow (TRY 13)**, N-(vinylbenzyl)acridone-benzyl methacrylate-Me methacrylate-methacrylic acid copolymer potassium salt prepd. in the presence of 3-mercaptopropionic acid, and dipropylene glycol showed vol.-av. particle size 70-100 nm, viscosity 10-40 mPa-s, change in particle diam. and viscosity after storing at 60° for 24 h 30-50 nm and 30-50 mPa-s, resp., and dispersing time (vol.-av. particle diam. $\leq 100 \text{ nm}$) $\leq 2 \text{ h}$.



一般式 (I)

對於63專利局發表專利內容，皆轉成英文檢索，如:摘要、概念、每一物質主旨,並能做全文下載。

Patent Information

Patent No.	Kind	Language	Date	Application No.	Date
JP 2016160331	PATENTPAK	A	Sep 5, 2016	JP 2015-39546	Feb 27, 2015

Priority Application

JP 2015-39546	Feb 27, 2015
---------------	--------------

Indexing

Coatings, Inks, and Related Products (Section42-12)

Concepts

Disperse systems Dispersing agents

aq. **pigment** dispersions with good dispersibility and stability for aq. ink compns.

Jet-printing inks

Substances

6358-31-2 C.I. **Pigment Yellow 74** 🔍

Page 26 in PATENTPAK

TRY 13; aq. **pigment** dispersions with good dispersibility and stability for aq. ink compns.

Technical or engineered material use; Uses

主題搜索範例(Aqueous Pigment): 互動式專利內文(全文直接下載)

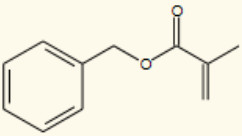
PAGE 19 / 31

ZOOM - +

DOWNLOAD PDF

Key Substances in Patent

CAS RN 2495-37-6

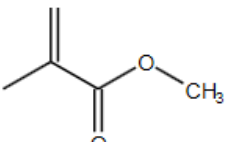


Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 19

CAS RN 80-62-6

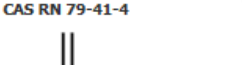


Search in SciFinder | View Detail

Analyst Markup Locations (1)

page 19

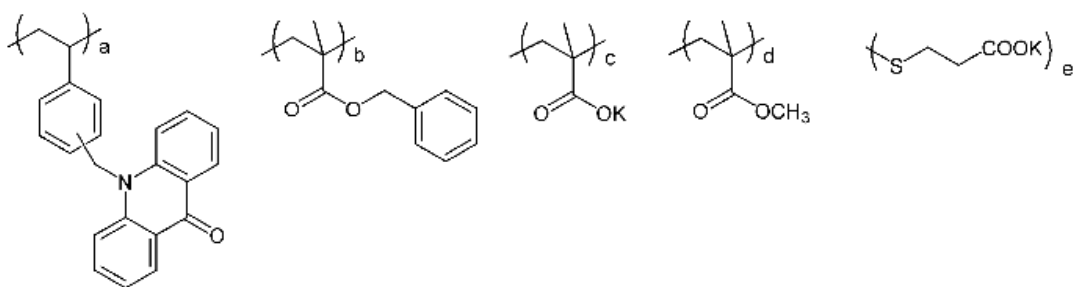
CAS RN 79-41-4



下記構造のポリマーからなる分散剤を合成した。

【0094】

【化8】



10

P-1

a : b : c : d : e = 5 : 37 : 25 : 31 : 2 (質量%) のランダムポリマー

20

【0095】

攪拌機、冷却管を備えた2000mlの三口フラスコにジプロピレングリコール198gを加え窒素雰囲気下で85℃に加熱した。

モノマーとして下記モノマーAを22.5g、ベンジルメタクリレート166.5g、メタクリル酸メチル139.53g、メタクリル酸を112.5g、連鎖移動剤として3-メルカプトプロピオン酸を8.97g、166gのジプロピレングリコールに溶解

2016 American Chemical Society. All rights reserved.

Substance reaction Research

Pigment Red 208



合成方法搜尋範例(C.I. Pigment Red 208):

The screenshot displays the SciFinder software interface. On the left, the 'Explore' and 'Saved Searches' tabs are visible, along with a list of search criteria under 'REFERENCES' and 'SUBSTANCES'. The main window is the 'Structure Editor', which shows the chemical structure of C.I. Pigment Red 208. The structure is a complex organic molecule with a central benzene ring fused to a naphthalene system, featuring various functional groups including a carboxylate ester, a diazo group, and a benzimidazole moiety. The structure is labeled 'product' and has the molecular formula $C_{29}H_{23}N_5O_5$ and a molecular weight of 523.55. A red text annotation '點選 尋找反應' (Click to find reaction) is overlaid on the right side of the structure. The 'Drawing Editor' panel on the right shows the 'Reaction' option selected. The bottom of the interface shows the chemical formula $C_{29}H_{23}N_5O_5$ and the molecular weight 523.55.

點選 尋找反應

合成方法搜尋範例(C.I. Pigment Red 208):

Reaction Structure substructure > reactions (8) 搜尋出8種合成 Pigment Red 208 合成方法

REACTIONS

Get References Tools Send to SciPlanner

Analyze **Refine**

Group by: No Grouping Sort by: Relevance

☐ 0 of 8 Reactions Selected

☐ 1. [View Reaction Detail](#) [Link](#) [Similar Reactions](#)

Single Step *Hover over any structure for more options.*

~52 ~43 86% ~14

Overview

Steps/Stages

1.1 R:

R: H₂SO₄, S: (CH₂OH)₂

1.2 R: KOH, S: (CH₂OH)₂

Notes

Reactants: 2, Reagents: 3, Solvents: 1, Steps: 1, Stages: 2, Most stages in any one step: 2

References

The synthesis of monoazo pigments derived from 5-(3'-hydroxy-2'-naphthoylamino)-benzimidazol-2-one

Quick View Other Sources

By Boruszczak, Zygmunt and Kraska, Jan

From Dyes and Pigments, 25(1), 59-67; 1994

合成方法搜尋範例(C.I. Pigment Red 208):

CAS Registry Number 31778-10-6

-85 -14

C₂₈ H₂₄ N₄ O₄

Benzoic acid, 2-[[2-[3-[[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthalenyl]diazenyl]-, butyl ester

Molecular Weight

523.54

Boiling Point (Predicted)

Value: 632.0±55.0 °C | Condition: Press: 760 Torr

Density (Predicted)

Value: 1.39±0.1 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

Value: 11.41±0.30 | Condition: Most Acidic Temp: 25 °C

Other Names

Benzoic acid, 2-[[[3-[[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthalenyl]azo]-, butyl ester (9CI)

Benzoic acid, α -[[2-hydroxy-3-[(2-oxo-5-benzimidazolyl)carbonyl]-1-naphthyl]azo]-, butyl ester (8CI)

5-[4- α -(Butoxycarbonyl)phenylazo]-3-hydroxy-2-naphthimido]-2-benzimidazolinone

C.I. 12514

C.I. Pigment Red 208

Graphitol Red HF 2B

HF 2B01

Hostaprint Red HF 2B32

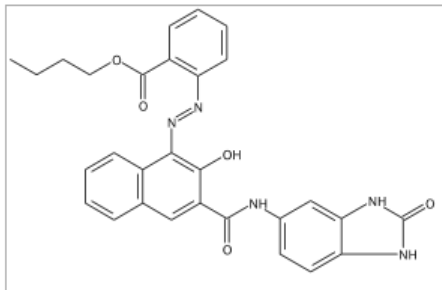
Novoperm Red HF 2B

Novoperm Red HF 2B01

PV Red HF 2B

Pigment Red 208

View less...



可直接獲取此物質資訊，文獻或商業來源

[Expand All](#) | [Collapse All](#)

► EXPERIMENTAL SPECTRA

IR

IR Properties

IR Absorption Spectrum

Value

[See spectrum](#)

Condition

Note

(1)WSS

IR Absorption Spectrum

[See spectrum](#)

(1)WSS

Notes

(1) WSS: Spectral data were obtained from Wiley Subscription Services, Inc. (US)

► PREDICTED PROPERTIES

Substance Research

Pigment Red 254



物質搜尋範例(C.I. Pigment Red 254):

Explore ▼

Saved Searches ▼

SciPlanner

Substance Identifier "pigment red 254 " > substances (1)

REFERENCES

Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

SUBSTANCES

Chemical Structure

Markush

Molecular Formula

Property

Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: SUBSTANCE IDENTIFIER ?

pigment red 254

Enter one per line.
Examples:
50-00-0
999815
Acetaminophen

Search

可直接在Substance Identifier 上，輸入pigment red 254

Contact Us | Legal

物質搜尋範例(C.I. Pigment Red 254):

Substance Identifier "pigment red 254 " > **substances (1)**

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools ▾

Analyze Refine

Sort by: CAS Registry Number ▾

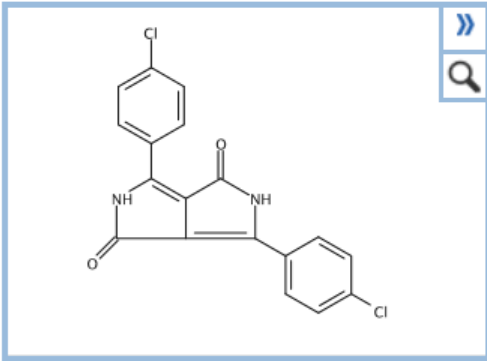
☐ 0 of 1 Substance Selected

Analyze by: ?
Substance Role ▾

Analytical Study 1
Biological Study 1
Formation, Nonpreparative 1
Miscellaneous 1
Occurrence 1
Preparation 1
Process 1
Properties 1

☐ 1. **84632-65-5** 🔍
~2804 📄 ~22 🧪

Pigment Red 254 有2804篇文獻與22個供應商



C₁₈ H₁₀ Cl₂ N₂ O₂
Pyrrolo[3,4-*c*]pyrrole-1,4-dione, 3,6-bis(4-chlorophenyl)-2,5-dihydro-

Click to view detail

▶ **Key Physical Properties**

物質搜尋範例(C.I. Pigment Red 254):

Substance Identifier "pigment red 254" > substances (1)

SUBSTANCES ?

Get References Get Reactions Get Commercial Sources Tools

Analyze Refine

Sort by: CAS Registry Number

Analyze by: Substance Role

Analytical Study 1

Biological Study 1

Formation, Nonpreparative 1

Miscellaneous 1

Occurrence 1

Preparation 1

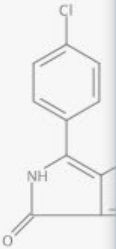
Process 1

Properties 1

0 of 1 Sub

1. 84632-65

~2804



Get Reactions

Limit results by reaction role:

- ☒ Product
- ☐ Reactant
- ☐ Reagent
- ☐ Reactant or reagent
- ☐ Catalyst
- ☐ Solvent
- ☐ Any role

可直接尋找 Pigment Red 254 為產物的合成步驟

Get Cancel

$C_{18}H_{10}Cl_2N_2O_2$
Pyrrolo[3,4-*c*]pyrrole-1,4-dione, 3,6-bis(4-chlorophenyl)-2,5-dihydro-

Key Physical Properties

javascript;

物質搜尋範例(C.I. Pigment Red 254):

Substance Identifier "pigment red 254" > substances (1) > get reactions (56)

尋找 **Pigment Red 254** 為產物的合成步驟共56個

REACTIONS ⓘ
Analyze **Refine**
Analyze by: ⓘ
Experimental Procedure
Experimental Procedures Not Available 30
Experimental Procedures Available 26
[Show More](#)

Get References Tools
Group by: No Grouping Sort by: Accession Number
0 of 56 Reactions Selected
13. [View Reaction Detail](#) ⓘ [Link](#)
Single Step *Hover over any structure for more options.*

Click to view detail

reaction products with pigments

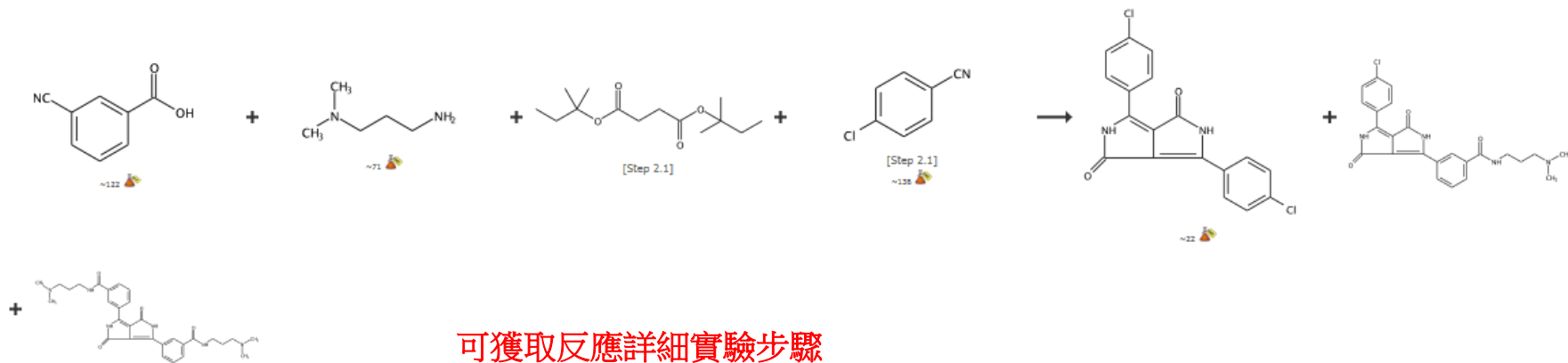
reaction products with azo compd.

Overview
Steps/Stages
1.1 R:HCl, S:H₂O, 3 h, rt → 90°C, pH 3.5

Notes
Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis(4-chlorophenyl)-2,5-dihydro- derivatized with 2,2-Azobis[N-(2-carboxyethyl)-2-methylpropanamide], Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

References
Surface-modified pigment preparations for use in coloring an org. material such as plastics, coatings or inks
Q Quick View **PATENTPAK** ⓘ
By Bugnon, Philippe and Nesvadba, Peter
From PCT Int. Appl., 2012089516, 05 Jul 2012

物質搜尋範例(C.I. Pigment Red 254):



Overview

Steps/Stages

- 1.1 R: SOCl_2 , S: PhMe, 50 h; 150 min, rt \rightarrow 95°C; 18 h, 90°C; 90°C \rightarrow reflux
- 1.2 75 min, reflux \rightarrow 90°C; 120 min, 100°C
- 2.1 R: $\text{NaOC}(\text{Et})\text{Me}_2$, S: HOOCMe_2Et , 4 h, 50°C; 50°C \rightarrow 105°C; 105°C; 105°C \rightarrow 50°C
- 2.2 H_2O , S: MeOH, 10 min, 0°C; 18 h, 0°C

Notes

- 2) unspecified catalyst used (stage 1), Reactants: 4, Reagents: 2, Solvents: 4, Steps: 2, Stages: 4, Most stages in any one step: 2

References

Dye compounds for improved red color filter composition

Quick View **PATENTPAK**
By Lenz, Roman et al
From PCT Int. Appl., 2009144115, 03 Dec 2009

Experimental Procedure

Step 1

Example 1004: 150 g of 3-cyanobenzoic acid are first introduced into 1000 ml of dry toluene under inert gas and heated to 50 °C, with stirring. To the resulting white suspension there are added, dropwise, 96 ml of thionyl chloride over a period of 150 minutes, the temperature being gradually increased to 95°C. Stirring is then carried out for a further 18 hours at 90 °C. The resulting brown solution is heated to reflux, and about 200 ml of a clear solution are distilled off under a gentle current of nitrogen. Cooling to 90 °C again is then carried out, and 106 g of 3-dimethylamino-1-propylamine are then added dropwise over 75 minutes, with stirring. Stirring is subsequently carried out for a further 120 minutes whilst refluxing gently (about 100°C). To the cooled reaction mixture there are added 500 ml of ethyl acetate and 500 ml of 2N sodium hydroxide solution and extraction is carried out. The aqueous phase is extracted a further three times using 300 ml of ethyl acetate each time; 60 ml of 30 % sodium hydroxide solution are added and extraction is carried out a further three times using 300 ml of ethyl acetate each time. The combined organic extracts are washed with 500 ml of saturated NaCl solution, dried over sodium sulfate and activated carbon and concentrated at 50°C using a rotary evaporator. Addition of 200 ml of methylene chloride to the residue and concentration are carried out a further three times. There are obtained 212.1 g of a clear brown oil of formula. ^1H NMR (300 MHz, CDCl_3): 9.03 (1 H, broad m, N-H); 8.04 (1 H, t, 1.4 Hz); 8.00 (1 H, dt, 7.8 and 1.4 Hz); 7.74 (1 H, dt, 7.8 and 1.4 Hz); 7.54 (1 H, t, 7.8 Hz); 3.55 (2H, dt, 6.0 and 4.7 Hz); 2.53 (2H, t, 5.8 Hz); 2.31 (6H, s); 1.77 (2H, m).

Step 2

Example 1006: 100 ml of tert-amyl alcohol are reacted under inert gas with 10.35 g of sodium at 130 °C (bath temperature) to form the corresponding alcoholate. Then a mixture, heated to 50 °C, of 13.8 g of 4-chlorobenzonitrile, 34.5 ml of succinic acid di-tert-amyl ester, 23.1 g of the nitrile of Example 1004 and 40 ml of tert-amyl alcohol is metered into the sodium tert-amylate over 4 hours, the temperature of the reaction mixture dropping to 105 °C. The resulting suspension is stirred for a further 4 hours and is then

物質搜尋範例(C.I. Pigment Red 254):

可獲取此物質供應商資料,包含純度、包材、交期等資料

Analyze

Analyze by:

Commercial Source

Chemieliva Pharmaceutical Product List2

HBCCChem Product List2

5A Pharmatech Product List1

abcr GmbH Product List1

Accel Pharmtech Product List1

AK Scientific Product Catalog1

AKos Out of Stock Catalog1

Ark Pharm Product List1

Atomax Chemicals Product List1

BOC Sciences Product List1

Sort by: Commercial Source

0 of 22 Commercial Sources Selected

Page: 1 of 2

Display Options

Commercial Source	Substance	Purity	Quantity	Purchasing Details	Stock Status	Ships Within
<input type="checkbox"/> 1. 5A Pharmatech Product List China Set Preference	84632-65-5 Pigment Red 254				Typically in stock	
<input type="checkbox"/> 2. abcr GmbH Product List Germany Set Preference	84632-65-5 Pigment Red 254		Grams	25.0 g, EUR 80.20		
<input type="checkbox"/> 3. Accel Pharmtech Product List United States Set Preference	84632-65-5 3,6-bis(4-chlorophenyl)-2,5-dihydro-Pyrrolo[3,4-c]pyrrole-1,4-dione	95-98%	Grams	25G 100G 500G		
<input type="checkbox"/> 4. AK Scientific Product Catalog United States Set Preference	84632-65-5 Pigment Red 254			Bulk Screening	Synthesis on demand	4 weeks
<input type="checkbox"/> 5. AKos Out of Stock Catalog Germany Set Preference	84632-65-5 Pyrrolo[3,4-c]pyrrole-1,4-dione, 3,6-bis(4-chlorophenyl)-2,5-dihydro-		Grams		Synthesis on demand	4 weeks
<input type="checkbox"/> 6. Ark Pharm Product List United States Set Preference	84632-65-5 3,6-Bis(4-chlorophenyl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione	95-98%	Grams	Order from Source 25 g, USD 105	Typically in stock	2 weeks

Polymer Reaction Research (EO-PO Polymer)



範例(EO-PO polymer: 產物):合成反應搜索

The screenshot displays the SciFinder software interface. On the left, the 'Explore' tab is active, showing search results for 'Research Topic "Aqueous PU resin" > references (265)'. Below this, there are sections for 'REFERENCES' and 'SUBSTANCES', each with a list of search criteria. The 'REACTIONS' section is also visible, showing 'Reaction Structure'.

The main window is the 'Structure Editor', which contains a large canvas for drawing chemical structures. The canvas shows two chemical structures: a three-membered ring with an oxygen atom (epoxide) and a four-membered ring with an oxygen atom (beta-lactone). The editor includes a toolbar with various drawing tools (atoms, bonds, rings, etc.) and a 'Drawing Editor' panel on the right. The 'Drawing Editor' panel has three radio buttons: 'Structure' (selected), 'Reaction', and 'Markush'. Below these, there is a section titled 'Get substances that match your query using:' with three radio buttons: 'Exact search', 'Substructure search' (selected), and 'Similarity search'. At the bottom of the 'Drawing Editor' panel are 'OK' and 'Cancel' buttons.

The bottom status bar of the Structure Editor shows the chemical formula $C_2H_4O \cdot C_3H_6O$ and the time 44.05 . 58.08.

範例(EO-PO polymer : 產物):合成反應搜索

REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

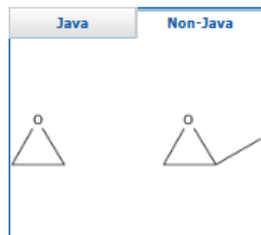
Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?


Structure Editor:



Click image to change structure or view detail.

Import CXF

Search

 Advanced Search ☐ Always Show

Search Type:

- ☒ Exact Structure
☐ Substructure
☐ Similarity

☐ Show precision analysis



Launch a SciFinder substance or reaction search directly from ChemBioDraw Ultra 14. [Learn More](#)

Characteristics

- ☐ Single component
☐ Commercially available
☐ Included in references

Classes

- ☐ Alloys
☐ Coordination compounds
☐ Incompletely defined
☐ Mixtures
☒ Polymers
☐ Organics, and others not listed

選擇反應形式POLYMER

範例(EO-PO polymer : 產物):合成反應搜索

Chemical Structure exact with limiters > substances (26642) > refine "exact" (15)

SUBSTANCES

Get References

Get Reactions

Get Commercial Sources

Tools

包含EO-PO為起始物 參與共聚
反應搜索到26642篇文獻

Create Keep Me Posted Alert

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Analyze Refine

Sort by: CAS Registry Number

0 of 26642 Substances Selected

Page: 1 of 1777

Sample Analysis

Substance Role

Uses ≥ 11972

Preparation ≥ 11647

Properties ≥ 4040

Biological Study ≥ 1756

Reactant or Reagent ≥ 1661

Process ≥ 1163

Prophetic in Patents ≥ 112

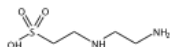
Analytical Study ≥ 108

Occurrence ≥ 79

Formation, Nonpreparative ≥ 40

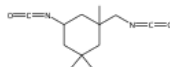
Show More

1. 1980887-13-5

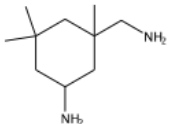


• Na

4098-71-9
C12 H18 N2 O1



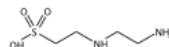
2855-13-2
C10 H12 N2



822-06-0
C4 H12 N2 O2

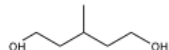


2. 1980887-11-3

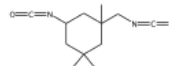


• Na

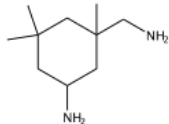
4457-71-0
C4 H14 O2



4098-71-9
C12 H18 N2 O1



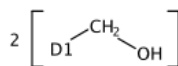
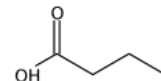
2855-13-2
C10 H12 N2



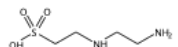
Click to view detail

3. 1980887-10-2

56743-27-2
C4 H12 O4

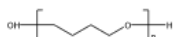


34730-59-1 (Component: 83111-01-7)
C4 H12 N2 O3 S . Na



• Na

25190-06-1
(C4 H8 O)n H2 O



4098-71-9
C12 H18 N2 O1

A CAS SOLUTION

範例(EO-PO polymer : 產物):合成反應搜索

Chemical Structure exact with limiters > substances (26642) > refine "exact" (15)

SUBSTANCES

Get References

Get Reactions

Get Commercial Sources

Tools

Create Keep Me Posted Alert

Send to SciPlanne

Analyze Refine

Sort by: CAS Registry Number

0 of 15 Substances Selected

Analyze by:

Substance Role

Properties 13

Preparation 8

Uses 8

Process 7

Biological Study 6

Analytical Study 5

Prophetic in Patents 4

Reactant or Reagent 4

Combinatorial Study 3

Formation, Nonpreparative 3

Show More

1. 1799500-53-0

~1

15448-47-2
 C_2H_4O



Absolute stereochemistry, Rotation (+).

75-21-8
 C_2H_4O



$(C_2H_4O \cdot C_2H_4O)_n$
INDEX NAME NOT YET ASSIGNED

4. 1706921-08-5

~1

15448-47-2
 C_2H_4O



R

2. 1799500-52-9

~1

16088-62-3
 C_2H_4O



Absolute stereochemistry, Rotation (-).

75-21-8
 C_2H_4O



$(C_2H_4O \cdot C_2H_4O)_n$
INDEX NAME NOT YET ASSIGNED

5. 1706921-04-1

~1

16088-62-3
 C_2H_4O

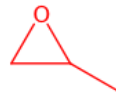


S

3. 1707286-19-8

~1

75-56-9
 C_2H_4O



75-21-8
 C_2H_4O



$(C_2H_4O \cdot C_2H_4O)_n$
Oxirane, 2-methyl-, polymer with oxirane, isotactic, triblock

6. 1294010-58-4

~1

75-56-9
 C_2H_4O



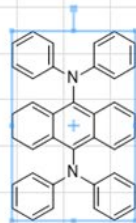
Use ChemDraw to Convert Chemical Structure to SciFinder



Undo Delete Ctrl+Z
Redo not available Shift+Ctrl+Z
Cut Ctrl+X
Copy Ctrl+C
Paste Ctrl+V
Clear Del
Select All Ctrl+A
Repeat SMILES Ctrl+Y
Copy As
Paste Special
Get 3D Model
Insert File...
Insert Object...
物件(O)

SMILES Alt+Ctrl+C
SLN
InChI
InChI Key
Formula: $C_{38}H_{30}N_2$
Exact Mass: 514.2409
Mol. Wt.: 514.6720
Decimals: 4
m/z: 514.2409 (100.0%), 515.2443
Elem. Anal.: C, 88.68; H, 5.88; N, 5.44
Paste

畫好結構，Edit並選擇Copy As選項，
選擇SMILES檔。



REFERENCES

Research Topic
Author Name
Company Name
Document Identifier
Journal
Patent
Tags

SUBSTANCES

Chemical Structure
Markush
Molecular Formula
Property
Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java



Import CXF

Search

Advanced Search ☒ Always Show

Characteristics

- ☐ Single component
- ☐ Commercially available
- ☐ Included in reference

Classes

- ☐ Alloys
- ☐ Coordination compounds
- ☐ Incompletely defined
- ☐ Mixtures
- ☐ Polymers
- ☐ Organics, and

Studies

- ☐ Analytical

Structure Editor

T

Add to editor by CAS Registry Number, SMILES, or InChI

Shortcut Keys

100%

Drawing Editor:

- ☒ Structure
- ☐ Reaction
- ☐ Markush

Get substances that match your query using:

- ☐ Exact search
- ☒ Substructure search
- ☐ Similarity search

OK

Cancel

**Add to editor by CAS
Number, SMILES, or InChI**



REFERENCES

Research Topic
 Author Name
 Company Name
 Document Identifier
 Journal
 Patent
 Tags

SUBSTANCES

Chemical Structure
 Markush
 Molecular Formula
 Property
 Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ?

Structure Editor:

Java Non-Java

Click to Edit

Import CXF

Search

Advanced Search ☒ Always Show

Characteristics ☐ Single component
☐ Commercially available
☐ Included in reference

Classes ☐ Alloys
☐ Coordination compounds
☐ Incompletely defined
☐ Mixtures
☐ Polymers
☐ Organics, and

Studies ☐ Analytical
☐ Biological

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Add to Editor

Enter CAS Registry Number, SMILES, or InChI:
C(C=CC=C5)=C2N(C6=CC=CC=C6)C7=CC=CC=C7
 Examples:
 50-00-0
 CCCO
 InChI=1S/C3H8O/c1-2-3-4/h4H,2-3H2,1H3

OK Cancel

Get substances that match your query using:
☐ Exact search
☒ Substructure search
☐ Similarity search

OK Cancel

Characteristics: ☐ Single component, ☐ Commercially available, ☐ Included in reference

Classes: ☐ Alloys, ☐ Coordination compounds, ☐ Incompletely defined, ☐ Mixtures, ☐ Polymers, ☐ Organics, and

Studies: ☐ Analytical, ☐ Biological

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 Journal
 Patent
 Tags

SUBSTANCES

Chemical Structure
 Markush
 Molecular Formula
 Property
 Substance Identifier

REACTIONS

Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE ⓘ

Structure Editor:



Import CXF

Search

Advanced Search ☒ Always Show

Characteristics ☐ Single component
☐ Commercially available
☐ Included in reference

Classes ☐ Alloys
☐ Coordination compounds
☐ Incompletely defined
☐ Mixtures
☐ Polymers
☐ Organics, and

Studies ☐ Analytical
☐ Biological

Structure Editor

Click and drag to select objects. Ctrl-click to select or deselect individual objects.

Structure Editor: ☒ Structure
☐ Reaction
☐ Markush

Get substances that match your query using:
☐ Exact search
☒ Substructure search
☐ Similarity search

OK
 Cancel

C₃₈H₃₀N₂ 514.67