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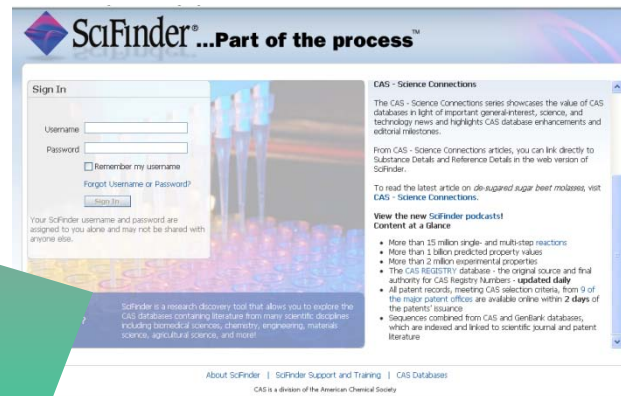
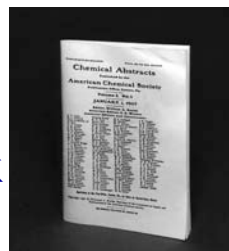
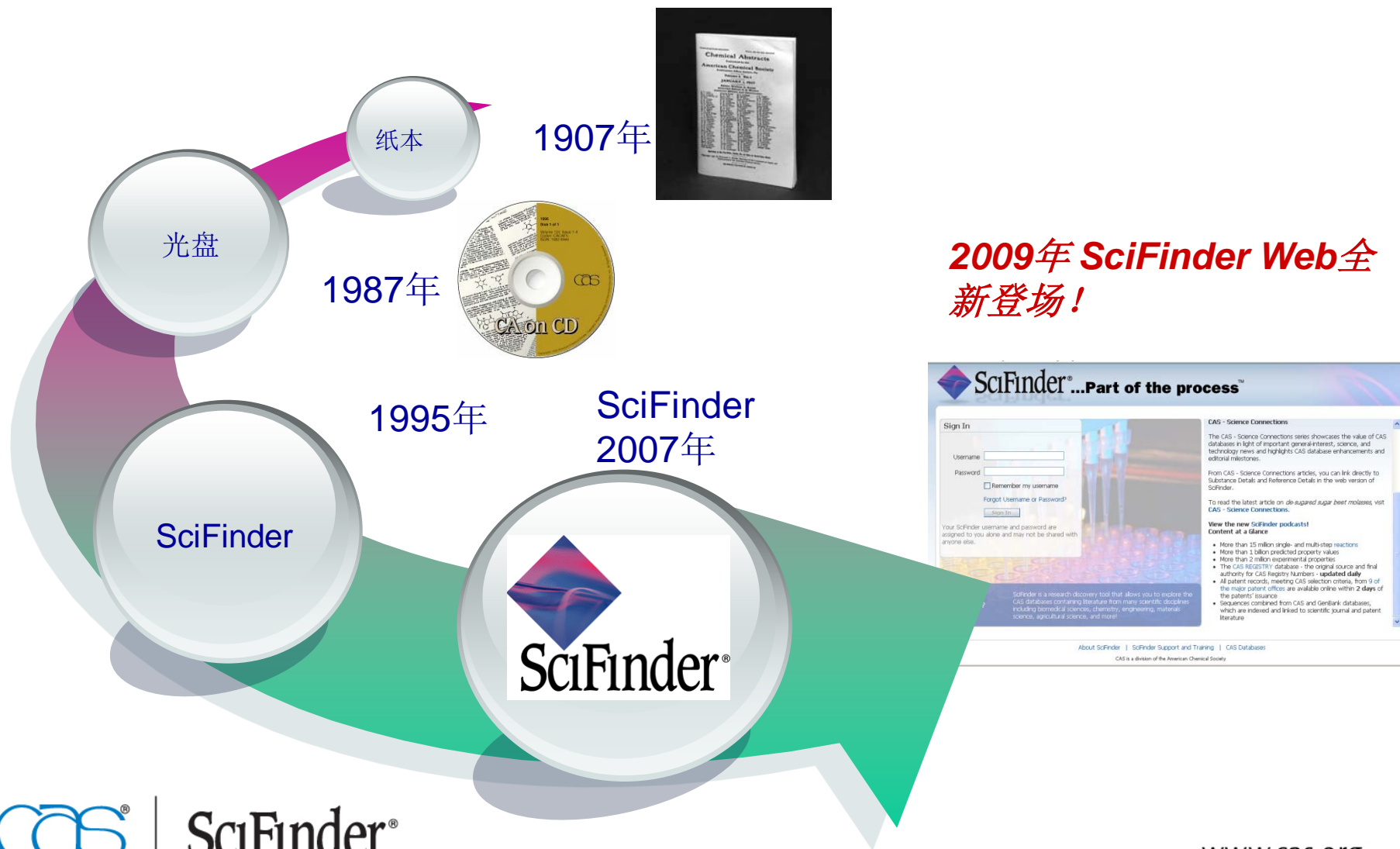
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SciFinder介绍----背景



SciFinder介绍----背景

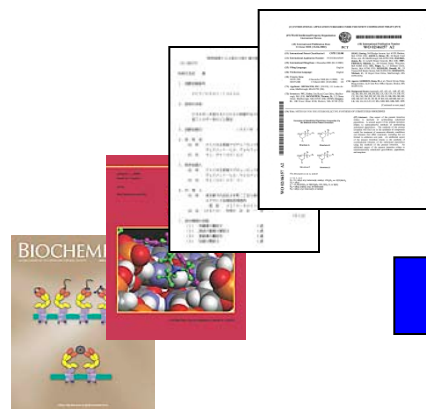
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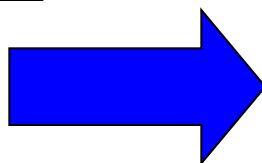
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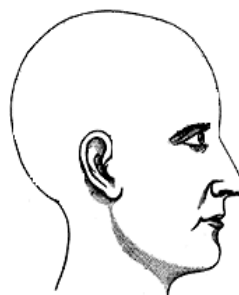
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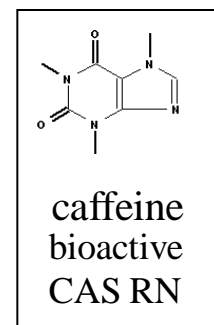
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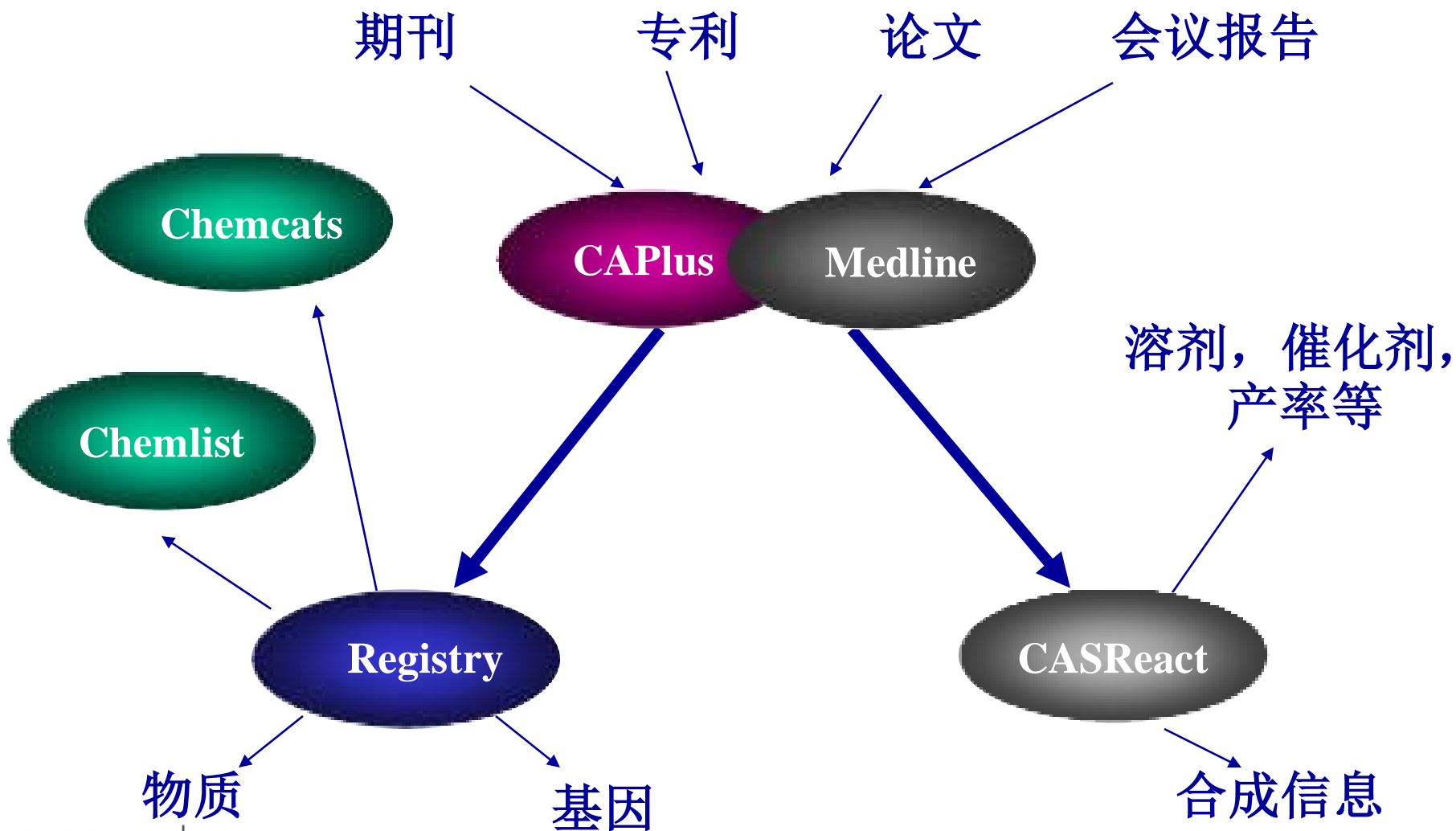


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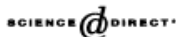
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CHEM. RES. CHINESE U. 2006, 22(1), 14–16

Fluorescence and Thermostability of Nanometer Porphyrin Trimer

SHI Ying-yan^{1,2}, FA Huan-bao¹, ZHENG Wen-qi¹, LI Di¹, SHAN Ning¹ and WANG Xing-qiao^{1,2*}

1. College of Chemistry, Jilin University, Changchun 130023, P. R. China;

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Received Feb. 28, 2005

A nanometer porphyrin trimer was firstly synthesized with 1,3-dibromopropane as a bridge-linked agent and the fluorescence property and thermostability were studied. The results show that the fluorescence property and thermostability of the trimer are different from those of monophyrin. The effects of the molecule structure on the optical property and the thermostability were also studied in detail.

Keywords Monophyrin; Porphyrin trimer; Fluorescence; Thermostability

Article ID 1005-9040(2006)01-014-03

Introduction

Porphyrin possesses some comparison with the porphyrin monomers are much attracting our properties in some aspects, such as energy transformation and electrochromic properties. Oligomeric porphyrins have been under intensive research for their potential applications in molecular electronic and optic fields. For instance, multiporphyrin tapes or arrays may serve as molecular wires^[1–5], molecular switches^[6–8], photo funnels^[9], information storage^[10], and third-order nonlinear optical materials^[11]. In order to understand the effects of the peripheral substitution groups and oligomerization of porphyrin on the properties, we studied the UV-Vis and fluorescence spectra, and thermostability of the porphyrin trimer synthesized via a convenient route by using 1,3-dibromopropane as a bridge-linked agent. The results show that the fluorescence and the thermostability of porphyrins can change significantly

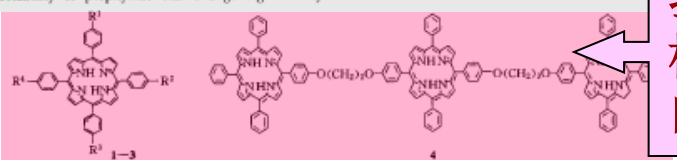


Fig. 1 The structures of porphyrin monomers 1–3 and the porphyrin trimer(4).

1. R¹ = OH, R² = R³ = H; 2. R¹ = R² = OH, R³ = H; 3. R² = O(CH₂)₃, R¹ = R³ = H.

* Supported by the National Natural Science Foundation of China(No. 20071014).

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of porphyrin peripheral substituents and the oligomer formation. The kind and the number of peripheral substituents have a tremendous influence on the fluorescence property of porphyrins. This investigation provides a valuable reference for the research of molecular wires and logic gate circuits in molecular electronics.

Experimental

Pyrrrole (Fluka Chemika-Biochemika) and 1,3-dibromopropane (reagent grade) were freshly distilled prior to use. DMF and anhydrous K₂CO₃ were dried. Other chemicals were of reagent grade. The UV-Vis spectra were recorded on a Cintra 10 e UV-Visible spectrometer(GBC, Australia). The fluorescence spectra were obtained with a Perkin Elmer LS55 Fluorescence spectrometer. The TG/DTA curves were measured by a NETZSCH STA 449C analyzer.

The syntheses of all porphyrins (see Fig. 1) have been described elsewhere^[11].

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Results and Discussion

1 UV-Vis Spectrum

The room temperature solution electronic absorption values are almost identical in Table 1. The characteristic absorption bands of porphyrins are represented by the Soret band in the visible region, and the other four absorption maxima around 516, 550, 590 and 645 nm can be attributed to the Q-bands, corresponding to $a_{1u}(\pi) \rightarrow e_g^*(\pi)^{12}$. This indicates that porphyrin monomers being linked by —CH₂— have little effect on the electron delocalization of a π -conjugated porphyrin system.

Table 1 UV-Vis absorption spectra data of porphyrins 1–4 in CH₂Cl₂

No.	Q band, λ /nm(10 ³ ϵ)				
	1	2	3	4	
1	418.40(0.3)	515.68(2.3)	547.68(1.8)	589.92(1.4)	647.52(1.2)
2	418.40(0.3)	515.68(1.0)	550.24(0.7)	589.92(0.4)	648.80(0.2)
3	418.40(0.4)	515.68(1.8)	552.80(1.3)	592.48(0.2)	648.80(0.6)
4	419.68(0.2)	518.24(0.1)	554.08(0.01)	593.76(-0.3)	648.80(-0.1)

2 Fluorescence Spectrum

Fig. 2 shows the fluorescence emission spectra of porphyrin monomers 1–3 and a porphyrin trimer. When porphyrins 1–4 were excited at 400 nm, the fluorescence emission peaks of porphyrins 1 and 2 lie around 471, 651 and 714 nm; the fluorescence emission peaks of porphyrins 3 and 4 are at 653 and 717 nm. The fluorescence emission peaks of porphyrins 1 and 2 at 471 nm can be assigned to the S₁ → S₀ transition and it is corresponding to the fluorescence emission peak at 418.4 nm of their electronic absorption spectra. The fluorescence emission peaks at the same position disappear in the fluorescence emission spectra of porphyrins 3 and 4. The fluorescence emission peaks at 650 and 714 nm of porphyrins 3 and 4 can be assigned to the S₁ → S₀ transition and correspond with Q(0, 0), Q(0, 1) of porphyrins 1–4^[12].

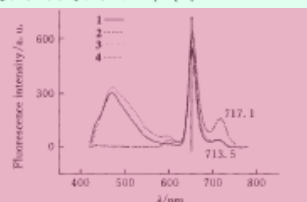


Fig. 2 The fluorescence emission spectra of porphyrin monomers 1–3 and a trimer(4) (excited at 400 nm).

The experimental results indicate that in dichloroethane, compared with those at 418 nm in the absorption spectrum, the fluorescence emission peak at 471 nm has several-nanometer displacement, which is caused by the lattice relaxation, that is, the electron has given its small part of energy to the crystal lattice by means of its interaction with crystal lattice in the form of heat, intensifying the thermal vibration of the

H₂DHDPP(2). The band around 420 nm is assigned to the Soret band which arises from the transition of $a_{1u}(\pi) \rightarrow e_g^*(\pi)$, and the other four absorption maxima around 516, 550, 590 and 645 nm can be attributed to the Q-bands, corresponding to $a_{2u}(\pi) \rightarrow e_g^*(\pi)^{12}$. This indicates that porphyrin monomers being linked by —CH₂— have little effect on the electron delocalization of a π -conjugated porphyrin system.

crystal lattice.

The main routes for the electrons in a conjugated system to transit from the excited states to the ground states are fluorescence radiation transition and nonradiation transition (interchange and system crossing). Compared with that of porphyrin 1, the fluorescence intensity of porphyrin 2 at 471 nm is stronger, for porphyrin 2 has two hydroxyphenyl groups at the meso-position, while porphyrin 1 has only one hydroxyphenyl group at the meso-position. Therefore, the different peripheral hydroxyphenyl groups have a tremendous influence in the forms of energy transition. The fluorescence emission peaks at 471 nm transit from a single excited state to the ground state. At 471 nm, along with the increase of porphyrin peripheral hydroxyphenyl groups, the non-radiation transition of electrons becomes weaker, while the fluorescence radiation transition becomes stronger. At the same position, the fluorescence emission peaks of porphyrins 3 and 4 nearly vanish because of the change of the porphyrin peripheral functional groups and polymerization. The non-radiation transition of electrons from the excited state to the ground state is the main form. This result shows that the porphyrin peripheral functional groups and polymerization have tremendous influence on the fluorescence property of porphyrins.

Fig. 3 shows the fluorescence excitation spectrum (monitored at 653 nm) and the emission spectrum of the trimer (excited at 400 or 327 nm) in CH₂Cl₂. The results in Fig. 3 confirm that different excitation wavelengths can only affect the fluorescence emission intensity, while they have no influence on peak position.

Fig. 4 shows the fluorescence excitation spectrum and the emission spectrum of the porphyrin trimer in different solvents, CH₂Cl₂ or DMF. It can be seen that the fluorescence intensity in DMF is stronger than that

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1. Fluorescence and thermostability of nanometer porphyrin trimer

摘要

By: Shi, Ying-yan; Fa, Huan-bao; Zheng, Wen-q; Li, Di; Shan, Ning; Wang, Xing-qiao

A nanometer porphyrin trimer was firstly synthesized with 1,3-dibromopropane as a bridge-linked agent and the fluorescence property and thermostability were studied. The results show that the fluorescence property and thermostability of the trimer are different from those of the mono-porphyrin. The effects of the mol. structure on the optical property and the thermostability were also studied.

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fluorescence and thermostability of porphyrins and nanometer porphyrin trimer

Properties

UV and visible spectra

of porphyrins and nanometer porphyrin trimer

Solvent polarity effect

on fluorescence and thermostability of porphyrins and nanometer porphyrin trimer

Supplementary Terms

porphyrin trimer nanometer bromopropane bridging fluorescence thermostability

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Properties

109-64-8

fluorescence and thermostability of nanometer porphyrin trimer with bridge-linking agent of

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130023

题录

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Results and Discussion
1 UV-Vis Spectrum

The room temperature solution electronic absorption values are almost identical in Table 1. The characteristic absorptions of porphyrins are represented by the UV-Vis spectra of compounds 3 and 4 with a typical set of Soret bands and Q-bands in the visible region, which are similar to those of H₂MHTPP(1) and trans-

Table 1 UV-Vis absorption spectra data of porphyrins 1-4 in CH₂Cl₂

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	λ	DP σ	λ	DP σ
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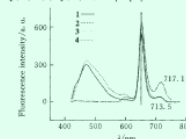


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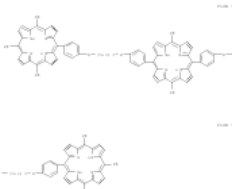
H₂DHDP(2). The band around 420 nm is assigned to the Soret band which arises from the transition of $a_{1g}(\pi) \rightarrow e_g^*(\pi)$, and the other four absorption maxima around 516, 550, 590 and 645 nm can be attributed to the Q-bands, corresponding to $a_{1g}(\pi) \rightarrow e_g^*(\pi)$ ^[1]. This indicates that porphyrin monomers being linked by -CH₂- have little effect on the electron delocalization of a π -conjugated porphyrin system. crystal lattice.

The main routes for the electrons in a conjugated system to transit from the excited states to the ground states are fluorescence radiation transition and non-radiation transition (interchange and system crossing). Compared with that of porphyrin 1, the fluorescence intensity of porphyrin 2 at 471 nm is stronger, for porphyrin 2 possesses two hydroxyphenyl groups at the meso-position, but porphyrin 1 has only one hydroxyphenyl group at the meso-position. Therefore, the different numbers of the porphyrin peripheral hydroxyphenyl groups result in the difference in the forms of energy releasing when electrons transit from a single excited state to the ground state. At 471 nm, along with the increase of porphyrin peripheral hydroxyphenyl groups, the non-radiation transition of electrons becomes weaker, while the fluorescence radiation transition becomes stronger. At the same position, the fluorescence emission peaks of porphyrins 3 and 4 nearly vanish because of the change of the porphyrin peripheral functional groups and polymerization. The non-radiation transition of electrons from the excited state to the ground state is the main form. This result shows that the porphyrin peripheral functional groups and polymerization have tremendous influence on the fluorescence property of porphyrins.

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1. Substance Detail
757977-32-5

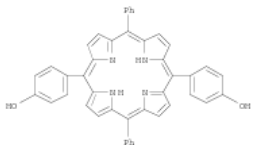


C138 H98 N12 O4

21H,23H-Porphine, 5,15-diphenyl-10,20-bis[4-(3-[4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)phenoxy]propoxy)phenyl]- (9C1)

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2. Substance Detail
147859-70-9

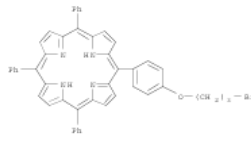


C44 H30 N4 O2

Phenol, 4,4'-(10,20-diphenyl-21H,23H-porphine-5,15-diyl)bis-

- ~15 References
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3. Substance Detail
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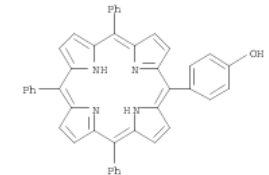


C47 H35 Br N4 O

21H,23H-Porphine, 5-[4-(3-bromopropoxy)phenyl]-10,15,20-triphenyl-

- ~22 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

4. Substance Detail
87345-22-0



C44 H30 N4 O

Phenol, 4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)-

- ~206 References
- Reactions
- Commercial Sources
- Regulatory Information
- Link

5. Substance Detail
109-64-8

Br-CH₂-CH₂-CH₂-Br

C3 H6 Br2

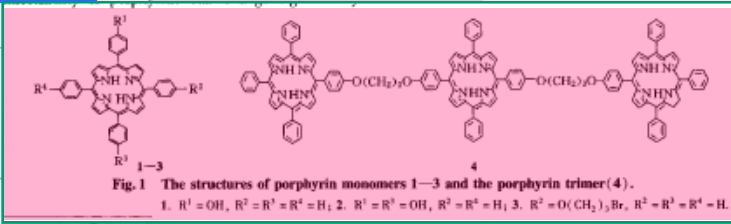
Propane, 1,3-dibromo-

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Substances	
87345-22-0 102202-47-1 147859-70-9 757977-32-5	fluorescence and thermostability of Properties
109-64-8	fluorescence and thermostability of nanometer porphyrin trimer with bridge-linking agent of Other use, unclassified; Uses

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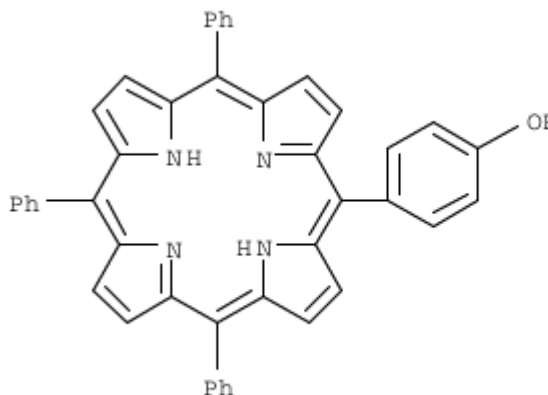
CAS Registry Number: 87345-22-0

C₄₄ H₃₀ N₄ O

Phenol, 4-(10,15,20-triphenyl-21H,23H-porphin-5-yl)-
5,10,15-Triphenyl-20-(4-hydroxyphenyl)porphyrin; 5-(4-Hydroxyphenyl)-10,15,20-triphenylporphine; 5-(4-Hydroxyphenyl)-10,15,20-triphenylporphyrin; 5-(4-Hydroxyphenyl)-10,15,25-triphenylporphyrin; 5-(p-Hydroxyphenyl)-10,15,20-triphenylporphyrin; meso-5-(4'-Hydroxyphenyl)-10,15,20-triphenylporphyrin

Component

Deleted CAS Registry Numbers: 869660-92-4



Experimental Properties: [Chemical](#) [Spectra](#) [Thermal](#)

Chemical Properties

Potential of Electrode Reaction

Value

See full text

Conditions

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Spectra Properties

Carbon-13 NMR Spectrum

Value

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Conditions

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Emission/Luminescence Spectrum

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IR Absorption Spectrum

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IR Spectrum

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Mass Spectrum

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UV and Visible

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Emission/Luminescence Spectrum

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UV and Visible Spectrum

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1 of 6

Thermal Properties

Melting Point

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Melting Point

>300 °C

Solv: (

Melting Point

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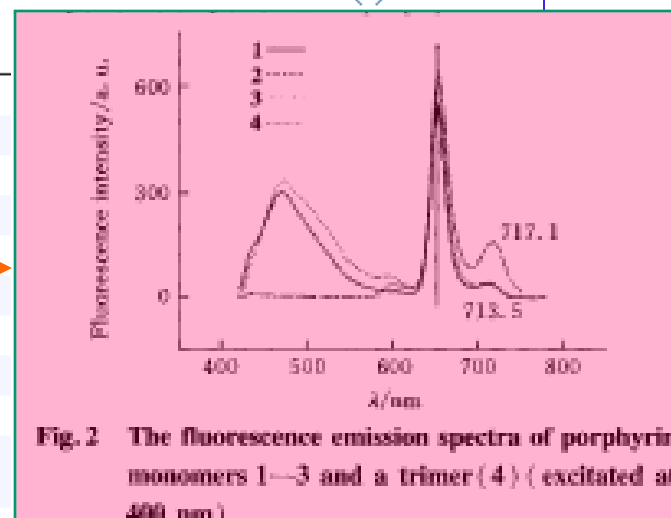


Fig. 2 The fluorescence emission spectra of porphyrin monomers 1–3 and a trimer (4) (excited at 400 nm).

(2) CAS

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- **SciFinder**中的反应检索

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(bold* = required)

CONTACT INFORMATION

First Name*:

Last Name*:

E-mail*:

Confirm E-mail*:

Phone Number:

Fax number:

Area of Research: Select one

Job Title: Select one

USERNAME AND PASSWORD

Username*: [Tips](#)

Password*:

Re-enter Password*:

SECURITY INFORMATION

Security Question*: Select one [Why?](#)

Answer*:

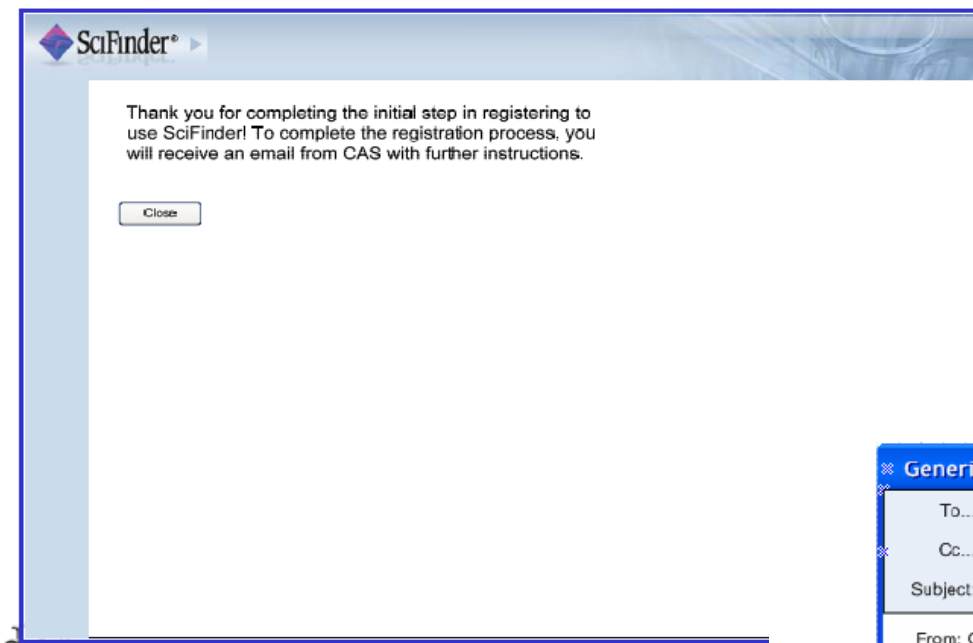
Callout 1: Email domain must match valid domain(s) and the entire address must be unique.

Callout 2: Username and password must meet minimum requirements and be unique.

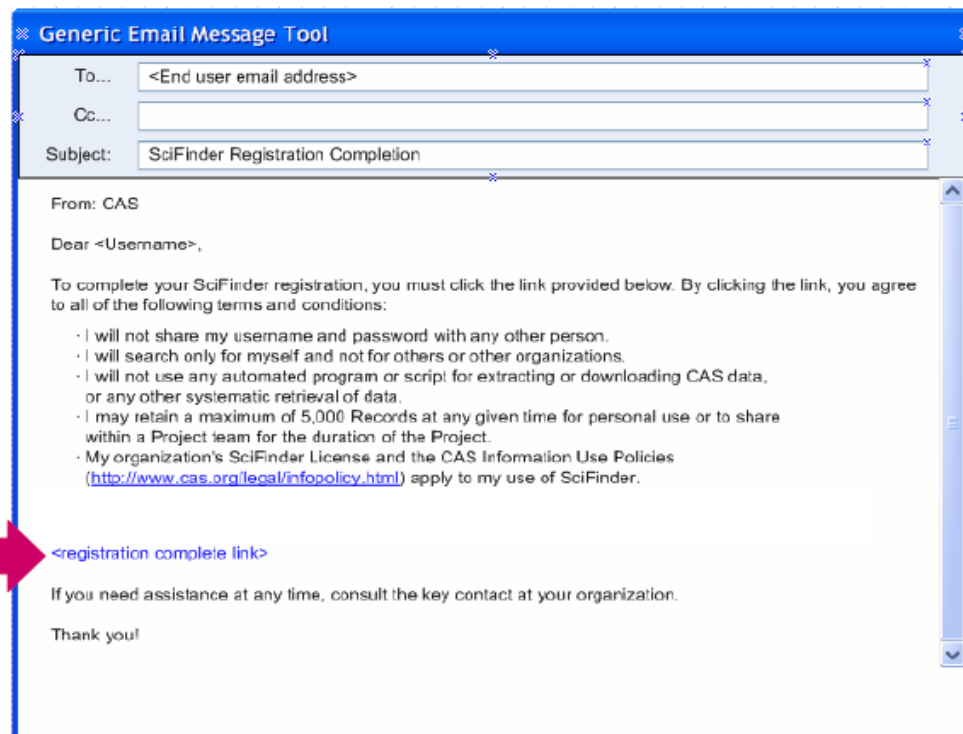
Callout 3:

- What is your favorite color?
- What is the name of the city where you grew up?
- What is the name of your favorite pet?
- What is your favorite musical instrument?
- What is your ideal vacation location?

对新ID的Email确认



需要点击邮件中的确认链接



使用这个链接登陆SciFinder



SciFinder的登陆界面



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Password

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Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.

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What is SciFinder?

SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!

<https://scifinder.cas.org>

Welcome to SciFinder!

60 Million: It's more than just a number

CAS REGISTRY today registered its 60 millionth substance, keeping pace with the rapid growth of worldwide chemical research. The substance was included in a Chinese patent application claiming compounds with potential therapeutic activity, submitted by the Institute of Materia Medica, Chinese Academy of Medical Sciences. For complete information, [Click Here](#).

Fast forward from ideas to results with the power of SciPlanner

CAS is excited to announce enhancements to your SciFinder experience. These enhancements are now available to you and all SciFinder users at your organization. As the new features are designed to improve efficiency and productivity, we encourage you to log in and try them out today!

SciFinder enhancements include:

- SciPlanner - a groundbreaking interactive workspace that allows researchers to more quickly identify synthesis options to design the best pathway and approaches

SciFinder 的主检索界面

文献，物质，反应检索入口，默认开始检索文献

在机构中寻找或添加联系人

The screenshot shows the SciFinder main search interface. At the top, there are three main navigation buttons: "Explore References", "Explore Substances", and "Explore Reactions". Below these, the user is logged in as "Verna Wong" and can "Sign Out". On the right side, there are links for "Saved Answer Sets", "Keep Me Posted Results", "NEW! S Planner", "My Connections", "Help", "History", and "Preferences".

The main search area is titled "Explore References" and includes a "Research Topic" search box with a "Search" button. Below the search box, there are examples of search terms: "The effect of antibiotic residues on dairy products" and "Photocyanation of aromatic compounds".

On the left side of the search area, there is a dropdown menu for "Research Topic" with the following options: "Author Name", "Company Name", "Document Identifier", "Journal", "Patent", and "Tags".

Below the search area, there are filters for "Publication Year(s)" and "Document Type(s)". The "Document Type(s)" filter includes checkboxes for: Biography, Book, Clinical Trial, Commentary, Conference, Dissertation, Editorial, Historical, Journal, Letter, Patent, Preprint, Report, and Review.

On the right side, there are three panels: "Saved Answer Sets" (listing various search results like "lipitor patent", "Polymyxin B - Bio-act", etc.), "Keep Me Posted Results" (showing "No profiles exist"), and "My Connections" (showing "No invitations to connect").

Annotations in Chinese are present:

- A blue box highlights the "Explore References", "Explore Substances", and "Explore Reactions" buttons, with an arrow pointing to the text "文献，物质，反应检索入口，默认开始检索文献".
- A blue box highlights the "My Connections" link in the top right, with an arrow pointing to the text "在机构中寻找或添加联系人".
- A blue box highlights the "Research Topic" dropdown menu, with an arrow pointing to the text "可用的检索方法".
- A blue box highlights the "Saved Answer Sets" panel, with an arrow pointing to the text "保存过的结果集".
- A blue box highlights the "Keep Me Posted Results" panel, with an arrow pointing to the text "邮件提醒结果集".

寻找和添加联系人

My Connections BETA + Invite Colleagues To Connect

Connections | **Invitations**

0 Connections | 0 Selected | Remove


You currently have no connections.

Establishing connections with colleagues within your organization is a key part of the SciFinder experience. My Connections lets you establish connections with colleagues within your organization with SciFinder references. To establish a connection, you must be connected to the organization of the colleague you wish to connect to. You can remove a connection at any time.

Invite Colleagues To Connect * Required

Enter the full or partial name of a colleague within your organization

Last Name: * **First Name:**



CAS is a division of the A

提纲

- **SciFinder**介绍
- **SciFinder**检索界面
- **SciFinder**中的文献检索
- **SciFinder**中的物质检索
- **SciFinder**中的反应检索

SciFinder包含的文摘数据库

CA plus(1907-至今)

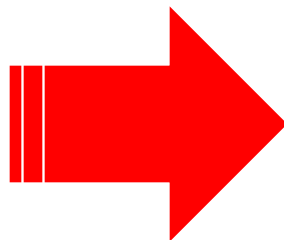
- 包含了**CA**纸本和光盘的所有内容。
- 涵盖了**98%**世界化学化工文献。
- **10000**多种期刊和**61**个专利发行机构的专利（含专利族）。除此之外，会议录、技术报告、图书、学位论文、评论、会议摘要、电子期刊、网络预印本；
- 每天更新

Medline

- 美国国立医学图书馆出品
- 生命科学医学相关
- 临床报告，毒理、病理学报告

可通过关键词、作者姓名、机构名称等查询，也可通过物质和反应链接

检索光催化技术用于污水处理相关的文献



随着工业的发展、城市规模的不断扩大，水污染成为威胁人类的健康和安全的一大难题。

光催化技术是污水处理技术发展的重要方向。

设置合适的关键词获得最为全面和相关的文献

获得光催化技术用于污水处理相关的参考文献
photocatalyst for wastewater

The screenshot shows the SciFinder web interface. At the top, there are navigation links for 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below this, a user is logged in as 'Verna Wong'. The main search area is titled 'Explore References' and contains a search bar with the text 'photocatalyst for wastewater'. To the right of the search bar is a 'Search' button. Below the search bar, there are examples of search results: 'The effect of antibiotic residues on dairy products' and 'Photocyanation of aromatic compounds'. A blue arrow points from the text '使用介词of, with, by, beyond来连接关键词' to the search bar. On the left side of the search bar, there is a dropdown menu with options: 'Research Topic', 'Author Name', 'Company Name', 'Document Identifier', 'Journal', 'Patent', and 'Tags'. Below the search bar, there are fields for 'Publication Year(s)' and 'Document Type(s)'. The 'Publication Year(s)' field has examples: '1995, 1995-1999, 1995-, -1995'. The 'Document Type(s)' field has checkboxes for 'Biography', 'Book', 'Dissertation', 'Editorial', 'Patent', and 'Preprint'.

Research Topic

Research Topic ⓘ

photocatalyst for wastewater

Search

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

使用介词of, with, by, beyond来连接关键词

Publication Year(s) ⓘ

Examples: 1995, 1995-1999, 1995-, -1995

Document Type(s) ⓘ

Biography Dissertation Patent
 Book Editorial Preprint

检索前，也可以提前限定一些内容，比如年限，文献类型等

设置合适的关键词获得最为全面和相关的文献

SciFinder® Explore References Explore Substances Explore Reactions

Welcome Verna Wong | Sign Out

Create Keep Me Posted Research Topic "photocatalyst for wastewater"

Research Topic Candidates

5 Topics 1 Selected

Select All Deselect All

Research Topic Candidates	References
<input type="checkbox"/> 285 references were found containing "photocatalyst for wastewater" as entered.	285
<input checked="" type="checkbox"/> 1990 references were found containing the two concepts "photocatalyst" and "wastewater" <u>closely associated with one another.</u>	1990
<input type="checkbox"/> 3893 references were found where the two concepts "photocatalyst" and "wastewater" were <u>present anywhere in the reference.</u>	3893
<input type="checkbox"/> 33021 references were found containing the concept "photocatalyst".	33021
<input type="checkbox"/> 403341 references were found containing the concept "wastewater".	403341

Get References

“Concept”表示做了同意词的扩展

“Closely associated with one another”表示同时出现在一个句子中

“were present anywhere in the reference”表示同时出现在一段话中

获得最为全面和相关的文献

文献记录数

可以快速浏览文献的内容，是否符合要求

文献分析限定工具

The screenshot displays the SciFinder search results page for the query "photocatalyst for wastewater". The interface includes a navigation bar with options like "Explore References", "Explore Substances", and "Explore Reactions". The search results are listed in a table with columns for "References", "Get Substances", "Get Reactions", "Get Related", "Tools", and "Send to SciPlanner".

Annotations on the screenshot include:

- A blue box around "1969 References" in the top left, with an arrow pointing to the text "文献记录数".
- A blue box around the first search result title, with an arrow pointing to the text "可以快速浏览文献的内容，是否符合要求".
- A blue box around the "Analysis" tab in the right sidebar, with an arrow pointing to the text "文献分析限定工具".
- A blue box around the abstract text of the first result, with an arrow pointing to the text "检索命中的字段".

The first search result is:

1. **Wastewater treatment over WO₃ photocatalyst combined with ozonation under visible light irradiation**
 By Nishimoto, S.; Mano, T.; Kameshima, Y.; Miyake, M.
 From Pacificchem 2010, International Chemical Congress of Pacific Basin Societies, Honolulu, HI, United States, December 15-20, 2010 (2010), ENVR-265. Language: English, Database: CAPLUS

Water treatment to remove org. pollutants from industrial process **waters** and **wastewaters** is an important issue worldwide. In recent years, TiO₂ **photocatalyst** combined with ozonation (i.e., oxidn. by ozone) under UV irradsn. has attracted considerable attention due to its high treatment efficiency. Some org. compds. are degraded little or slowly by photocatalysis or ozonation alone, but combining these two methods considerably enhances pollutant removal from **wastewater**. From an economic perspective, it is desirable to reduce the energy consumed by the ozone generator in the process. Thus, applying visible-light-responsive **photocatalysts** that utilize solar energy to **water** treatment will enable more economic **water** treatment. In the present study, we accordingly investigated the effect of combining WO₃ **photocatalyst** and ozone under visible light irradsn. (O₃/vis/WO₃) on **wastewater** treatment. The O₃/vis/WO₃ treatment exhibited a much higher total org. carbon removal than ozonation alone. Bare WO₃ was found to function as a visible-light-responsive **photocatalyst** for decompn. of org. compds. in the presence of ozone, which readily reacts with photoexcited electrons in the conduction band of WO₃.

The second search result is:

2. **Synthesis and application of novel mesoporous-assembled SrTi_xZr_{1-x}O₃-based nanocrystal photocatalysts for azo dye degradation**
 By Khunrattanaphon, Pattharin; Chavadej, Sumaeth; Sreethawong, Thammanoon
 From Chemical Engineering Journal (Amsterdam, Netherlands) (2011), 170(1), 292-307. Language: English, Database: CAPLUS

In this work, novel mesoporous-assembled SrTi_xZr_{1-x}O₃ nanocrystal **photocatalysts** were successfully synthesized by a sol-gel process with the aid of a structure-directing surfactant under mild conditions. The photocatalytic activity of the synthesized **photocatalysts** for degrading Acid Black (AB) diazo dye used as a model contaminant in textile **wastewater** was investigated by varying Ti-to-Zr molar fraction, calcination conditions, and Pt loading. The synthesized **photocatalysts** were systematically characterized by TG-DTA, N₂ adsorption-desorption anal., XRD, UV-visible spectroscopy, SEM-EDX, TEM-EDX, TPR, and H₂ chemisorption. The photocatalytic activity results showed that without Pt loading, the mesoporous-assembled SrTi_xZr_{1-x}O₃ **photocatalyst** with a Ti-to-Zr molar fraction of 0.9:0.1 (i.e. SrTi_{0.9}Zr_{0.1}O₃) calcined at 700 °C for 4 h provided a max. degrading rate const. as compared to the other SrTi_xZr_{1-x}O₃ **photocatalysts**. The optimum Pt loading of 1 wt.% by a single-step sol-gel method on the mesoporous-assembled SrTi_{0.9}Zr_{0.1}O₃ **photocatalyst** was found to greatly increase the degrading rate const. of the AB dye. Furthermore, the calcination temp. was found to significantly affect the degrading rate const. of the Pt-loaded mesoporous-assembled SrTi_{0.9}Zr_{0.1}O₃ **photocatalyst**.

The right sidebar shows an "Analysis" panel with a table of authors and their corresponding counts:

Author Name	Count
Zhao Jincal	14
Liu Hong	13
Tanaka Keiichi	13
Taoda Hiroshi	12
Fujishima Akira	11
Liu Wei	11
Ma Wanhong	11
Song Limin	11
Fu Xianzhi	10
Hidaka Hisao	10

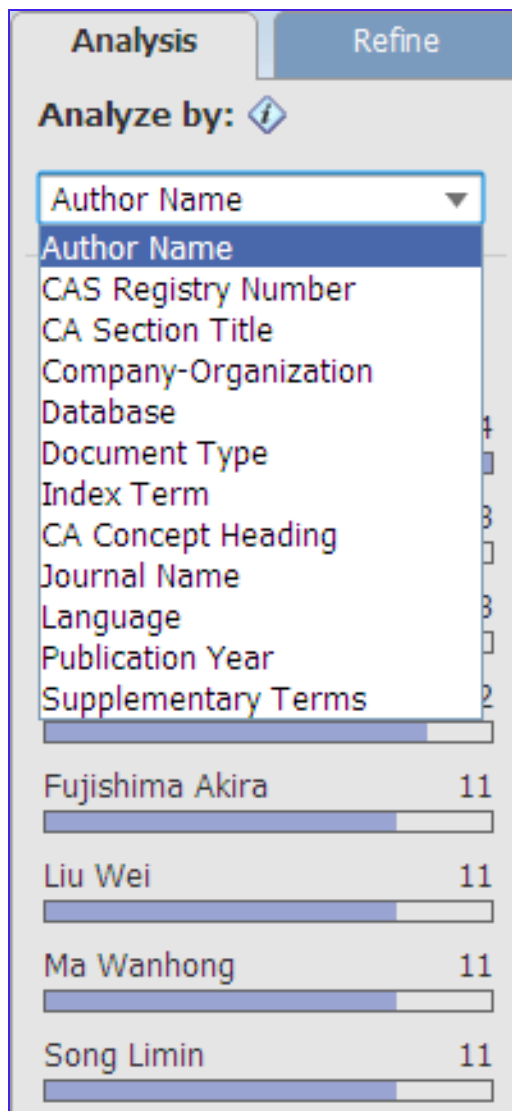
At the bottom of the sidebar, there is a "Show More" button and a "Categorize" section.

SciFinder中强大的文献的后处理功能，帮助我们缩小文献范围

SciFinder为文献分析提供：

12种分析方法
7种限定工具

包括索引词，学科，作者名，机构名，文献类型，期刊名称，出版年限，出版语言等。



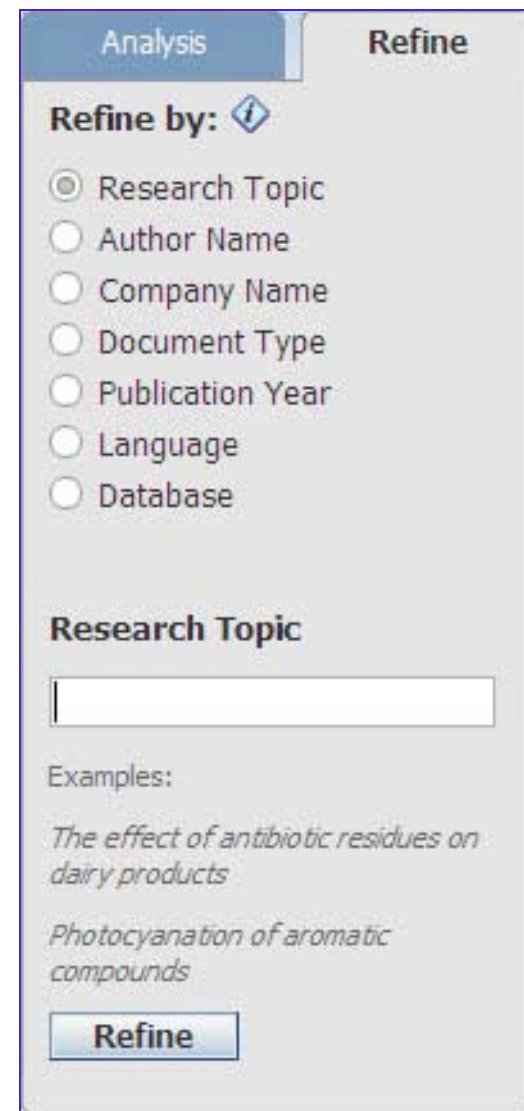
Analysis Refine

Analyze by: ⓘ

Author Name

Author Name
CAS Registry Number
CA Section Title
Company-Organization
Database
Document Type
Index Term
CA Concept Heading
Journal Name
Language
Publication Year
Supplementary Terms

Fujishima Akira	11
Liu Wei	11
Ma Wanhong	11
Song Limin	11



Analysis **Refine**

Refine by: ⓘ

Research Topic
 Author Name
 Company Name
 Document Type
 Publication Year
 Language
 Database

Research Topic

Examples:

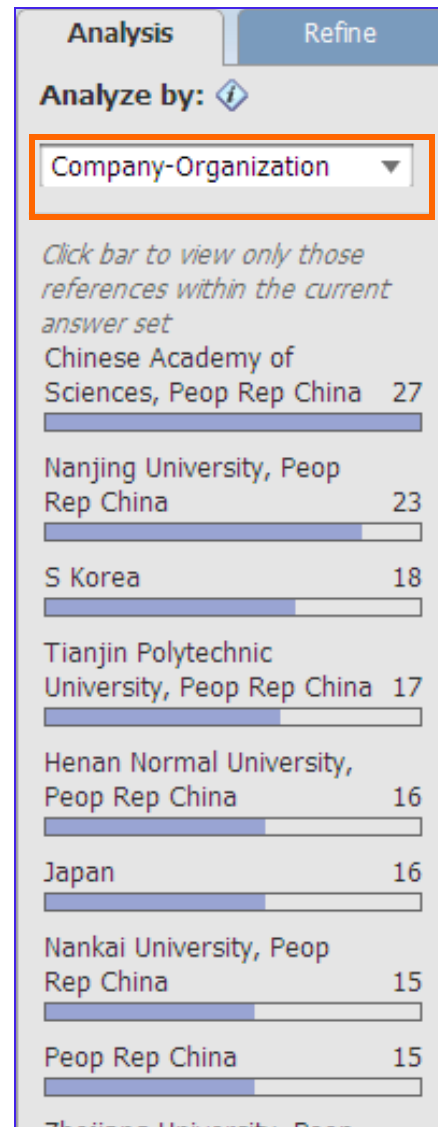
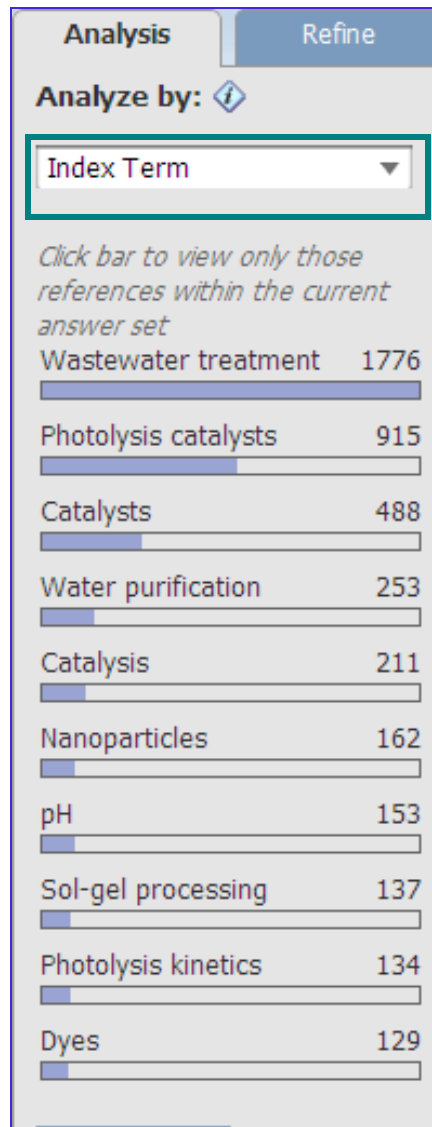
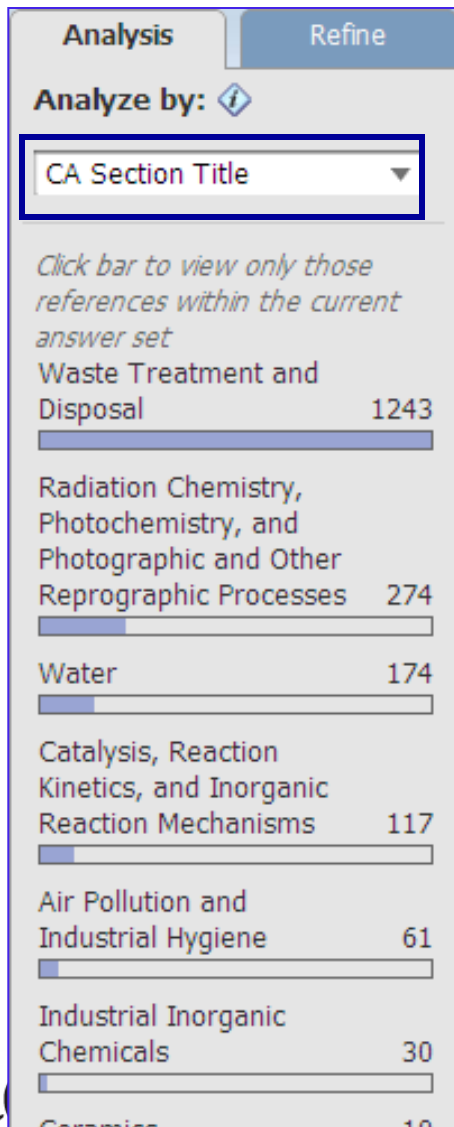
The effect of antibiotic residues on dairy products

Photocyanation of aromatic compounds

Refine

对文献进行多角度分析

- 这些文献涉及了哪些领域？
- 文献中出现了哪些重要概念？
- 哪些机构的研究处于领先水平？



对文献进行限定，缩小范围

通过文献类型直接获取专利

Analysis
Refine

Refine by: ⓘ

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

Document Type(s)

- Biography
- Book
- Clinical Trial
- Commentary
- Conference
- Dissertation
- Editorial
- Historical
- Journal
- Letter
- Patent
- Preprint
- Report
- Review

Refine

Explore References
Explore Substances
Explore Reactions

Welcome Verna Wong | Sign Out

Create Keep Me Posted > Research Topic "photocatalyst for wastewater" > references (1969) > refine "Patents only" (696)

References
Get Substances
Get Reactions
Get Related
Tools
Send to SciPlanner

696 References
0 Selected
Save Print Export

Select All
Deselect All
Sort by: Accession Number
Answers per Page [15]
1 2 3 4 5 6 ... 47

1. **Nanoscale titanyl pyrophosphate photocatalyst and its preparation method**
 By Zhao, Wanting
 From Faming Zhuanni Shenqing (2011), CN 102029168 A 20110427. Language: Chinese, Database: CAPLUS
 The title **photocatalyst** consists of titanyl pyrophosphate ultrafine powders with particle size of 10-60 nm. The title method comprises (1) using surfactant-contg. deionized **water** or anhyd. ethanol as solvent, adding Ti source, and stirring to obtain 0.1-1.1 mol/L Ti-contg. soln. A, (2) adding 0.5-5 mol/L alk. soln. under stirring, and stirring to form yellow or white oily suspension B, (3) adding 1-5 mol/L hydrogen peroxide soln. into the suspension B, and stirring to obtain oily suspension C, (4) dissolving P source in deionized **water** or anhyd. ethanol to obtain 0.1-1.1 mol/L P-contg. soln., adding into the suspension C, stirring for 5-60 min, aging at 15-30°C for 0.5-3 days, ultrasonically washing with deionized **water** and anhyd. ethanol, centrifuging, and repeating washing and centrifuging for 3-6 times, and (5) drying the slurry at 80-150°C for 1-5 h, calcining at 300-500°C for 2-6 h, and ball-milling.

Substances Reactions Citings Full Text Link Comments Tags

2. **Photoelectrocatalytic method for treatment of organic wastewater using photoelectric rotary disk with sharp conical structure as photoanode**
 By Jia, Jinping; Li, Kan; Yang, Chen; Wang, Yalin
 From Faming Zhuanni Shenqing (2011), CN 102030387 A 20110427. Language: Chinese, Database: CAPLUS
 The title method comprises: (1) adopting stainless steel or Ti disk as substrate, and processing the substrate to form sharp conical structure, (2) lowering titania **photocatalyst** on the substrate, forming photoelec. rotary disk on rotating shaft to be used as photoanode, and connecting the rotating shaft with motor, (3) placing Cu sheet cathode at the inner wall of the reaction tank and opposite to the photoanode, and connecting with the neg. electrode of DC power source via wire, (4) adjusting the voltage of the DC power source to start the motor, and adjusting the rotation speed of the photoanode to form a layer of liq. film on the photoanode, (5) irradiating the photoanode with excitation source (UV lamp or solar light), and (6) sampling, analyzing the removal ratio of org. matter in **wastewater**, and completing the treatment of refractory org. **wastewater**. The invention can greatly reduce the light absorption by org. **wastewater**, increase the surface area of photoanode, reinforce mass transfer, and increase the utilization ratio of excitation light and photoelectrocatalytic degradn. efficiency.

Substances Reactions Citings Full Text Link Comments Tags

3. **Preparation method of Bi-containing perovskite type photocatalyst, and its application in photocatalytic degradation of p-chlorophenol-containing wastewater**
 By Hu, Ruisheng; Jia, Haxia; Xu, Na; Bai, Yaqin
 From Faming Zhuanni Shenqing (2011), CN 102019184 A 20110420. Language: Chinese, Database: CAPLUS
 The title prepn. method includes (1) dissolving Fe(NO₃)₃·9H₂O, Bi(NO₃)₃·5H₂O, La(NO₃)₃·nH₂O with 2mol/L nitric acid soln. to obtain transparent soln., where the mol. ratio of Fe(NO₃)₃·9H₂O to Bi(NO₃)₃·5H₂O to La(NO₃)₃·nH₂O to nitric acid is 1:0.1-0.98:0.02-0.9:20, (2) prep. 0.5mol/L citric acid soln., where the mol. ratio of Fe(NO₃)₃·9H₂O to citric acid is 1:4. (3) adding the citric acid soln. into the transparent soln. stirring at room temp. for 10min, and const. temp.

SciFinder将文献依不同类型做分类，列出所有 index，可自由勾选能更容易找到感兴趣的主题

直接定位到感兴趣的污染物

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ
All	Formed, removed, & other substances (939)	1 2 3 4 ... 6
General chemistry	Environment (89)	Select All Desele
Technology	Pollutants (578)	<input checked="" type="checkbox"/> Methyl orange
Catalysis	Geology & soil chemistry (73)	<input checked="" type="checkbox"/> Methylene blue
Physical chemistry	Substances in geology & astronomy (1)	<input checked="" type="checkbox"/> Phenol
Environmental chemistry		<input checked="" type="checkbox"/> Rhodamine B
Synthetic chemistry		<input type="checkbox"/> Titanium dioxide
Polymer chemistry		<input type="checkbox"/> TOC (total organic carbon) 27
Genetics & protein chemistry		<input type="checkbox"/> Carbon 24
Biology		<input type="checkbox"/> Organic compounds 19
Analytical chemistry		<input type="checkbox"/> 4-Chlorophenol 13
Biotechnology		<input type="checkbox"/> Hydrogen peroxide 13
		<input type="checkbox"/> Reactive brilliant red X-3B 13
		<input type="checkbox"/> Benzene 12
		<input type="checkbox"/> Orange II 12
		<input type="checkbox"/> Toluene 11
		<input type="checkbox"/> Tetrabutyl titanate 10

Environmental chemistry > Pollutants > 4 Index Term(s) Selected

OK Cancel

甲基橙、亚甲基蓝
苯酚
罗丹明B
.....

SciFinder将文献依不同类型做分类，列出所有 index，帮助您获得新的创造灵感

可选择的催化剂有哪些？

Categorize ⓘ

1. Select a heading and category. 2. Select index terms of interest.

Category Heading ⓘ	Category ⓘ	Index Terms ⓘ	Terms ⓘ
All	Catalysts (889)	1 2 3 4 ... 9	Click 'x' to remove the category
General chemistry	Catalysis (13)	Select All Deselect All	Selected Terms'
Technology		<input checked="" type="checkbox"/> Titania	Terms > Catalysts (3
Catalysis		<input checked="" type="checkbox"/> Zinc oxide 119	Terms)
Physical chemistry		<input type="checkbox"/> Silica 100	
Environmental chemistry		<input type="checkbox"/> Carbon 70	
Synthetic chemistry		<input type="checkbox"/> Platinum 54	
Polymer chemistry		<input checked="" type="checkbox"/> Tungsten oxide (WO ₃) 51	
Genetics & protein chemistry		<input type="checkbox"/> Silver 48	
Biology		<input type="checkbox"/> Anatase 46	
Analytical chemistry		<input type="checkbox"/> Iron 46	
Biotechnology		<input type="checkbox"/> Cadmium sulfide 41	
		<input type="checkbox"/> Ferric oxide 39	
		<input type="checkbox"/> Alumina 33	
		<input type="checkbox"/> Tin dioxide 28	
		<input type="checkbox"/> Copper 27	
		<input type="checkbox"/> Silica gel 26	
		<input type="checkbox"/> Iron oxide (Fe ₃ O ₄) 25	

Catalysis > Catalysts > 3 Index Term(s) Selected

OK Cancel

氧化钛
氧化锌
氧化钨

这是您感兴趣，打算研究的催化剂

您不了解，但感兴趣的催化剂

从文献中获取更多的信息

2. Synthesis and application of novel mesoporous-assembled SrTi_xZr_{1-x}O₃-based nanocrystal photocatalysts for azo dye degradation

By Khunrattanaphon, Pattharin; Chavadej, Sumaeth; Sreethawong, Thammanoon

From Chemical Engineering Journal (Amsterdam, Netherlands) (2011), 170(1), 292-307. Language: English, Database: CAPLUS

In this work, novel mesoporous-assembled SrTi_xZr_{1-x}O₃ nanocrystal **photocatalysts** were successfully synthesized by a sol-gel process with the aid of a structure-directing surfactant under mild conditions. The photocatalytic activity of the synthesized **photocatalysts** for degrdn. of Acid Black (AB) diazo dye used as a model contaminant in textile **wastewater** was investigated by varying Ti-to-Zr molar fraction, calcination conditions, and Pt loading. The synthesized **photocatalysts** were systematically characterized by TG-DTA, N₂ adsorption-desorption anal., XRD, UV-visible spectroscopy, SEM-EDX, TEM-EDX, TPR, and H₂ chemisorption. The photocatalytic activity results showed that without Pt loading, the mesoporous-assembled SrTi_xZr_{1-x}O₃ **photocatalyst** with a Ti-to-Zr molar fraction of 0.9:0.1 (i.e. SrTi_{0.9}Zr_{0.1}O₃) calcined at 700 °C for 4 h provided a max. degrdn. rate const. as compared to the other SrTi_xZr_{1-x}O₃ **photocatalysts**. The optimum Pt loading of 1 wt.% by a single-step sol-gel method on the mesoporous-assembled SrTi_{0.9}Zr_{0.1}O₃ **photocatalyst** was found to greatly increase the degrdn. rate const. of the AB dye. Furthermore, the calcination temp. was found to significantly affect the degrdn. rate const. of the Pt-loaded mesoporous-assembled SrTi_{0.9}Zr_{0.1}O₃ **photocatalyst**.

✚ Substances ▲ Reactions 📄 ~0 Citings 📄 Full Text 🔗 Link 💬 0 Comments 🏷️ 0 Tags



在摘要里可以看到这种纳米晶体光催化剂用于降解偶氮染料的最佳比例、温度、时间

6. Preparation of TiO₂/attapulgite composite catalyst and photocatalytic degradation of reactive scarlet

By Li, Zhilin; An, Qingzhen

From Huagong Huanbao (2011), 31(1), 82-85. Language: Chinese, Database: CAPLUS

Using attapulgite as carrier and TiOSO₄ as titanium source, the TiO₂/attapulgite composite catalyst with 10 nm of anatase TiO₂ particle was prepd. by ultrasonic dispersion-repptn. process. The composite catalyst was characterized by XRD, TEM and X-ray energy spectrometer. The optimum prepn. conditions are as follows: mass ratio of attapulgite to TiO₂ 1:3.0 and calcination temp. 450°C. When the initial mass concn. of the reactive scarlet soln. is 30 mg/L, the dosage of the TiO₂/attapulgite composite catalyst is 2 g/L and the reaction time of degrdn. under UV is 40 min, the degrdn. rate of reactive scarlet is 98.2%, which is far higher than that on TiO₂. The degrdn. rate of reactive scarlet is 87.0% after irradiation under sunlight with the composite catalyst for 160 min.

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摘要里可以看到这种氧化钛/硅镁土复合催化剂的制备方法

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8. Studies on photodegradation of two commercial dyes in aqueous phase using different photocatalysts

By: Kansal, S. K.; Singh, M.; Sud, D.

We studied the photocatalytic degrdn. of Methyl orange (MO) and Rhodamine 6G (R6G) in aq. phase. Photocatalytic activity of various semiconductors such as TiO₂, ZnO, SnO₂, ZnS, and CdS was investigated. An attempt was made to study the effect of process parameters viz., amt. of catalyst, concn. of dye, and pH on photocatalytic degrdn. of MO and R6G was carried out by irradiating the aq. solns. of dyes contg. photocatalysts with UV and solar light. The rate of decolorization was estd. from residual concn. spectrophotometrically. Similar expts. were carried out by varying pH (2-10) and initial concn. of dye (5-200 mg/L). The max. decolorization (>90%) of dyes occurred under UV/solar system and it was found that COD redn. takes place at a faster rate under solar light. In case of R6G, highest decolorizing efficiency was achieved with lower dose of catalyst (0.5 g/L) than MO (1 g/L) under similar conditions. The performance of photocatalytic system employing ZnO/solar light was observed to be better than ZnO/UV system.

Indexing

Waste Treatment and Disposal (Section 60-2) ⓘ

Section cross-reference(s): 22, 40, 41, 74

Source

Journal of Hazardous Materials
Volume 141
Issue 3
Pages 581-590
Journal
2007

Abstract

The present study involves the photocatalytic degradation of Methyl Orange (MO) and Rhodamine 6G (R6G), employing heterogeneous photocatalytic process. Photocatalytic activity of various semiconductors such as titanium dioxide (TiO₂), zinc oxide (ZnO), stannic oxide (SnO₂), zinc sulphide (ZnS) and cadmium sulphide (CdS) has been investigated. An attempt has been made to study the effect of process parameters viz., amount of catalyst, concentration of dye and pH on photocatalytic degradation of MO and R6G. The experiments were carried out by irradiating the aqueous solutions of dyes containing photocatalysts with UV and solar light. The rate of decolorization was estimated from residual concentration spectrophotometrically. Similar experiments were carried out by varying pH (2-10), amount of catalyst (0.25-2.0 g/l) and initial concentration of dye (5-200 mg/l). The experimental results indicated that the maximum decolorization (more than 90%) of dyes occurred with ZnO catalyst and at basic pH and the maximum adsorption of MO was noticed at pH 4 and of R6G at pH 10. The percentage reduction of MO and R6G was estimated under UV/solar system and it was found that COD reduction takes place at a faster rate under solar light as compared to UV light. In case of R6G, highest decolorizing efficiency was achieved with lower dose of catalyst (0.5 g/l) than MO (1 g/l) under similar conditions. The performance of photocatalytic system employing ZnO/solar light was observed to be better than ZnO/UV system.

Keywords: Decolorization; Azo dye; Methyl Orange; Rhodamine 6G; Photocatalysis

Article Outline

1. Introduction
2. Experimental methods
 - 2.1. Materials

Concepts ⓘ

Substances ⓘ

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Concepts ⓘ

Wastewater treatment

decolorization; photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

Adsorption

of dye onto photocatalyst; photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

UV and visible spectra

of dyes; photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

Dyes	Photolysis catalysts
Photolysis kinetics	Solar UV radiation
Textiles	UV radiation

photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

Substances ⓘ

1306-23-6 Cadmium sulfide (CdS), uses
1314-13-2 Zinc oxide (ZnO), uses
1314-98-3 Zinc sulfide (ZnS), uses
13463-67-7 Titanium oxide (TiO₂), uses
18282-10-5 Stannic oxide (SnO₂)

photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

Catalyst use; Uses

547-58-0 Methyl orange
989-38-8 Rhodamine 6G

photocatalytic degrdn. of Methyl orange and Rhodamine 6G in aq. phase using different photocatalysts

Physical, and
Properties;

CAS Registry Number: 547-58-0
(Component: 502-02-3)

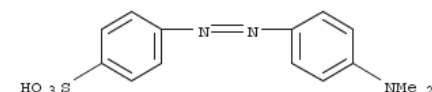
C14 H15 N3 O3 S . Na

Benzenesulfonic acid, 4-[2-[4-(dimethylamino)phenyl]diazanyl]-, sodium salt (1:1)

Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt (9CI); Benzenesulfonic acid, p-[[p-(dimethylamino)phenyl]azo]-, sodium salt (8CI); Orange III (6CI); 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; Acid Orange 52; Albion Methyl Orange; C.I. 13025; C.I. Acid Orange 52; Diazoben; Eniamethyl Orange; Gold orange; Helianthine; Helianthine B; KCA Methyl Orange; Methyl Orange B; Methyl orange; Orange 3; Sodium 4-(dimethylamino)azobenzene-4'-sulfonate; Sodium 4-[4-(dimethylamino)phenylazo] benzenesulfonate; Sodium 4'-(dimethylamino)azobenzene-4-sulfonate; Sodium p-[[p-(dimethylamino)phenyl]azo] benzenesulfonate; Sodium p-dimethylaminoazobenzene-sulfonate; Tropaeolin D

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8. Studies on photodegradation of two commercial dyes in aqueous phase using different photocatalysts

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 2007
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双酚A奶瓶：对食品安全再敏感些

2011年03月02日 08:59:01 来源：新京报 【字号 大小】 【收藏】 【打印】 【关闭】

很多有关产品缺陷的信息，都是“出口转内销”。我国研究者在世界上最早得出了“双酚A对男性性功能有危害”的直接证据。为何监管部门没能在国内率先行动，是什么原因导致我们的监管总是慢半拍？

据报道，欧盟认为含双酚A奶瓶会诱发性早熟，从3月1日起，将禁止生产含化学物质双酚A（BPA）的婴儿奶瓶。实际上，这并不是欧盟刚刚作出的决定，在去年11月25日，欧盟食物链和动物健康委员会（SCFCAH）就通过了相关决定。

卫生部官员昨日也表示，目前中国正在清理包装材料，并出台了征求意见稿。征求意见稿中规定，未来婴幼儿奶瓶不能使用双酚A。

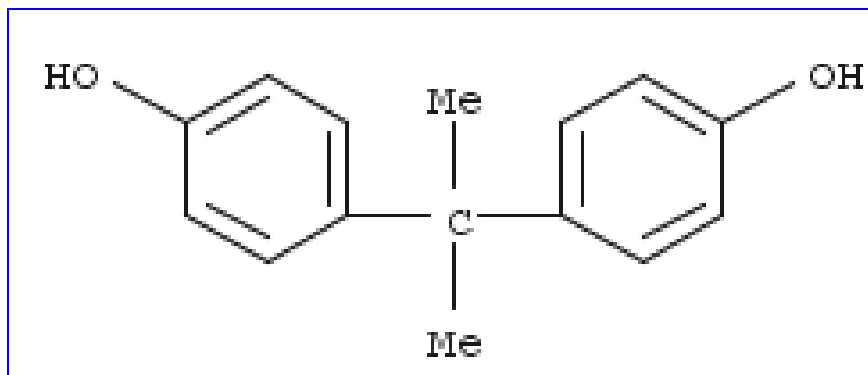
有关部门虽然出台了征求意见稿，但反应已稍显滞后，含有双酚A的奶瓶还在商场出售。在历经了三聚氰胺等食品安全风波之后，民众对于与食品相关的安全格外敏感，一有相关的消息，就会格外紧张。

其实，在欧盟宣布对含双酚A的塑料奶瓶全面禁止之前，已有不少国家和地区对此类产品作了禁止性规定。2008年，加拿大第一个宣布在所有食品包装和容器（包括奶瓶）上禁用双酚A，澳大利亚也从2010年7月1日起逐渐淘汰含双酚A的婴儿奶瓶；后来美国许多州和大型零售商，包括沃尔玛在内采取了同样的步骤。



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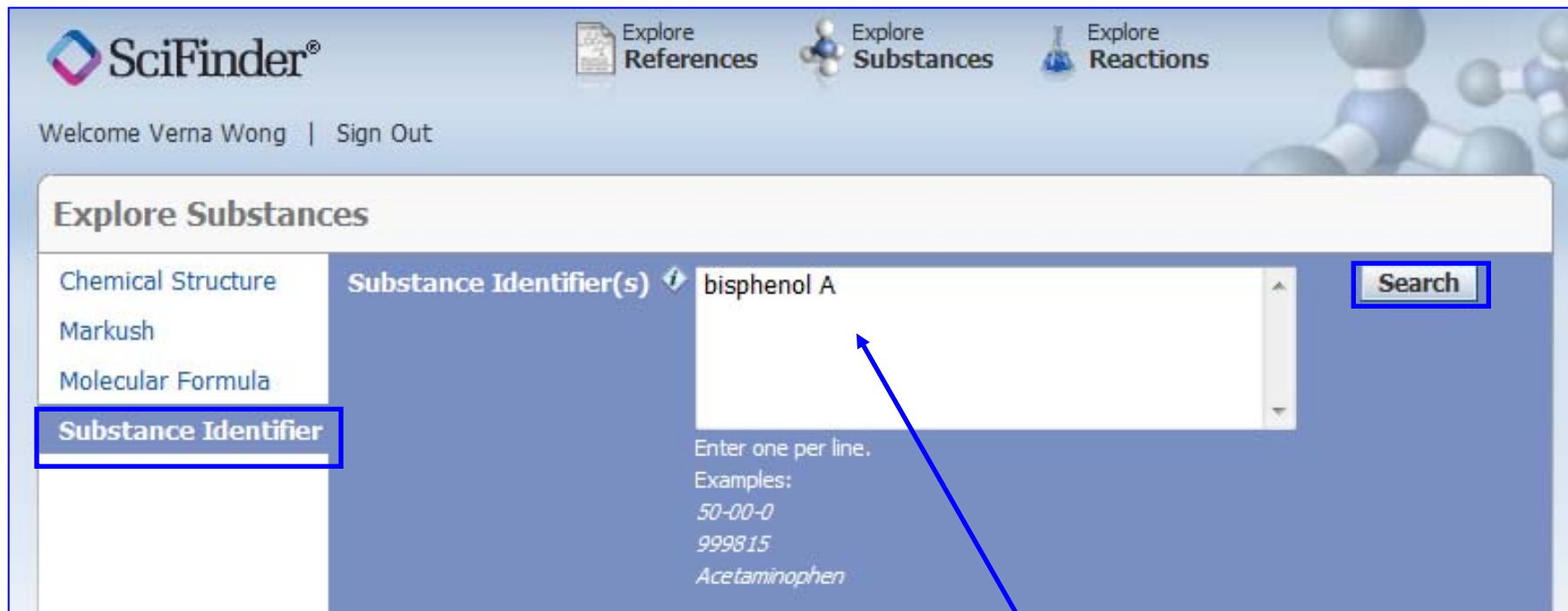
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双酚A（bisphenol A; BPA）



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Substance Identifier(s)

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Acetaminophen

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Phenol, 4,4'-(1-methylethylidene)bis-

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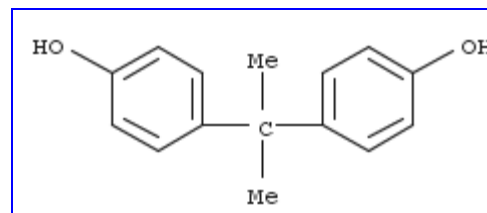
Phenol, 4,4'-(1-methylethylidene)bis-

Phenol, 4,4'-isopropylidenedi- (8CI); (4,4'-Dihydroxydiphenyl) dimethylmethane; 2,2-Bis(4-hydroxyphenyl)propane; 2,2-Bis(p-hydroxyphenyl)propane; 2,2-Di(4-hydroxyphenyl)propane; 2,2-Di(4-phenylol)propane; 2,2'-Bis(4-hydroxyphenyl)propane; 4,4'-(1-Methylethylidene)bisphenol; 4,4'-(Propane-2,2-diyl)diphenol; 4,4'-Isopropylidenebis[phenol]; 4,4'-Isopropylidenediphenol; 4,4'-Methylethylidenebisphenol; B 0494; BPA; BPA 154; BPA 157; BPA-M; Bis(4-hydroxyphenyl)dimethylmethane; Bis(p-hydroxyphenyl)propane; Bisphenol A; Dian; Diano; Diphenylolpropane; HT 3082; Hidorin F 285; Hidorin F 568; Ipognox 88; Isopropylidenebis(4-hydroxybenzene); NSC 1767; NSC 17959; Parabis; Parabis A; Pluracol 245; Rikabanol; p,p'-Bisphenol A; p,p'-Dihydroxydiphenylpropane; p,p'-Isopropylidenebisphenol; p,p'-Isopropylidenediphenol; β,β'-Bis(p-hydroxyphenyl)propane

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Biological Study	✓	✓	✓	✓
Combinatorial Study	✓	✓		
Formation, Nonpreparative	✓	✓	✓	✓
Miscellaneous	✓	✓	✓	✓
Occurrence	✓	✓	✓	✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓		✓	
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

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Bioconcentration Factor	344	pH 2 Temp: 25 °C	(79)	
Bioconcentration Factor	344	pH 3 Temp: 25 °C	(79)	
Bioconcentration Factor	344	pH 4 Temp: 25 °C	(79)	
Bioconcentration Factor	344	pH 5 Temp: 25 °C	(79)	
Bioconcentration Factor	344	pH 6 Temp: 25 °C	(79)	

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Half-Life (Biological)	See full text	1 of 4	(18) CAS	
LC50	See full text		(23) CAS	
Median Lethal Dose(LD50)	4040 mg/kg	Organism: rat Route: oral	(26) CAS	
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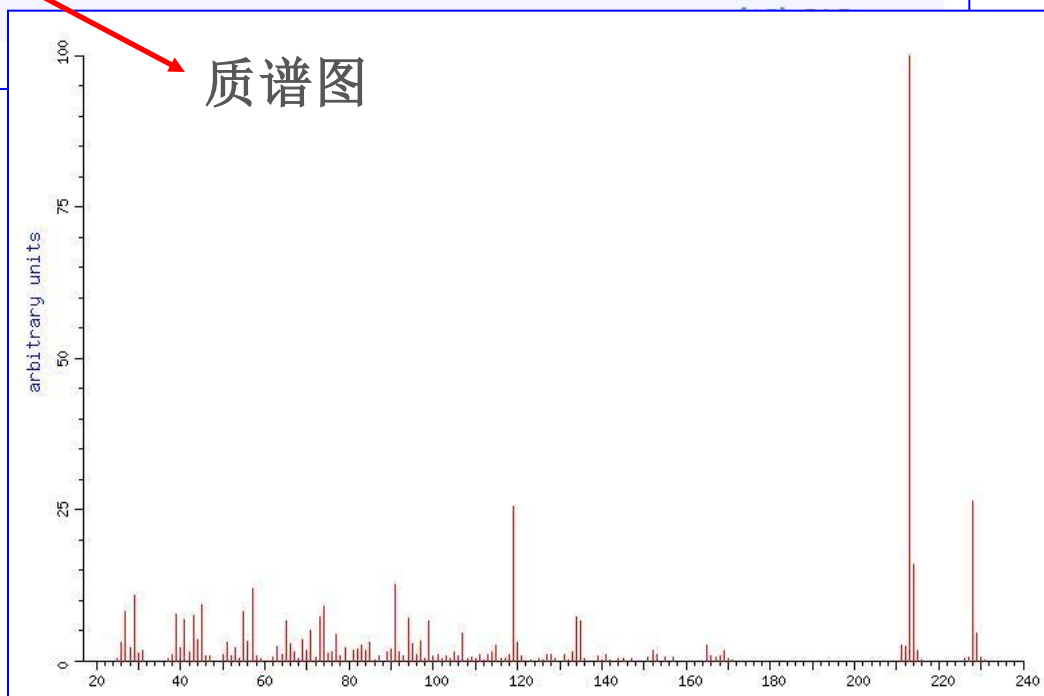


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IR Spectrum	See full text		(22) CAS
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Mass Spectrum	See spectrum		(13) WSS
Mass Spectrum	See spectrum		(13) WSS
Mass Spectrum	See spectrum		(14) AIST
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16. **A recombinant peroxisome proliferator response element-driven luciferase assay for evaluation of potential environmental obesogens**

By Wang, Ya-Fen; Chao, How-Ran; Wu, Chia-Hsin; Tseng, Chu-Han; Kuo, Ya-Ting; Tsou, Tsui-Chun
From Biotechnology Letters (2010), 32(12), 1789-1796. Language: English, Database: CAPLUS


A recombinant Huh7-PPRE-Luc cell line for analyzing the peroxisome proliferator response element (PPRE)-driven luciferase activity was established. The cells exhibited a good dose-response induction in PPRE-driven luciferase activity by three subtypes of peroxisome proliferator-activated receptor (PPAR) agonists as well as by a retinoid X receptor agonist, 9-cis-retinoic acid. Among five environmental chems. tested, benzyl Bu phthalate and bisphenol induced PPRE-driven luciferase activation in Huh7-PPRE-Luc cells and caused adipogenic differentiation of 3T3-L1 cells. This recombinant Huh7-PPRE-Luc cell line would be useful for screening potential environmental obesogens with PPAR activity.

 Substances  Reactions  Citing  Full Text  Link  0 Comments  0 Tags

17. **Generation of reactive oxygen species in sperms of rats as an earlier marker for evaluating the toxicity of endocrine-disrupting chemicals**

By Minamiyama, Yukiko; Ichikawa, Hiroshi; Takemura, Shigekazu; Kusunoki, Hiroshi; Naito, Yuji; Yoshikawa, Toshikazu
From Free Radical Research (2010), 44(12), 1398-1406. Language: English, Database: CAPLUS

Bisphenol A (BPA) and diethylstilbestrol (DES) have been reported to cause sperm toxicity. To identify an earlier marker of toxicity of environmental substances or food additives, this study detd. whether the levels of reactive oxygen species (ROS) in sperms could serve as indexes for the prediction of sperm toxicity and quality. Male Wistar rats were given drinking water contg. various doses of BPA or DES for 8 wk. Some rats were treated with 0.45% N-acetyl cysteine (NAC) for 2 days prior to the administration of DES or BPA. Administration of BPA or DES to rats for 1 wk dose-dependently increased the prodn. of ROS, even at doses and time points which had no effect on sperm motility. 4-Hydroxy-2-nonenal modified proteins increased in sperms 8 wk after BPA or DES treatment. NAC reversed oxidative stress and prevented the loss of sperm function in the DES or BPA-treated group. During observation, changes in the sperm motility, sperm count and morphol. were not correlated to the increase in ROS levels. These results suggest that ROS levels may be used as an early indicator of sperm count and quality decreases which result from chronic toxicity.


 Substances  Reactions  Citing  Full Text  Link  0 Comments  0 Tags


18. **In vitro effects of Bisphenol A on sperm motility characteristics in Perca fluviatilis L. (Percidae; Teleostei)**

By Hatef, A.; Alavi, S. M. H.; Linhartova, Z.; Rodina, M.; Policar, T.; Linhart, O.

Analysis

Refine

Analyze by: 

Author Name 

Click bar to view only those references within the current answer set

Soto Ana M	33
Sonnenschein Carlos	28
Vom Saal Frederick S	24
Iguchi Taisen	19
Morita Masatoshi	16
Rubin Beverly S	15
Lee Jae Seong	14
Tsutsumi Osamu	14
Arizono Koji	13
Ashby John	13

Show More

Categorize

More detailed analysis based on CAS indexing

双酚A分析方法方面的文献

References Get Substances Get Reactions Get Cited Get Citing Get Full Text Combine Answer Sets

1872 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number ↓ Answers per Page [15] 1 2 3 4 5 6 ... 125 Display: — = ≡

1. **Direct determination of bisphenol A in water by derivative synchronous fluorimetry** **衍生化荧光**
 By Ding, Bo; Yin, Pinghe; Liu, Yufang; Li, Qiang
 From Fenxi Ceshi Xuebao (2010), 29(11), 1190-1193. Language: Chinese, Database: CAPLUS
 The detn. of bisphenol A (BPA) soln. mixed with β -cyclodextrin (β -CD) was studied by deriv. synchronous fluorescence spectrometry. The expt. results indicated that the deriv. synchronous fluorescence spectra of mixt. and matrix were sepd. absolutely, and the matrix effect was eliminated. The effects of pH, amt. of β -CD and salinity on the deriv. synchronous fluorescence intensity were studied. A novel method was developed for the detn. of BPA by deriv. synchronous fluorescence spectrometry. The calibration curve of BPA was linear in the range of 1.5-500 μ g·L⁻¹ with a detection limit of 0.46 μ g·L⁻¹. The method was successfully used in the direct detn. of BPA in tap water, bottled water and pond water. The spiked recoveries were in the range of 94%-104% with RSDs of 0.76% -4.4%.
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

2. **Voltammetric determination of bisphenol A in food package by a glassy carbon electrode modified with carboxylated multi-walled carbon nanotubes** **玻璃碳电极**
 By Li, Junhua; Kuang, Daizhi; Feng, Yonglan; Zhang, Fuxing; Liu, Mengqin
 From Microchimica Acta (2011), 172(3-4), 379-386. Language: English, Database: CAPLUS
 A highly sensitive and mercury-free method for detn. of bisphenol A (BPA) was established using a glassy carbon electrode that was modified with carboxylated multi-walled carbon nanotubes. A sensitive oxidn. peak is found at 550 mV in linear sweep voltammograms at pH 7. Based on this finding, trace levels of bisphenol A can be detd. over a concn. range that is linear from 10 nM to 104 nM, the correlation coeff. being 0.9983, and the detection limit (S/N = 3) being 5.0 nM. The method was successfully applied to the detn. of BPA in food package.
 Substances Reactions Citing Full Text Link 0 Comments 0 Tags

3. **Aptamer-modified anodized aluminum oxide-based capacitive sensor for the detection of bisphenol A** **电容传感器**
 By Kang, Bongkeun; Kim, Joo Hyoung; Kim, Soyoun; Yoo, Kyung-Hwa
 From Applied Physics Letters (2011), 98(7), 073703/1-073703/3. Language: English, Database: CAPLUS
 We describe a rapid, sensitive, and low-cost method to detect bisphenol A (BPA) using an anodized aluminum oxide-based capacitive sensor. BPA is detected by measuring the change in capacitance caused by the biospecific binding of BPA with a BPA aptamer that is immobilized on the electrode surface. For a soln. contg. 100 pM BPA, the capacitance decreased by approx. 3%. In addn., we fabricated a capacitive sensor array and demonstrated that BPA in environmental samples can be measured using our capacitive sensor. (c) 2011 American Institute of Physics.

Analysis Refine

Analyze by:

Author Name

Click bar to view only those references within the current answer set

Calafat Antonia M	24
Nakazawa Hiroyuki	21
Hosoya Ken	19
Ye Xiaoyun	16
Barcelo Damia	15
Morita Masatoshi	13
Needham Larry L	13
Hamada Fumio	12
Kubo Takuya	12
watabe roshiyuki	12

Show More

Categorize

More detailed analysis based on CAS indexing

获得双酚A合成制备方法

Reactions Get References Find Additional Reactions Combine Answer Sets

109 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: ↓ Answers per Page [50] 1 2 3 ▶

Display:

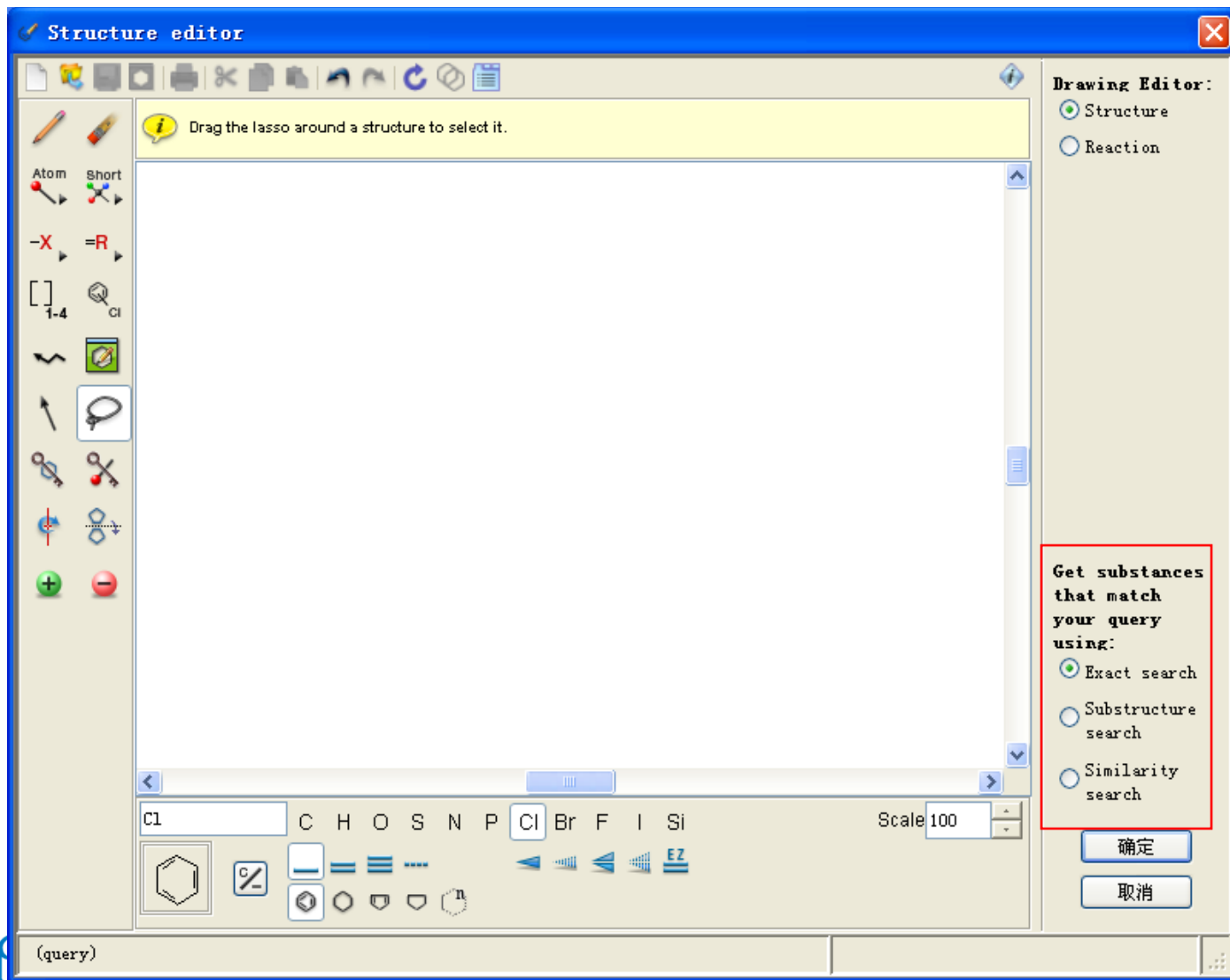
1. View Reaction Detail [Link](#) Similar Reactions
Single Step *Hover over any structure for more options.*

The reaction shows the synthesis of Bisphenol A. On the left, a phenol molecule (a benzene ring with an -OH group) and an acetone molecule (H₃C-C(=O)-CH₃) are shown with a plus sign between them. An arrow points to the right, where the product, Bisphenol A, is shown. Bisphenol A consists of two phenol rings connected to a central carbon atom, which is also bonded to two methyl groups (-Me).

▼ Overview

Steps/Stages	Notes
1.1 C:Polysorb1, C:19351-18-9, 338K	flow system, industrial, Reactants: 2, Catalysts: 2, Steps: 1, Stages: 1, Most stages in any one step: 1
	References Method for production of high purity bisphenol A By Kiedik, Maciej et al From Pol., 199315, 30 Sep 2008 Full Text

SciFinder结构绘制工具



可选择

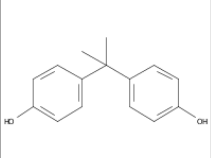
精确结构检索、
亚结构检索、
相似结构检索

使用结构检索可以获得双酚A衍生物的信息

Explore Substances

Chemical Structure

Markush
Molecular Formula
Substance Identifier



Click image to change structure or view detail

Search type: Exact Structure Substructure Similarity

Show precision analysis

Characteristic(s)

Single component
 Commercially available
 Included in reference(s)

当需要去检索物质的衍生物时，可以使用亚结构检索，Substructure。

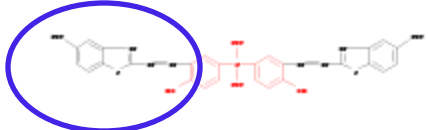
Substances

4647 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] 1 2 3 4 5 6 ... 310

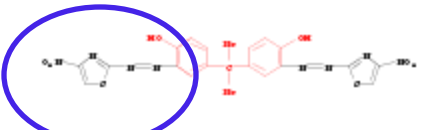
View:

1. Substance Detail
1264194-12-8



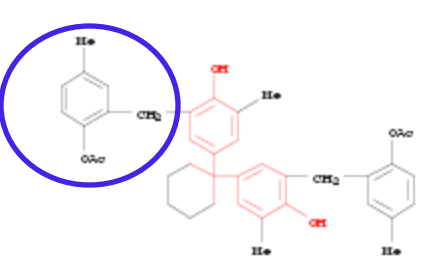
C₃₁ H₂₆ N₆ O₂ S₂
INDEX NAME NOT YET ASSIGNED


2. Substance Detail
1264194-10-6



C₂₁ H₁₆ N₈ O₆ S₂
INDEX NAME NOT YET ASSIGNED

3. Substance Detail
1263289-83-3



 CAS is a division of the A

理化性质限定工具

可以通过理化性质限定物质，选择特定的理化性质，输入数值范围，点击**Refine**

Analysis
Refine

Refine by: ⓘ

- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value** NEW
- Reference Availability
- Atom Attachment

Select Properties

Refine by Property Value ⓘ

1. Select one or more properties. Click each property to display value options.

Properties - 1 selected

Experimental

- Boiling Point
- Melting Point

Predicted

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Acceptor/Donor Sum
- Koc
- logD
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility
- Molar Volume

2. Specify values and limits.

Values - Experimental Boiling Point

Specify range (degrees C):

to

Min: -273.0 Max:

Pressure (Torr):

to

Min: 0.0 Max:

Include substances with no value for the specified properties

Refine-Atom Attachment 获得结构中特定修饰情况

Refine下的Atom Attachment工具，帮助科研工作者了解结构中各个位点的可修饰性

Analysis
Refine

Refine by: ⓘ

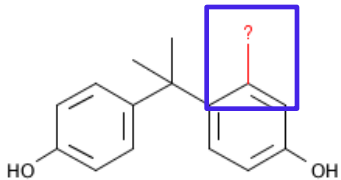
- Chemical Structure
- Isotope-Containing
- Metal-Containing
- Commercial Availability
- Property Availability
- Property Value
- Reference Availability
- Atom Attachment

Select Attachments

Refine by Atom Attachment ⓘ

1. Click an atom to display the attachments present at that site.
2. Select attachment(s) of interest.

Substructure



Atom Attachments

Select All Deselect All

<input type="checkbox"/> H or None	4461
<input type="checkbox"/> C	93
<input type="checkbox"/> O	67
<input type="checkbox"/> Cl	11
<input type="checkbox"/> Br	10
<input type="checkbox"/> Hg	2
<input type="checkbox"/> N	1
<input type="checkbox"/> F	1
<input type="checkbox"/> Other	1
<input type="checkbox"/> A - Any (not H)	185
<input checked="" type="checkbox"/> Q - Any (not C,H)	92
<input type="checkbox"/> Ak - Alkyl chain	70
<input type="checkbox"/> X - Halogen	22
<input type="checkbox"/> M - Metal	2
<input type="checkbox"/> Hy - Heterocycle	1

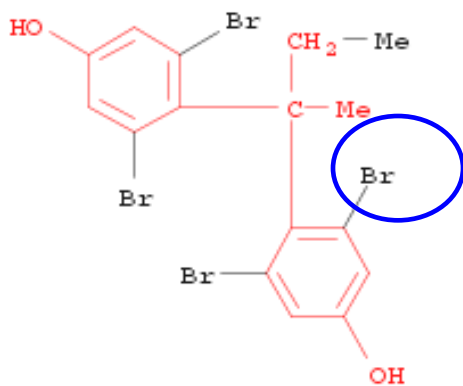
? = Q

Refine
Cancel

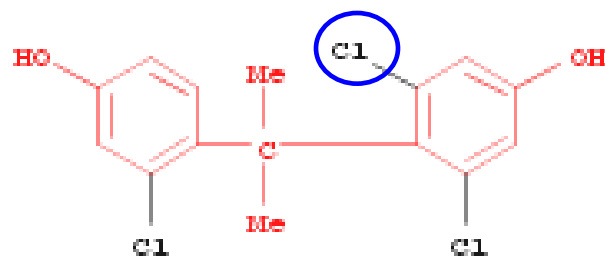
获得特定位置上为非C,H的衍生物

特定位置上为非C,H的任何元素

20. Substance Detail
897091-57-5



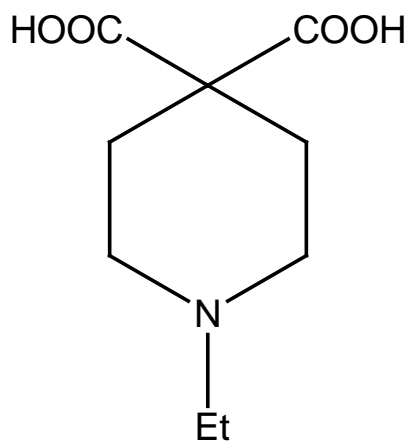
10. Substance Detail
1033261-02-7



15. Substance Detail
929102-14-7



可进行相似结构检索



SciFinder中的相似结构检索，帮助获得在结构上存在相似的物质。

Explore Substances

Chemical Structure Chemical Structure ⓘ

Markush

Molecular Formula

Substance Identifier

HOOC COOH

Et

Search

Click image to change structure or view detail

Search type: ⓘ

- Exact Structure
- Substructure
- Similarity

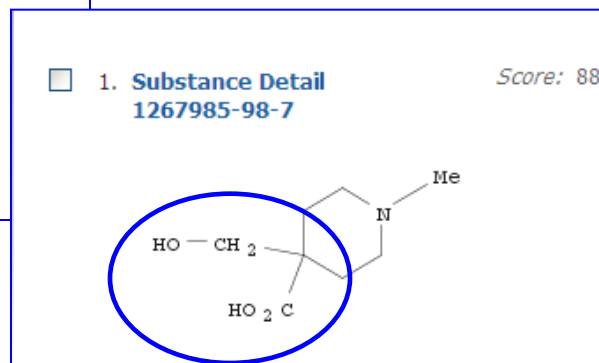
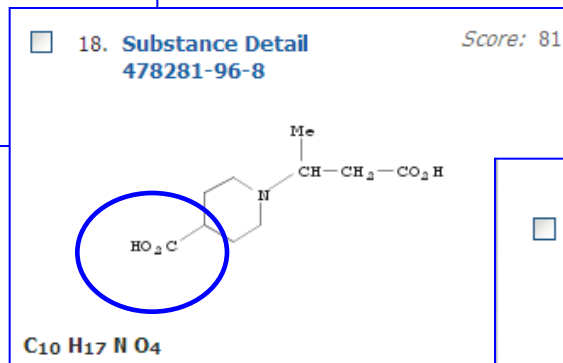
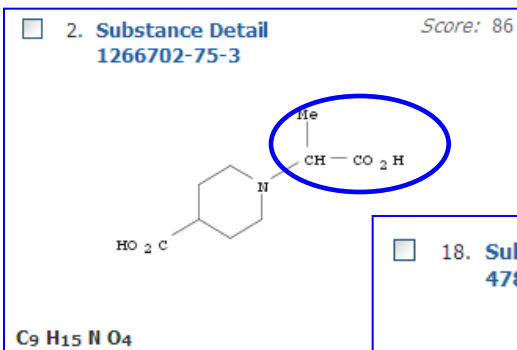
Show precision analysis

相似结构检索可获得相似度在60分以上的物质

Similarity Candidates	
6 Candidates 2 Selected	
Select All Deselect All	
Similarity Candidates	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input checked="" type="checkbox"/> 85-89	8
<input checked="" type="checkbox"/> 80-84	16
<input type="checkbox"/> 75-79	62
<input type="checkbox"/> 70-74	229
<input type="checkbox"/> 65-69	658
<input type="checkbox"/> 0-64 (least similar)	2603
<input type="button" value="Get Substances"/>	

与原结构存在以下的区别：

取代基位置变化
取代基变化
母体结构变化



SciFinder中的Markush结构检索

在专利中描述物质的方式

➤ 特定物质[Specific Substance]:

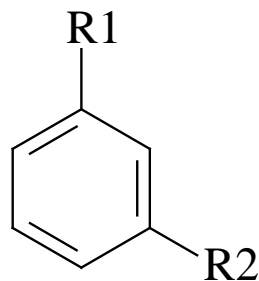
以特定化学结构所陈述的特定物质，会被标示CAS No.

➤ 预测性物质[Prophetic Substance]:

使用Markush结构所陈述的预测物质，一个Markush可以陈述上百或上千的化学物质

Patent 中所陈述的预测物质，不会被标示CAS No.

Markush检索，能检索到通过结构检索检不到的专利



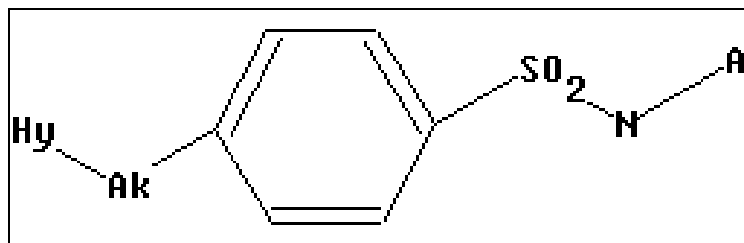
R1 = H, Br, Cl, I

R2 = Br, Cl, I, —CH₂—halogen, —CH(CH₃)—halogen,

Br, Cl, F, I

Br, Cl, F, I

SciFinder中的Markush结构检索



SciFinder中的Markush检索能帮助做初步的专利评估。

The screenshot shows the SciFinder interface. At the top, there are navigation links: 'Explore References', 'Explore Substances', and 'Explore Reactions'. Below the navigation, it says 'Welcome Sam Yu | Sign Out'. The main section is titled 'Explore Substances'. On the left, there is a sidebar with options: 'Chemical Structure', 'Markush' (highlighted with a 'NEW' badge), 'Molecular Formula', and 'Substance Identifier'. The 'Markush' option is selected, and the chemical structure diagram from the previous image is displayed in the main area. Below the structure, there is a 'Search' button. At the bottom, there is a 'Search type:' section with two radio buttons: 'Allow variability only as specified' (selected) and 'Substructure'.

Markush直接检索包含该通式结构的专利

SciFinder®

Welcome Sam Yu | Sign Out

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help
Keep Me Posted Results | History
My Connections | Preferences

Create Keep Me Posted | Markush substructure > references (1451)

References | Get Substances | Get Reactions | Get Cited | Get Citing | Get Full Text | Combine Answer Sets

1451 References | 0 Selected | Keep Selected | Remove Selected | Remove Duplicates | Add Tags | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [20] | 1 2 3 4 5 6 ... 73 | Display: [icon]

1. **Preparation of substituted 1H-pyrazolo[3,4-d]pyrimidin-6-amine compounds as antitumor agents**
By Hill, Jason; Ali, Syed M.; Ashwell, Mark; Tandon, Manish; Lapierre, Jean-Marc; Namdev, Nivedita; Nicewonger, Robert; Moussa, Magdi; Yang, Rui-Yang
From PCT Int. Appl. (2010), WO 2010078430 A1 20100708. Language: English, Database: CAPLUS
The present invention relates to substituted 1H-pyrazolo[3,4-d]pyrimidin-6-amine compds. I [R1, R2, R4 = H, (un) substituted alkyl; or R1 and R2, together with the atoms they attach to, form 5-6 membered ring (optionally unsatd. and optionally contg. 1-4 heteroatoms); Z = (CH2)_m, C(O), C(O)C(O), C(O)O, etc.; R = (un)substituted alkyl, alkoxy, aryloxy, etc.; m = 0-4; w = 1-2] and methods of synthesizing these compds. Over two-hundred compds. I were prepd. E.g., a 3-step synthesis of II, starting from tert-Bu 1,2,3,4-tetrahydroquinolin-3-ylcarbamate and 2-(trimethylsilyl)phenyl trifluoromethane...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

2. **Phenylalkyl-imidazole-bisphosphonate compounds**
By Cotesta, Simona; Jahnke, Wolfgang; Rondeau, Jean-Michel; Weiler, Sven; Widler, Leo
From PCT Int. Appl. (2010), WO 2010076258 A1 20100708. Language: English, Database: CAPLUS
(Unsubstituted or substituted phenyl)-alkyl-substituted [(imidazol-1-yl)-1-hydroxy-1-phosphono-ethyl]-phosphonic acids I (R1, R2 = H, (un)substituted phenylalkyl, ester, salt, etc.), as well as methods or processes for their manuf., their use in the manuf. of pharmaceutical formulations, their use in the treatment of diseases, methods of using them in the treatment of diseases, pharmaceutical formulations encompassing them and/or the compds. for use in the treatment of diseases, are disclosed. The compds. are able to inhibit excessive or inappropriate bone resorption.

Analysis | Refine

Analyze by: [Author Name](#)

Click bar to view only those references within the current answer set

Miller Andrew	14
Shih Neng Yang	11
Whittaker Mark	11
Moussy Alain	10
Quan Mimi Lifan	10
Zhu Bing Yan	10
Chakravarty Prasun K	9
Dorsch Dieter	9

SciFinder中的物质检索能帮助您

获得物质的CAS号,理化性质,图谱信息

获得物质的合成方法,分析方法,药理毒理信息

获得物质的所有衍生物

进行结构查新

查询物质的专利保护状态

提纲

- **SciFinder**介绍
- **SciFinder**的检索界面
- **SciFinder**中的文献检索
- **SciFinder**中的物质检索
- **SciFinder**中的反应检索

SciFinder包含的反应数据库

CAS React (1840—至今)

期刊, **专利**中涉及的有机、有机金属、无机、生化反应。

2600万单步, 多步反应。

1300万制备信息。

周更新。

可通过反应式检索, 可通过物质、文献链接。

反应检索入口

反应检索入口

SciFinder®

Welcome Verna Wong | Sign Out

Explore References | Explore Substances | **Explore Reactions**

Explore Reactions

Reaction Structure | Reaction Structure ⓘ

Click to Edit

Search

Solvent(s) ⓘ | Select Solvents

Non-participating ⓘ
Functional Group(s)

Number of Steps ⓘ

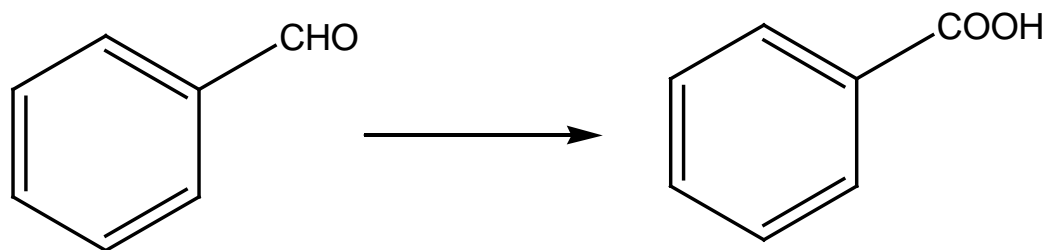
Classification(s) ⓘ

Examples: 1, 1 - 3, 1 - 3

CAS is a div

as.org

使用反应定义工具定义反应



精确反应检索帮助
获得特定物质之间的
反应，点击确定

可以提前设定反应的溶剂以及不参与反应的官能团

可以自定义一些反应溶剂以及不参与反应的官能团。

SciFinder®
Welcome Verna Wong | Sign Out

Explore References | Explore Substances | Explore Reactions

Explore Reactions

Reaction Structure | Reaction Structure

reactant | product

Click image to change structure or view detail

Search type: Allow variability only as specified Substructure

Solvent(s)

Non-participating Functional Group(s)

Solvent Hierarchy
[View Solvent List]

0 Selected | Select All | Deselect All

- Inorganic solvents
 - Ammonia
 - Ammonia-15N
 - Ammonia-d3
 - Water
 - Water-17O
 - Water-18O
 - Water-d
 - Water-d2
 - Water-d2-18O
 - Water-t
 - Water-t2

Find: Next Previous

View: All 217

0 Selected | Clear Selections

- Acetal
- Acetyl
- Acid Halide
- Acyclic Alkene
- Acyclic Ketone
- Acylmetal
- ALCOHOLS
- Aldehyde
- pi-Alkene
- ALKENES
- Alkyl Halide

Reactions must have all selections any selection

在SciFinder中能获得全面的反应集合

Create Keep Me Posted Reaction Structure structure variable only at spe... > reactions (292) > keep analysis "Experimental Procedure" (6)

Reactions Get References Combine Answer Sets

6 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: Relevance (New) ↓ Answers per Page [15]

Display:

1. View Reaction Detail Link Similar Reactions

Single Step Hover over any structure for more options.

96%

▼ Overview

Steps/Stages	Notes
1.1 R: NiCl ₂ , R: NaOCl, S: H ₂ O, S: CH ₂ Cl ₂ , 0°C; 5 min, 0°C; 2 h, 0°C; 2 h, rt	Reactants: 1, Reagents: 2, Solvents: 2, Steps: 1, Stages: 1, Most stages in any one step: 1

References

An Efficient and Practical System for the Catalytic Oxidation of Alcohols, Aldehydes, and α,β -Unsaturated Carboxylic Acids
By Grill, Joseph M. et al
From Journal of Organic Chemistry, 71(25), 9291-9296; 2006
 Full Text

▼ Experimental Procedure **NEW**

The Journal of Organic Chemistry

General/Typical Procedure: Procedure A: Standard procedure for the oxidation of primary alcohols and aldehydes. A 500 mL flask was charged with NiCl₂ hexahydrate (0.27 g, 1.14 mmol) and water (5 mL) and allowed to dissolve. A primary alcohol or an aldehyde (45 mmol) was added followed by dichloromethane (15 mL). The reaction was cooled in an ice bath after reaching homogeneity and cold bleach (300 mL) was added in a steady stream over 5 minutes. A fine black precipitate formed immediately. The resulting slurry was stirred for 2 hours at 0°C and 2 hours at room temperature. The slurry was then acidified with 2 M hydrochloric acid until the aqueous layer was strongly acidic by pH paper. The aqueous layer was extracted with diethyl ether (3 x 100 mL). The combined organic extracts were dried over anhydrous MgSO₄ and filtered. Removal of the solvent by rotary evaporation and brief high vacuum gave the crude product. The purities could generally be improved to greater than 98% by distillation of the crude product or by recrystallization in the case of solids. Benzoic acid, yield 5.28 g, 96%. ¹H NMR(CDCl₃): δ 7.49 (t, ³J_{HH} = 7.4 Hz, 2H), 7.63 (t, ³J_{HH} = 7.4 Hz, 1H), 8.14 (d, ³J_{HH} = 7.4 Hz, 2H), 12.02 (broad, 1H). ¹³C NMR (CDCl₃): δ 128.8, 129.5, 130.5, 134.1, 172.9. MS (ESI) m/z = 121 [M-H]⁻. CAS# [65-85-0].

Analysis Refine

Analyze by:

Catalyst

Click bar to view only those reactions within the current answer set

145698-90-4	1
MgBr ₂ -Et ₂ O	1

Show More

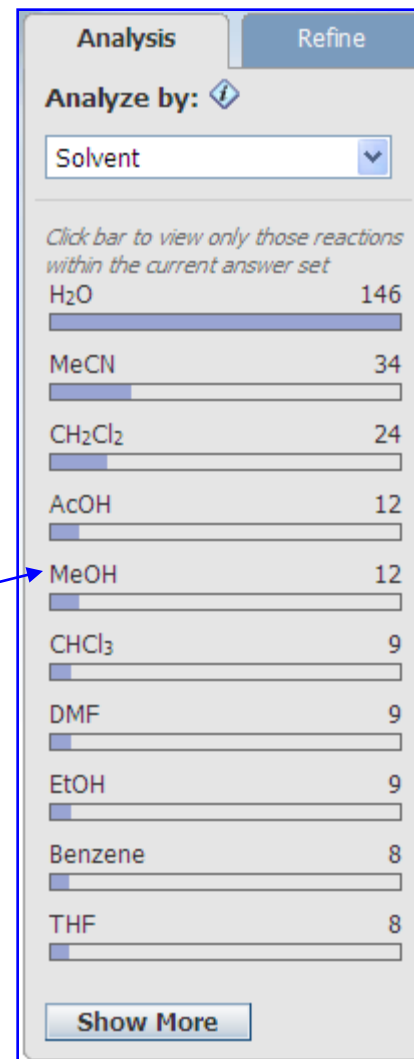
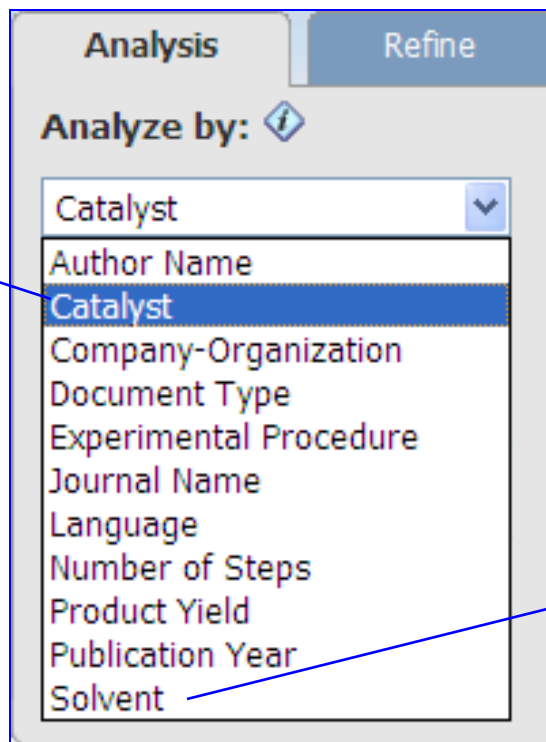
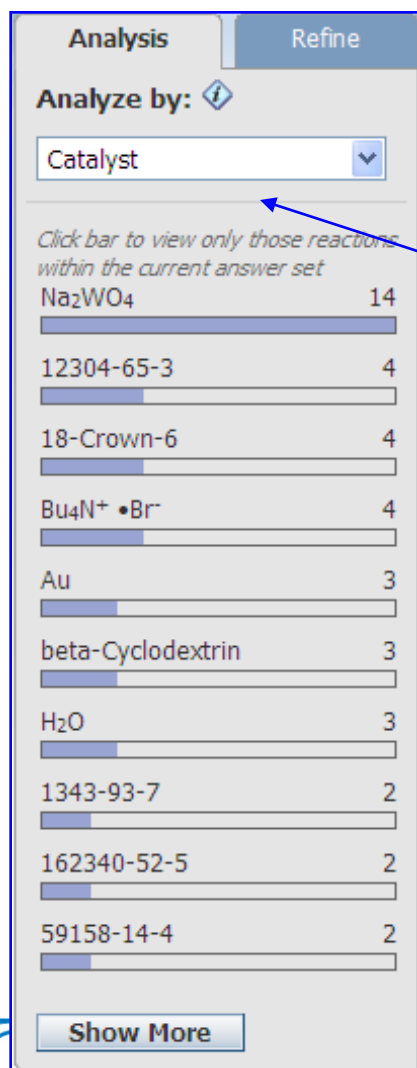
反应条件及文献出处

详细的反应过程信息

CAS is a

www.cas.org

反应检索中的分析功能



催化剂分析，用于找到经济型催化剂

溶剂分析，用于找到低毒性催化剂

反应检索中的限定功能

Analysis Refine

Refine by: ⓘ

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Product Yield:

%
Upper Limit
Example: 80

%
Lower Limit
Example: 20

Include answers that have no product yield

Refine

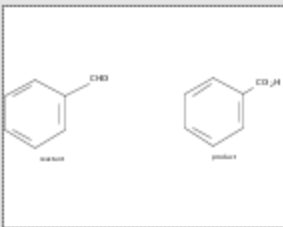
产率
限定

Analysis Refine

Refine by: ⓘ

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Reaction Structure:



Click image to change structure or view detail

Search type: **Allow variability only as specified**

Refine

Analysis Refine

Refine by: ⓘ

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Reaction Classification(s):

- Biotransformation
- Catalyzed
- Chemoselective
- Combinatorial
- Electrochemical
- Gas-phase
- Non-catalyzed
- Photochemical
- Radiochemical
- Regioselective
- Stereoselective

Refine

反应类
型限定

相似反应的获取

1. View Reaction Detail [Link](#) [Similar Reactions](#)
Single Step *Hover over any structure for more options.*

[Overview](#)

对于单步反应，可以进行相似反应检索

相似反应检索，依据和反应中心的相似程度，查询反应中心彼此相似的反应。

选择相似级别

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (7869)
- Medium - Reaction centers plus adjacent atoms and bonds (3436)
- Narrow - Reaction centers plus extended atoms and bonds (2843)

对于选择是全部反应中检索相似反应，还是在当前结果集中检索相似反应

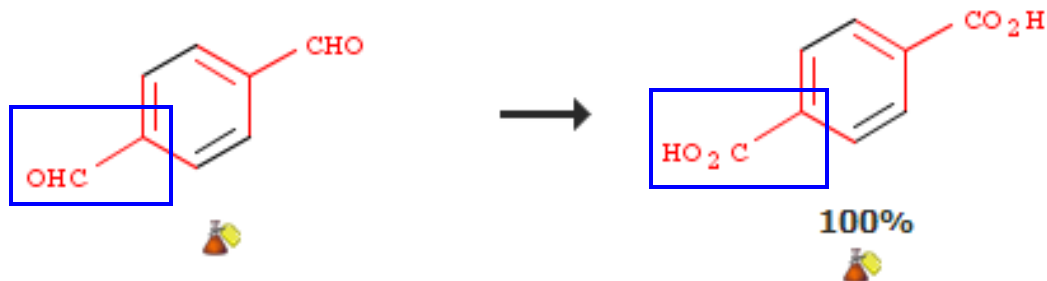
选择相似反应的相似限制

Broad: 仅反应中心相似

Medium: 反应中心及附属原子和键

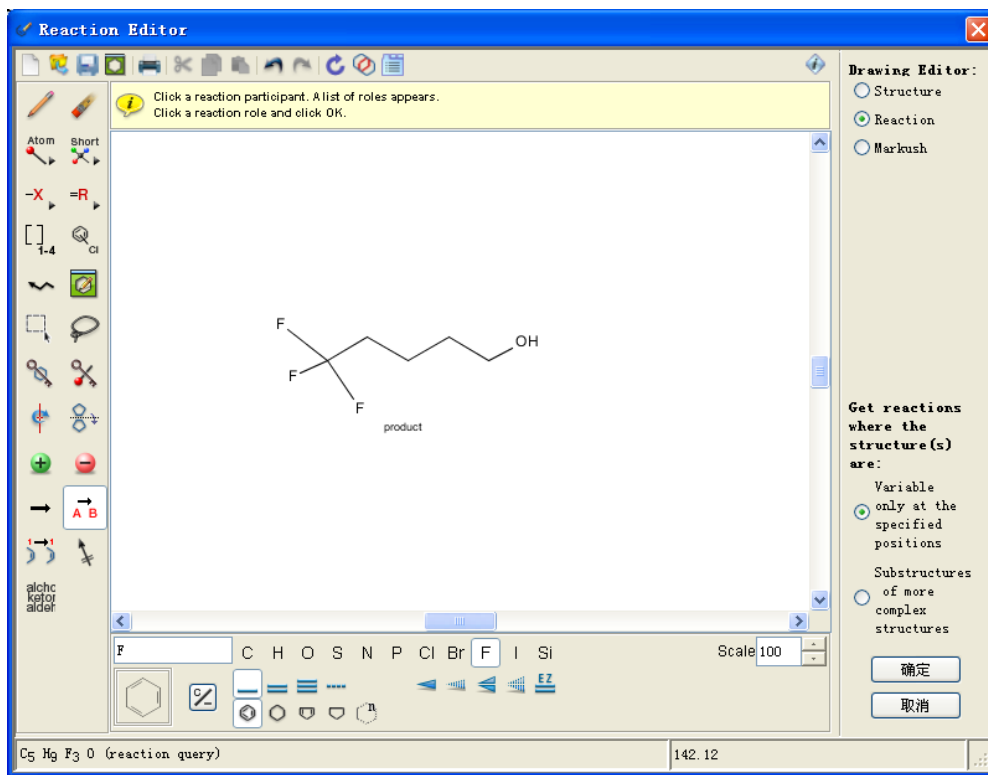
Narrow: 反应中心及扩展的原子和键

10. View Reaction Detail Link Similar Reactions
Single Step *Hover over any structure for more options.*



► Overview

获得物质的合成制备信息



通过SciFinder检索该物质的合成路线。但是没有找到具体的反应。

SciFinder Web能查询更多的物质制备信息。

SciFinder®

Explore References

Explore Substances

Explore Reactions

Welcome Verna Wong | Sign Out

Create Keep Me Posted Reaction Structure structure variable only at spe... > reactions (0)

Reactions

Find Additional Reactions

Combine Answer Sets

0 Reactions 0 Selected



Explore Reactions resulted in 0 reactions Return Find Additional Reactions

CAS®

SciFi



CAS is a division of the American Chemical Society


获得物质的合成制备信息

Reactions  Get References  Combine Answer Sets


1 Reaction 0 Selected Keep Selected Remove Selected

1 additional reaction has been added to your answer set.

Select All Deselect All Sort by: Accession Number  




1. Reaction Detail  Link

\longrightarrow HO - (CH₂)₄ - CF₃









4 references

SciFinder中没有收录该物质的合成路线，但是能获得该物质合成制备的文献，需通过全文才能获得反应。




SciFinder®  Explore References  Explore Substances  Explore Reactions








Welcome Sam Yu | Sign Out








Create Keep Me Posted Reaction Structure structure variable only at spe... > reactions (0) > find additional reactions (1) > get references (4)

References  Get Substances  Get Reactions  Get Cited  Get Citing  Get Full Text  Combine Answer Sets

4 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

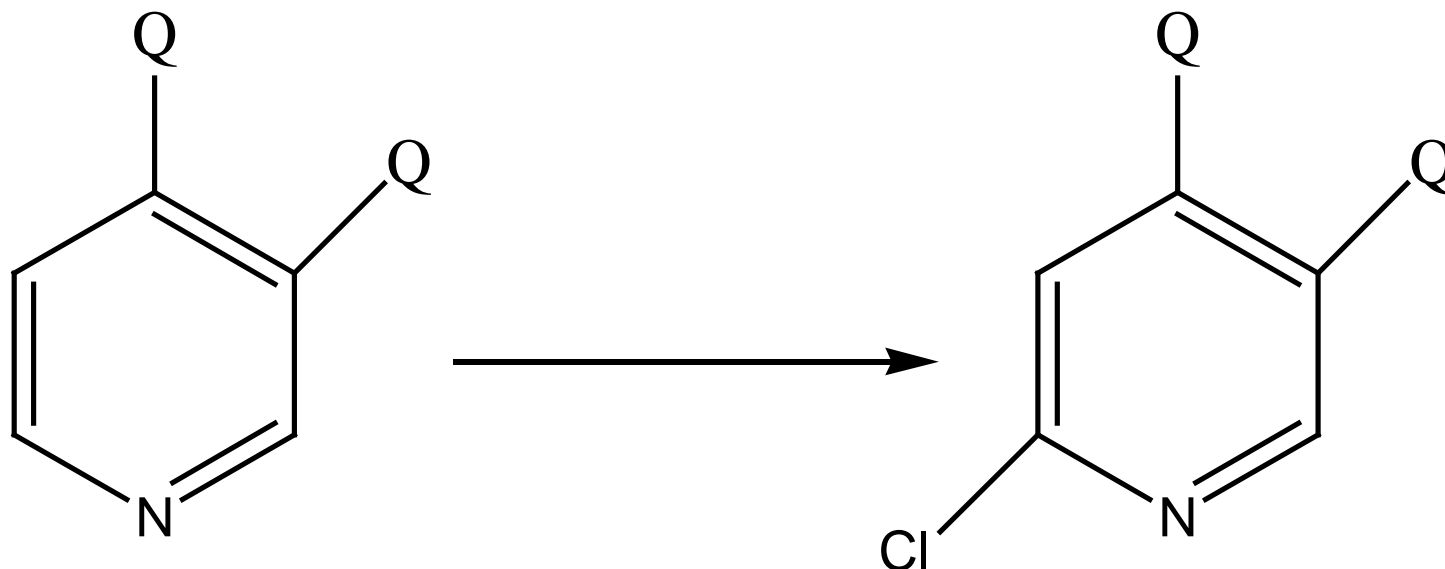
Select All Deselect All Sort by: Accession Number   Answers per Page [20] Display: 

1. Preparation of fused imidazolidine derivatives as inhibitors of cartilage matrix degradation
By Funabashi, Yasunori; Takizawa, Masayuki; Morimoto, Shinji; Notoya, Kohei
From PCT Int. Appl. (2002), WO 2002092606 A1 20021121. Language: Japanese, Database: CAPLUS
The title compds. I [R1 = (S)nR2, etc.; n = 0 - 2; R2 = H, (un)substituted hydrocarbon, etc.; R5 = H, (un)substituted hydrocarbon, etc.; the moiety represented by II in I is Q1, etc.; R6 = H, (un)substituted hydrocarbon, etc.; A = Q2, etc.; R10 = H, ZR15, etc.; Z = SO2, etc.; R15 = (un)substituted hydrocarbon, etc.; R11 = H, (un)substituted hydrocarbon] are prepd. A process for prepg. I is disclosed. Compds. of this invention in vitro at 0.1 μM gave 20% to 55% inhibition of MMP-13 prodn. Formulations are given.
 Substances  Reactions  Citing  Full Text  Link  0 Comments  0 Tags

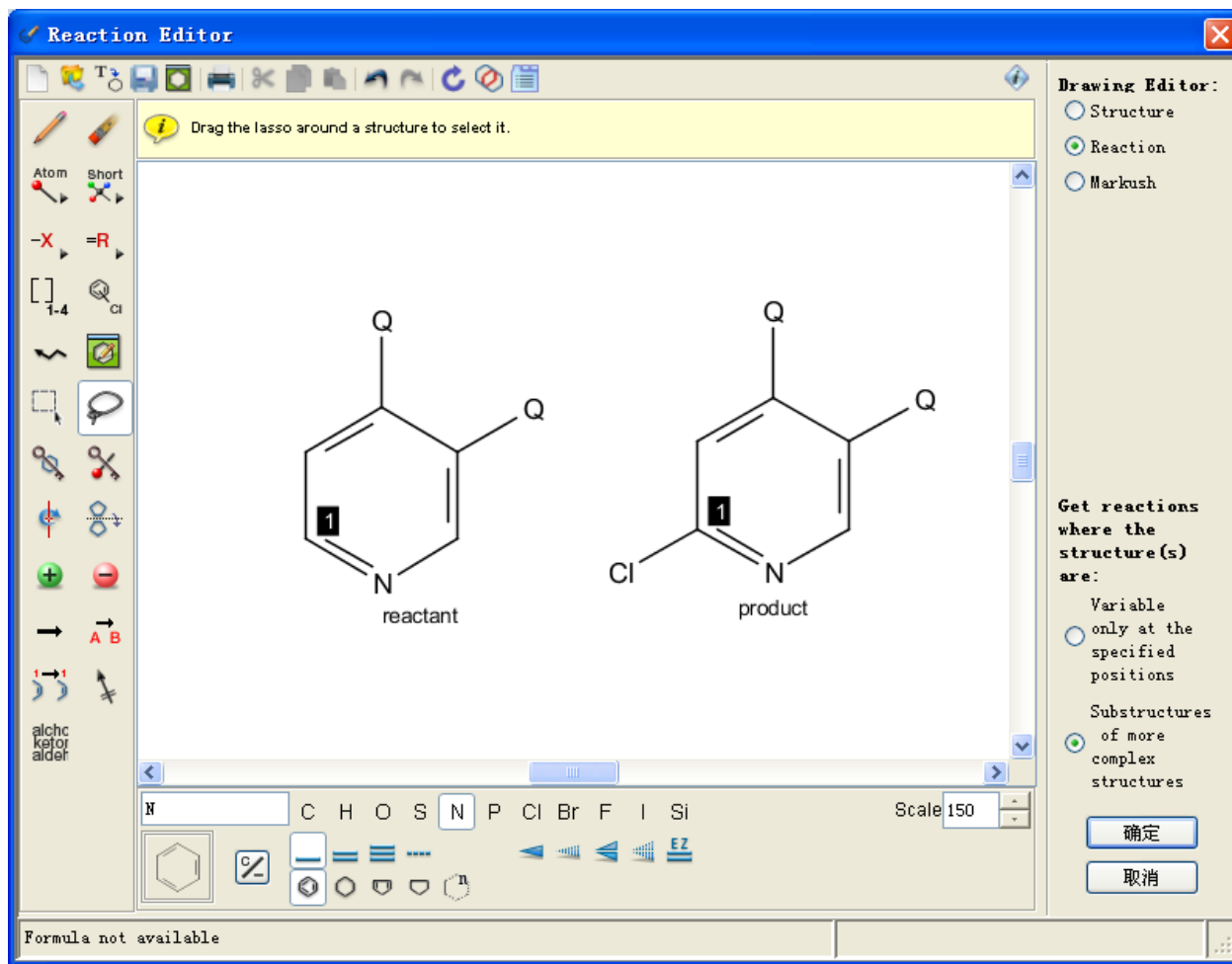
2. When is a trifluoromethyl group more lipophilic than a methyl group? Partition coefficients and selected chemical shifts of aliphatic alcohols and trifluoroalcohols
By Muller, Norbert
From Journal of Pharmaceutical Sciences (1986), 75(10), 987-91. Language: English, Database: CAPLUS
Octanol-water partition coeffs. were detd. for 12 trifluoromethylated aliph. alc. and their unfluorinated counterparts. The latter values were derived from measurements using the benzyl alc.-water solvent system after developing an appropriate correlation equation. Incidentally, an empirical equation was found which allows the partition coeff. of an unsubstituted alc. to be estd. given the mol. formula and b.p. Trifluorination strongly enhances lipophilicity only when the trifluoromethyl group is in the α-position. The enhancement is barely measurable for the β- and γ-(trifluoromethyl) al...
 Substances  Reactions  Citing  Full Text  Link  0 Comments  0 Tags

反应检索---检索对反应位置和原子有特定要求的反应

- 吡啶环的3,4位存在任意的非C,H原子或基团
- 检索在6位引入Cl的反应



定义反应结构




大多数科研工作者，刚开始都会画成这样。

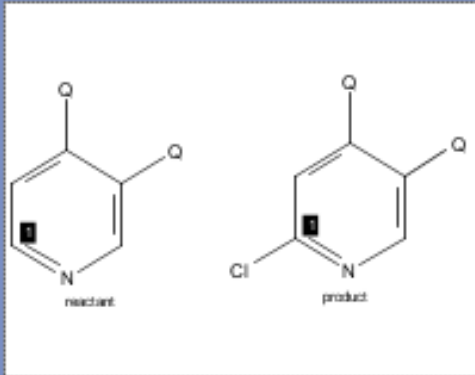
但是，这样足够吗？

尝试SciFinder中的初步检索。

亚结构检索，帮助获得所有的相关反应

Explore Reactions


Reaction Structure Reaction Structure 



reactant product

Click image to change structure or view detail

Search

Search type:  Allow variability only as specified
 Substructure

SciFinder中的反应筛选

Reactions Get References Find Additional Reactions Combine Answer Sets

3245 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: [dropdown] [down arrow] Answers per Page [15] 1 2 3 4 5 6 ... 217 [right arrow]

Display:

我们获得3200+ 条反应.

筛选的第一步是点击“ONE REACTION PER REFERENCE”. 这项功能将重复的记录合并

Reactions Get References Find Additional Reactions Combine Answer Sets

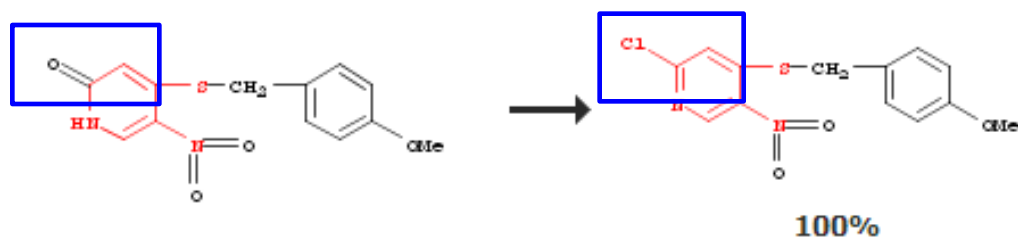
3245 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: [dropdown] [down arrow] Answers per Page [15] 1 2 3 4 5 6 ... 16 [right arrow]

Display: (230 Reactions)

简单的看一下这些反应

30. ▲22 Hits in this Reference ▲Similar Reactions
Single Step Hover over any structure for more options.

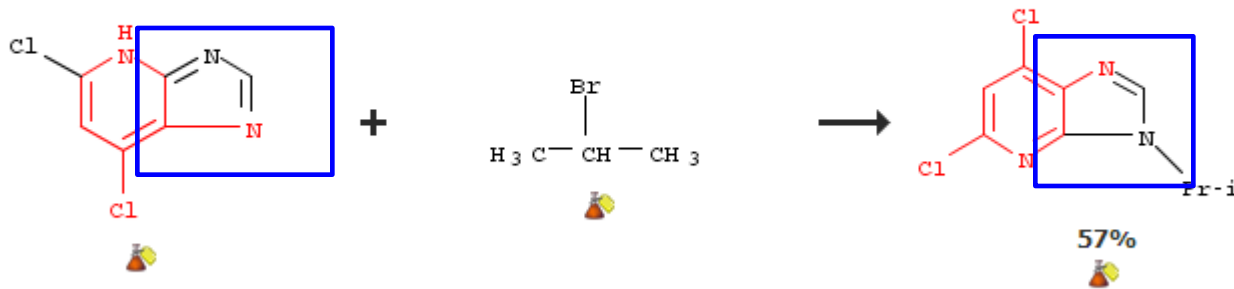


► Overview

第一条获取符合我们的要求

第二条，吡啶环系发生破坏，不是我们想要的

35. ▲5 Hits in this Reference ▲Similar Reactions
Single Step Hover over any structure for more options.



► Overview

反应中的Refine工具，添加环锁定

Analysis
Refine

Refine by:

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification
- Excluding Reaction Classification
- Non-participating functional groups

Reaction Structure:

Click image to change structure or view detail

Search type: **Substructure**

Refine

Click a ring system to block it from further ring fusion.
Click a chain to block it from ring formation.

Get reactions where the structure(s) are:

- Variable only at the specified positions
- Substructures of more complex structures



环锁定工具，当使用亚结构检索时，不允许发生稠环。

锁定环后的结果

Reactions Get References Combine Answer Sets

1063 Reactions 0 Selected Keep Selected Remove Selected

Select All Deselect All Sort by:

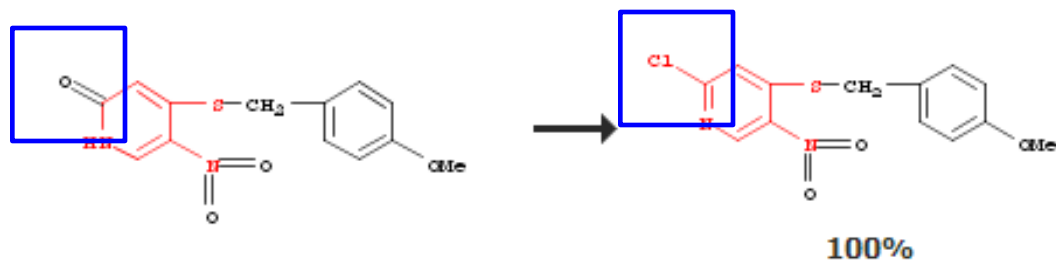
2. **▲ 2 Hits in this Reference** Similar Reactions
Single Step *Hover over any structure for more options.*

90%

这条反应，原来的6位上就有Cl，不符合我们的要求

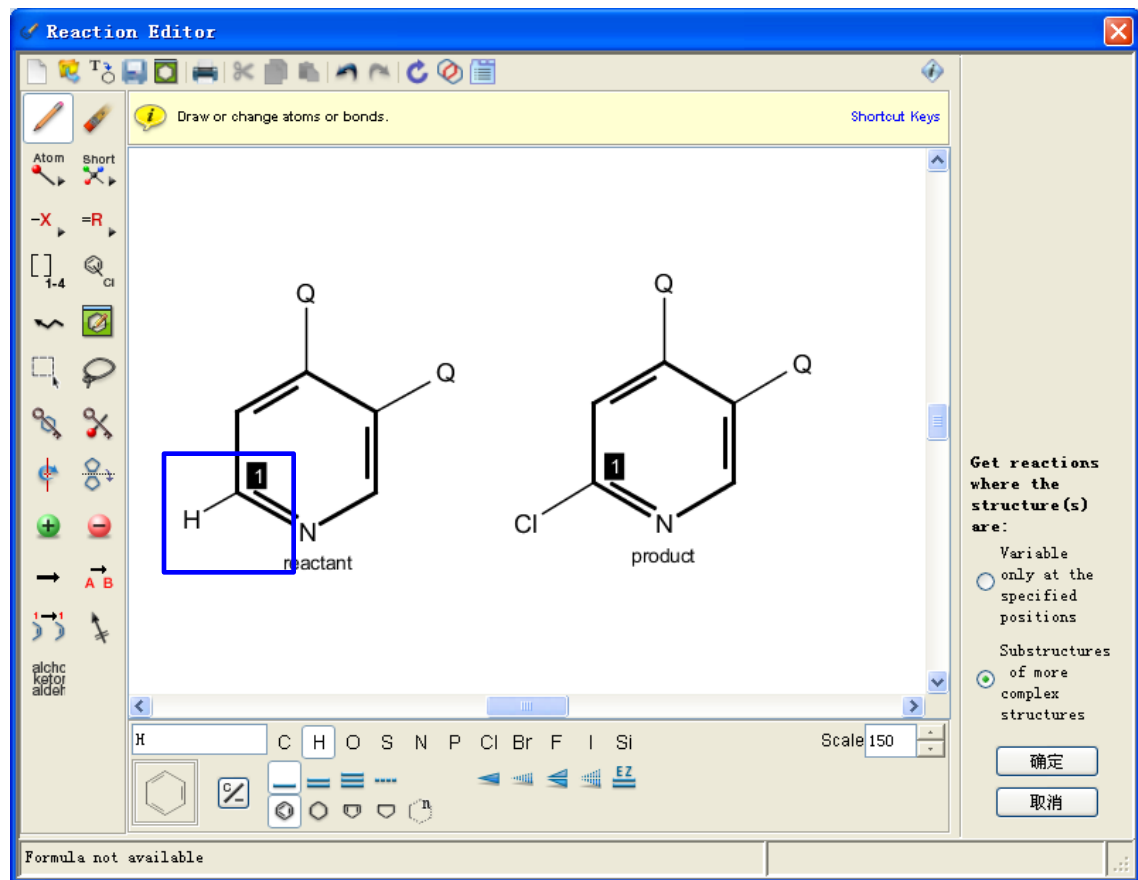
这条，或许满足我们的要求，这里需要大家思考，到底需要什么类型的反应，如果只想获得从H变成Cl的。

25. **▲ 17 Hits in this Reference** Similar Reactions
Single Step *Hover over any structure for more options.*



► Overview

继续使用Refine



Analysis **Refine**

Refine by: [?](#)

Reaction Structure

Product Yield

Number of Steps

Reaction Classification

Excluding Reaction Classification

Non-participating functional groups

Reaction Structure:

Click image to change structure or view detail

Search type: **Substructure**

Refine

这是我们要的反应

Reactions Get References Combine Answer Sets

69 Reactions 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: [v] [d] Answers per Page [15] 1 2 [▶]

Display: [▲] [▼] (15 Reactions) [⌂] [⚙]

4. ▲ 4 Hits in this Reference
3 Steps *Hover over any structure for more options.*

所有的反应都符合我们的
结构要求

在吡啶环的6位存在H到Cl
的变化

16. ▲ 5 Hits in this Reference
2 Steps *Hover over any structure for more options.*

▶ Overview

▶ Experimental Procedure **NEW**

一些值得思考的问题

- 并不是所有的科研工作者，一开始就能准确的定义反应结构
- 建议先大致浏览下反应结果集，然后去思考如何去除我们不想要的反应。
- 使用**Analyze/Refine**工具，或其他的检索策略，去除不想要的反应。

SciPlanner功能帮助制定逆合成路线

SciFinder®

Welcome Michelle Tang | Sign Out

Explore References | Explore Substances | Explore Reactions

Research Topic: Search

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

Publication Year(s):
Examples: 1995, 1995-1999, 1995-, -1995

NEW SciPlanner

Saved Answer Sets

- suoliuhua
- 瘦肉精
- 依法韦仑
- 帕尼单抗
- 失水山梨醇酯
- 依法韦仑多晶型
- 药物多晶型与生物利用度
- 204255-11-8达菲
- suoliuhua all
- advair
- Autosaved Reference Set

View All

Import

什么是SciPlanner?

1. **SciPlanner**是一个特定的工作区域，可以让用户用一种更加直接的方式去组织、管理检索结果。
2. 文献、物质、反应信息都可以传送到**SciPlanner**，并在其中进行自由组织，增强可视化效果。
3. **SciPlanner**可以辅助进行逆合成路线的制定。

在SciPlanner面板上逆推出源于简单起始原料的合成路线

SciPlanner
SciPlanner_04_19_2011_151715

Workspace Edit View GoTo

A novel, highly enantioselective ketone alkylation reaction mediated by chiral zinc aminoalkoxides
By Tan, Lushi et al
From *Angewandte Chemie, International Edition*, 38, 1433-7851, 711-713, 1999

Improved process for preparation of efavirenz
From *PCT Int. Appl.*, 2011007367, Jan 20, 2011

Trifluoromethyl-promoted homocamptothecins: Synthesis and biological activity
By Zhu, Lingqian et al
From *European Journal of Medicinal Chemistry*, 45, 0223-5234, 2726-2732, 2010

Preparation of substituted nitrogen heterocycles for treating various diseases
From *PCT Int. Appl.*, 2009121033, Oct 01, 2009

Clear References

A novel, highly enantioselective ketone alkylation reaction mediated by chiral zinc aminoalkoxides
Improved process for preparation of efavirenz

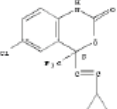
以PDF文件导出，可以看到整条合成路线

SciPlanner_05_03_2011_145024.pdf - Adobe Acrobat Pro

文件(F) 编辑(E) 视图(V) 文档(D) 注释(C) 表单(R) 工具(T) 高级(A) 窗口(W) 帮助(H)

创建 合并 协作 安全 签名 表单 多媒体 注释

1 / 7 139% 查找



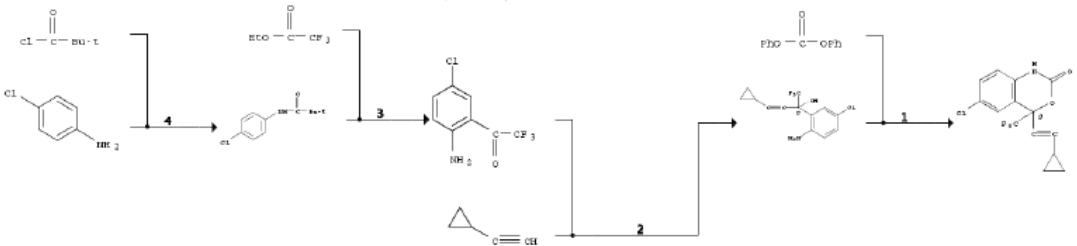
A novel, highly enantioselective ketone alkylation reaction mediated by chiral zinc aminoalkoxides
By Tan, Lushi et al
From *Angewandte Chemie, International Edition*, 38, 1433-7851, 711-713, 1999

SciFinder®

Improved process for preparation of efavirenz
From *PCT Int. Appl.*, 2011007367, Jan 20, 2011

Trifluoromethyl-promoted homocamptothecins:
Synthesis and biological activity
By Zhu, Lingjian et al
From *European Journal of Medicinal Chemistry*, 45, 0223-5234, 2726-2732, 2010

Preparation of substituted nitrogen heterocycles for treating various diseases
From *PCT Int. Appl.*, 2009121033, Oct 01, 2009



Page 1

以及详细的反应信息、物质信息和文献信息

SciFinder® Reaction Information		Notes	Yield
Reaction Stages			
20	1.1 R:DBU, S:THF, rt, 2 h, 60°C	Reactants: 2, Reagents: 1, Solvents: 1, Steps: 1, Stages: 1	98%

References

Improved pro
By Singh, Giri
From PCT Int

Reaction Stages	
21	1.1 R:BuMg S:THF

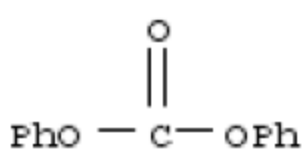
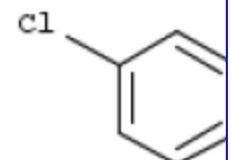
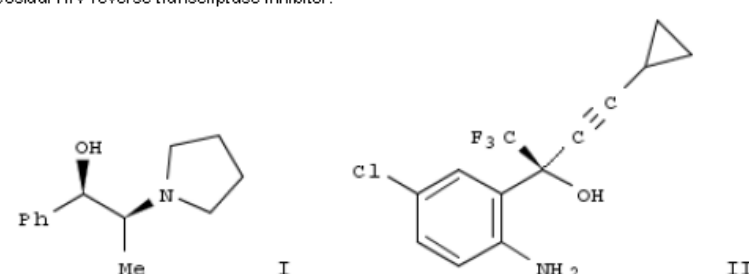
References

A novel, high
By Tan, Lushi
From Angew

Reaction Stages	
22	1.1 R:NaOH 25°C; 25°C

References

Trifluoromethyl
By Zhu, Lingji
From Europe

SciFinder® Reaction Information		Page 4
102-09-0	106-47-8	154598-52-4
 <p>C₁₃H₁₀O₃ Carbonic acid, diphenyl ester ~2001 References Reactions Commercial Sources Regulatory Information Link Copyright © 2011 American Chemical Society (ACS). All Rights Reserved.</p>	 <p>C₆H₆ClN Benzenamine, 4-chloro ~14690 References Reactions Commercial Sources Regulatory Information Link Copyright © 2011 American Chemical Society (ACS). All Rights Reserved.</p>	<p>A novel, highly enantioselective ketone alkylation reaction mediated by chiral zinc aminoalkoxides By Tan, Lushi; Chen, Cheng-yi; Tillyer, Richard D.; Grabowski, Edward J. J.; Reider, Paul J. From: Angewandte Chemie, International Edition (1999), 38(5), 711-713, Language: English, Database: CAPLUS, DOI:10.1002/(SICI)1521-3773(19990301)38:5<711::AID-ANIE711>3.0.CO;2-W</p> <p>A method for asym. alkylation of ketoanilines using chiral zinc aminoalkoxides was developed. Stereocontrol was provided by use of norephedrine derivs., e.g. I, as chiral auxiliaries in the prepn. of the active catalyst. Structural variations with achiral additives used were found to influence the enantioselectivities. This stereoselective alkylation was demonstrated in prepn. a key intermediate (II) used in the synthesis of Efavirenz, a potent nonnucleosidal HIV reverse transcriptase inhibitor.</p>  <p>Copyright © 2011 American Chemical Society (ACS). All Rights Reserved.</p>
		<p>Trifluoromethyl-promoted homocamptothecins: Synthesis and biological activity By Zhu, Lingjian; Miao, Zhenyuan; Sheng, Chunquan; Guo, Wei; Yao, Jianzhong; Liu, Wenfeng; Che, Xiaoying; Wang, Wenyu; Cheng, Pengfei; Zhang, Wannian From: European Journal of Medicinal Chemistry (2010), 45(7), 2726-2732, Language: English, Database: CAPLUS, DOI:10.1016/j.ejmech.2010.02.051</p> <p>The homocamptothecin (hCPT) represents a new class of topoisomerase inhibitor which combines enhanced plasma stability and strong antitumor activity. Fluorine imparts desirable characteristics to drugs by modulating both the pharmacokinetics and pharmacodynamic properties of a drug. Therefore, in an attempt to improve the antitumor activity of homocamptothecins, seven new 7-trifluoromethylated homocamptothecin derivs. I (R7 = CF₃, R9 = H, R10 = H, Cl, OMe, Br, CF₃, OH; R7 = CF₃, R9 = OMe, R10 = H) were prepd. by proline-catalyzed Friedlander annulation. The antitumor activity in vitro and in vivo on cancer cell lines, and inhibitory properties of topoisomerase I-mediated DNA cleavage of compds. I (R7 = CF₃, Me, R9 = H, R10 = H) were evaluated. Several of these trifluoromethylated hCPT derivs., i.e. I (R7 = CF₃, R9 = H, R10 = Cl, OMe, H), possessed higher in vitro antitumor activity than topotecan (TPT). Esp., compd. I (R7 = CF₃, R9 = H, R10 = H) showed effective in vivo antitumor activity comparable to that of TPT.</p>

SciFinder中的反应检索能帮助您

进行反应定义, 自定义不反应的基团

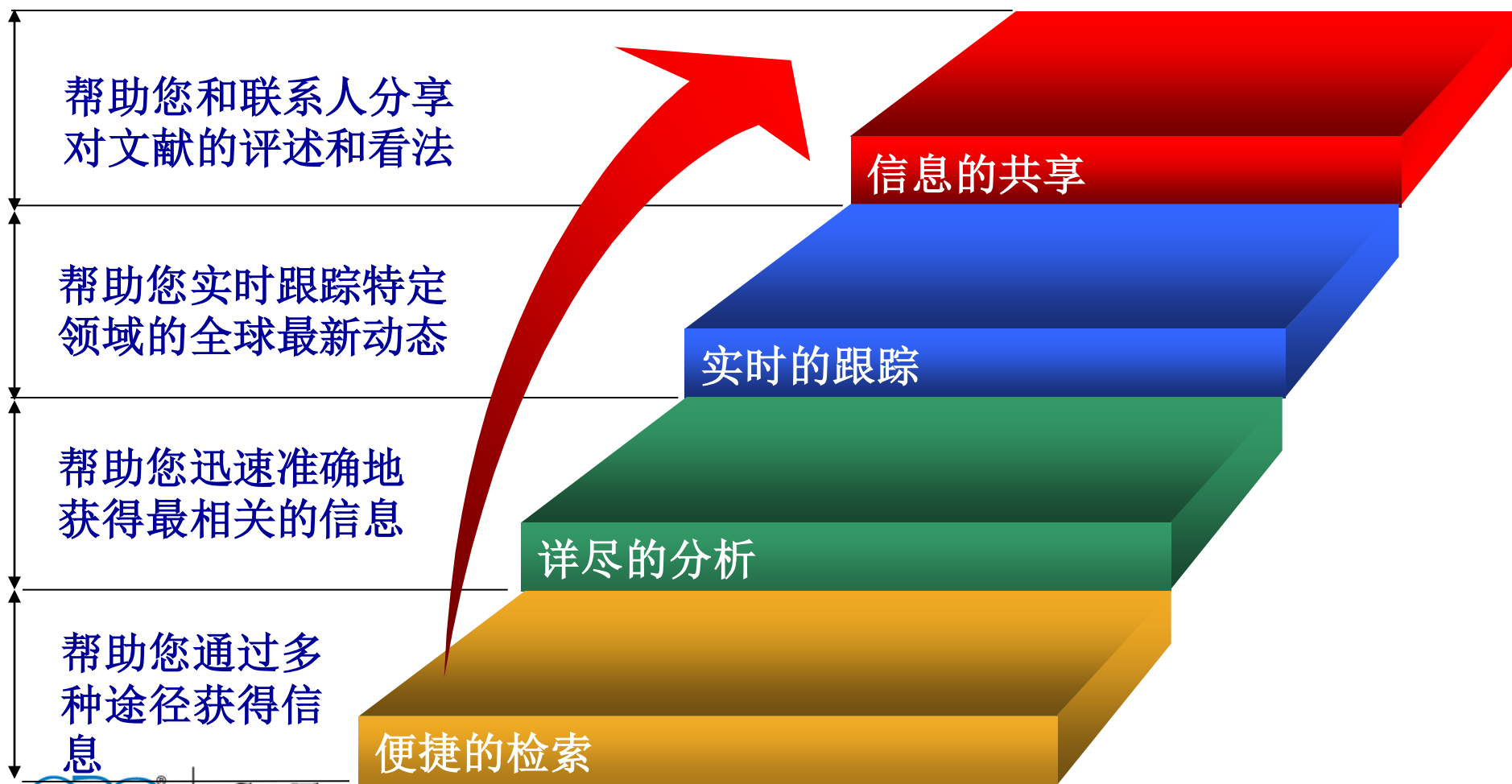
查看反应操作过程, 系统分析溶剂/催化剂等信息

获得没有被收录的反应对应的文献

获得反应中心相似的反应

利用SciPlanner功能帮助制定逆合成路线

SciFinder 帮您实现从检索到分析，到跟踪，到共享的飞跃





CAS 100th Anniversary Celebration

CAS databases streamline the investigative process allowing you to take an idea and rapidly find the important and necessary information before you forget about the idea or it loses its excitement. That really is invaluable."

— Dr. Robert Grubbs

2005 Nobel Laureate in Chemistry

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罗伯特·格拉布

2005年诺贝尔化学奖获得者

Thanks for attention!

For more information please contact : <http://www.igroup.com.cn/cas/>

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王 薇

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Email: verna@igroup.com.cn