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- SciFinder的检索界面
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- SciFinder中的反应检索

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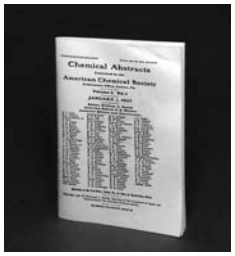

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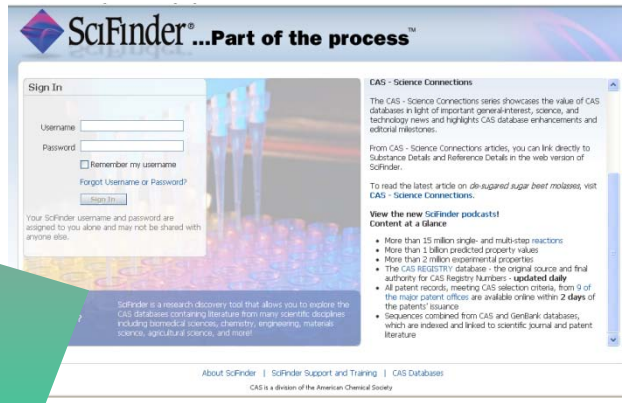

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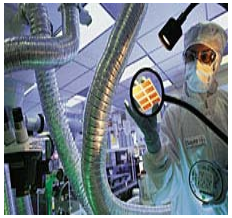

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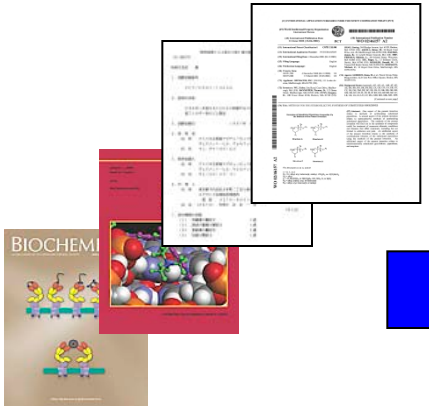

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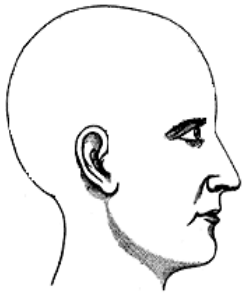

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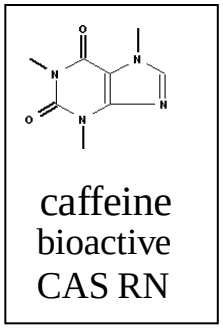

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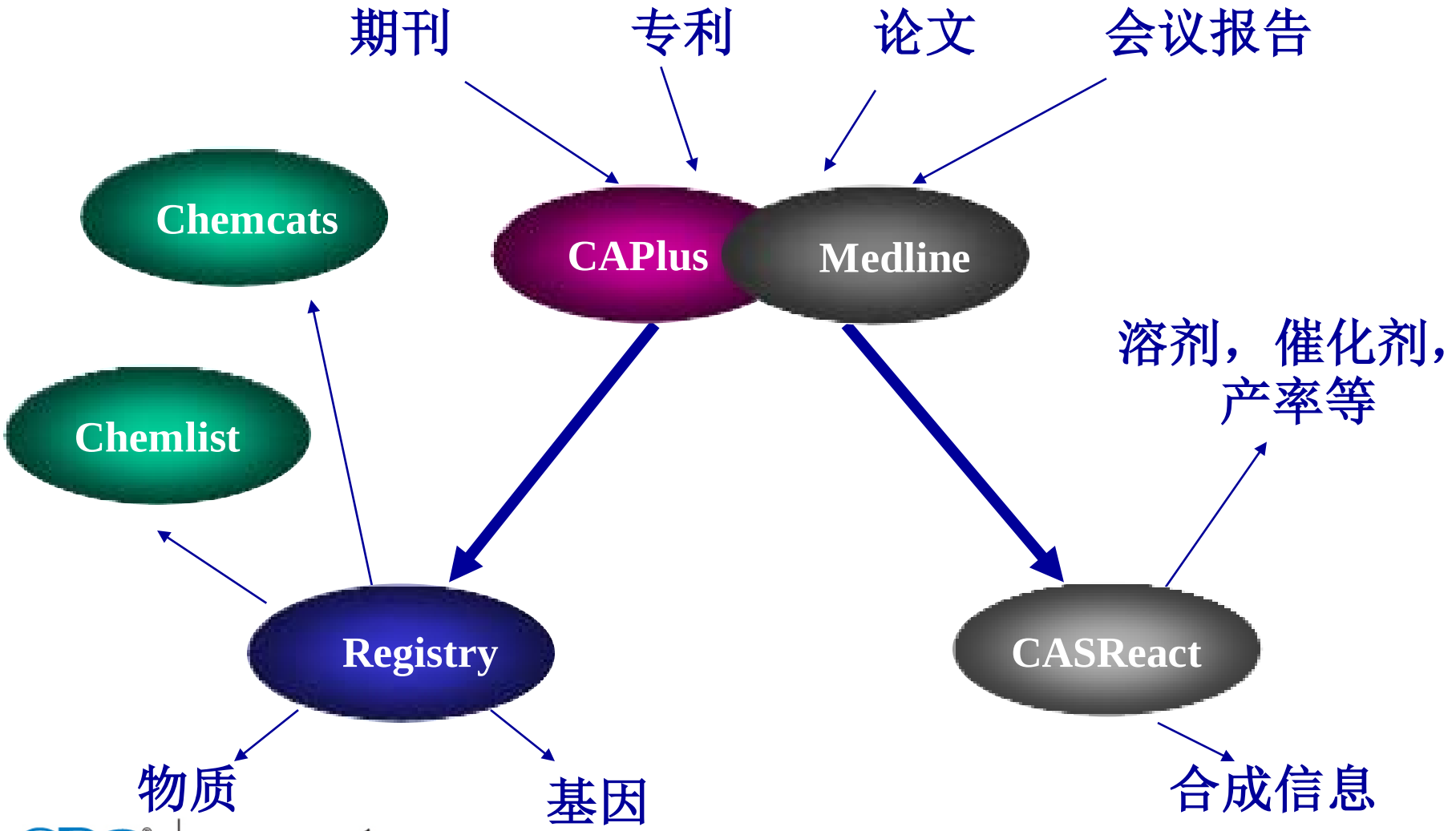

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Fluorescence and Thermostability of Nanometer Porphyrin Trimer

SHI Ying-yan[1,2], FA Huan-bao[1], ZHENG Wen-qi[1], LI Di[1], SHAN Ning[1] and WANG Xing-qiao[1]**
1. *College of Chemistry, Jilin University, Changchun* 130023, *P. R. China*;
2. *Departement of Base Science, Jilin Institute of Architecture and Civil Engineering, Changchun* 130021, *R. R. China*

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 monoporphyrin. The effects of the molecule structure on the optical property and the thermostability were also studied in detail.

Keywords Monoporphyrin; Porphyrin trimer; Fluorescence; Thermostability
Article ID 1005-9040(2006)-01-014-03

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Introduction

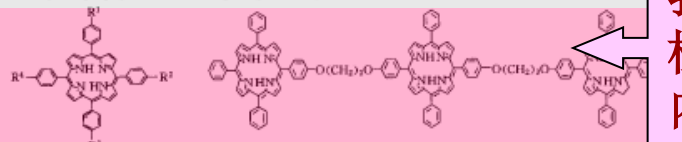
Porphyrin possesses some comparison with the porphyrin gomers are much attracting ow properties in some aspects, suc gy transformation and electro years, Oligomeric porphyrins have been under intensive research for their potential applications in molecular electronic and optic fields. For instance, multiporphyrin 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[8]. 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

of porphyrin peripheral substitu- the oligomer formation. The kind mmetry of a molecular structure mendous influence on the fluores- tability of porphyrins. This inves- uilable reference for the research olecular wires and logic gate cir- cuits in molecular electronics.

Experimental

Pyrrole(Fluka Chemika-Biochemika) and 1,3-dibromopropane (reagent grade) were freshly distilled prior to use. DMF and anhydrous K_2CO_3 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 been described elsewhere[11].



1—3 4

Fig. 1 The structures of porphyrin monomers 1—3 and the porphyrin trimer(4).
1. R^1 = OH, R^2 = R^3 = R^4 = H; 2. R^1 = R^5 = OH, R^2 = R^4 = H; 3. R^2 = $O(CH_2)_3Br$, R^1 = R^3 = R^4 = H.

* Supported by the National Natural Science Foundation of China(No. 20071014).
** To whom correspondence should be addressed. E-mail: wangxingqiao@mail.jlu.edu.cn

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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 characf porphyrins are represented by the ompounds **3** and **4** with a typical set Q-bands in the visible region, those of H_2MHTPP(**1**) and *trans*-H_2DHDPP(**2**). The band around 420 nm is assigned to the Soret band which arises from the transition of $a_{1u}(\pi)$—$e_g^*(\pi)$, and the other four absorption maxima around 516, 550, 590 and 645 nm can be attributed to the Q-bands, corresponding to $a_{2u}(\pi)$—$e_g^*(\pi)$[12]. This indicates that porphyrin monomers being linked by —CH_2— 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 CH_2Cl_2

	et band, λ/nm($10^5\varepsilon$)	Q band, λ/nm($10^4\varepsilon$)			
	418.40(0.3)	515.68(2.3)	547.68(1.8)	589.92(1.4)	647.52(1.2)
	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 emi and **2** at 471 nm can be as sition and it is correspo 418.4 nm of their electron the fluorescence emission at the same position disap sion peaks at 650 and 714 be assigned to the $S_1 \longrightarrow S_0$ transition and correspond with Q(0, 0), Q(0, 1) of porphyrins **1**—**4**[13].

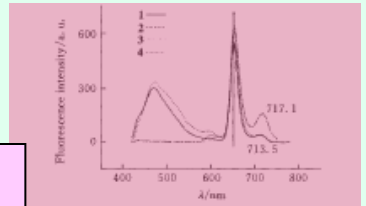

Fig. 2 The fluorescence emission spectra of porphyrin monomers 1—3 and a trimer(4)(excited at nm).

The experimental results indicate that in dichlo- ethane, compared with those at 418 nm in the ab- tion spectrum, the fluorescence emission peak at 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 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 por- oxyphenyl groups at the *me-* **1** has only one hydroxyphe- on. Therefore, the different peripheral hydroxyphenyl nce in the forms of energy ransit from a single excited 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 CH_2Cl_2. 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, CH_2Cl_2 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-qi; 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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UV and visible spectra

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porphyrin trimer nanometer bromopropane bridging fluorescence thermostability

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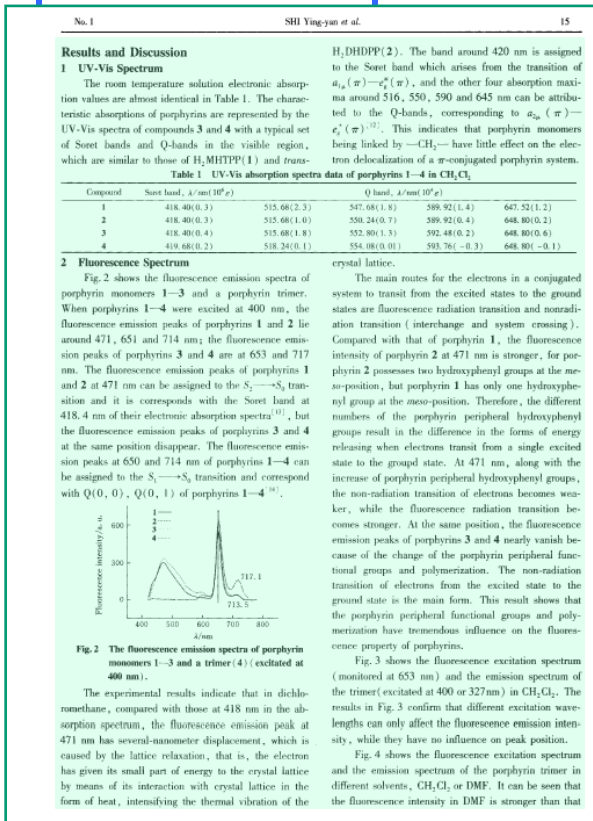

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Results and Discussion

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 H_2MHTPP(**1**) and *trans*-H_2DHDPP(**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 $a_{2u}(\pi)\rightarrow e_g^*(\pi)$[17]. This indicates that porphyrin monomers being linked by —CH_2— have little effect on the electron delocalization of a π-conjugated porphyrin system.

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Compound	Soret band, λ/nm($10^5\varepsilon$)	Q band, λ/nm($10^4\varepsilon$)			
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)

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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** 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 groupd 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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Fig. 4 shows the fluorescence excitation spectrum and the emission spectrum of the porphyrin trimer in different solvents, CH_2Cl_2 or DMF. It can be seen that the fluorescence intensity in DMF is stronger than that

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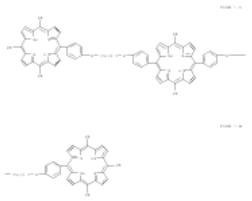
757977-32-5



$C_{138}H_{98}N_{12}O_4$

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

~3 References
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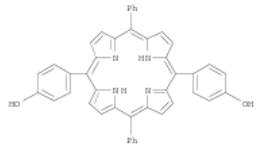

$C_{44}H_{30}N_4O_2$

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

~15 References
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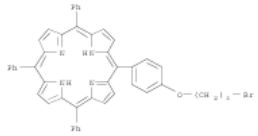

$C_{47}H_{35}BrN_4O$

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

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Reactions
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4. Substance Detail
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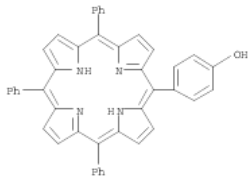

$C_{44}H_{30}N_4O$

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

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5. Substance Detail
109-64-8

$C_3H_6Br_2$

Propane, 1,3-dibromo-

~4,720 References
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Concepts

Fluorescence — Thermal stability

fluorescence and thermostability of porphyrins and nanometer porphyrin trimer

Porphyrins

fluorescence and thermostability of porphyrins and nanometer porphyrin trimer

Properties

UV and visible spectra

of porphyrins and nanometer porphyrin trimer

Solvent polarity effect

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Supplementary Terms

porphyrin trimer nanometer bromopropane bridging fluorescence thermostability

Substances

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fluorescence and thermostability of

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109-64-8

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

Other use, unclassified; Uses

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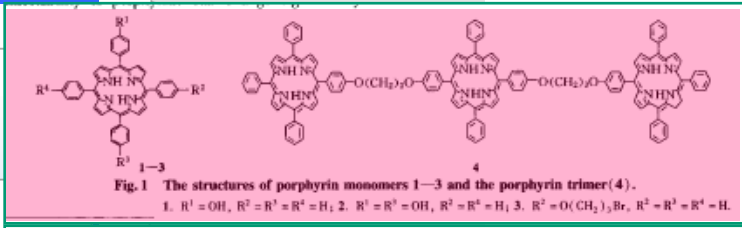

Fig. 1 The structures of porphyrin monomers 1—3 and the porphyrin trimer(4).
1. R^1 = OH, R^2 = R^3 = R^4 = H; 2. R^1 = R^3 = OH, R^2 = R^4 = H; 3. R^2 = $O(CH_2)_3Br$, R^2 = R^3 = R^4 = H.

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CAS Registry Number: 87345-22-0

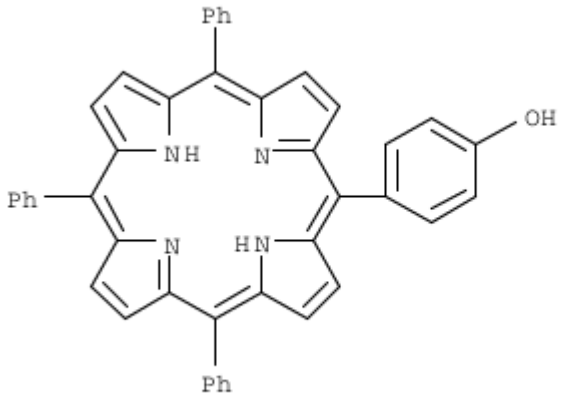
$C_{44}H_{30}N_4O$

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

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Spectra Properties	Value	Conditions
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Emission/Luminescence Spectrum	See full text	
IR Absorption Spectrum	See full text	1 of 7
IR Spectrum	See full text	1 of 2
Mass Spectrum	See full text	1 of 10
NMR Spectrum	See full text	1 of 2
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UV and Visible Emission/Luminescence Spectrum	See full text	1 of 2
UV and Visible Spectrum	See full text	1 of 6

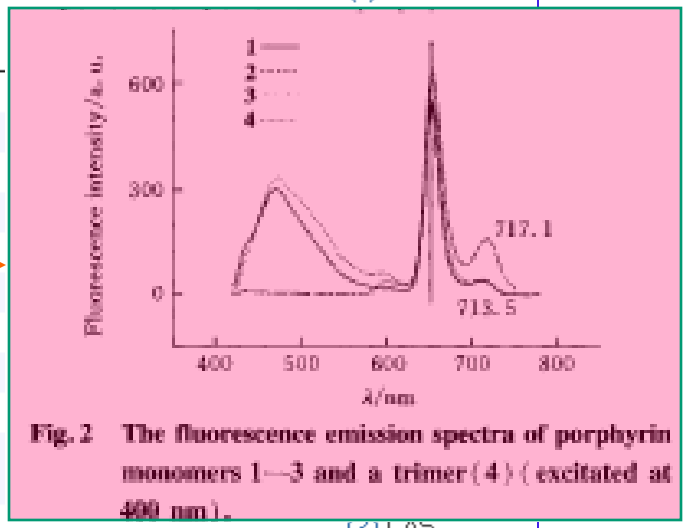

Fig. 2 The fluorescence emission spectra of porphyrin monomers 1—3 and a trimer (4) (excited at 400 nm).

(2) CAS

Thermal Properties	Value	Condi
Melting Point	>300 °C (decomp)	
Melting Point	>300 °C	Solv: (
Melting Point	>300 °C	Solv: (
Melting Point	220 °C	

Table 1 UV-Vis absorption spectra data of porphyrins 1—4 in CH_2Cl_2

Compound	Soret band, λ/nm($10^5\varepsilon$)	Q band, λ/nm($10^4\varepsilon$)			
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)

(1) CAS

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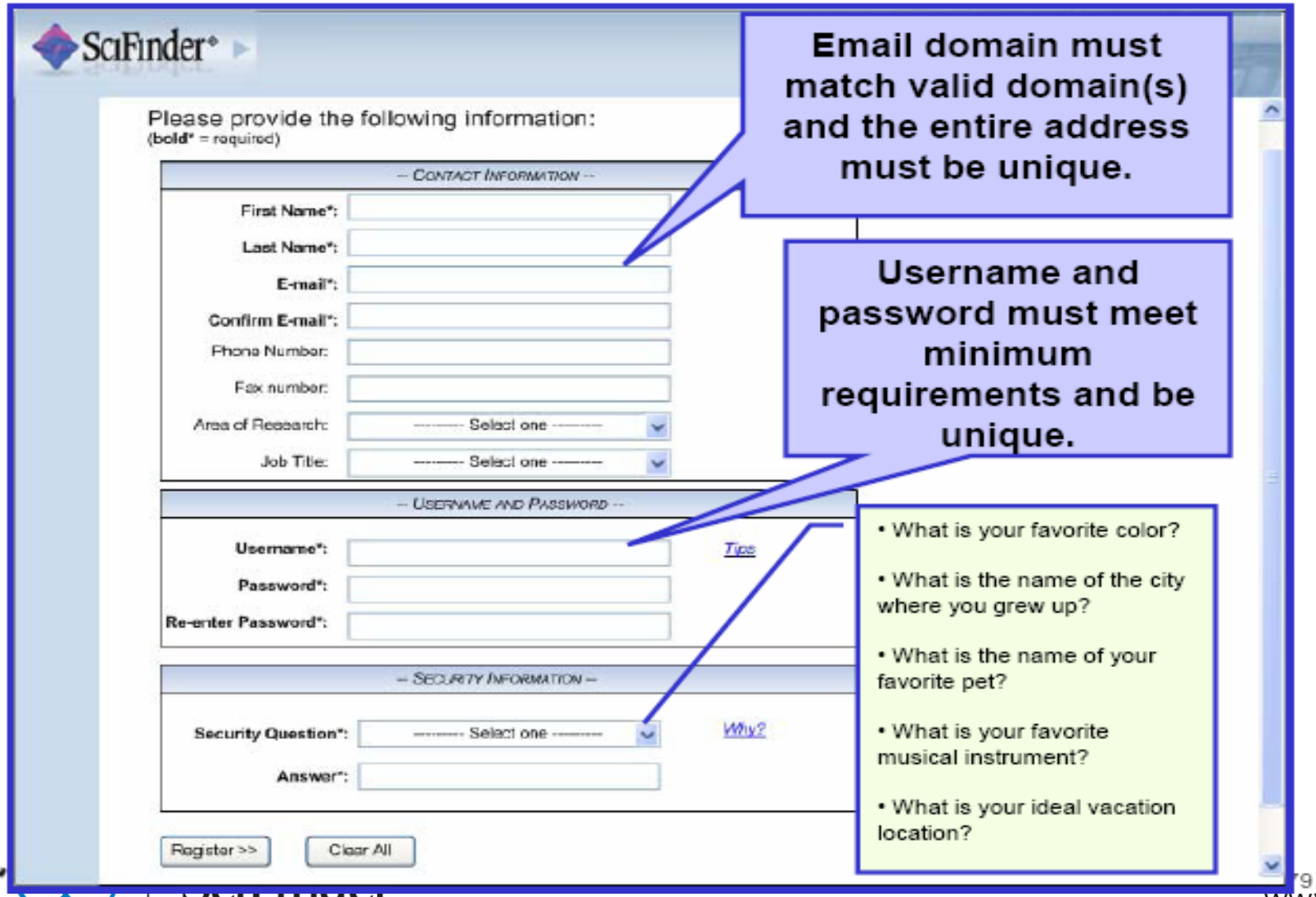

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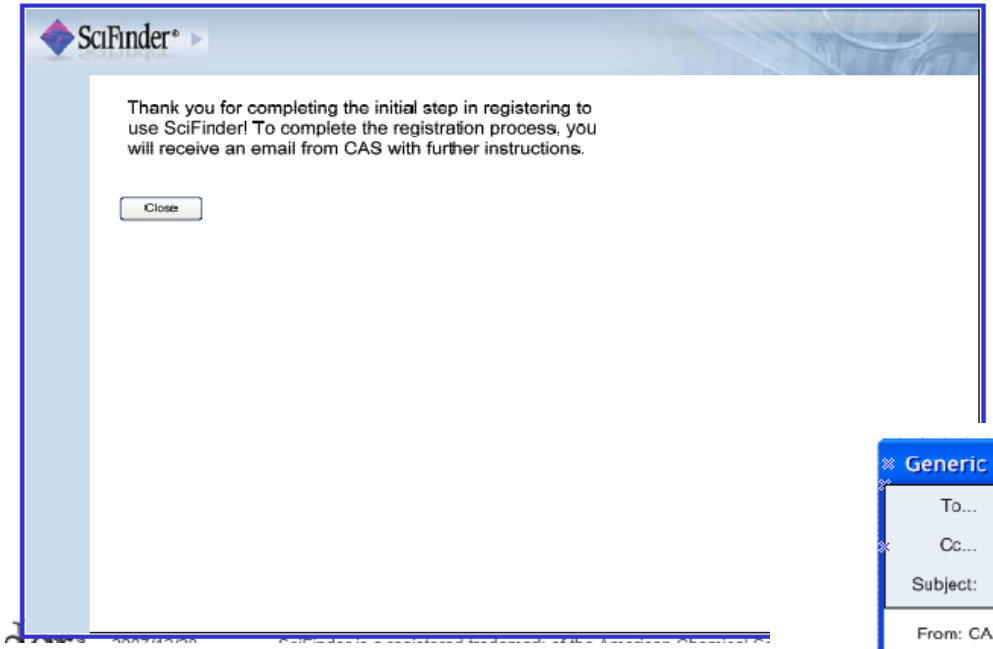

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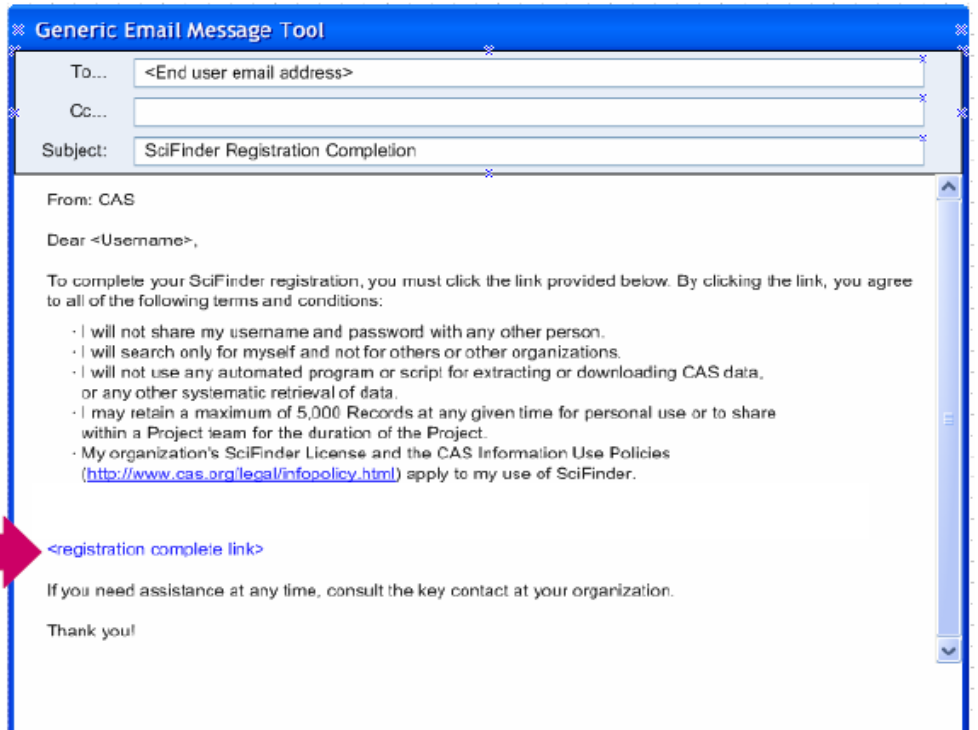

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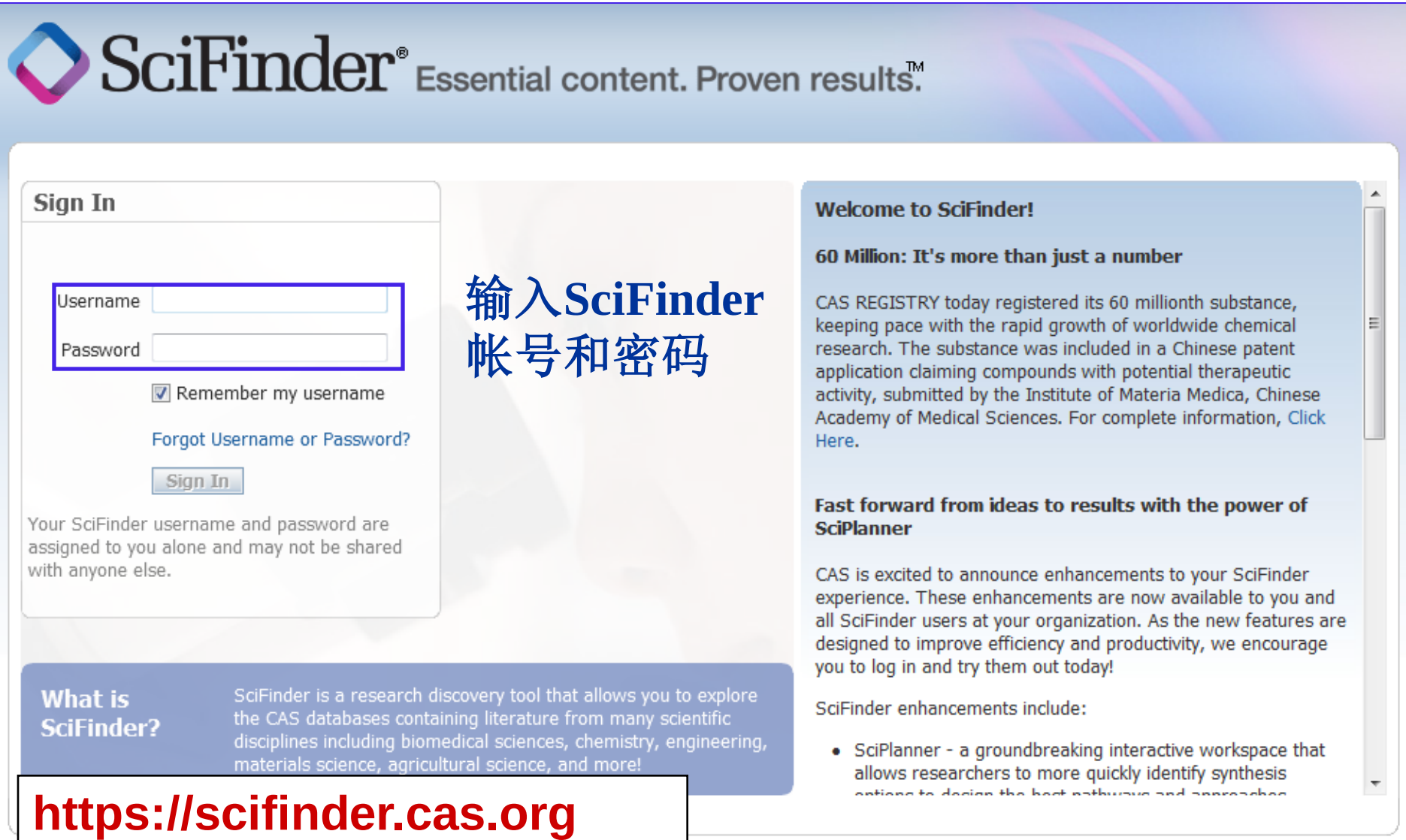

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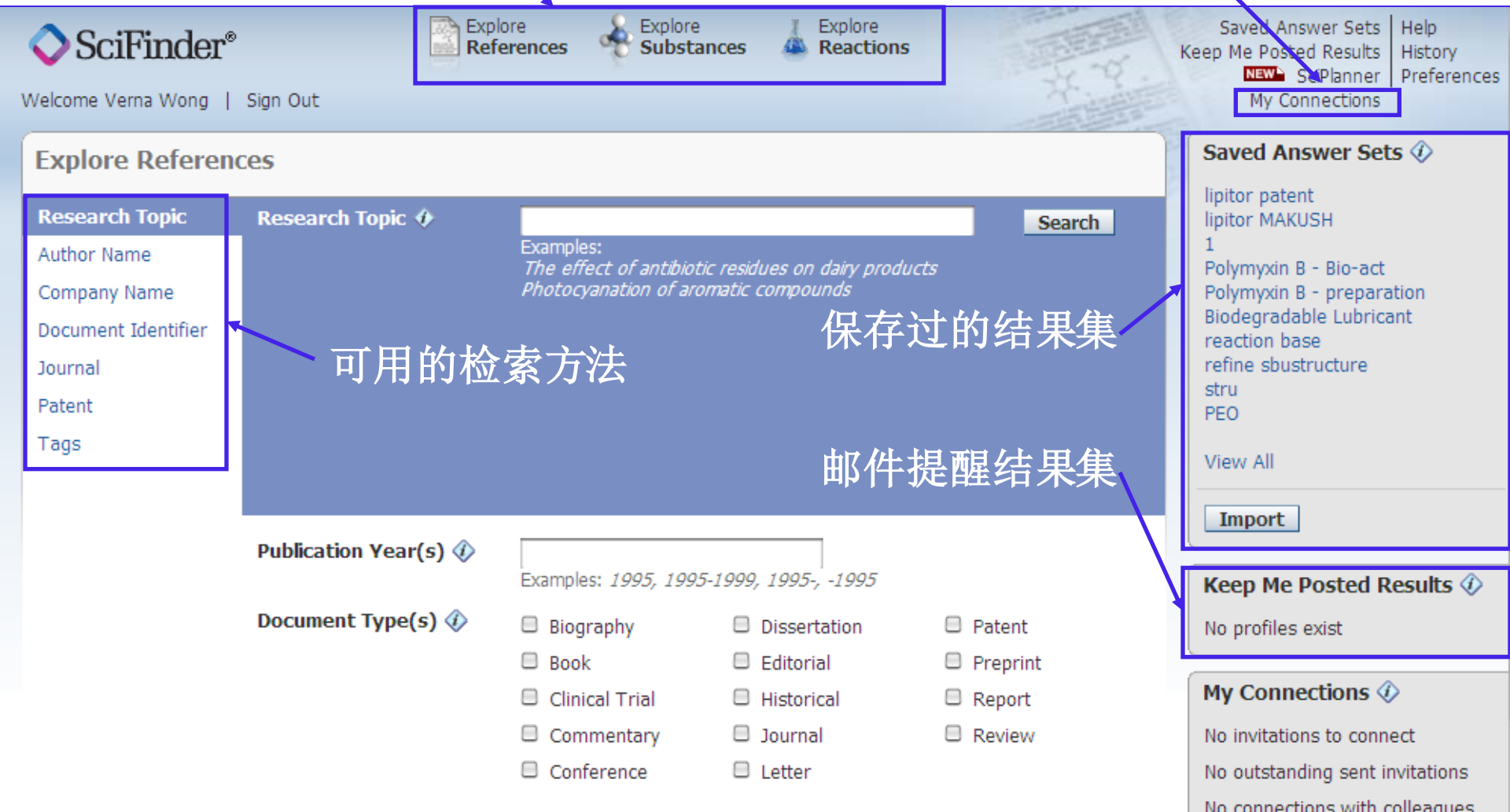

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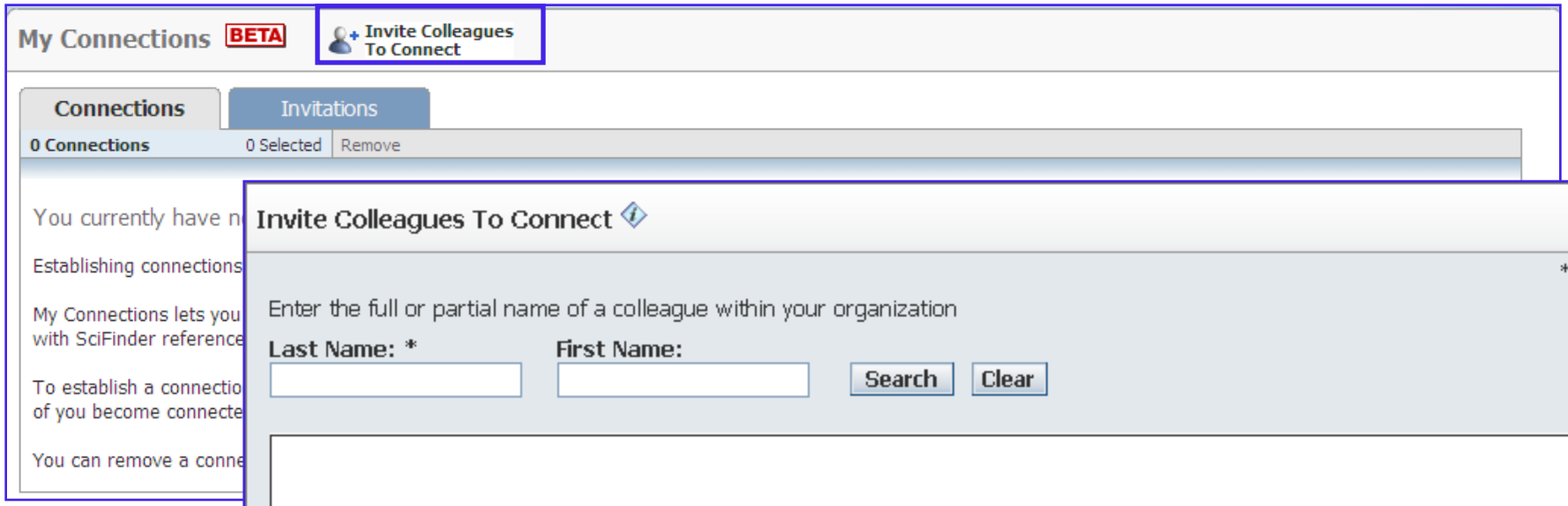

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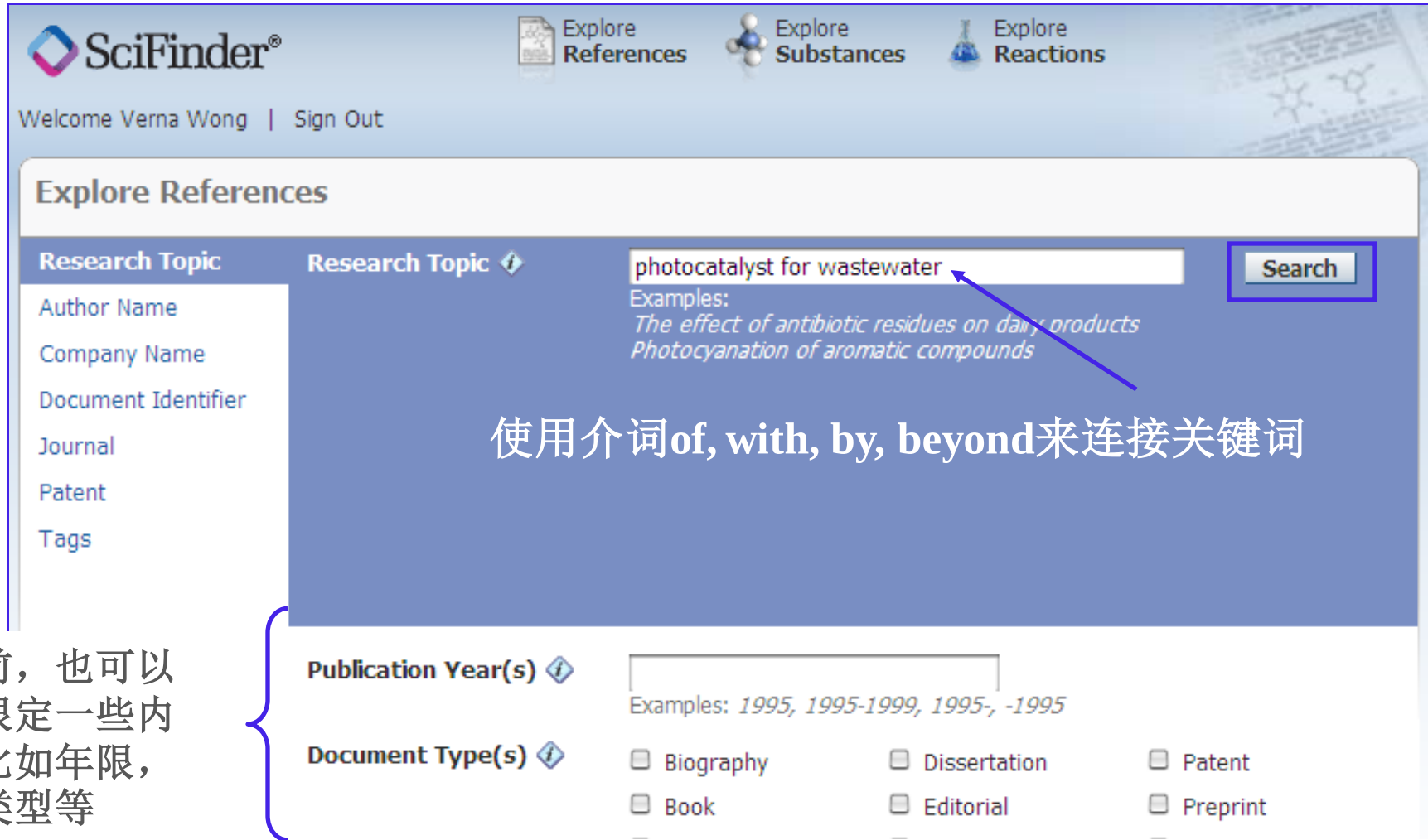

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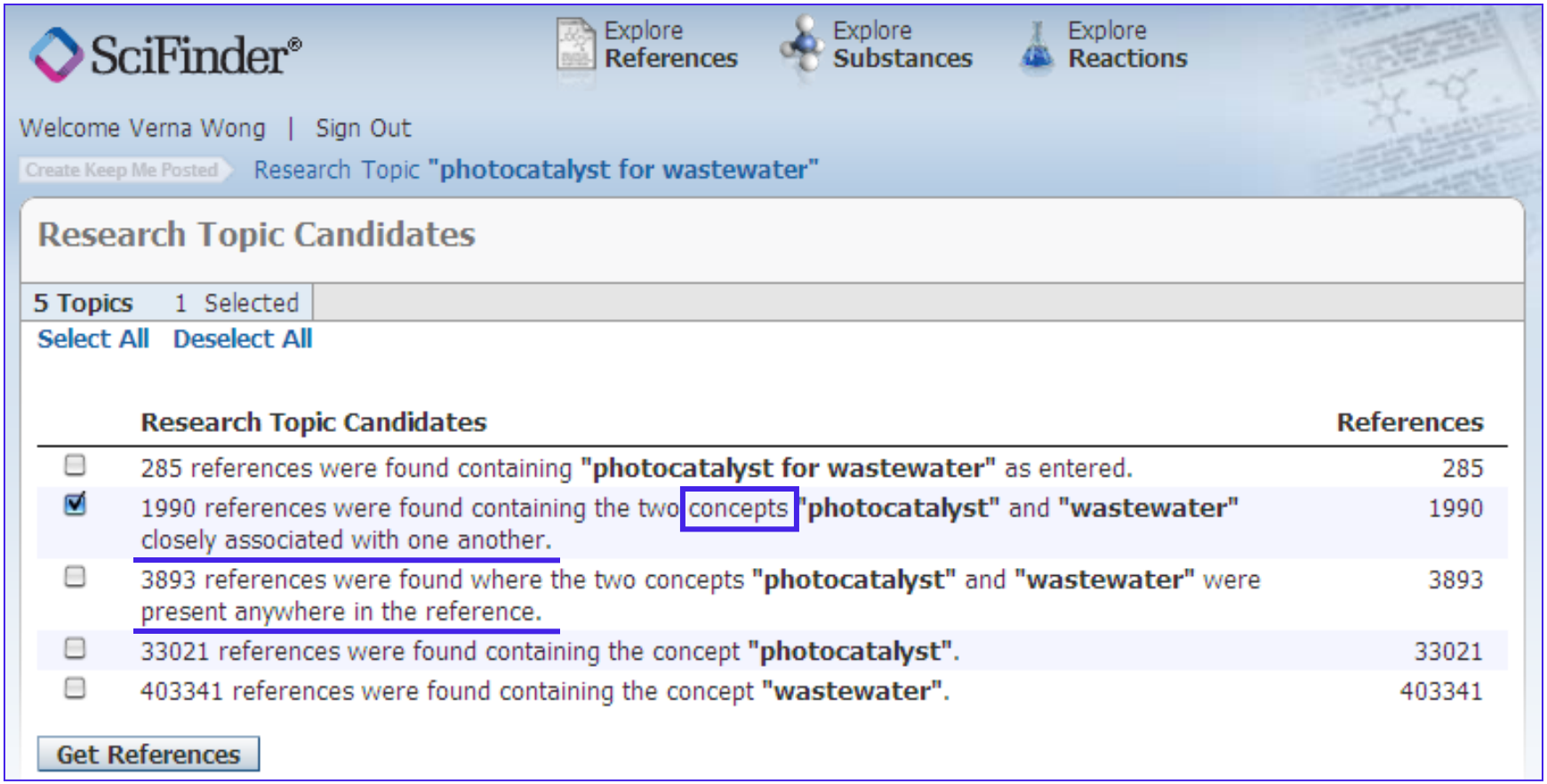

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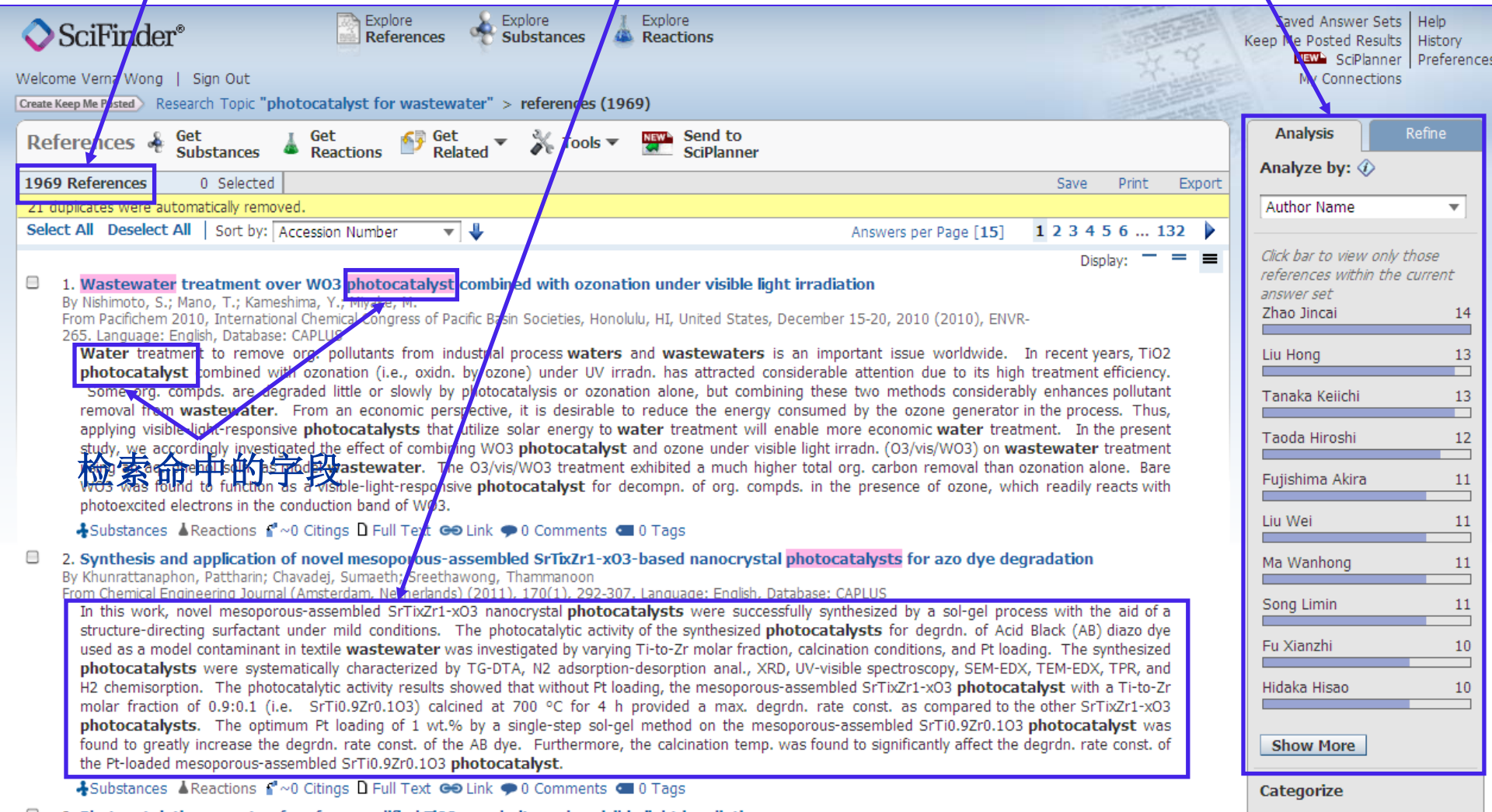

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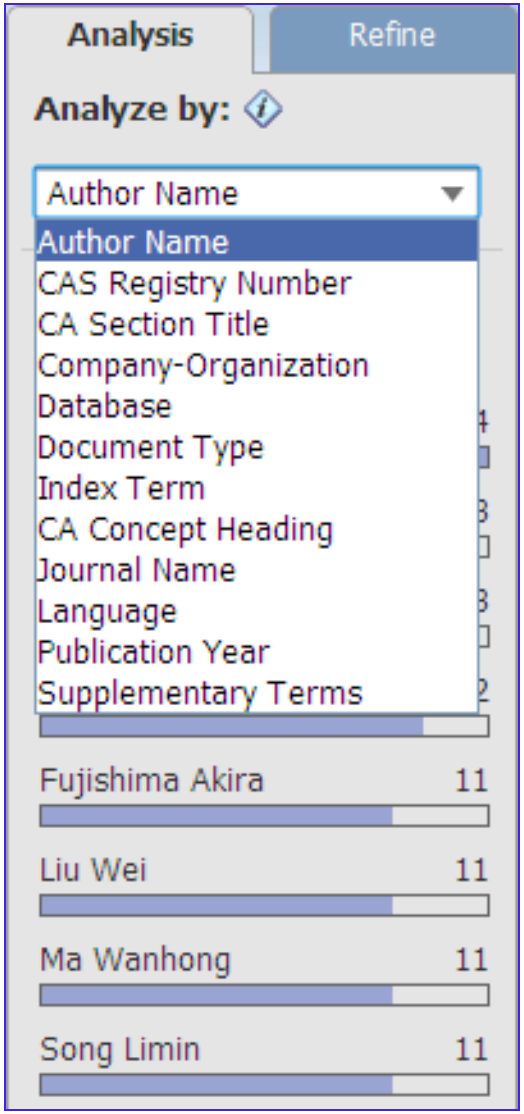

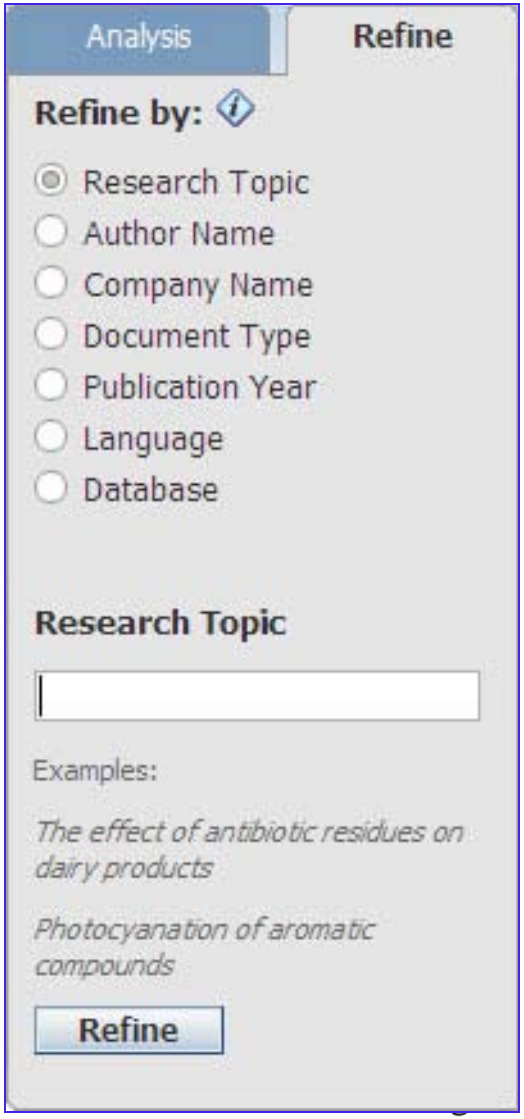

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Display:

1. **Nanoscale titanyl pyrophosphate photocatalyst and its preparation method**
By Zhao, Wanting
From Faming Zhuanli 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.
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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 Zhuanli 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) lowing 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 degrdn. efficiency.
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3. **Preparation method of Bi-containing perovskite type photocatalyst, and its application in photocatalytic degradation of p-chlorophenol-containing wastewater**
By Hu, Ruisheng; Jia, Haixia; Xu, Na; Bai, Yaqin
From Faming Zhuanli Shenqing (2011), CN 102019184 A 20110420. Language: Chinese, Database: CAPLUS
The title prepn. method includes (1) dissolving $Fe(NO_3)_3 \cdot 9H_2O$, $Bi(NO_3)_3 \cdot 5H_2O$, $La(NO_3)_3 \cdot nH_2O$ with 2mol/L nitric acid soln. to obtain transparent soln., where the mol. ratio of $Fe(NO_3)_3 \cdot 9H_2O$ to $Bi(NO_3)_3 \cdot 5H_2O$ to $La(NO_3)_3 \cdot nH_2O$ to nitric acid is 1:0.1-0.98:0.02-0.9:20, (2) prepg. 0.5mol/L citric acid soln., where the mol. ratio of $Fe(NO_3)_3 \cdot 9H_2O$ 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.

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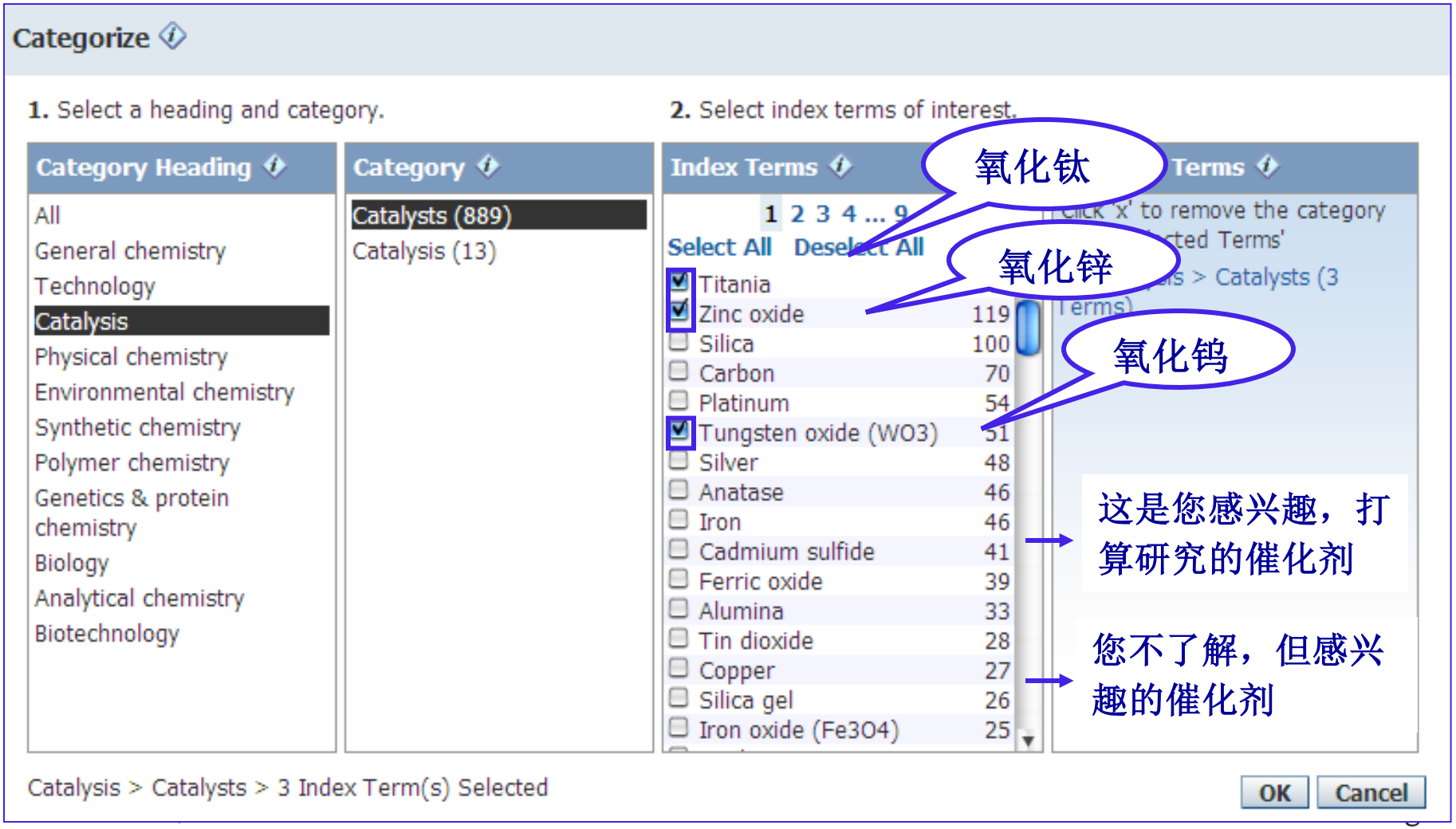

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2. **Synthesis and application of novel mesoporous-assembled SrTixZr1-xO3-based nanocrystal photocatalysts for azo dye degradation**
By Khunrattanaphon, Pattharin; Chavadej, Sumaeth; Sreethawong, Thammanoon
From Chemical Engineering Journal (Amsterdam, Netherlands) (2011), 170(1), 292-307. Language: English, Database: CAPLUS

In this work, novel mesoporous-assembled SrTixZr1-xO3 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 SrTixZr1-xO3 **photocatalyst** with a Ti-to-Zr molar fraction of 0.9:0.1 (i.e. SrTi0.9Zr0.1O3) calcined at 700 °C for 4 h provided a max. degrdn. rate const. as compared to the other SrTixZr1-xO3 **photocatalysts**. The optimum Pt loading of 1 wt.% by a single-step sol-gel method on the mesoporous-assembled SrTi0.9Zr0.1O3 **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 SrTi0.9Zr0.1O3 **photocatalyst**.

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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 irradn. under sunlight with the composite catalyst for 160 min.

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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 process parameters viz., amt. of catalyst, concn. of dye, and pH on photocatalytic degrdn. of MO an carried out by irradiating the aq. solns. of dyes contg. photocatalysts with UV and solar light. The ra estd. from residual concn. spectrophotometrically. Similar expts. were carried out by varying pH (2- 2.0 g/L) and initial concn. of dye (5-200 mg/L). The max. decolorization (>90%) of dyes occurred v basic pH and the max. adsorption of MO was noticed at pH 4 and of R6G at pH 10. The percentage estd. under UV/solar system and it was found that COD redn. takes place at a faster rate under sola light. In case of R6G, highest decolorizing efficiency was achieved with lower dose of catalyst (0.5 g similar conditions. The performance of photocatalytic system employing ZnO/solar light was obsd. t system.

Indexing

Waste Treatment and Disposal (Section 60-2)

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

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

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S.K. Kansal[a], , , M. Singh[b] and D. Sud[c]

[a]Department of Chemical Engineering and Technology, Panjab University, Chandigarh 160014, India

[b]Department of Chemical Technology, Sant Longowal Institute of Engineering and Technology, Longowal 148106, Sangrur, Punjab, India

[c]Department of Chemistry, Sant Longowal Institute of Engineering and Technology, Longowal 148106, Sangrur, Punjab, India

Received 2 May 2006; revised 11 July 2006; accepted 11 July 2006. Available online 21 July 2006.

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 (TiO_2), zinc oxide (ZnO), stannic oxide (SnO_2), 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

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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 kinetics
Textiles
Photolysis catalysts
Solar UV radiation
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, e
Properties;

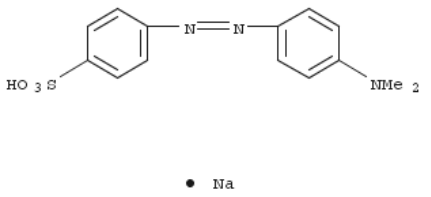
CAS Registry Number: 547-58-0
(Component: 502-02-3)

C14 H15 N3 O3 S . Na

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

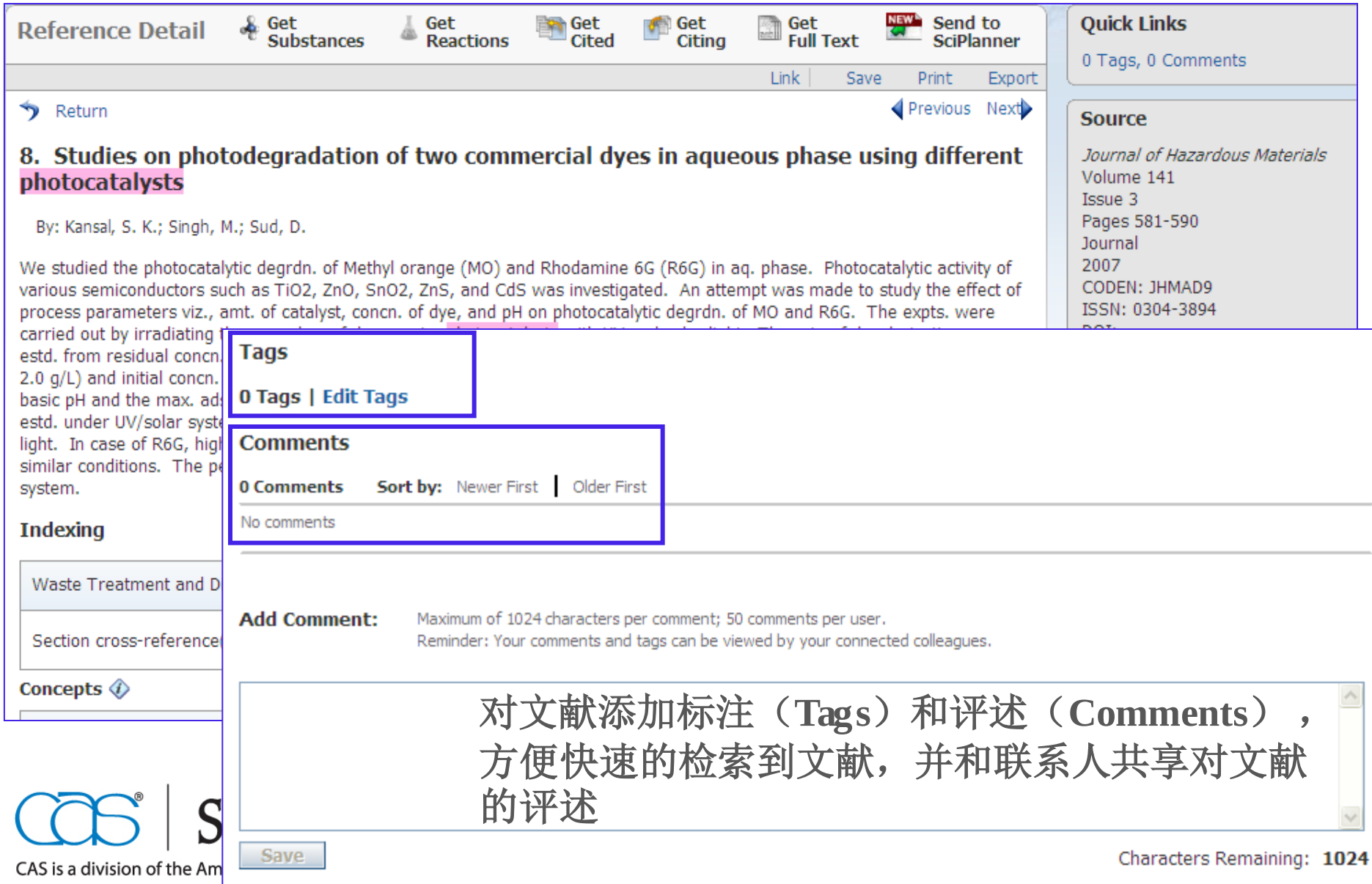
Benzenesulfonic acid, 4-[[4-(dimethylamino)phenyl]azo]-, sodium salt (9CI); Benzenesulfonic acid, p-[[p-(dimethylamino)phenyl] azo]-, sodium salt (8CI); Orange III (6CI); 4-Dimethylaminoazobenzene-4'-sulfonic acid sodium salt; Acid Orange 52; Albion Methyl Orange; C.I. 13025; C.I. Acid Orange 52; Diazoben; 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-dimethylaminoazobenz enesulfonate; Tropaeolin D

Deleted CAS Registry Numbers: 1342-24-1; 66777-17-1



~5,688 References

可以用中文对文献进行标注或者评述



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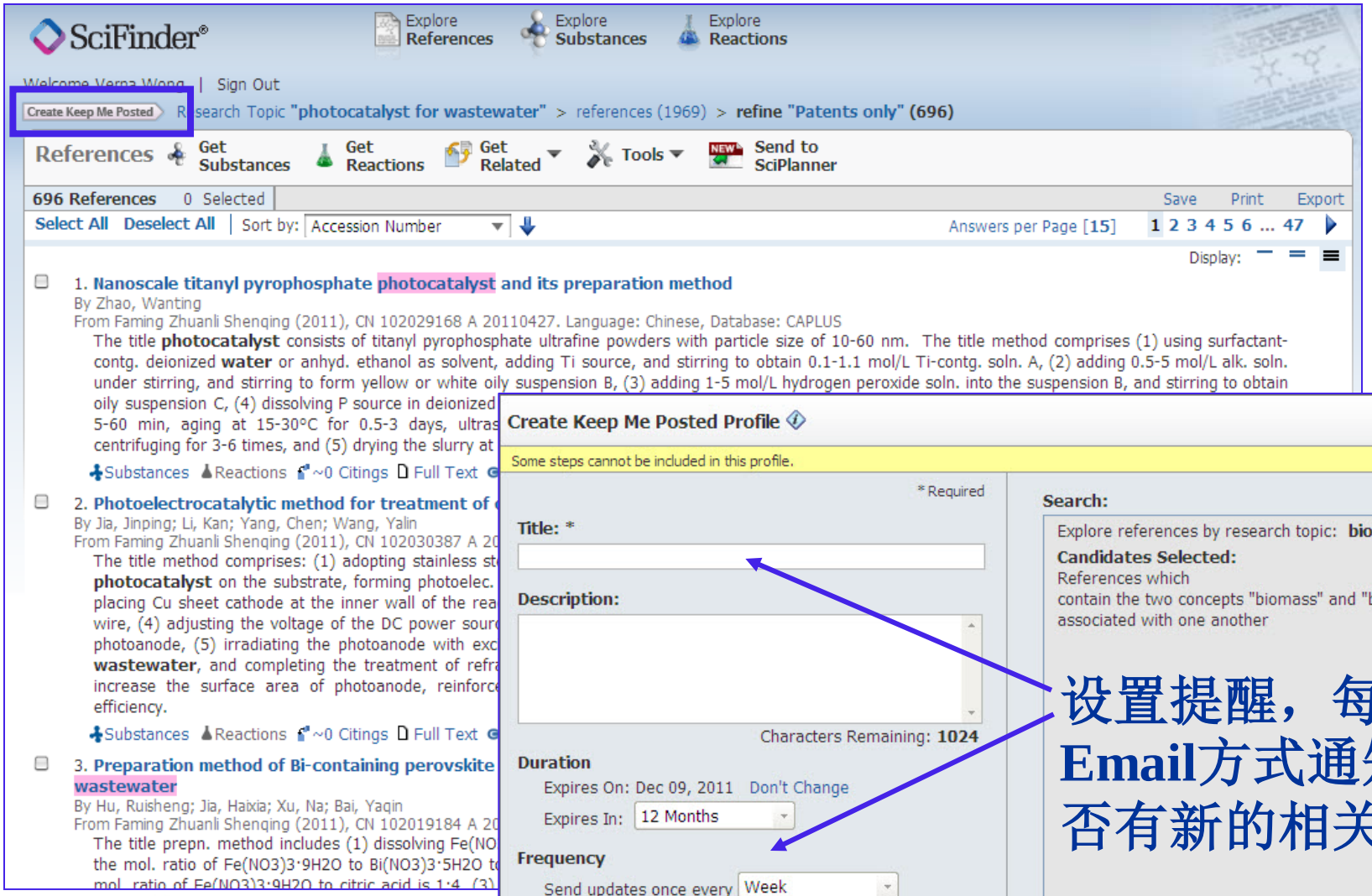

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在SciFinder中检索双酚A的信息

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。

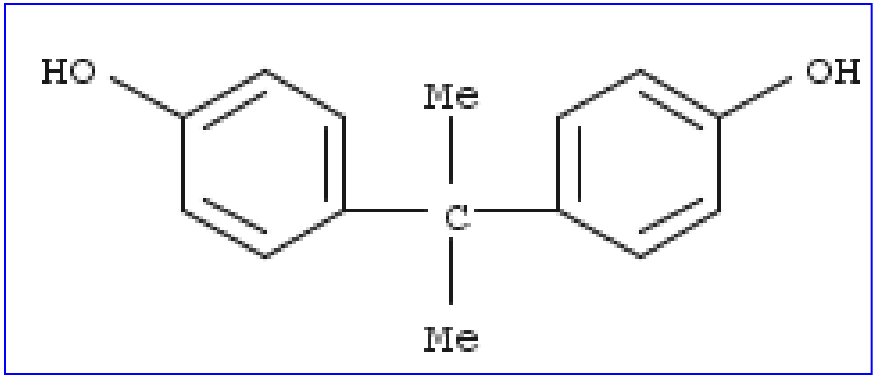
卫生部官员昨日也表示，目前中国正在清理包装材料，并出台了征求意见稿。征求意见稿中规定，未来婴幼儿奶瓶不能使用双酚A。

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。

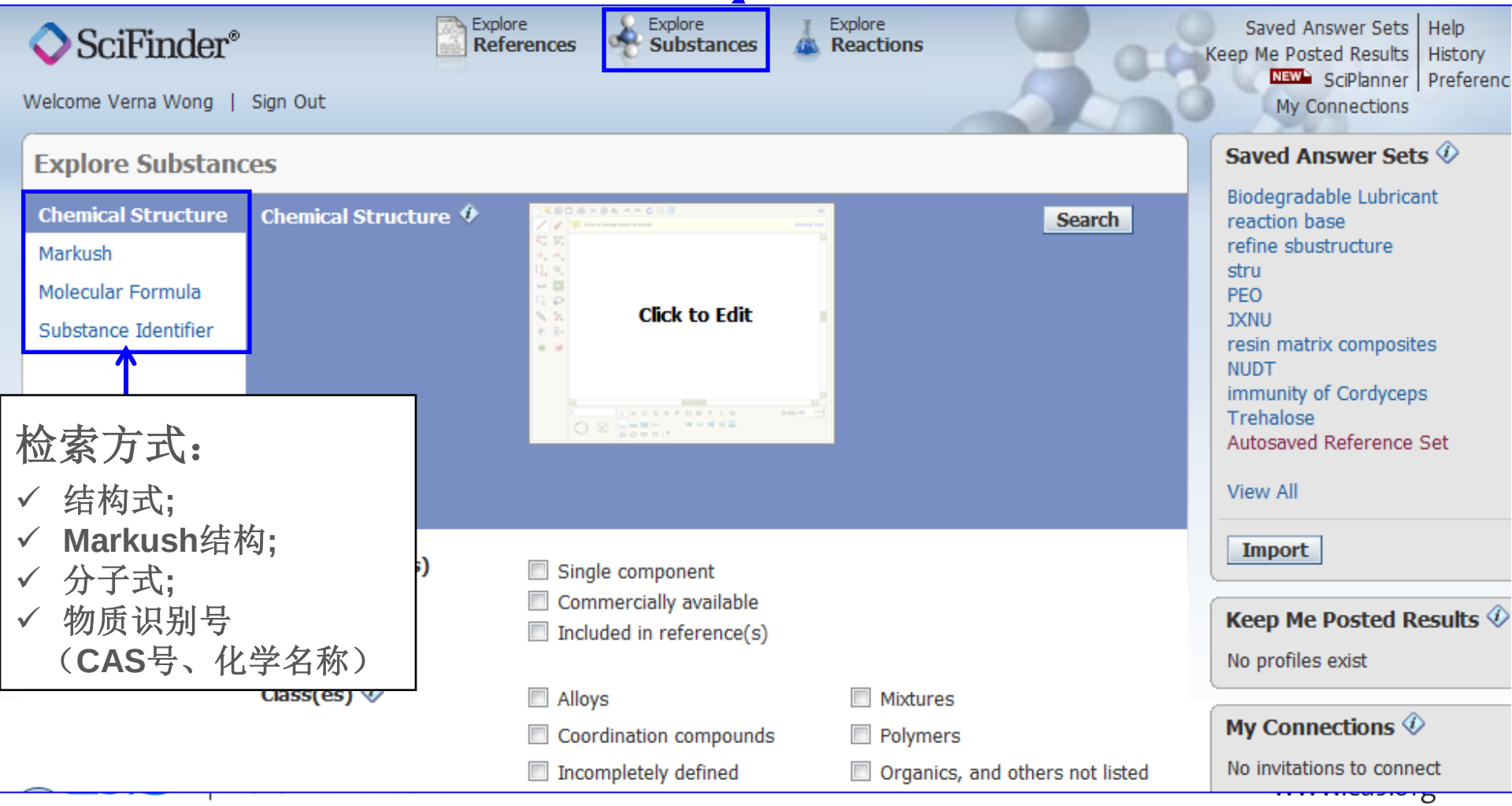
其实，在欧盟宣布对含双酚A的塑料奶瓶全面禁止之前，已有不少国家和地区对此类产品作了禁止性规定。2008年，加拿大第一个宣布在所有食品包装和容器（包括奶瓶）上禁用双酚A，澳大利亚也从2010年7月1日起逐渐淘汰含双酚A的婴儿奶瓶；后来美国许多州和大型零售商，包括沃尔玛在内采取了同样的步骤。

在SciFinder中检索双酚A的信息

- 你是否知晓欧盟已全面禁用含双酚A的奶瓶？
- 你了解双酚A吗？
- 你想了解双酚A的毒副作用吗？
- 你想知道目前双酚A最新的检测手段吗？



简明的物质检索入口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Chemical Structure
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Molecular Formula
Substance Identifier
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Saved Answer Sets
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reaction base
refine sbustructure
stru
PEO
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NUDT
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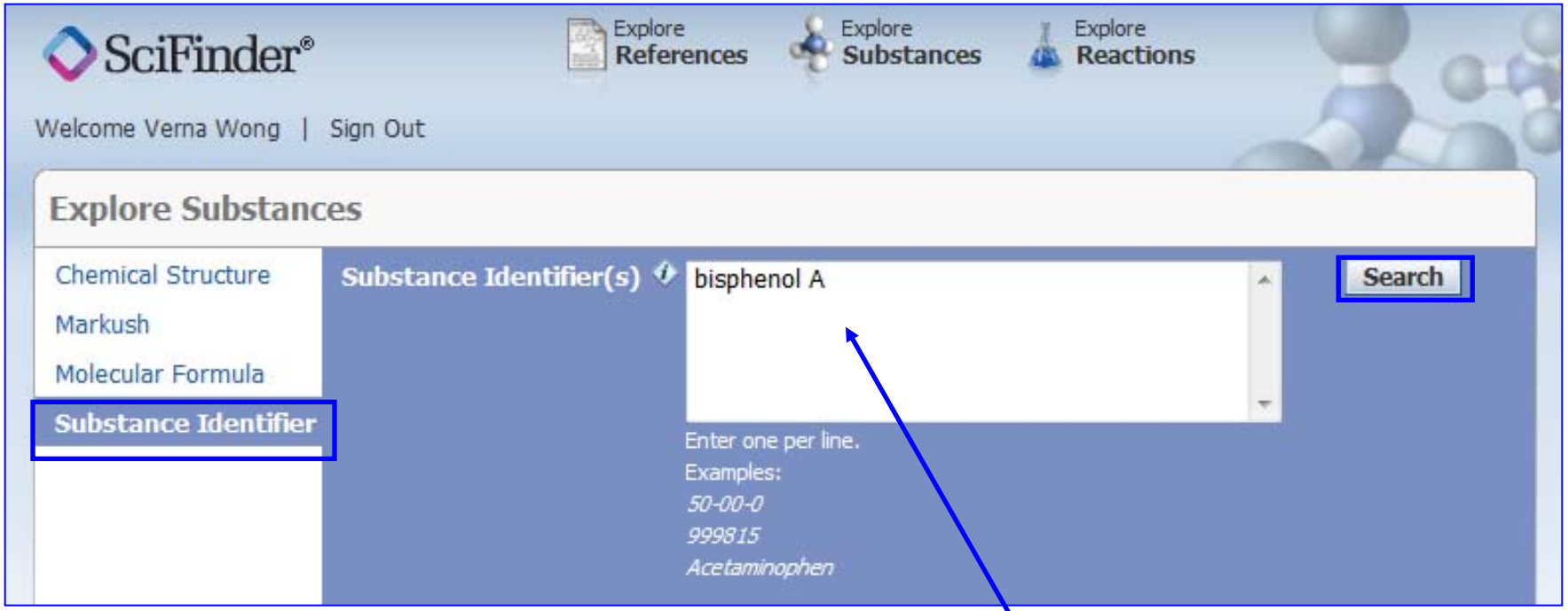
Trehalose
Autosaved Reference Set
View All
Import
Single component
Commercially available
Included in reference(s)
Alloys
Coordination compounds
Incompletely defined
Mixtures
Polymers
Organics, and others not listed
Keep Me Posted Results
No profiles exist
My Connections
No invitations to connect
检索方式：
✓ 结构式;
✓ Markush结构;
✓ 分子式;
✓ 物质识别号
（CAS号、化学名称）

通过物质标示符（名称，CA号，俗名，商品名）找物质

双酚A（ bisphenol A; BPA）



这里可以通过输入物质的名称，CA号，俗名，商品名，来进行检索

轻松获得双酚A的记录

通过物质的标准菜单，可以获得和物质有关的所有内容——文献、反应、供应商信息、全球管制信息都可以任意链接到。

Substance Detail获得和双酚A有关的所有详细信息

SciFinder中收录双酚A的详细信息

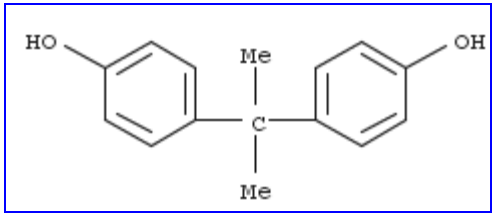
CAS Registry Number: 80-05-7

$C_{15}H_{16}O_2$

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

Deleted CAS Registry Numbers: 27360-89-0; 37808-08-5; 137885-53-1; 146479-75-6



双酚A的CAS号、分子式、结构式、化学名、别名

网上获取物质CAS号的途径有多种，只有通过CAS的平台**SciFinder**、**STN**获得的CAS号才是唯一准确可靠的。

按照CAS Role分类的专利、非专利文献列表。对某类文献感兴趣，仅需点击交叉处的v即可方便快捷地获取。

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Combinatorial Study	✓	✓		
Formation, Nonpreparative	✓	✓	✓	✓
Miscellaneous	✓	✓	✓	✓
Occurrence	✓	✓	✓	✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓		✓	
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

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Predicted Properties: Biological Chemical Density Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Condition	Note
Bioconcentration Factor	344	pH 1 Temp: 25 °C	(79)
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)

Top

Experimental Properties: Biological Chemical Density Interface Lipinski and Related Spectra Structure-related Thermal

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 11	(2) CAS
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
NOAEL/LOAEL	See full text	1 of 10	(68) CAS
Toxic Equivalence Factors	See full text		(74) CAS

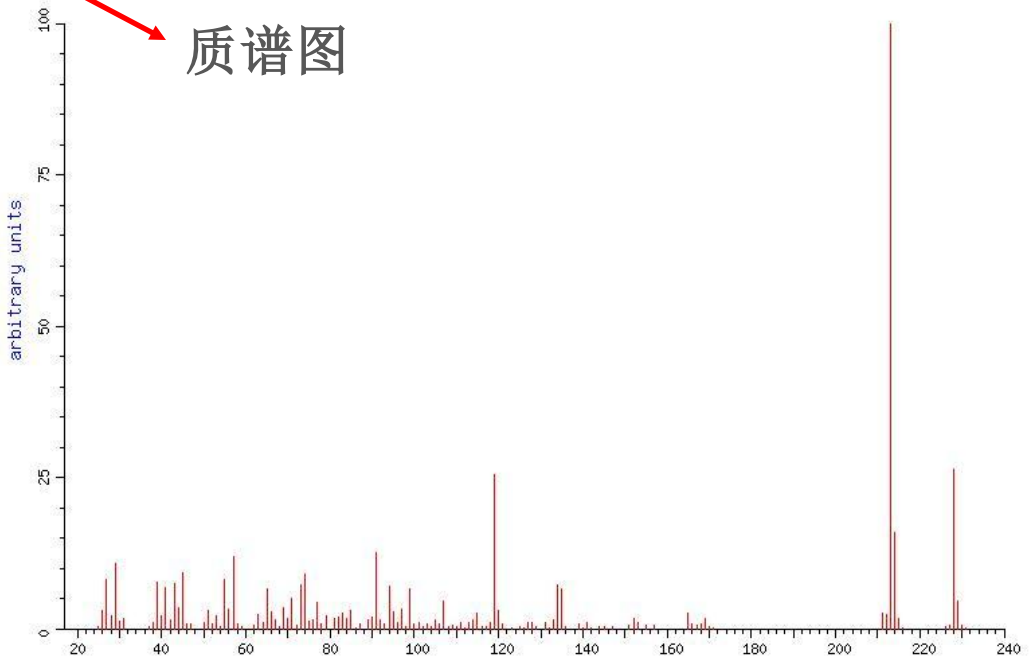
Top

实验数据，可以看到原始文献对应的链接

来源于文献报导的谱图信息

IR Absorption Spectrum	See spectrum		(13) WSS
IR Absorption Spectrum	See spectrum		(13) WSS
IR Absorption Spectrum	See full text	1 of 5	(20) CAS
IR Emission/Luminescence Spectrum	See full text		(21) CAS
IR Spectrum	See full text		(22) CAS
Mass Spectrum	See spectrum		(13) WSS
Mass Spectrum	See spectrum		(13) WSS
Mass Spectrum	See spectrum		(13) WSS
Mass Spectrum	See spectrum		(14) AIST
Mass Spectrum	See full text	1 of 49	(25) CAS
NMR Spectrum	See full text		
Proton NMR Spectrum	See spectrum		

质谱图



可以直接点击查看谱图，也可以去原文中查找更详细的谱图数据。

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Display:

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

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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
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Ashby John	13

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

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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 1.5-500μg·L-1 with a detection limit of 0.46μg·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
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获得双酚A合成制备方法

Reactions | Get References | Find Additional Reactions | Combine Answer Sets

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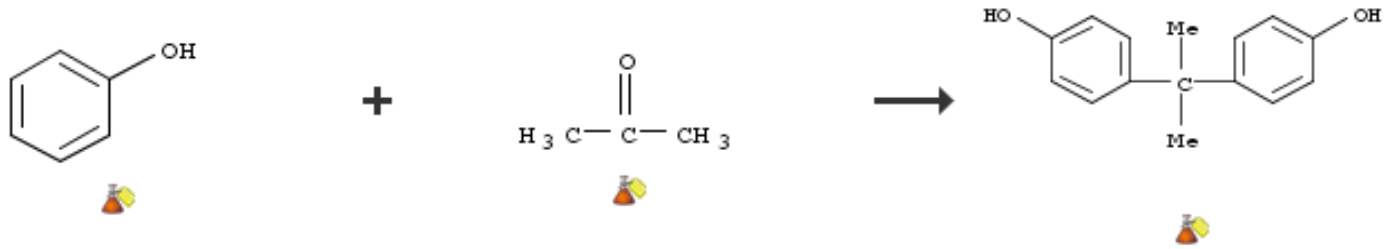
Display:

1. View Reaction Detail | Link | Similar Reactions

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



Overview

Steps/Stages

1.1 C:Polysorb1, C:19351-18-9, 338K

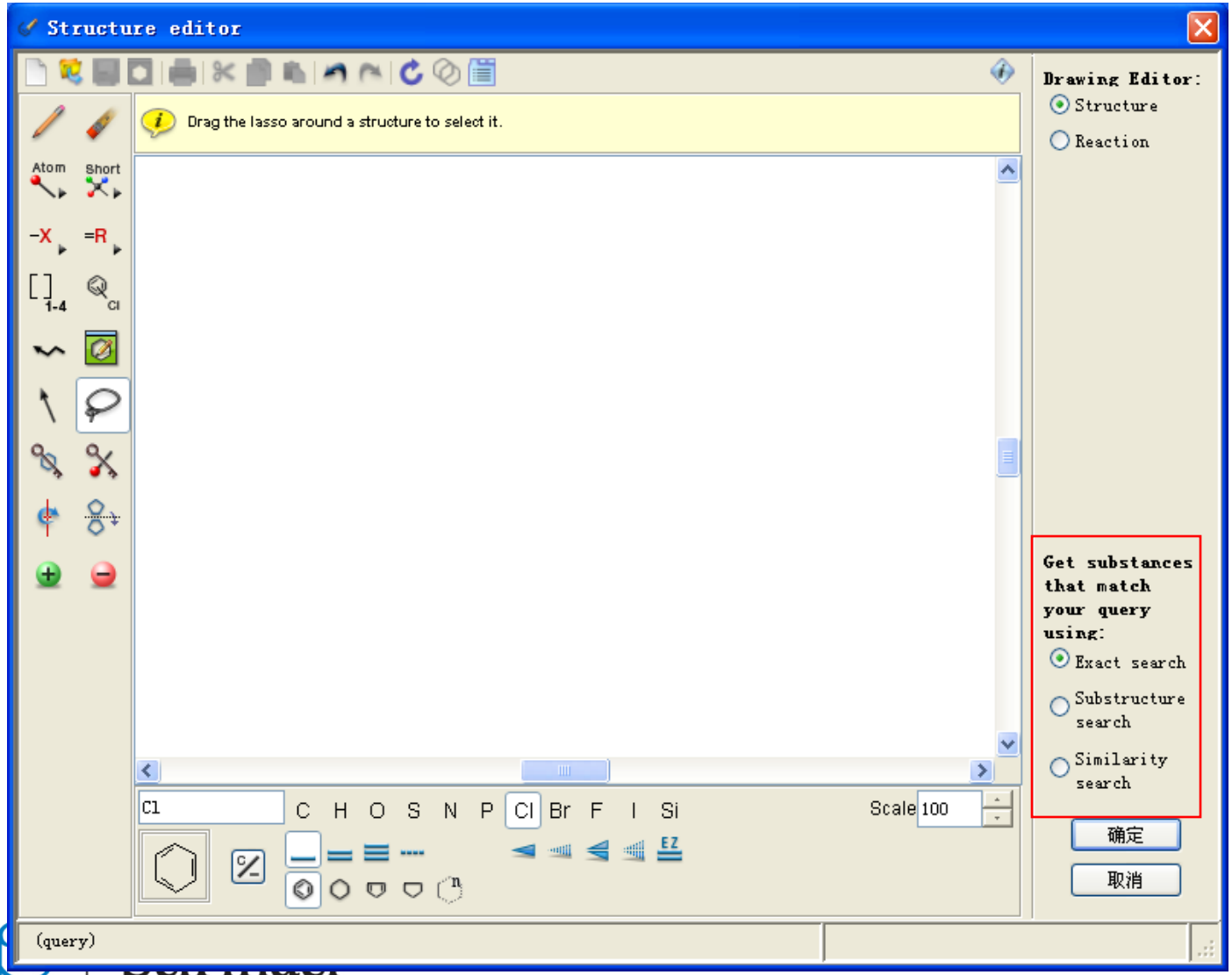
Notes

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

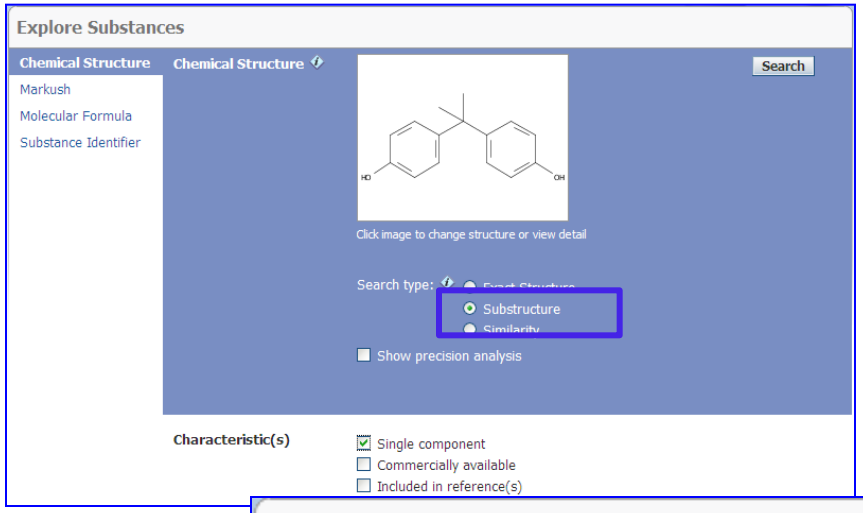
SciFinder结构绘制工具



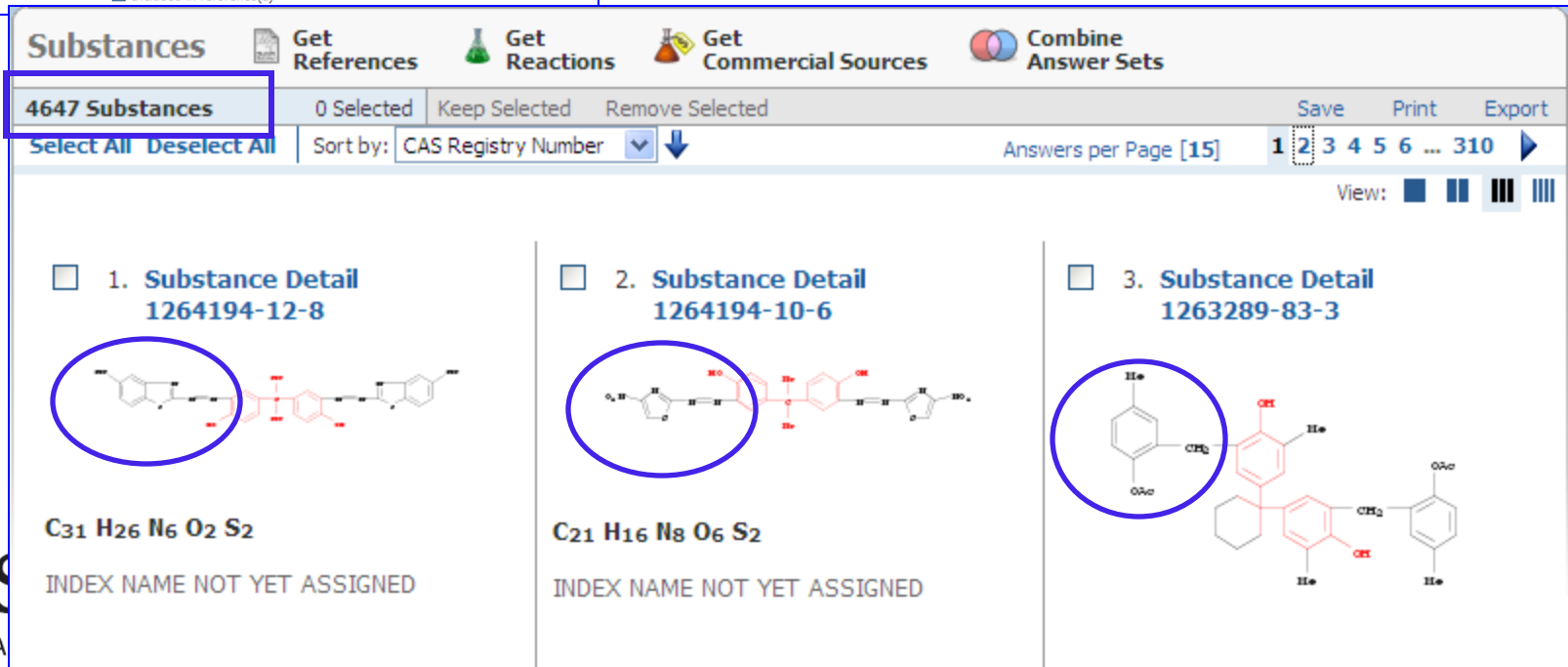
可选择

精确结构检索、亚结构检索、相似结构检索

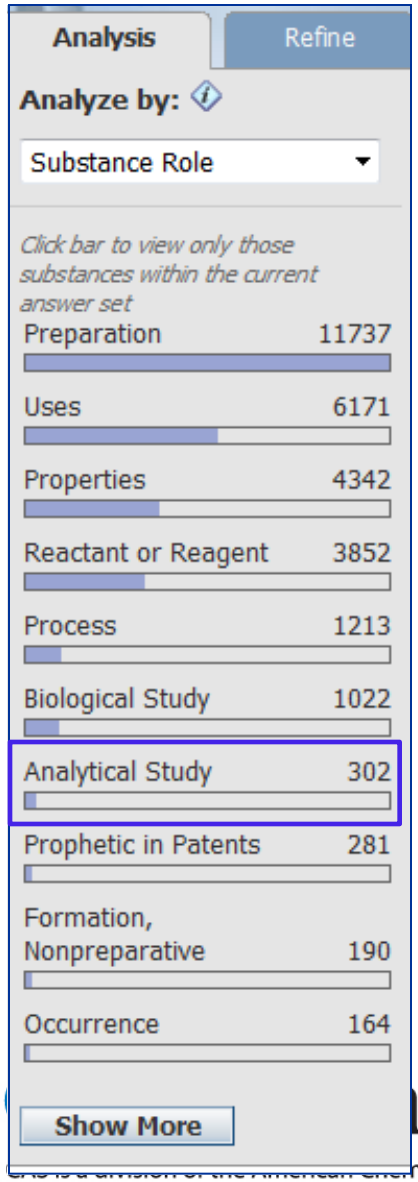
使用结构检索可以获得双酚A衍生物的信息



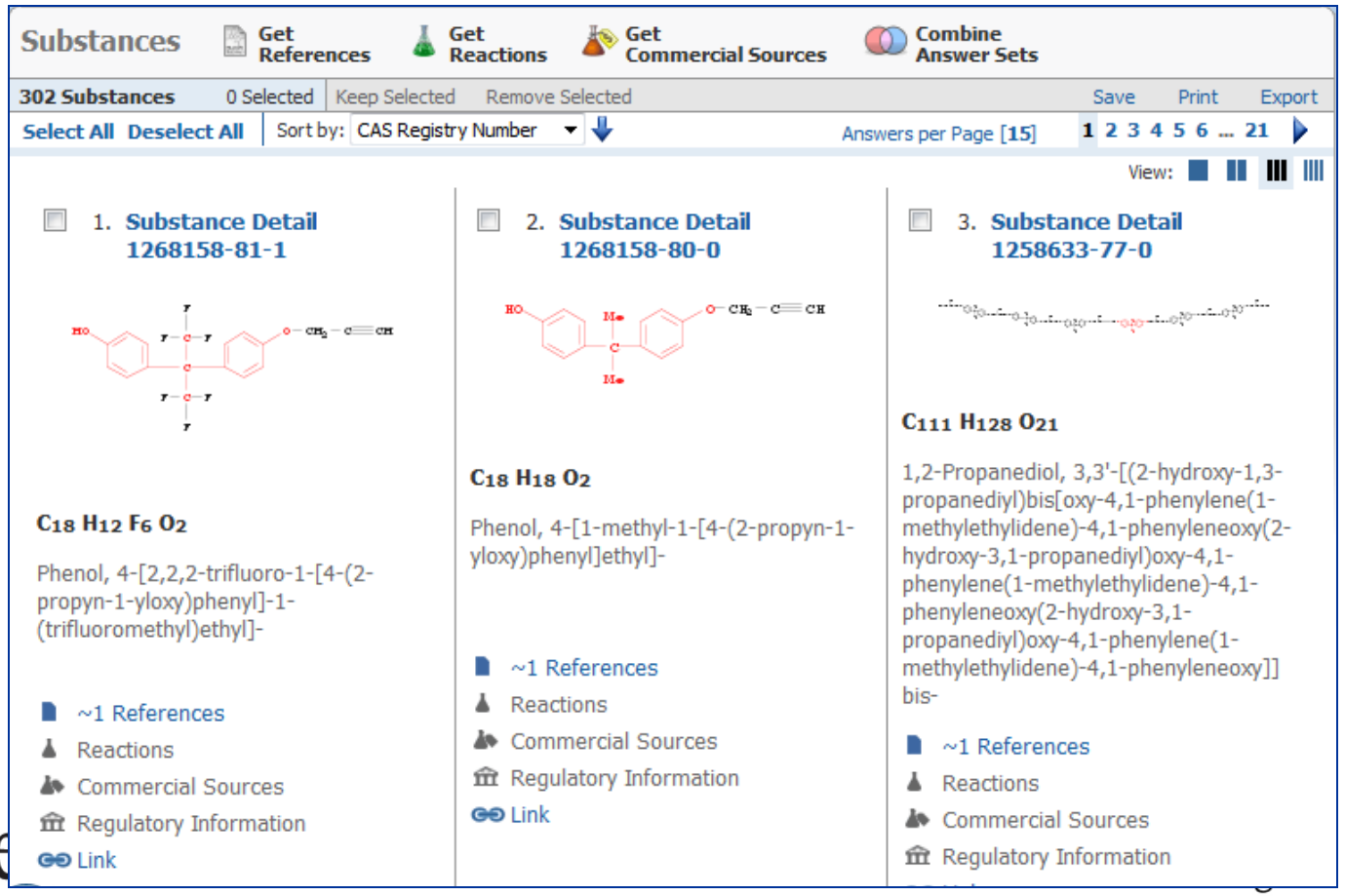
当需要去检索物质的衍生物时，可以使用亚结构检索，**Substructue**。



结构检索中的分析功能

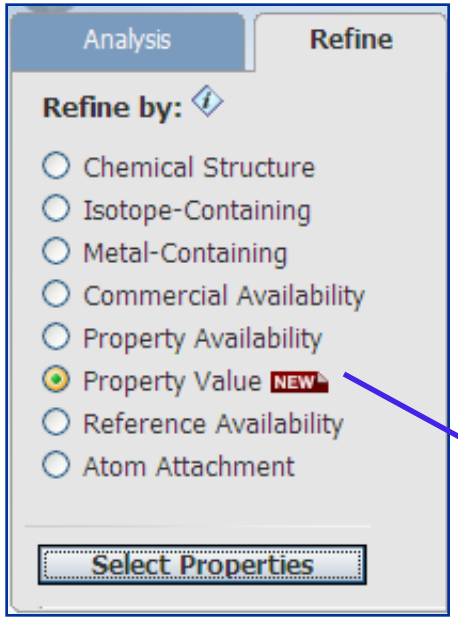


Substance Role分析，帮助获得具有特定研究报道的物质

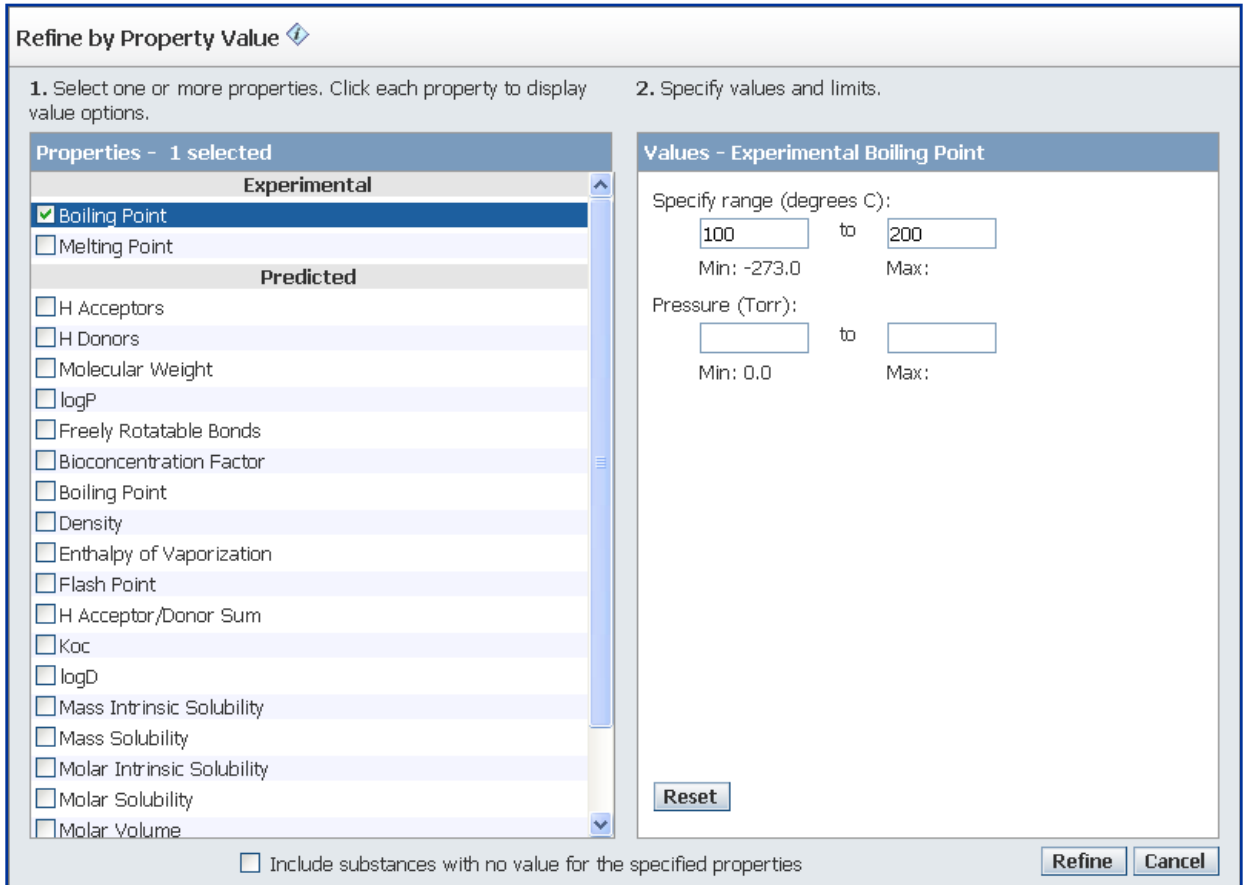


nical Society

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**



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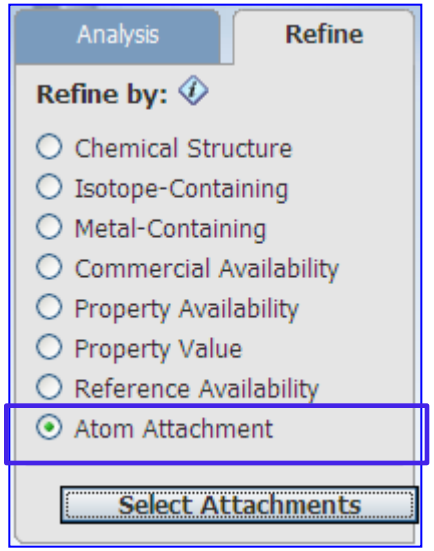
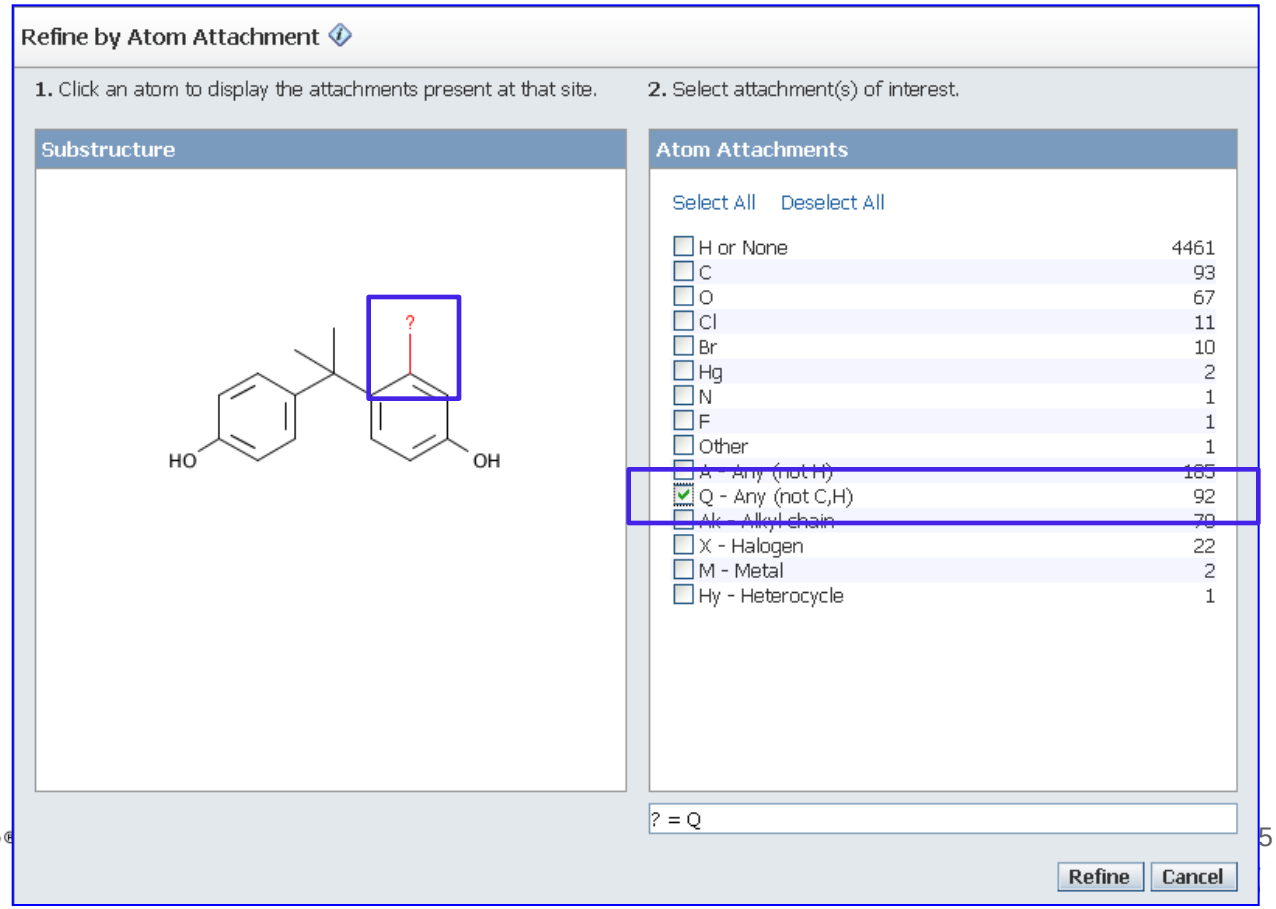
Refine-Atom Attachment获得结构中特定修饰情况



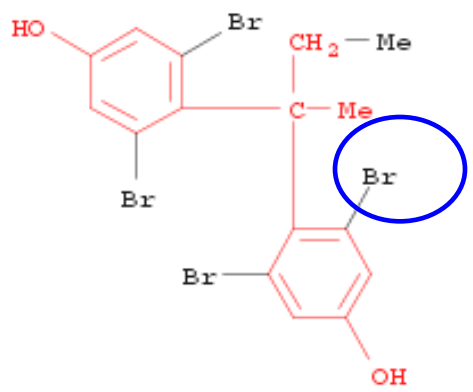
Refine下的Atom Attachment工具，帮助科研工作者了解结构中各个位点的可修饰性



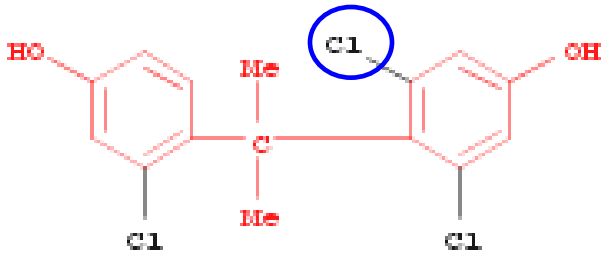
获得特定位点上为非C,H的衍生物

特定位点上为非C,H的任何元素

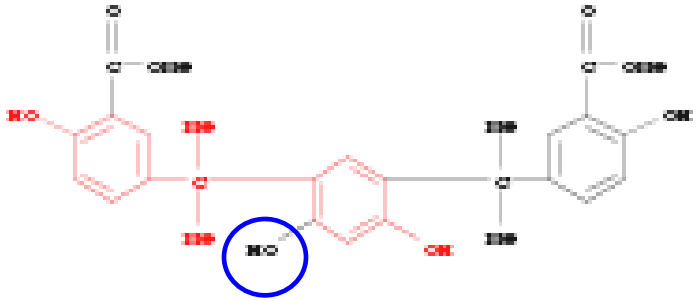
20. Substance Detail
897091-57-5



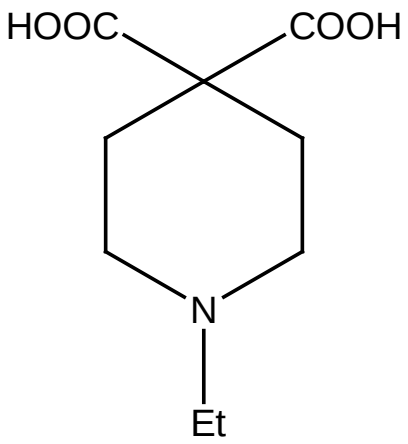
10. Substance Detail
1033261-02-7



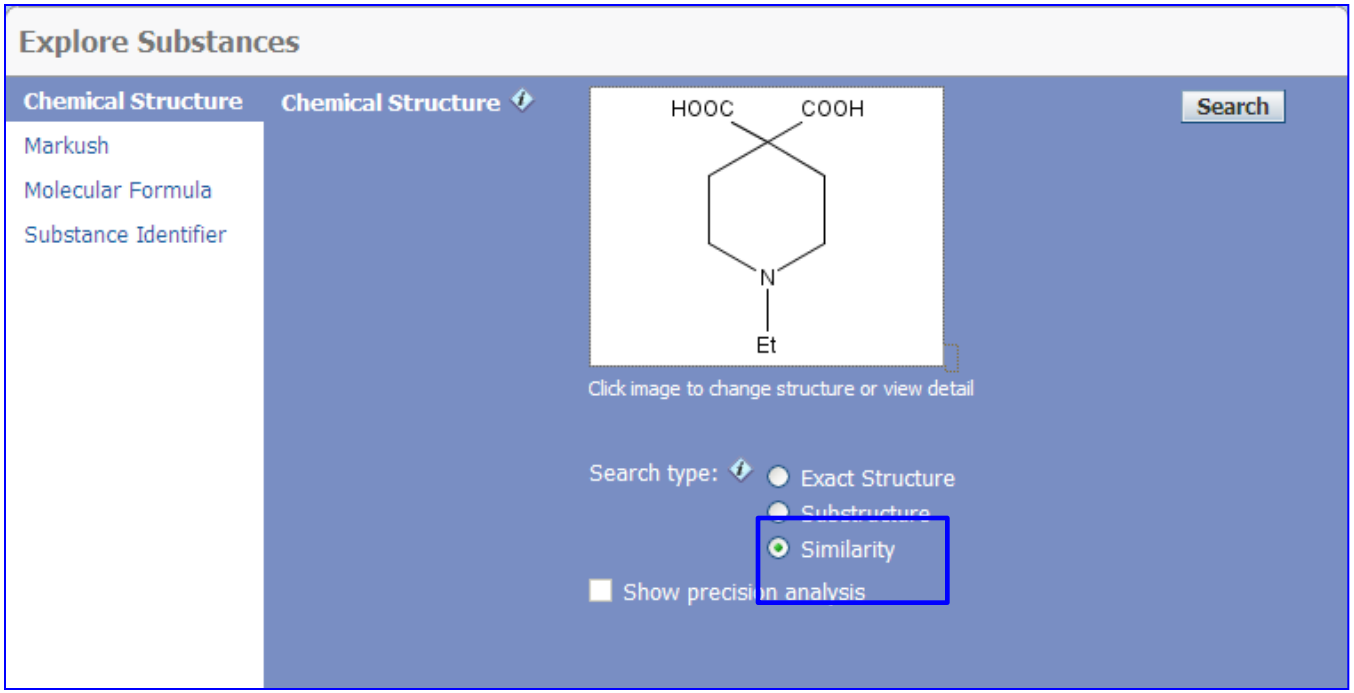
15. Substance Detail
929102-14-7



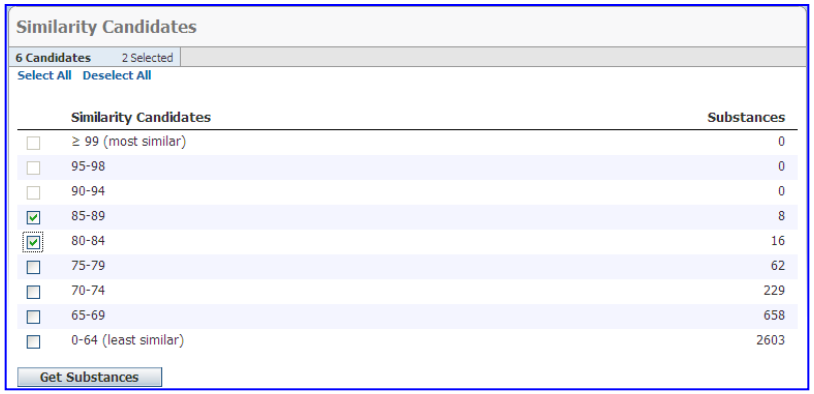
可进行相似结构检索



SciFinder中的相似结构检索，帮助获得在结构上存在相似的物质。

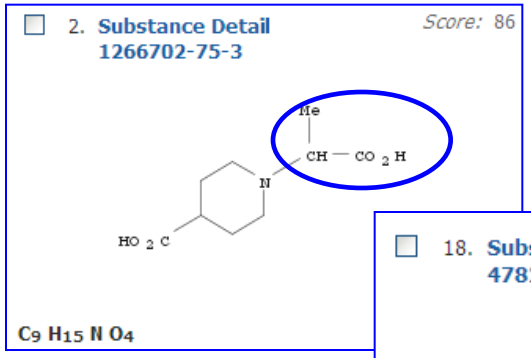


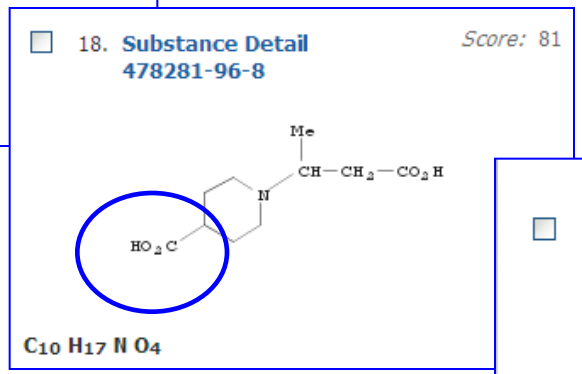
相似结构检索可获得相似度在60分以上的物质

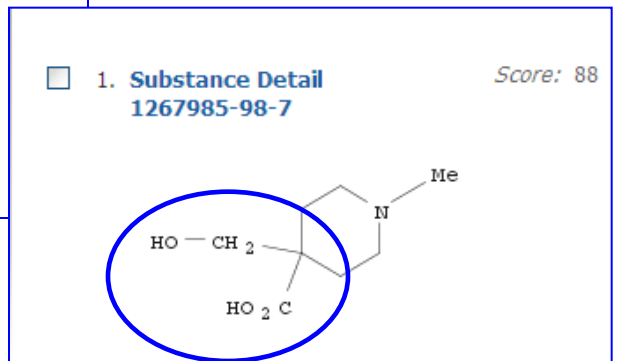


与原结构存在以下的区别：

取代基位置变化
取代基变化
母体结构变化







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SciFinder中的Markush结构检索

在专利中描述物质的方式

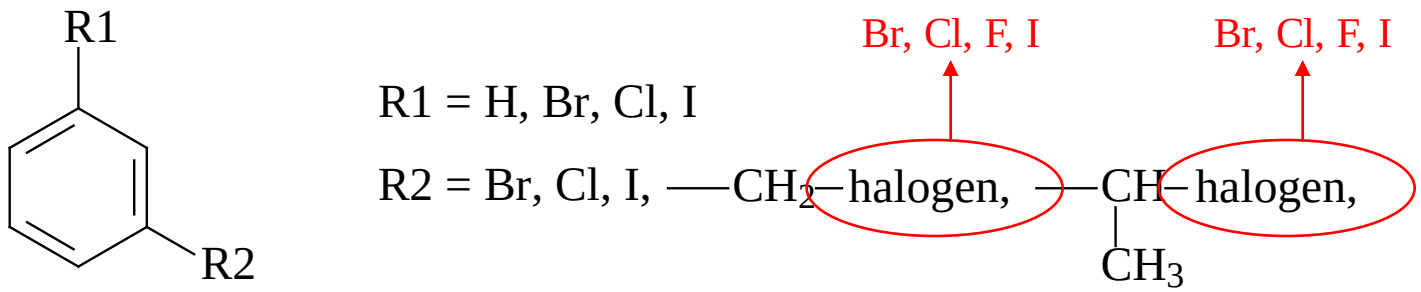
- 特定物质[Specific Substance]：

  以特定化学结构所陈述的特定物质，会被标示CAS No.

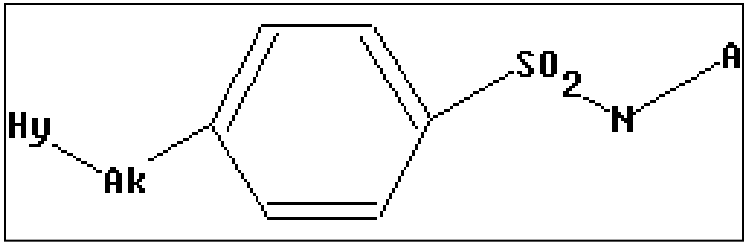
- 预测性物质[Prophetic Substance]：

  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.

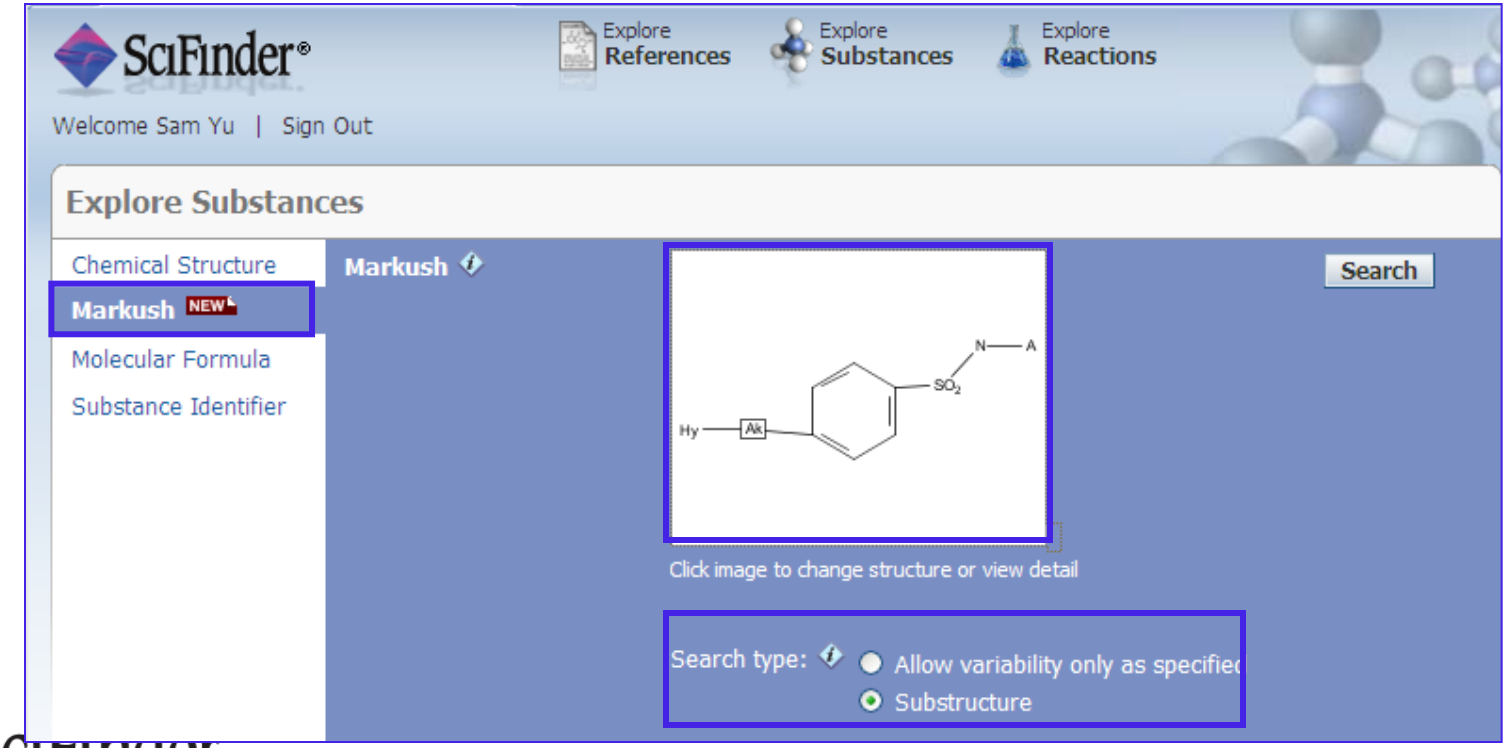
Markush检索，能检索到通过结构检索检不到的专利



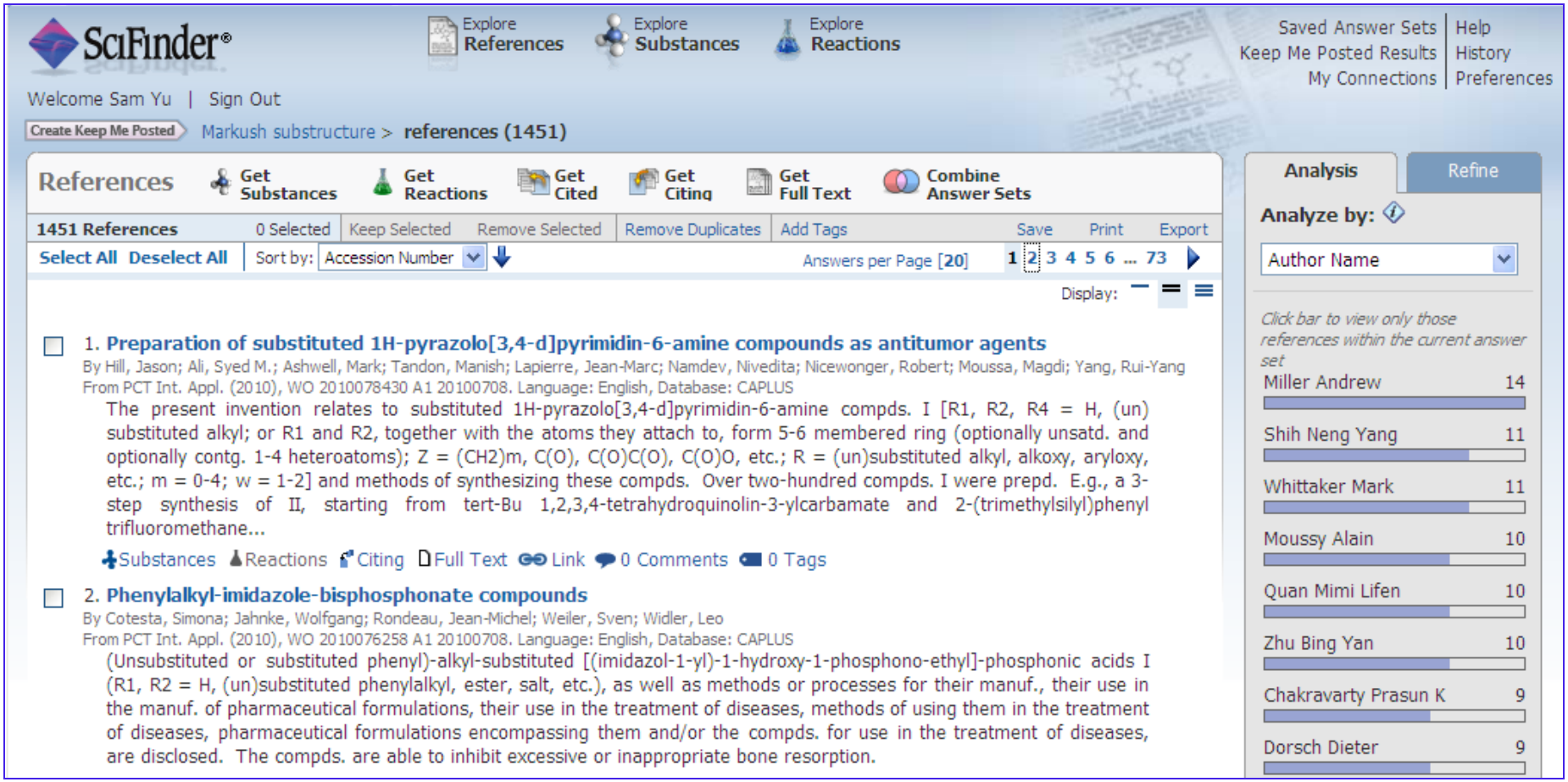
SciFinder中的Markush结构检索



SciFinder中的Markush检索能帮助做初步的专利评估。



Markush直接检索包含该通式结构的专利



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

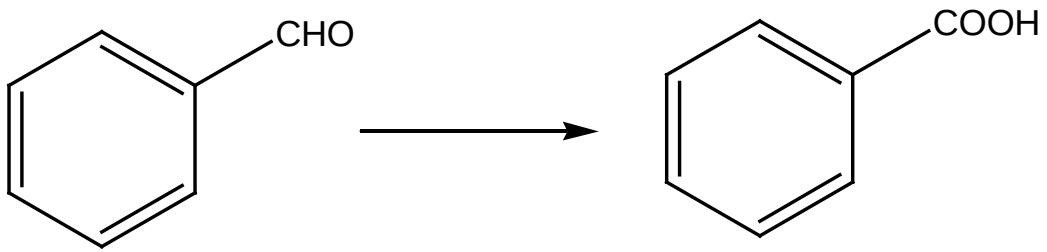
CAS React（1840－至今）
期刊，专利中涉及的有机、有机金属、无机、生化反应。
2600万单步，多步反应。
1300万制备信息。
周更新。

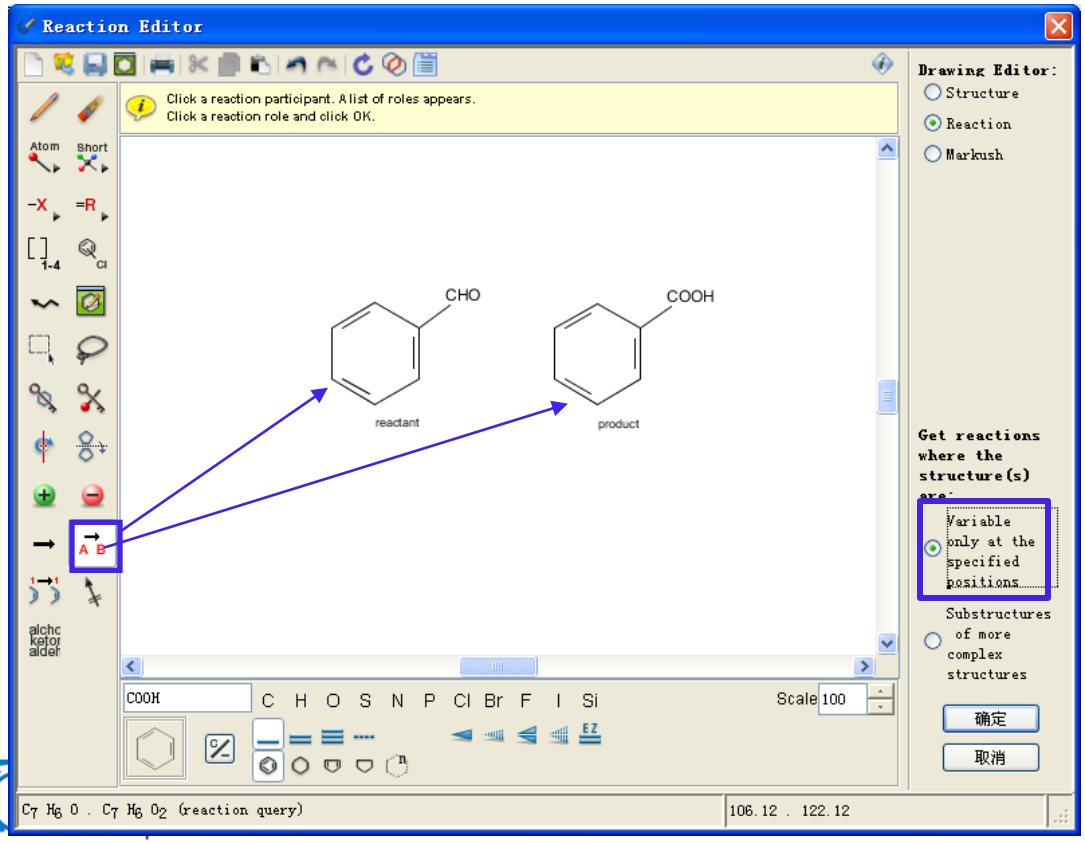
可通过反应式检索，可通过物质、文献链接。

反应检索入口


反应检索入口
SciFinder®
Explore References
Explore Substances
Explore Reactions
Welcome Verna Wong | Sign Out
Explore Reactions
Reaction Structure
Reaction Structure
Search
Click to Edit
点击，进入画图版
Solvent(s)
Select Solvents
Non-participating Functional Group(s)
Select Groups
Number of Steps
Examples: 1, 1 - 3, 1 -, - 3
Classification(s)

使用反应定义工具定义反应

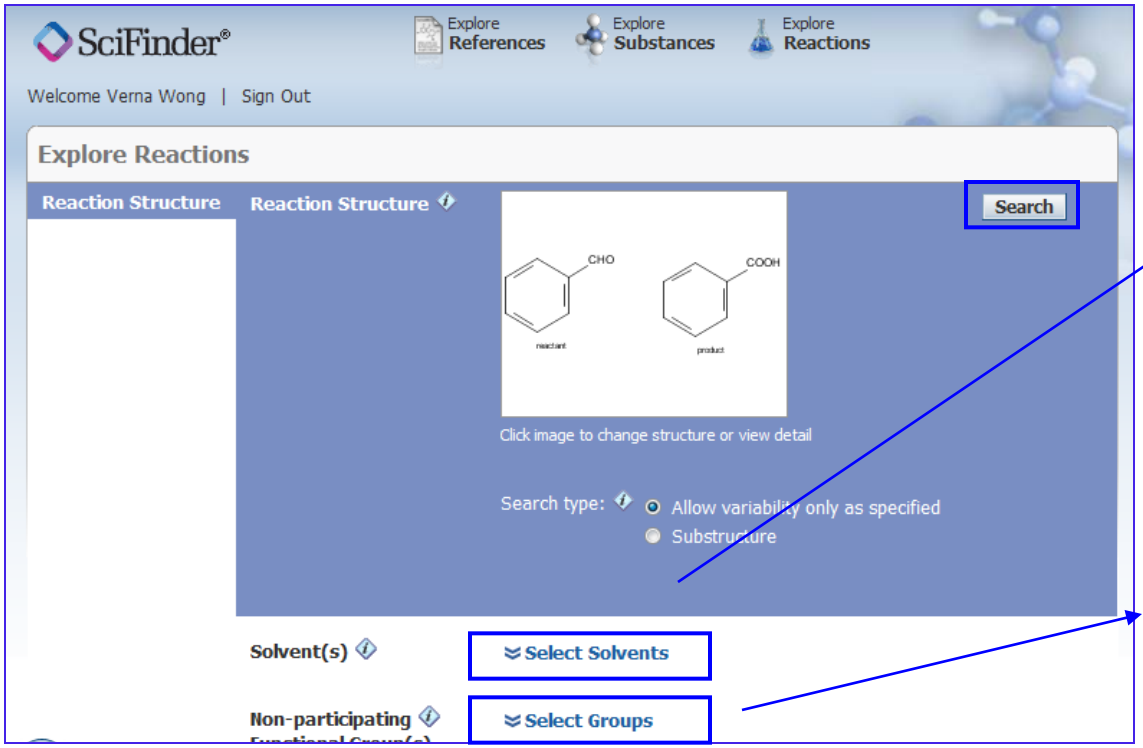


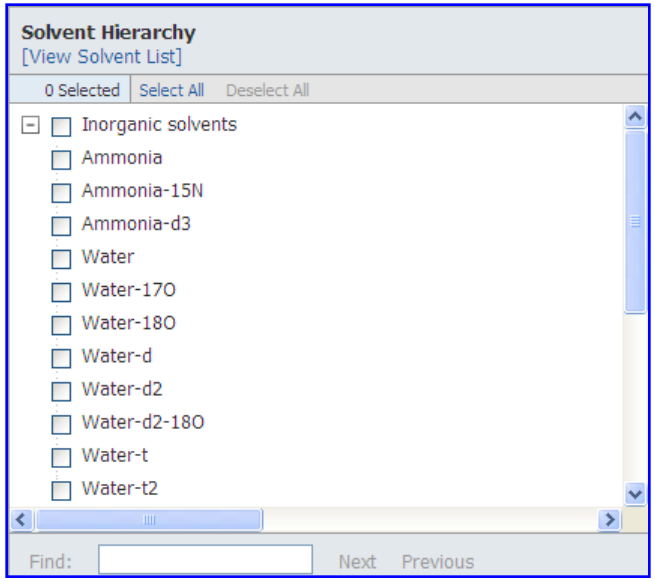


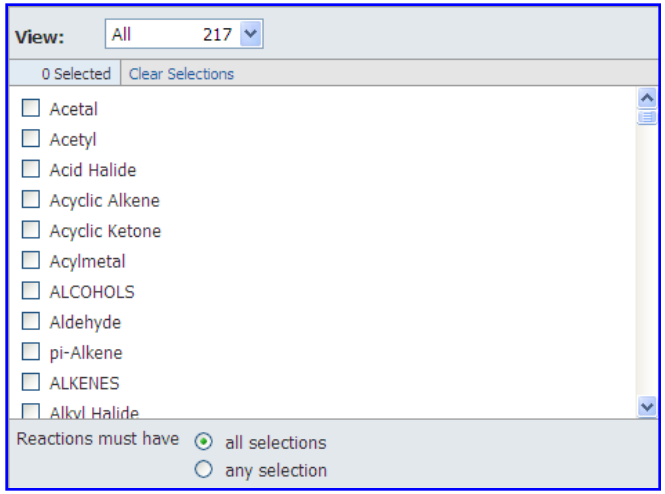
精确反应检索帮助获得特定物质之间的反应，点击确定

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。







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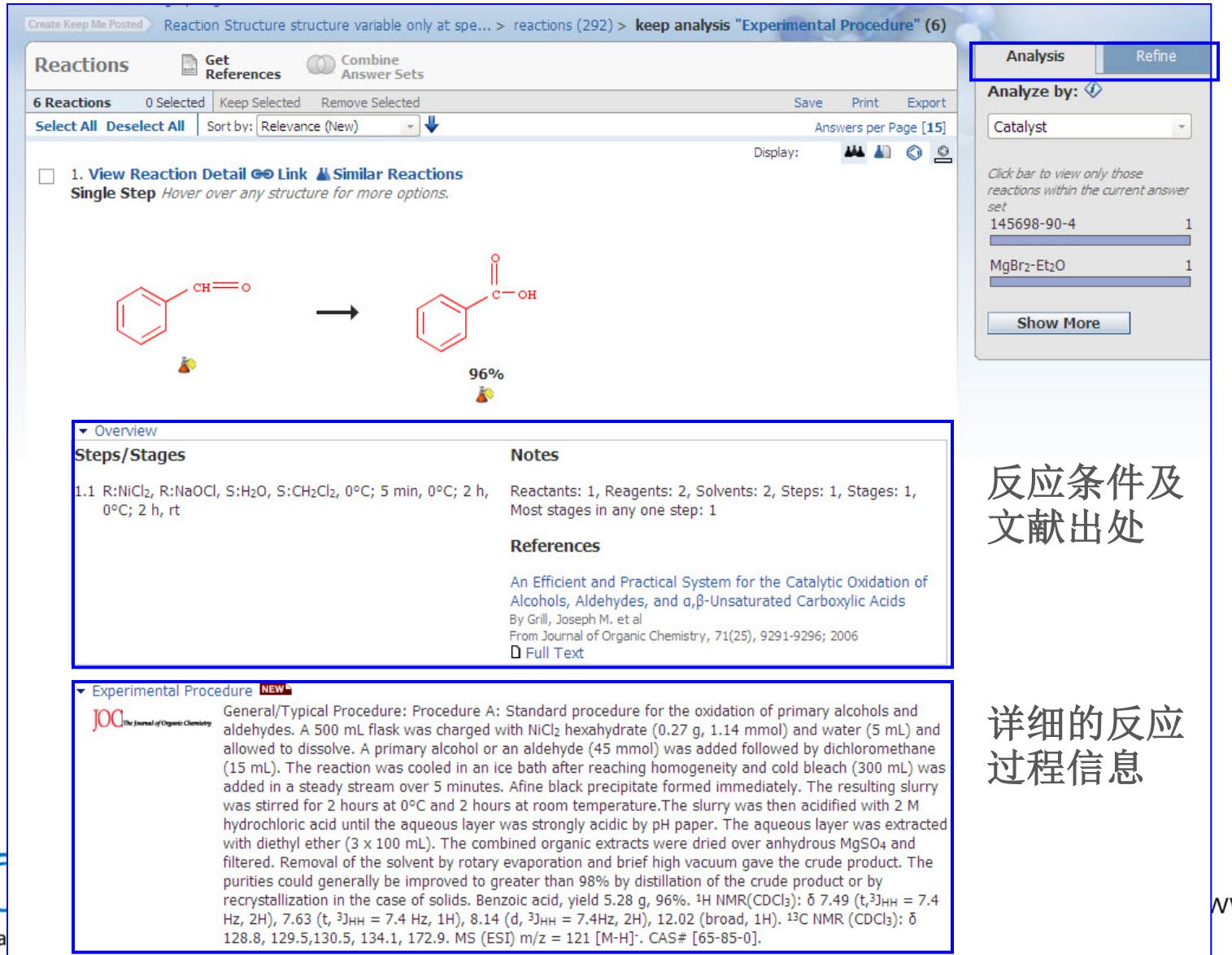
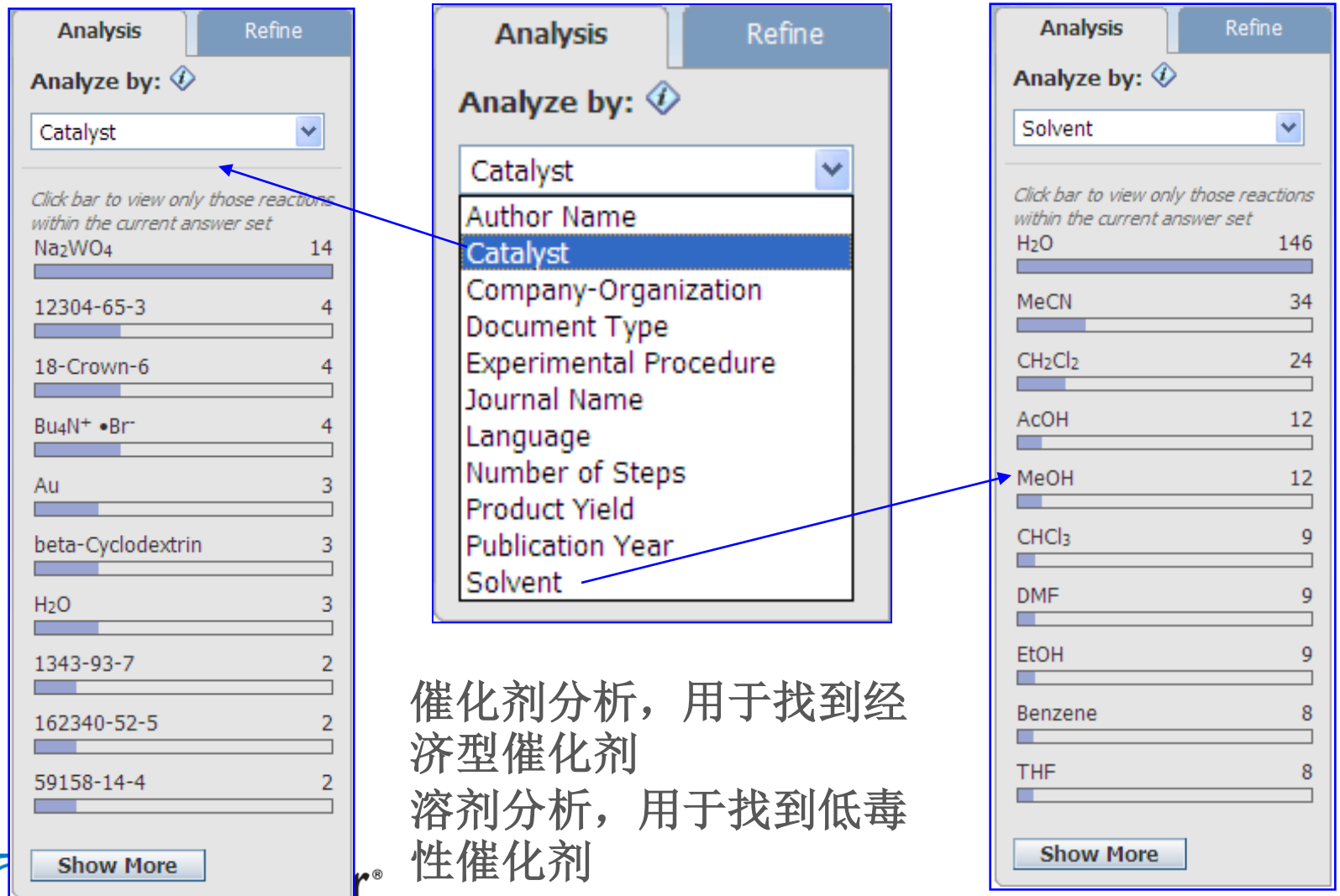
在SciFinder中能获得全面的反应集合



反应条件及文献出处

详细的反应过程信息

反应检索中的分析功能

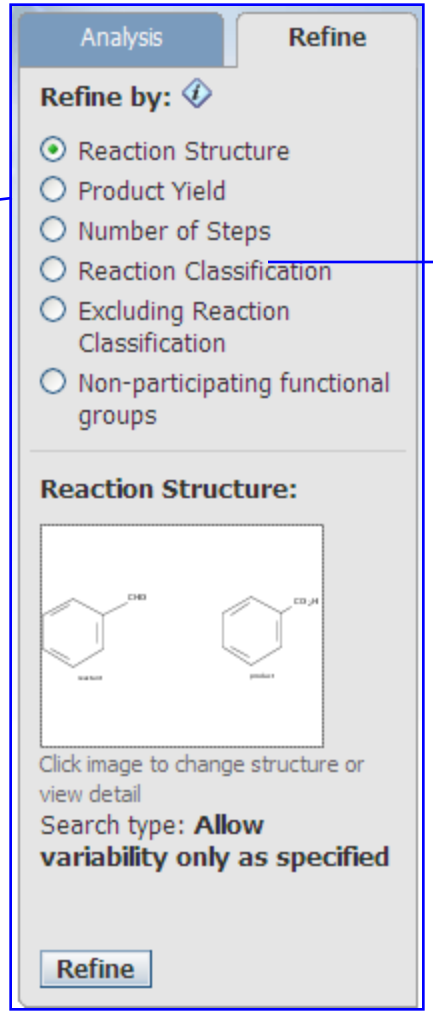


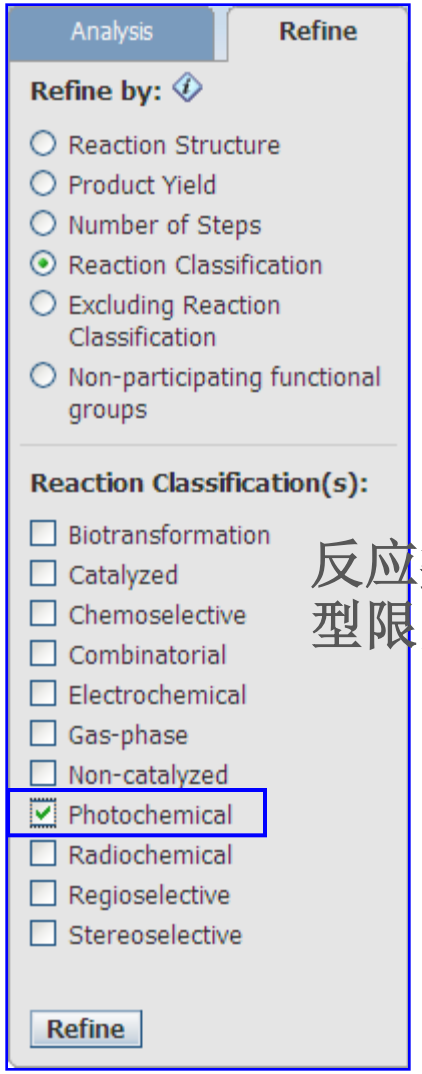
催化剂分析，用于找到经济型催化剂

溶剂分析，用于找到低毒性催化剂

反应检索中的限定功能

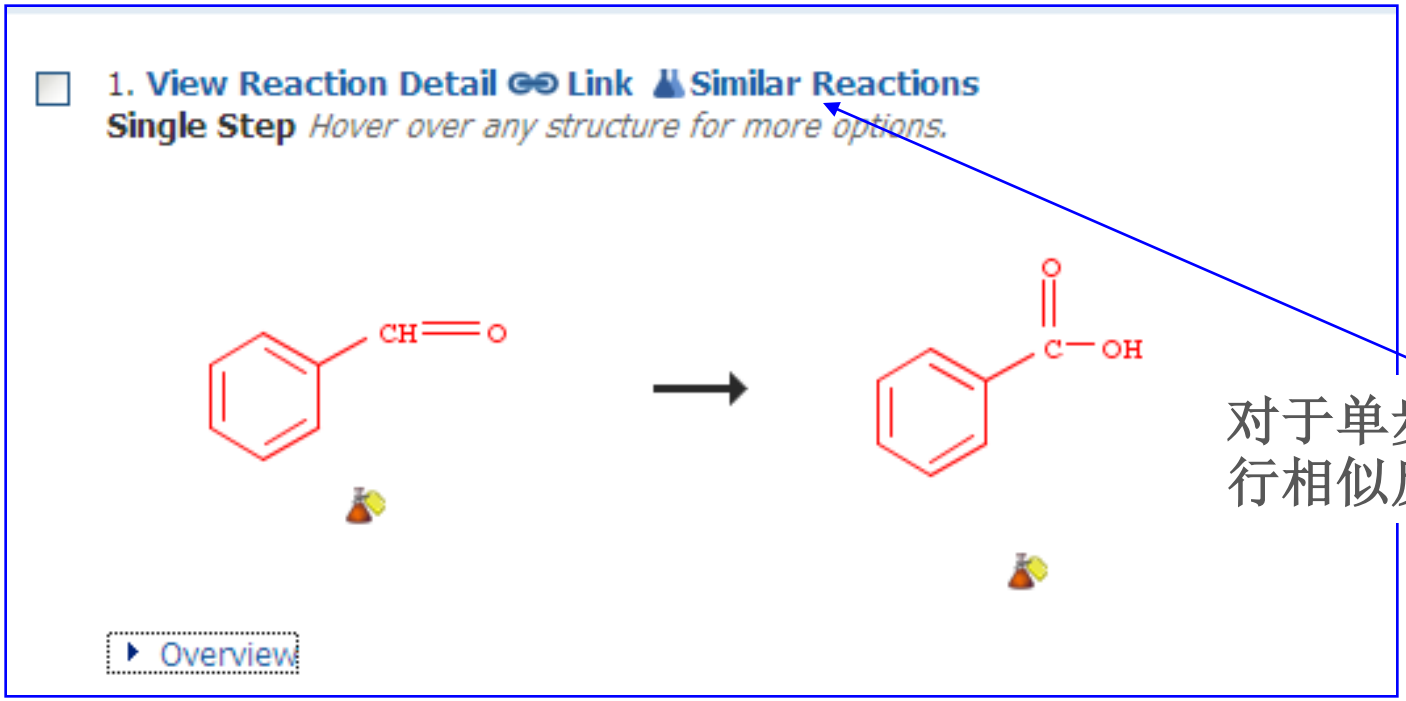
产率限定





反应类型限定

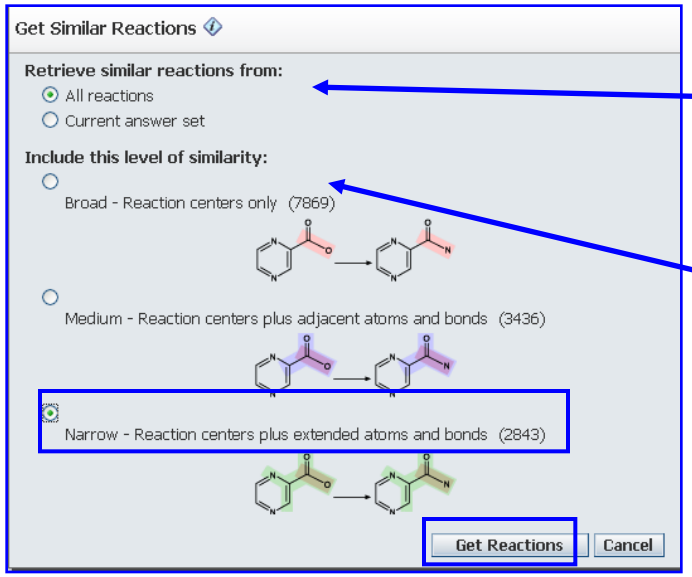
相似反应的获取



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



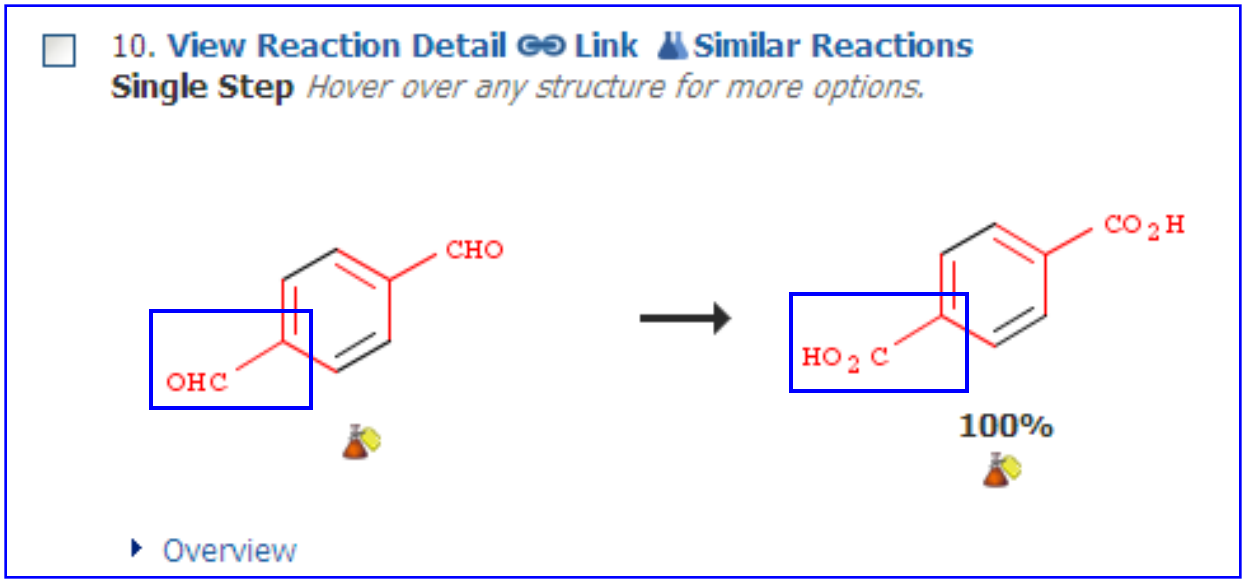
对于选择是全部反应中检索相似反应，还是在当前结果集中检索相似反应

选择相似反应的相似限制

Broad： 仅反应中心相似

Miedum： 反应中心及附属原子和键

Narrow： 反应中心及扩展的原子和键



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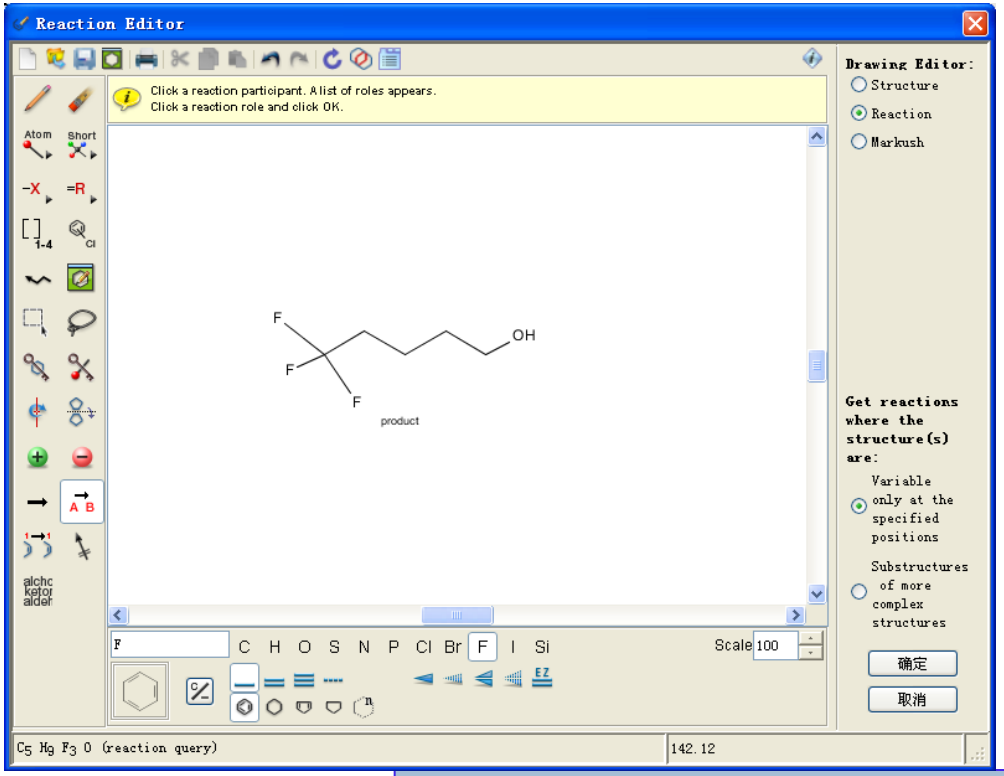
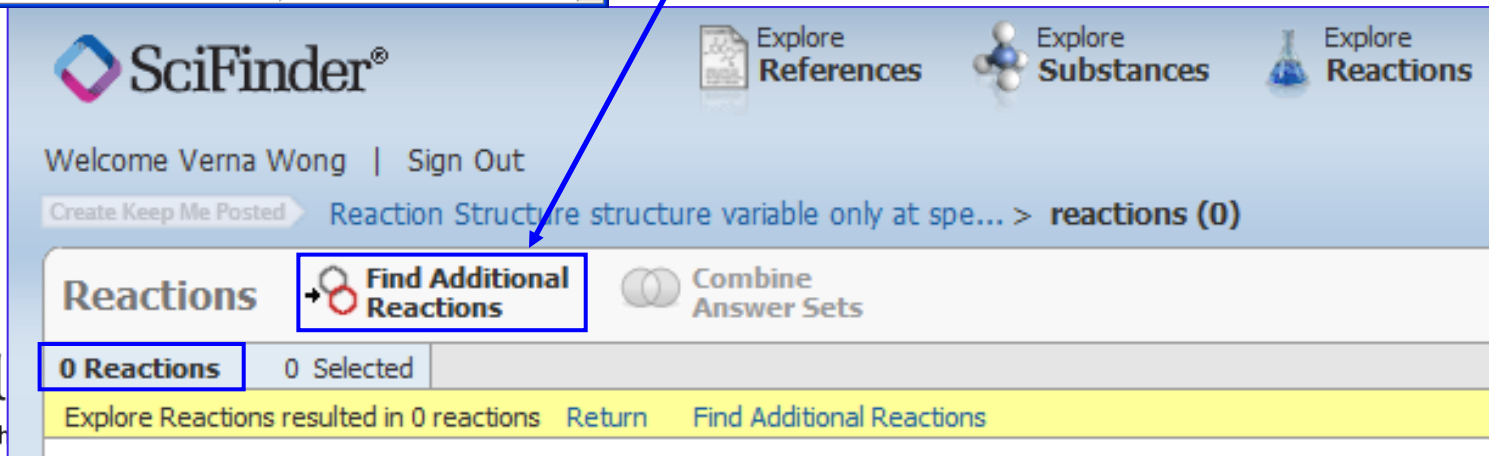
获得物质的合成制备信息



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。



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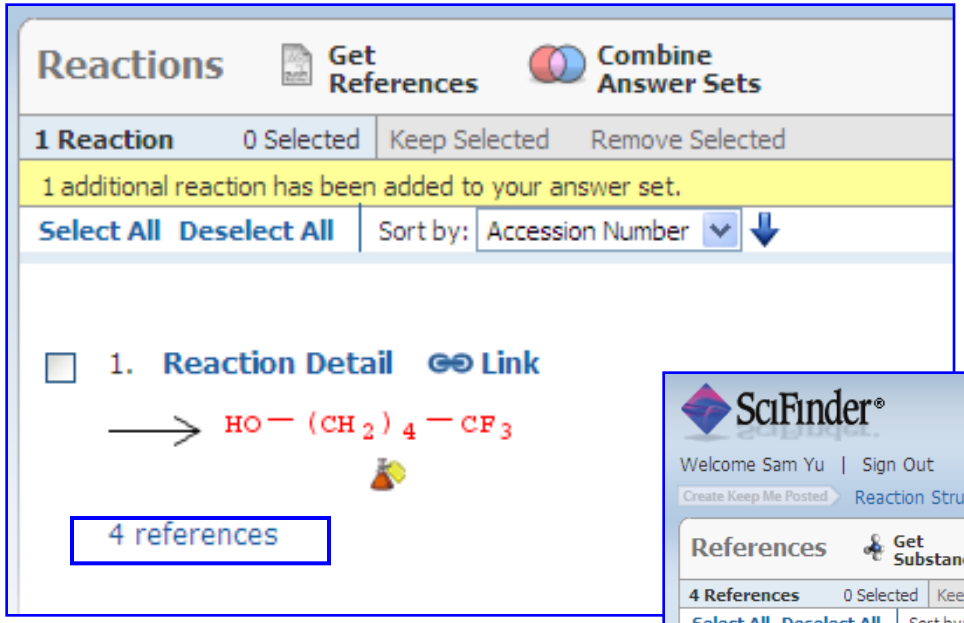
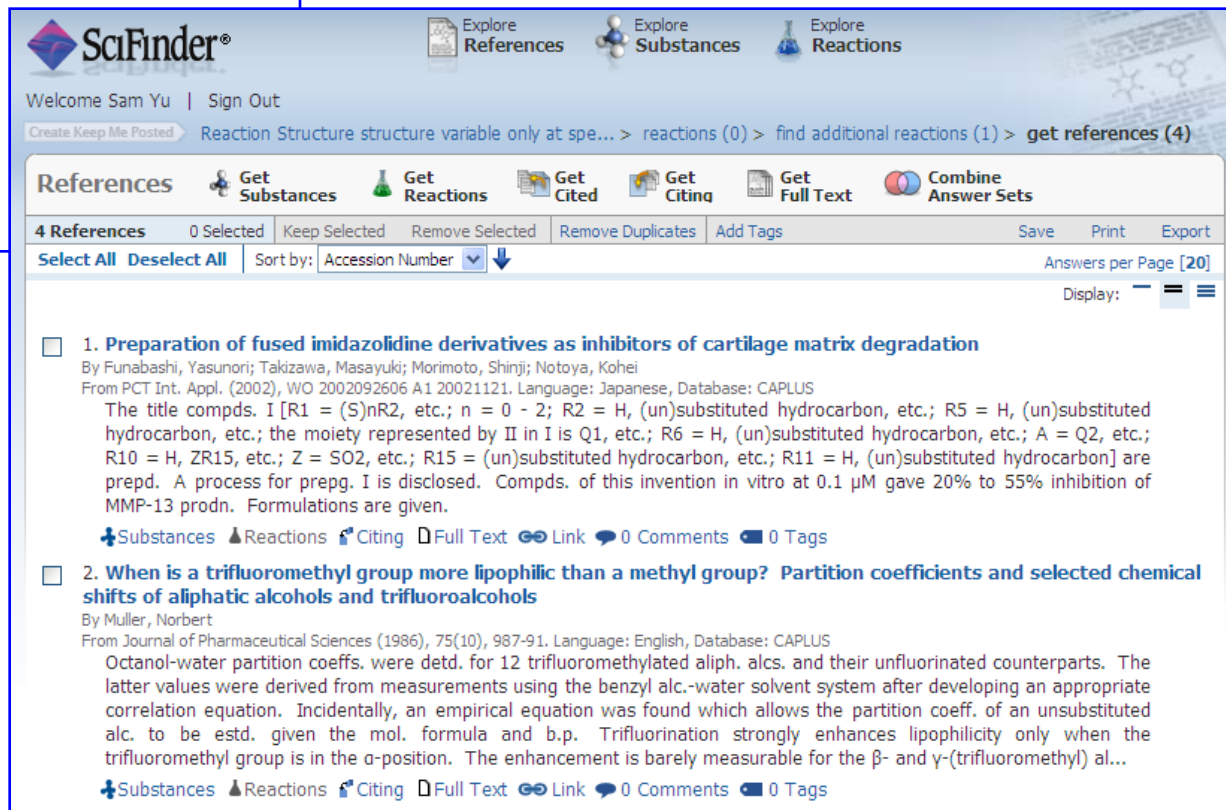
获得物质的合成制备信息



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。



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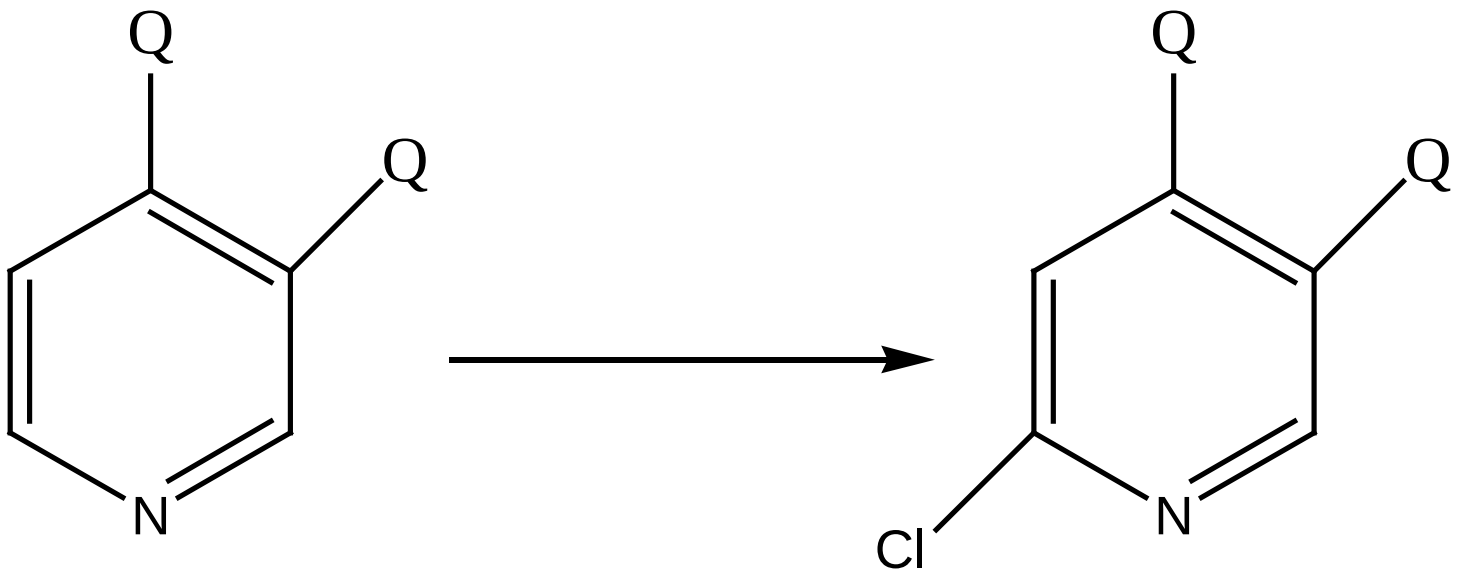
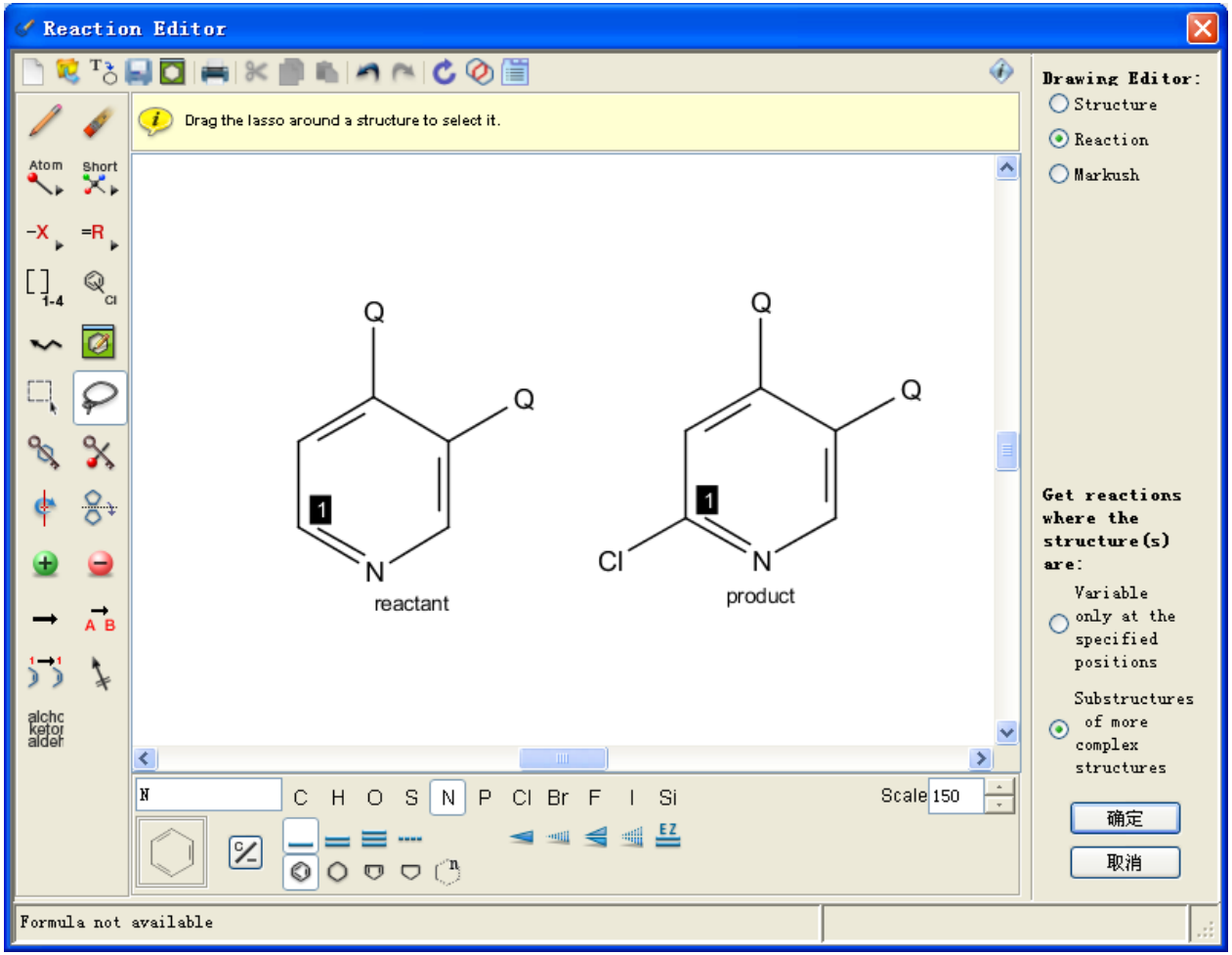
反应检索---检索对反应位置和原子有特定要求的反应

- 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

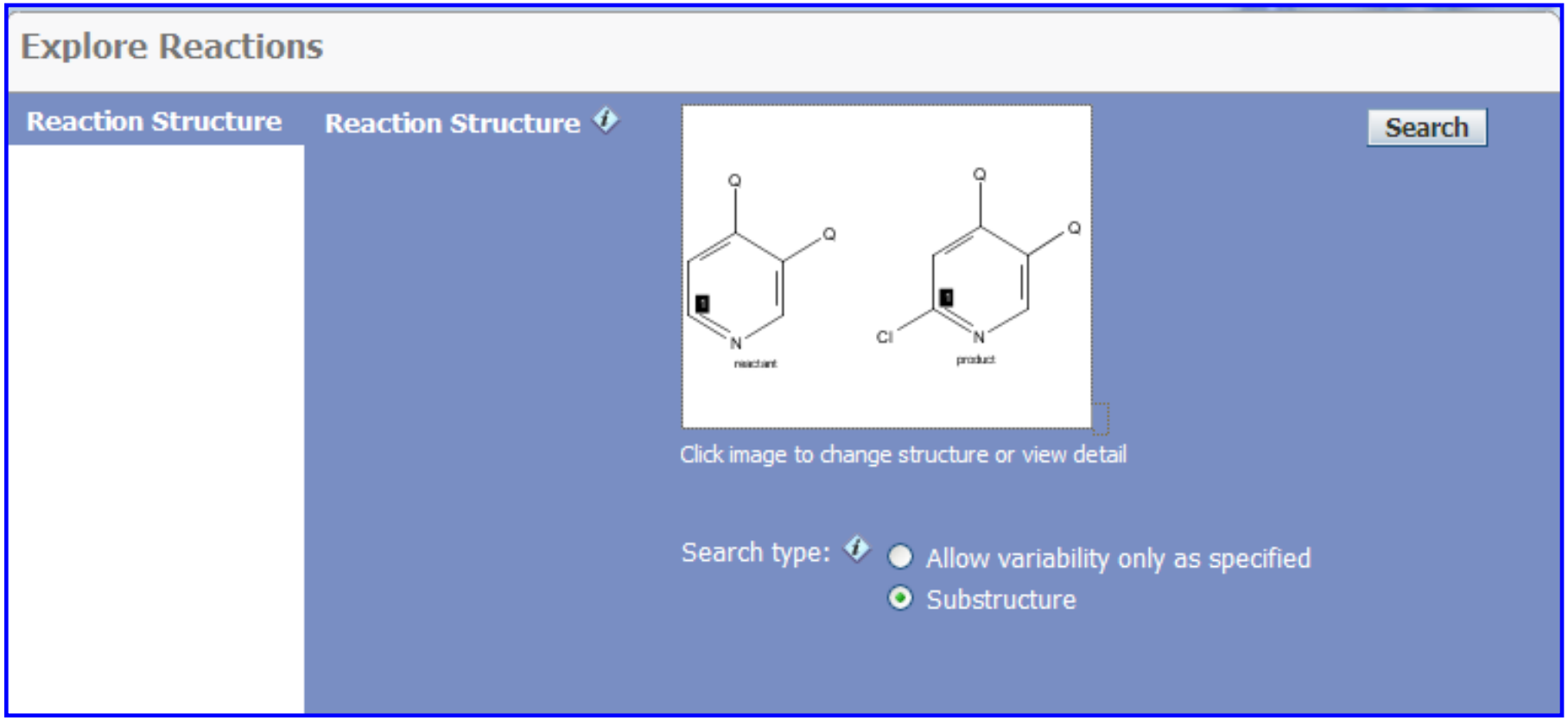


大多数科研工作者，刚开始都会画成这样。

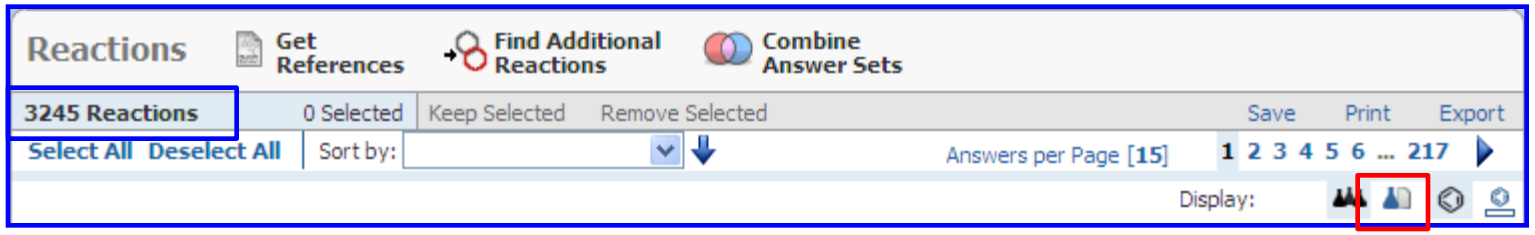
但是，这样足够吗？

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

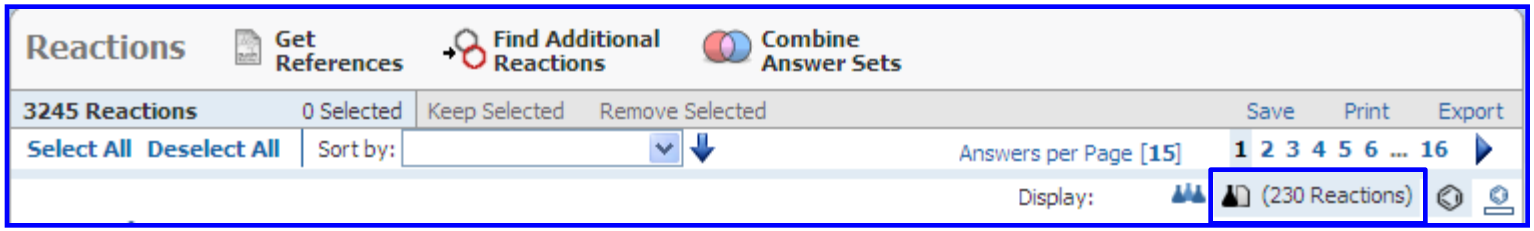


SciFinder中的反应筛选



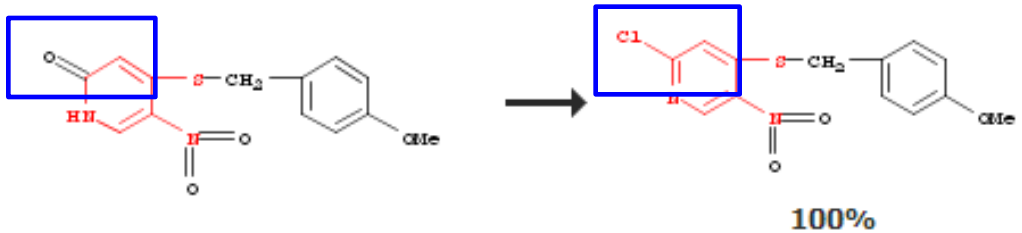
我们获得3200+ 条反应.

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



简单的看一下这些反应

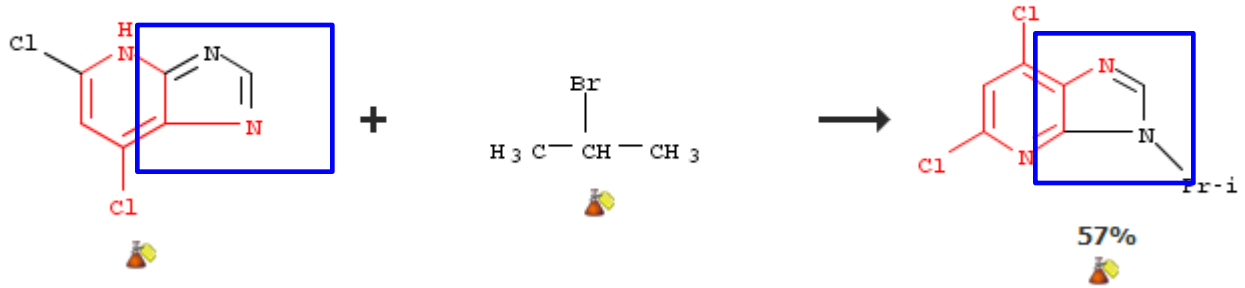
30. 22 Hits in this Reference Similar Reactions
Single Step *Hover over any structure for more options.*



Overview

第一条获取符合我们的要求

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



Overview

第二条，吡啶环系发生破坏，不是我们想要的

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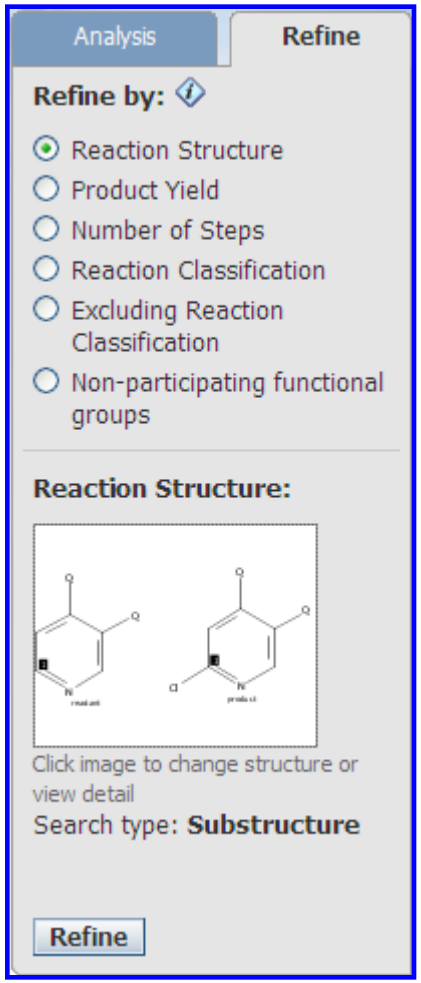
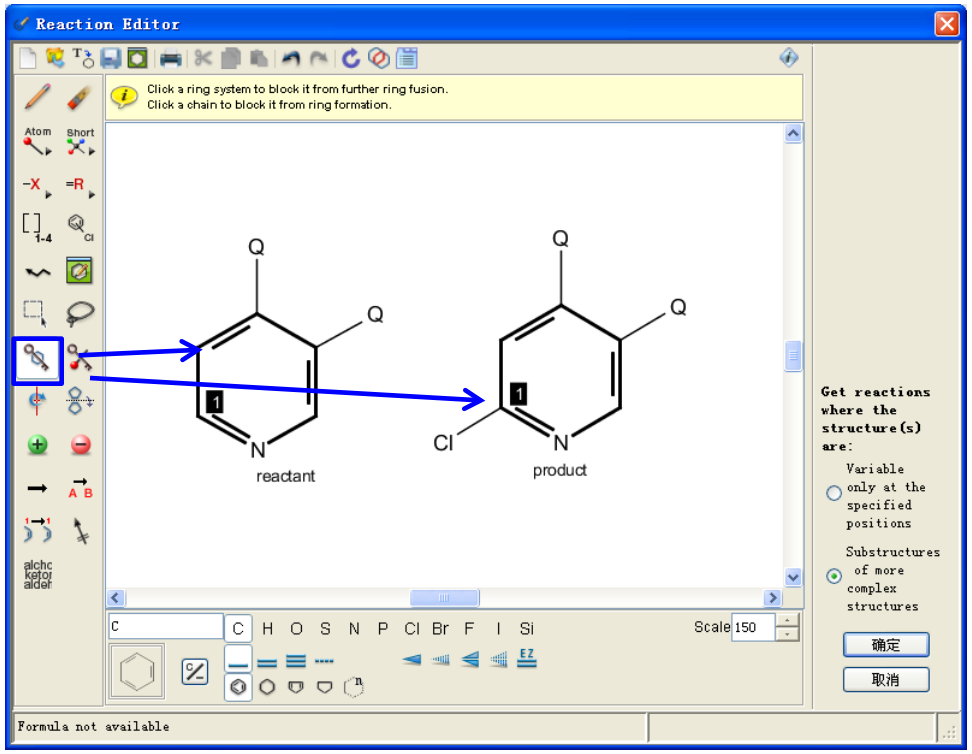
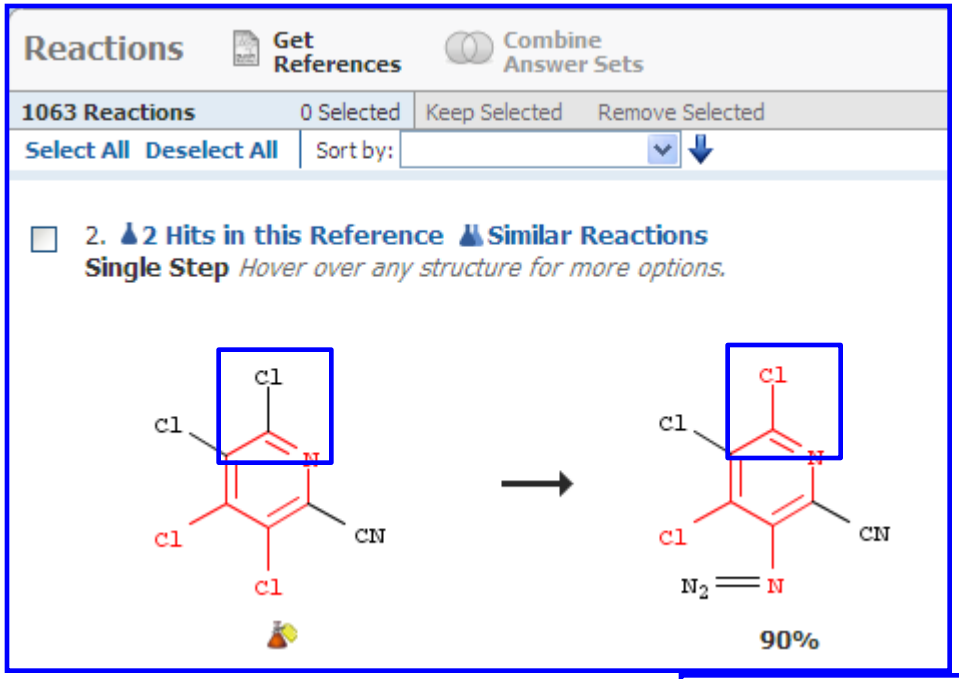
反应中的Refine工具，添加环锁定





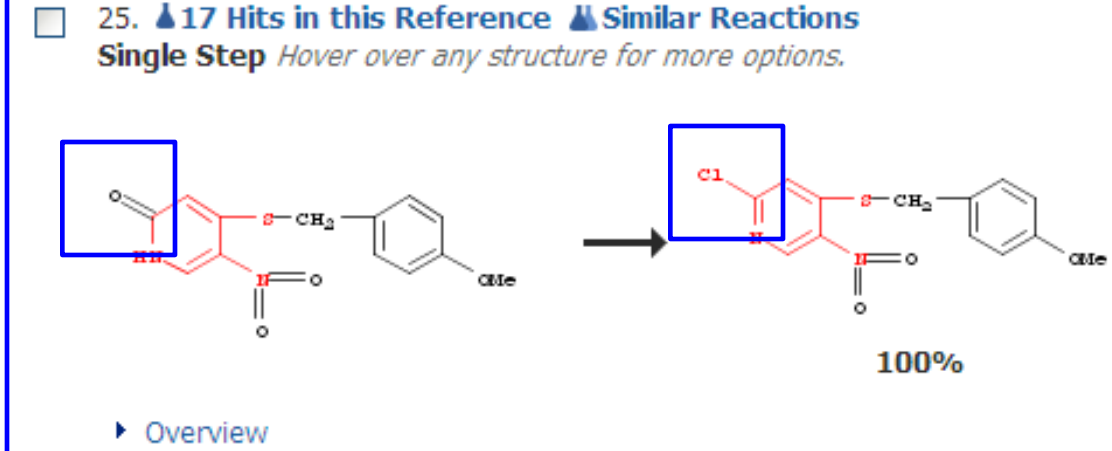
环锁定工具，当使用亚结构检索时，不允许发生稠环。

锁定环后的结果



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。



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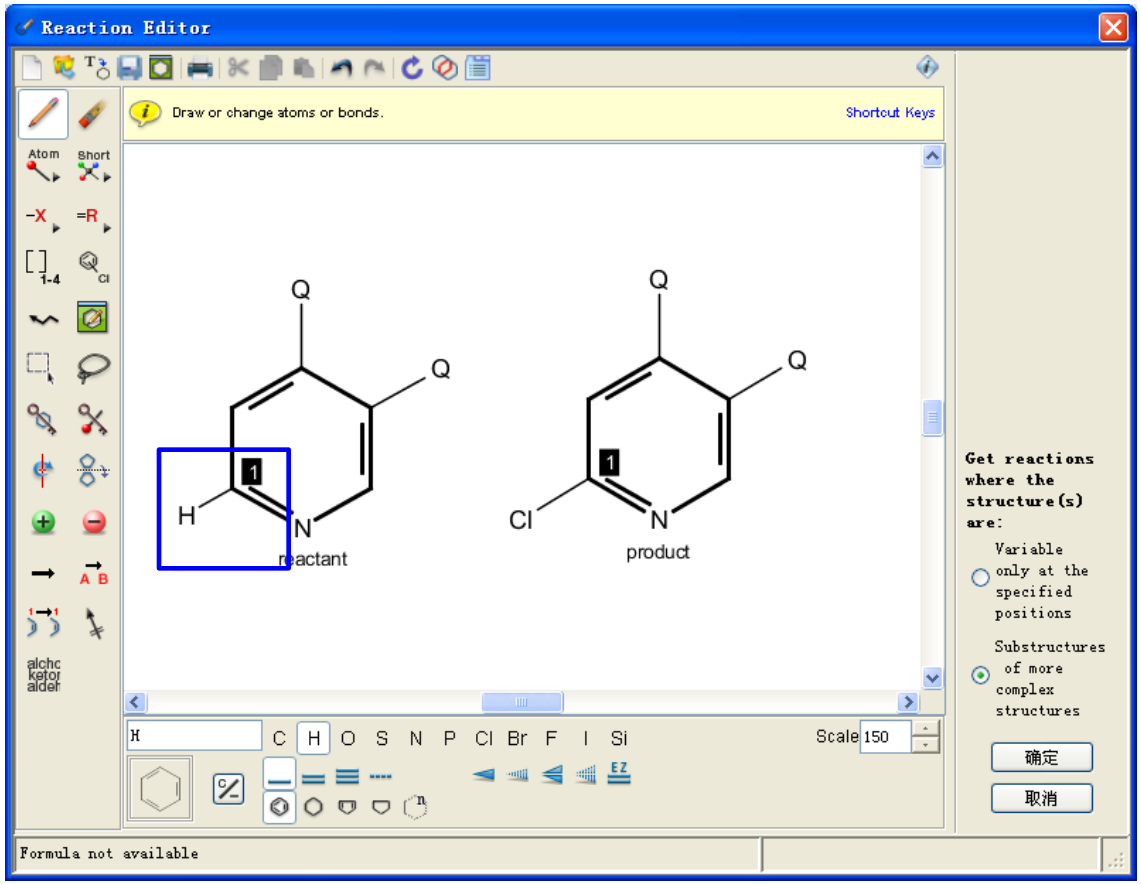
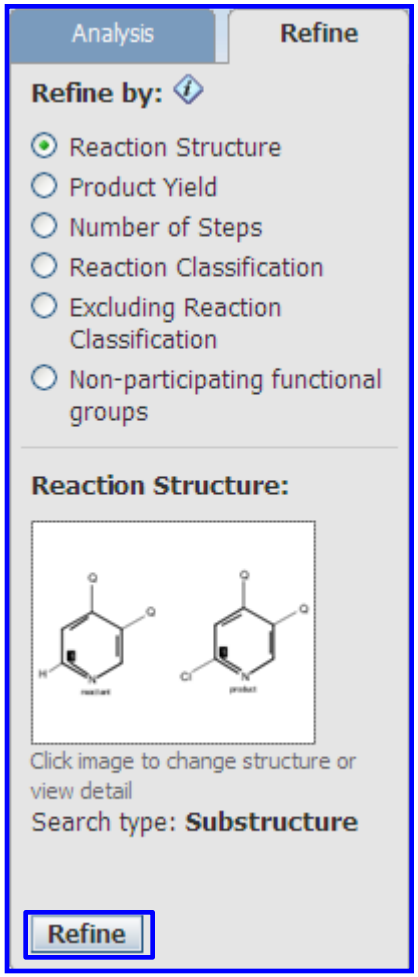
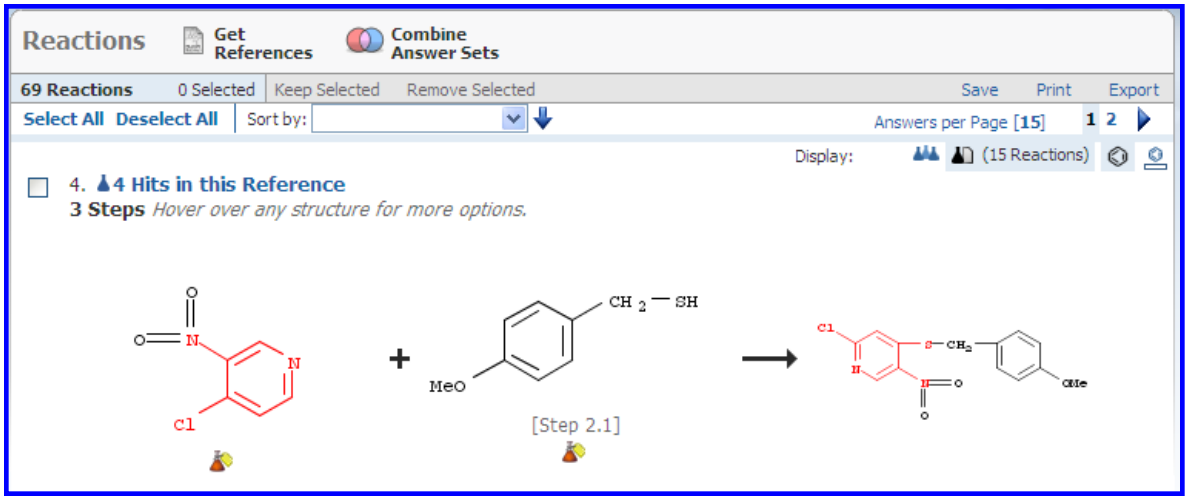
继续使用Refine


Reaction Editor
Draw or change atoms or bonds.
Shortcut Keys
Q
Q
H
N
1
reactant
Q
Q
Cl
N
1
product
Get reactions where the structure(s) are:
Variable only at the specified positions
Substructures of more complex structures
C H O S N P Cl Br F I Si
Scale 150
确定
取消
Formula not available

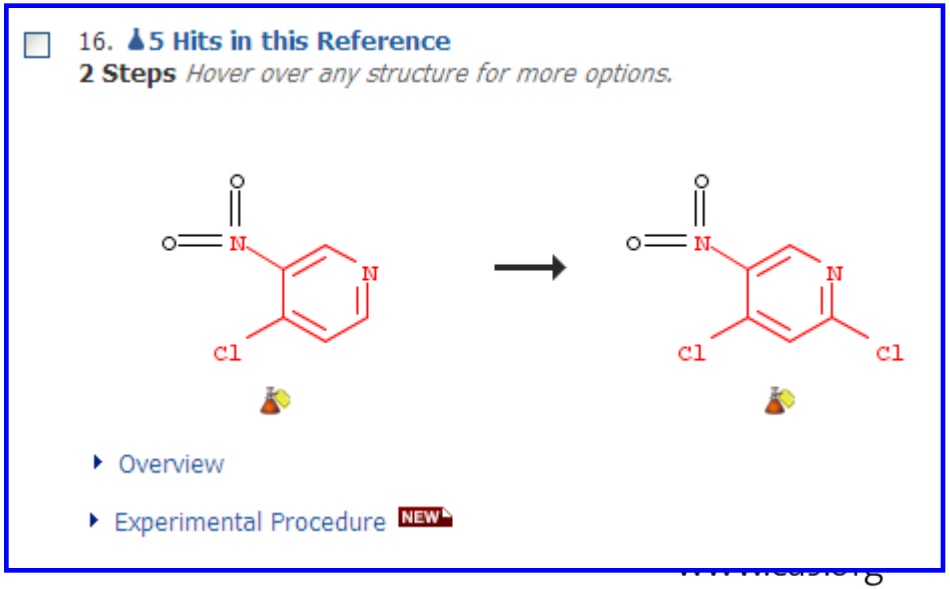

Analysis
Refine
Refine by:
Reaction Structure
Product Yield
Number of Steps
Reaction Classification
Excluding Reaction Classification
Non-participating functional groups
Reaction Structure:
Click image to change structure or view detail
Search type: Substructure
Refine

这是我们想要的反应



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



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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

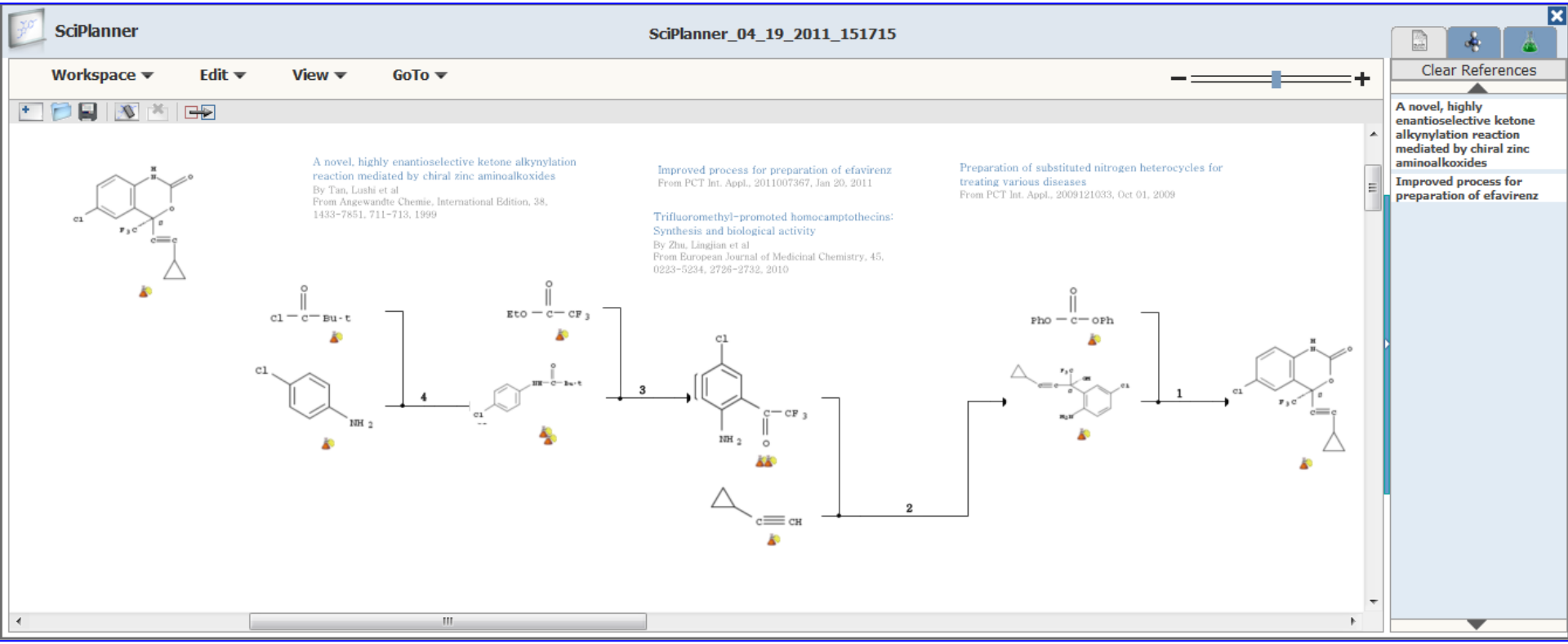
什么是SciPlanner?

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



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)

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1 /7 139% 查找

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Page 1

A novel, highly enantioselective ketone alkynylation 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

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

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

以及详细的反应信息、物质信息和文献信息

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Reaction Information

Reaction	Stages	Notes	Yield
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 proc
By Singh, Giri
From PCT Int

Reaction	Stages
21	1.1 R:BuMg S:THF

References

A novel, highl
By Tan, Lushi
From Angewe

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

References

Trifluoromethy
By Zhu, Lingji
From Europes

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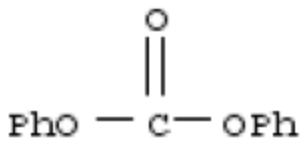
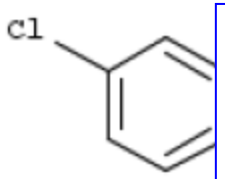
102-09-0	106-47-8	154598-52-4
		
$C_{13}H_{10}O_3$ Carbonic acid, diphenyl ester ~2001 References Reactions Commercial Sources Regulatory Information Link	C_6H_6ClN Benzenamine, 4-chlor ~14690 References Reactions Commercial Sources Regulatory Information Link	
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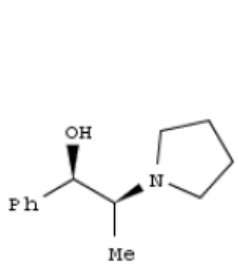
References

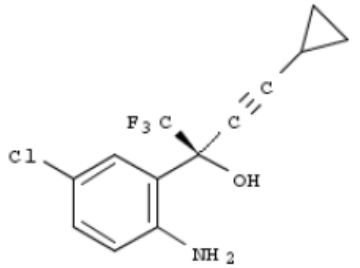
A novel, highly enantioselective ketone alkynylation reaction mediated by chiral zinc aminoalkoxides

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

A method for asym. alkynylation 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 alkynylation was demonstrated in prepg. a key intermediate (II) used in the synthesis of Efavirenz, a potent nonnucleosidal HIV reverse transcriptase inhibitor.



I



II

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Trifluoromethyl-promoted homocamptothecins: Synthesis and biological activity

By Zhu, Lingjian; Miao, Zhenyuan; Sheng, Chunquan; Guo, Wei; Yao, Jianzhong; Liu, Wenfeng; Che, Xiaoying; Wang, Wenya; 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

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.

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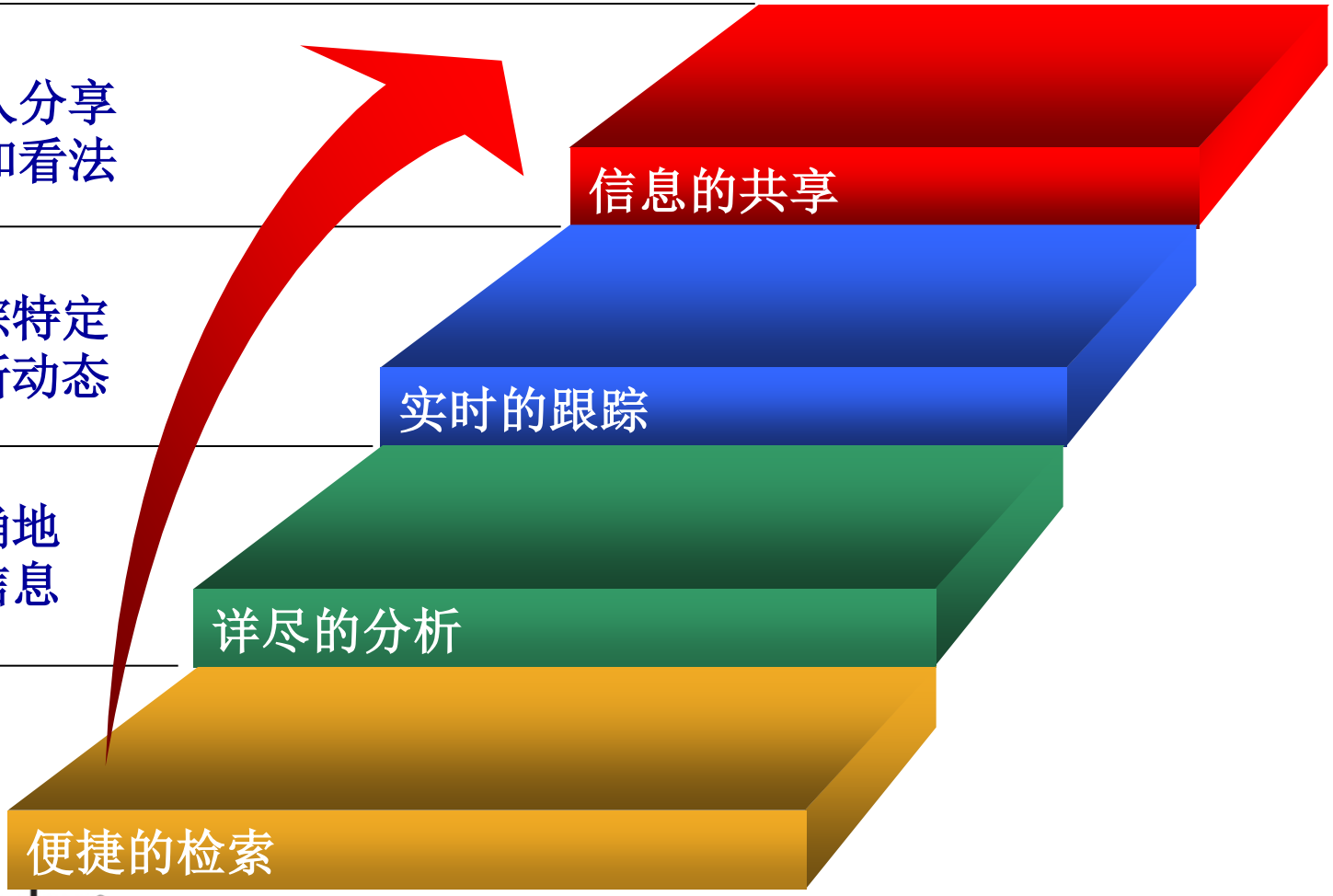
帮助您通过多种途径获得信息



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邮编： 510030

王 薇

Tel:(020)83274076

Email: verna@igroup.com.cn