



SciFinder®

SFoW Training

CAS Representative-TW, 許傳奇




What is the “Competitiveness” of the 21 Century ?

Bill Gates: ***Speed !***

- 接受資訊的速度！
- 管理資訊的速度！
- 運用資訊的速度！



A division of the American Chemical Society

- CAS, the global leader in chemical information, and a division of the American Chemical Society
- Provides the most comprehensive databases of disclosed research in chemistry and related sciences, including the world's largest collection of substance information, the CAS REGISTRYSM (Gold Standard)
- Indexes and summarizes chemistry-related information from scientific journals, patents, conference proceedings, and other pertinent documents.
- Products & Services :  **SciFinder[®]**  **STN[®]**  **SCIENCE IP[®]**
The CAS Search Service



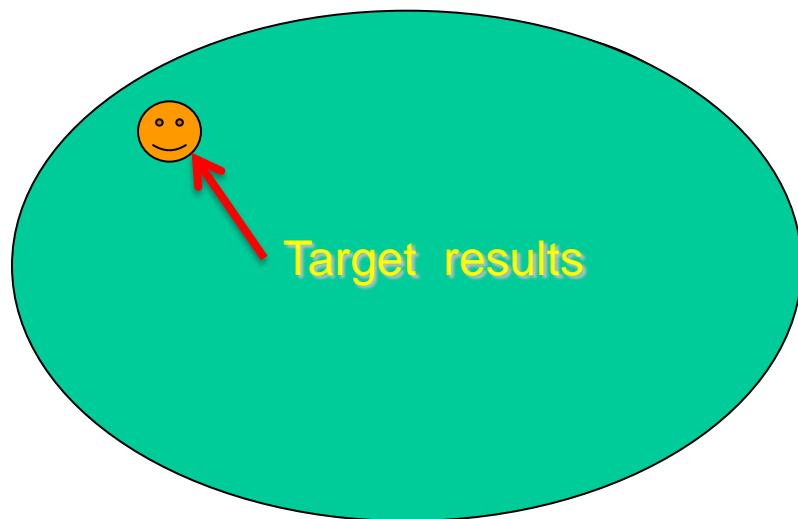


A division of the American Chemical Society

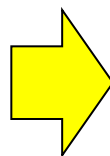
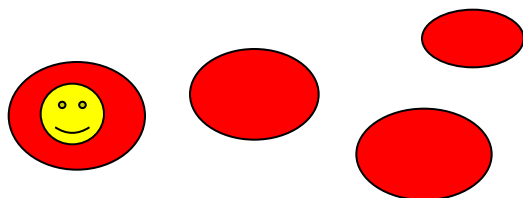
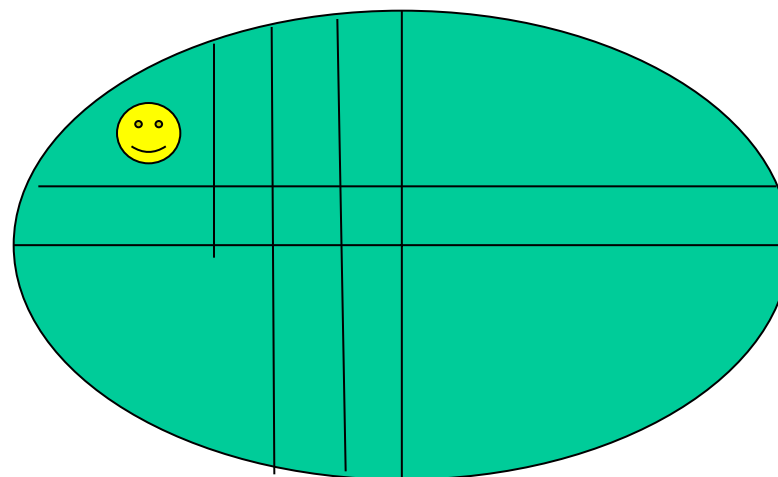
- Around 900 PhD involve in the reference editing.
- More than 10,000 organizations around the world use SciFinder.



Step 1.
Completely



Step 2.
Analyze/Refine



We cannot search parts of Full Text

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**}

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

2. Department of Base Science, Jilin Institute of Architecture and Civil Engineering, Changchun 130021, P. 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 monophyrin. The effect of the trimer on the fluorescence property and thermostability were also studied in detail.

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

Introduction

Porphyrin possesses some unique properties. In comparison with the porphyrin monomer, porphyrin oligomers are much attracting owing to their much better properties in some aspects, such as light harvest, energy transformation and electron transition. In recent years, Oligomeric porphyrins with various structures 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

along with the change of the peripheral substitution groups and oligomerization of porphyrin. This investigation provides an available reference for the research on photosynthesis, molecular wires and logic gate circuits in molecular electronics.

Experimental

Pyrolo(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].

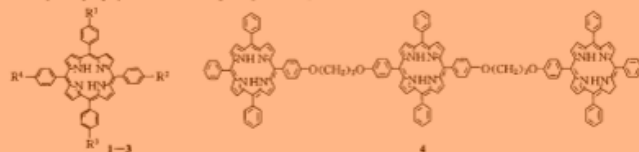


Fig. 1 The structures of porphyrin monomers 1–3 and the porphyrin trimer(4).

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

Results and Discussion

1 UV-Vis Spectrum

The room temperature solution electronic absorption values are almost identical in Table I. 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-

H₂DHDP(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.

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

Compound	Soret band, $\lambda/\text{nm}(10^3\epsilon)$		Q band, $\lambda/\text{nm}(10^3\epsilon)$			
	λ	ϵ	λ	ϵ	λ	ϵ
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 S₂ → S₀ transition and it corresponds with the Soret band at 418.4 nm of their electronic absorption spectra^[12], but the fluorescence emission peaks of porphyrins 3 and 4 at the same position disappear. The fluorescence emission peaks at 650 and 714 nm of porphyrins 1–4 can be assigned to the S₁ → S₀ transition and correspond with Q(0, 0), Q(0, 1) of porphyrins 1–4^[12].

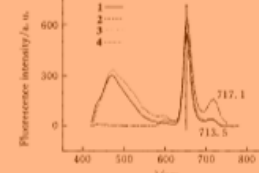


Fig. 2 The fluorescence emission spectra of porphyrin monomers 1–3 and a trimer(4) (excited at 400 nm).

The experimental results indicate that in dichloromethane, 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

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 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.

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.

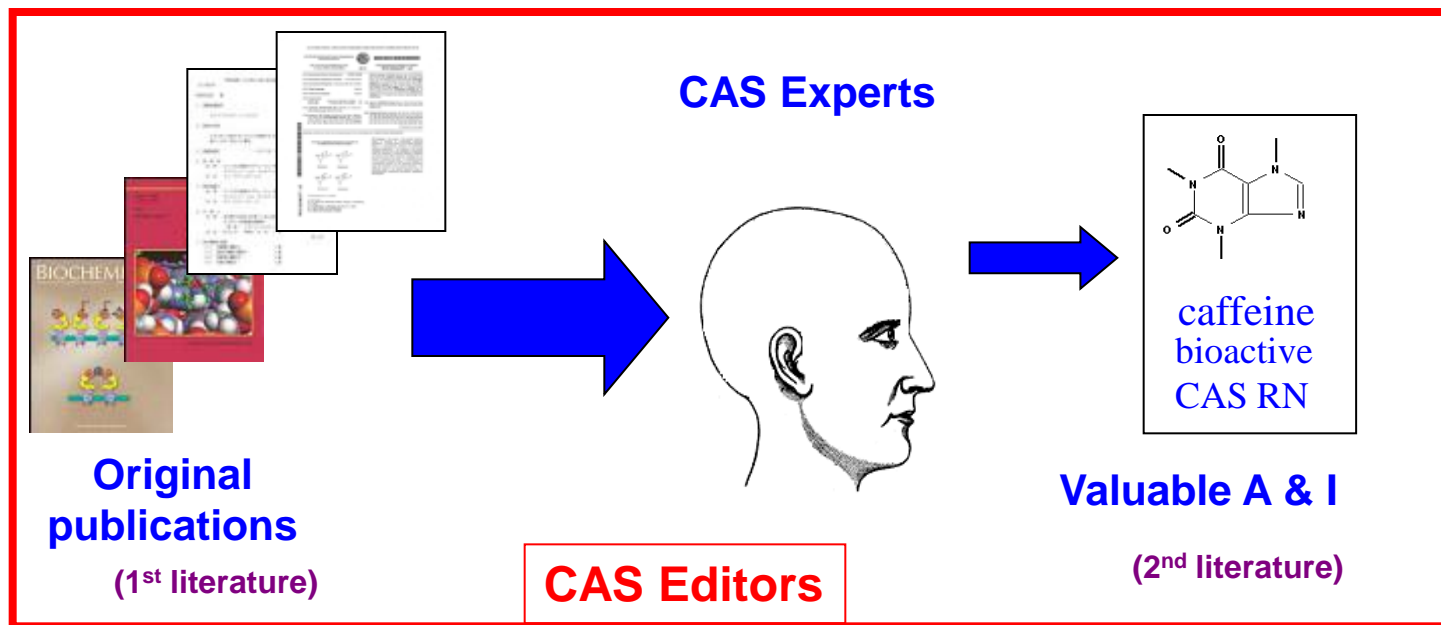
Fig. 4 shows the fluorescence excitation spectrum and the emission spectrum of the porphyrin trimer in different solvents, CH₂Cl₂ or DMF. It can be seen that the fluorescence intensity in DMF is stronger than that

CAS Workflow : Human Indexing

Establish the Largest, Authority and Reliability database around the world!



Science & Tech.



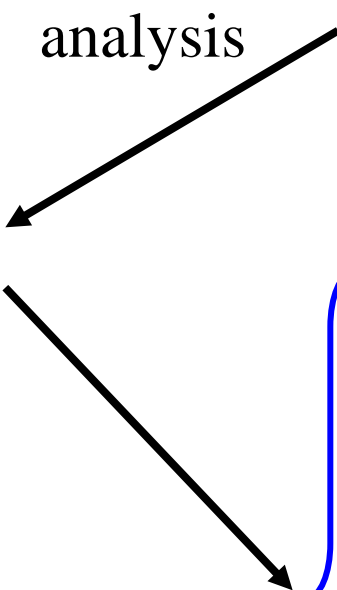
Scientists



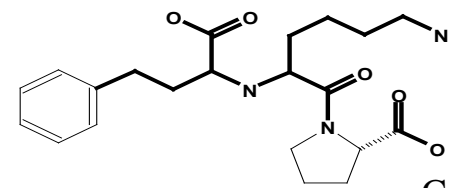
EX: Patent analysis by Human Indexing



Dr. Bruce Benjamin



PCT		WORLD INTELLECTUAL PROPERTY ORGANIZATION International Bureau	
INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)			
(51) International Patent Classification 7 : C12N 15/31, C07K 14/81, C11D 3/33, 3286		A2	(11) International Publication Number: WO 00/01826
(21) International Application Number: PCT/US99/15246		(43) International Publication Date: 13 January 2000 (13.01.00)	
(22) International Filing Date: 7 July 1999 (07.07.99)		(81) Designated States: AE, AL, AM, AT, AT (Utility model), AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, CZ (Utility model), DE, DE (Utility model), DK, DK (Utility model), EE, EE (Utility model), ES, FI, FI (Utility model), GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KR, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LU (1-7/MD), MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK (Utility model), SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, HE, HU, IT, LI, NL, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TO).	
(30) Priority Data: 00/091,911 7 July 1998 (07.07.98) US		(71) Applicant (for all designated States except US): THE PROCTER & GAMBLE COMPANY [US/US]; One Procter & Gamble Plaza, Cincinnati, OH 45202 (US).	
(72) Inventors; and (75) Inventors/Applicants (for US only): SAUNDERS, Charles, Winston [US/US]; 3501 Carlsbad Court, Fairfield, OH 45014 (US), CORREA, Paul, Elliott [US/US]; 5755 Dry Ridge Road, Cincinnati, OH 45232 (US), SUN, Yiping [US/US]; 7589 Lakota Springs Drive, West Chester, OH		Published Without international search report and to be republished upon receipt of that report.	



CAS RN 2835-34-8

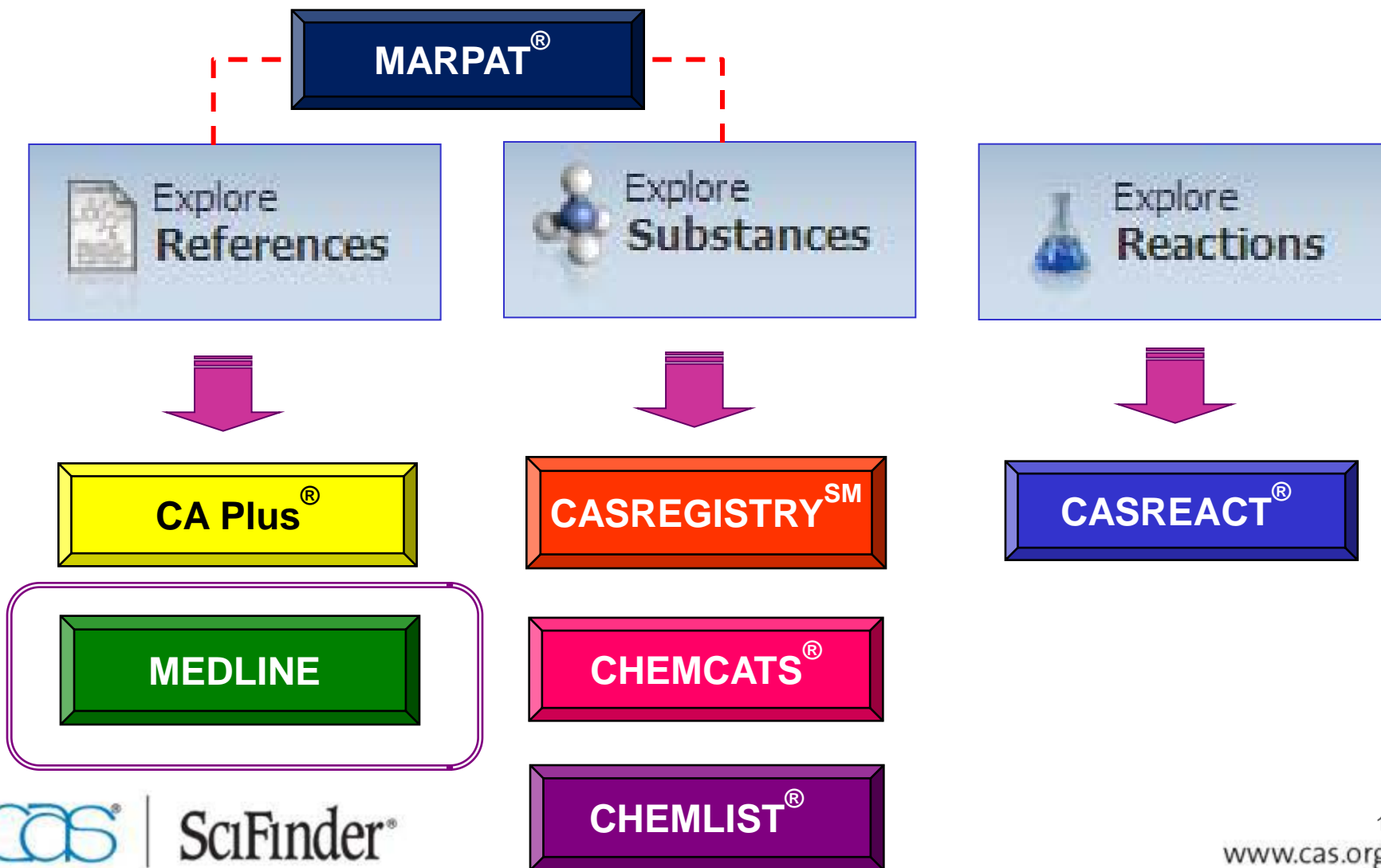
Protein Sequence

```

1 MFPTIPLSRL FDNAMLRAHR LHQLAFDTYQ EFEEA YIPKE QKYSFLQNPQ
51 TSLCFSESIA TPSNREETQQ KSNLELLRIS LLIQSWLEP VQFLRSVFAN
101 SLVYGASDSN VYDLLKDL EE GIQTL MGRLE DGS PRTGQIF KQYTSKFDNT
151 SHND DALLKN YGLLYCFR KD MDK VETFLRI VQCRSVEGSC GF
    
```





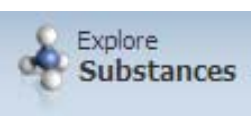






- Somatotropin CAS RN 154907-93-4
- Animal gene *pac43*
- Oncogenes
- Neoplasm inhibitors
- Liver neoplasm

Database in SciFinder: 3 types and 7 databases



Coverage, content in glance

<http://www.cas.org/expertise/cascontent/ataglance/index.html>

Type	Database	Content and coverage
 Explore References	  	<ul style="list-style-type: none"> • Early 1800s to present • >33 million references from 61 patent authorities worldwide and >10,000 major scientific journals • >19 million references from MEDLINE® • MARPAT from 1988 to present, spanning 61 patent authorities
 Explore Substances	   	<ul style="list-style-type: none"> • >56 million organic and inorganic substances • >62 million sequences • >2.9 billion predicted and experimental properties, spectra, and data tags, plus • >42.2 million proton NMR spectra 1957 to present, plus selected substances back to the early 1900s • Commercial source information from >1,100 suppliers for >44 million substances • Regulatory information for more than 275,000 substances • >350 k records with more than 831 k searchable Markush structures (updated daily)
 Explore Reactions		<ul style="list-style-type: none"> • 1840 to present • >13.6 million synthetic preparations • >28 million single- and multi-step reactions

CAplus (Early 1800s-)

CAS databases cover patents from **61** patent authorities around the world !!



- ▶ Canadian Intellectual Property Office (CIPO)
- ▶ European Patent Office (EPO)
- ▶ French Patent Office (INPI - Institut National de la Propriete Industrielle)
- ▶ German Patent Office (DPMA)
- ▶ Japanese Patent Office (JPO)
- ▶ Russian Patent Office (ROSPATENT - Russian Agency for Patents and Trademarks)
- ▶ United Kingdom Intellectual Property Office (UK-IPO)
- ▶ United States Patent & Trademark Office (USPTO)
- ▶ World Intellectual Property Organization (WIPO).

Worldwide coverage of many scientific disciplines

Biochemistry-

- Agrochemical regulators
- Biochemical genetics
- Fermentation
- Immunochemistry
- Pharmacology

.....

Organic chemistry-

- Amino acids
- Biomolecules
- Carbohydrates
- Organometallic compounds
- Steroids

.....

Macromolecular chemistry-

- Cellulose, lignin, paper
- Coatings, inks
- Dyes, organic pigments
- Synthetic elastomers
- Textiles, fibers

.....

Applied chemistry-

- Air pollution
- Ceramics
- Essential oils, cosmetics
- Fossil fuels
- Ferrous metals, alloys

.....

Physical, inorganic, analytical chemistry-

- Surface chemistry
- Catalysts
- Phase equilibrium
- Nuclear phenomena
- Electrochemistry
- Crystallography and Liquid Crystals

.....

CAS REGISTRY (1957-)

- The **world's largest** collection of organic and inorganic **substance information**
- Consists more than **56** million **organic and inorganic substances** and **62** million **sequences**
 - * *Organic compounds*
 - * *Inorganic compounds*
 - * *Metals*
 - * *Alloys*
 - * *Minerals*
 - * *Coordination compound*
 - * *Nonstructurable materials (UVCBs)*
 - * *Organometallics*
 - * *Elements*
 - * *Isotopes*
 - * *Nuclear Particles*
 - * *Proteins and Nucleic*
 - * *Polymers*

Experimental and predicted property information

SciFinder	Experimental	Predicted
Properties	4.3 million (for 2.8 million substances)	3 billion (for 46.2 million substances)
Spectra	721,000 (for 488,000 substances)	44.1 million ¹³C-NMR and 44.1 million ¹H-NMR (available in SciFinder)
Data Tags	10.3 million (for 3.3 million substances)	N/A

Update: 2/7/2011

CASREACT (1840-) : sources

- **CAS**
 - Journals from **1985**-present
 - Patents from **1991**-present
- **InfoChem (which supplies the VINITI/ZIC database)**
 - Journals from 1974-1991
 - Patents 1982-1991
- **INPI (data from the French Core Reactions Database)**
 - **1840**-1985

CHEMLIST (1979-)

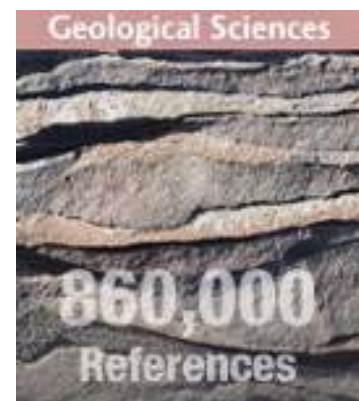
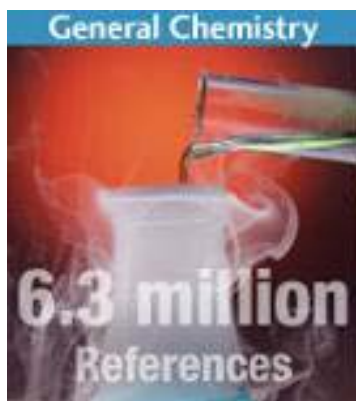
- An electronic collection of thousands of chemical substances that are regulated in key markets across the globe
- **More than 275,000** substances
- **Inventories and lists** information in the key market around the world
- Update more than 50 new substances each week

CHEMCATS (1995-)

- Quickly find the catalog information you need.
- You will find the following contact information (depending upon the supplier):
 - * Catalog name
 - * Order number
 - * Chemical and trade names
 - * CAS Registry Number
 - * Chemical structure
 - * Grade information
 - * Pricing terms
 - * Packaging and availability information
 - * Supplier contact information
 - Company name and address
 - Phone and fax number
 - E-mail
 - Web address

SciFinder, including

- Chemistry ;
- Biomedical / Life Science ;
- Material ;
- Engineering ;
- Agricultural Science and more...



SciFinder Web <https://scifinder.cas.org>



<https://scifinder.cas.org/>

Sign In

Username

Password

Remember my username

[Forgot Username or Password?](#)

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

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!

Welcome to SciFinder

NEW! The new web version of SciFinder makes access to SciFinder even more essential to your scientists research process. Some of the **new features** include:

- Direct links to data
- Keep Me Posted enhancements
- Improved search precision
- Session history retention
- Index term linking

Visit www.cas.org for more information about the latest release.

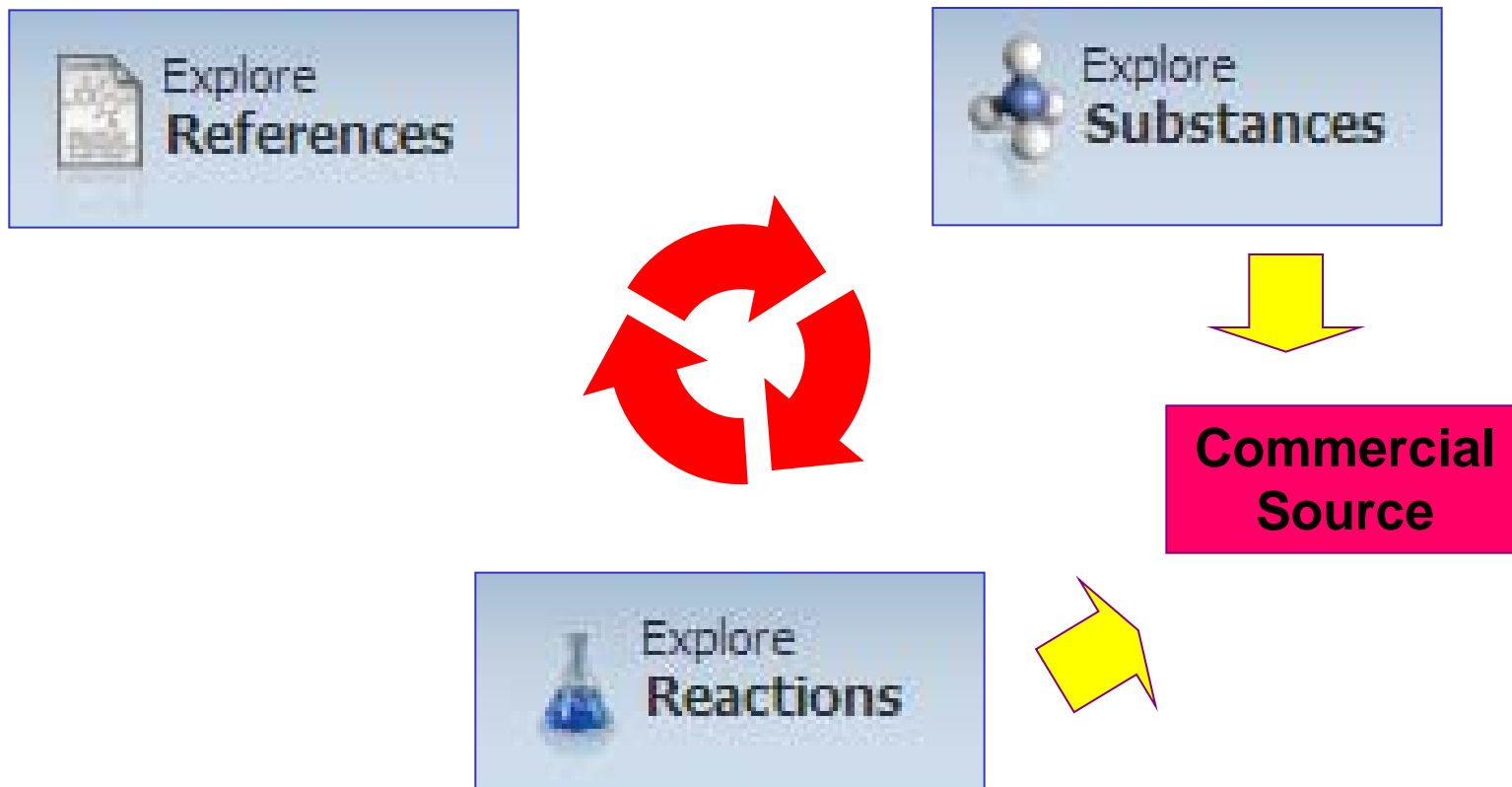
CAS - Science Connections

The CAS - Science Connections series showcases the value of CAS databases in light of important general-interest, science, and technology news and highlights CAS database enhancements and editorial milestones.

From CAS - Science Connections articles, you can link directly to Substance Details and Reference Details in the web version of SciFinder.

To read the latest article on *Charles Darwin and radiometric*

Free Thinking, Search & Play !!



License Agreement~



Welcome Coach Hsu | [Sign Out](#)

License Agreement

As a SciFinder Authorized User, I acknowledge the following:

I have been assigned a unique loginid/password and will not share my loginid/password with any other person.

I will search only for myself and not for others or other organizations.

I will not use any automated program or script for extracting and downloading CAS data, or any other systematic retrieval of data.

I may retain **a maximum of 5,000 Records at any given time** for personal use or to share within a Project team for the duration of the Project.

My company's SciFinder License and the [CAS Information Use Policies](#) apply to my use of SciFinder.

I will contact my SciFinder Key Contact if I have any questions.

Learn more about SFoW online !

 https://cas.csod.com/lms/catalog/main_o.aspx?tab_page_id=-67

~FREE~

每月皆有線上課程可供讀者自行上網登記參與。



CAS | **Learning Solutions**
CAS is a division of the American Chemical Society

Home Learning Login Create Account

Welcome to your resource center for CAS learning events and materials.
If you have a CAS Learning Solutions account, click Login below. If you don't, click Cre

LOGIN

CREATE ACCOUNT

CALENDAR

SEARCH TRAINING

Learn more about SFoW online !



<http://www.igrouptaiwan.com/online/CAS/SciFinder%20Web/>

Index of /online/CAS/SciFinder Web

<u>Name</u>	<u>Last modified</u>	<u>Size</u>	<u>Description</u>
Parent Directory		-	
系統公告/	07-Dec-2010 15:26	-	
Advanced Training/	29-Nov-2010 15:29	-	
Basic Training/	29-Nov-2010 09:37	-	
How To Use SFoW/	26-Nov-2010 14:03	-	
SFoW中文使用說明/	26-Nov-2010 13:51	-	
Tutorial (Eng.)/	29-Oct-2009 10:06	-	

Apache/2.2.10 (Fedora) Server at www.igrouptaiwan.com Port 80

~FREE~

CAS台灣代表自行建立之相關檔案，供台灣研究人員使用!!

What can we do when access is slowed?

- Double check the connection to SFoW server:

Hostname: scifinder.cas.org

- Update the version of Browser and JAVA
- Turn off unused program or Web page
- Alternative browser, ex. [FireFox](#), [Safari](#)

What do we do for customers in Taiwan?

- Training, including Basic and Advance.
- OSS, On-Site Service.
- Consultant, ex. Case study, products and information service.
- Event hosting and invitation.
- Others.



追隨？不如領導！

Leader! or Follower?

美國化學文摘社(CAS)-台灣代表

CAS: www.cas.org 、 TW: www.igrouptaiwan.com

Contact us if you need further information ~

鄭淮辰 許傳奇 蘇甯棻 趙婉婷

Tel : (02) 2707 6611# 221, 226~228

Fax : (02) 2705 0482

email : cas.tw@igrouptaiwan.com

