

SciFinder 的學習心得與使用成果

前言：

其實當初為了決定作業的主題我猶豫了很久，直到看到這一篇新聞。國貿系的學生都能自學製毒，但反省自己，藥學系讀到大三連簡單的 Amphetamine 都不會合成，更別提 Morphine、Heroin。看到老師上課示範使用 SciFinder 幾個很強大的功能，所以想要用 SciFinder 寫一個屬於自己 Amphetamine 的反應？

大學生曠課忙製毒 寫毒製程只花2分鐘

自由時報 自由時報 - 2011年11月22日 下午12:49

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大學生曠課忙製毒 寫毒製程只花2分鐘

【自由時報記者沈繼昌、陳怡靜／楊梅報導】大學生缺錢，網路學製毒賺外快！2分鐘內流利寫下製毒過程，承辦警員大嘆，腦筋雖好卻用在不正當的地方。

台北海洋技術學院國貿系三年級學生潘奕誠，夥同同齡友人余晨愷租屋製毒，歷經多次試驗失敗，最近終於製成500公克安毒，黑市價格近百萬元，準備販售時被查獲。

沒有前科的21歲潘嫌，坦承缺錢製毒，以前在綽號「小李」男子那兒看過製毒過程，認為並不難，與余嫌一拍即合。

警方在桃園縣楊梅市中山南路某12樓出租公寓內，逮捕2人，並起出瓦斯爐、氨水、鹽酸、活性炭、感冒藥、攪拌器等大批製毒工具與原料，安毒成品500公克、半成品18公克。

警方說，2人在「小李」介紹下租屋居住，潘嫌從網路與相關書籍獲得製毒方法，記錄成筆記後，2人花費20萬元購買製毒工具，今年8月間嘗試製毒，期間多次因比例、步驟不對，安毒無法結晶，製毒過程產生惡臭，2人還買香薰以香水噴霧降低異味。

新聞報導：大學生製毒「還沒賣就被捕」上網學技術花20萬租屋買機具
蘋果日報 - 2011年11月22日 上午11:53

新聞報導：大學生製毒！還沒賣 就被逮了
東森新聞 - 2011年11月22日 上午11:17

新聞報導：大學生製毒 出貨前被逮
自由時報 - 2011年11月22日 上午4:31

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顯示更多

STEP1: 總之既然明確知道要搜索以知物質，當然最先使用 **Explore Substance**。

SciFinder - Explore Substances - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

Welcome SYANGTYAN HUANG | Sign Out

Add KMP Alert Substance Identifier "Amphetamine" > substances (0)

Explore Substances

Chemical Structure
Markush
Molecular Formula
Substance Identifier

Substance Identifier(s) Amphetamine Search

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

Saved Answer Sets
Morphine006-1
Morphine005
Morphine004
Morphine003
morphine001
morphine 000
morphine00
heroin 00
Autosaved Reaction Set
View All
Import

Keep Me Posted Results
No profiles exist

STEP2: 其實 SciFinder 的資料庫很強大，但是每次使用資料庫，每家業者都喜歡自己編號，如同 SciFinder 自己有一個 CAS Registry Number，有時查詢未知的 Substances 只會出現 CAS Registry Number 和結構，結構類似的會讓人困惑。

SciFinder®

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Substance Identifier "Amphetamine" > substances (1) > 300-62-9

Substance Detail

CAS Registry Number: 300-62-9

C₉H₁₃N

Benzeethanamine, α-methyl-

Benzeethanamine, α-methyl-, (±)-; Phenethylamine, α-methyl-, (±)- (8CI); (±)-1-Phenyl-2-aminopropane; (±)-Desoxynorephedrine; (±)-Phenylisopropylamine; (±)-α-Methylphenethylamine; (±)-α-Methylphenylethylamine; (±)-β-Phenylisopropylamine; 1-Benzylethylamine; 1-Methyl-2-phenylethylamine; 1-Phenyl-2-aminopropane; 1-Phenyl-2-propanamine; 1-Phenyl-2-propylamine; 2-Amino-1-phenylpropane; 3-Phenyl-2-propylamine; Actedron; Adderall; Adderall XR; Adipam; Alodene; Amfetamine; Amphetamine; Anorexine; Benzebar; Benzedrine; Benzolone; Desoxynorephedrine; Elastonin; Fenopromin; Finam; Isomayne; Isomyn; Mecodrin; NSC 22159; Norephedrine; Norydrine; Obesin; Obesine; Oktedrin; Ortedrine; Percomon; Phenamine; Phenedrine; Profamina; Propisamine; Racemic Amphetamine; Raphetamine; Rhinalator; SLI 381; Simpatedrin; Simpatina; Sympamine; Sympatedrine; Weckamine; dl-α-Methylphenethylamine; α-Methyl-β-phenylethylamine; α-Methylbenzeethanamine; α-Methylphenethylamine; α-Methylphenylethylamine; β-Aminopropylbenzene; β-Phenylisopropylamine

Deleted CAS Registry Numbers: 60-15-1;17108-96-2;96332-84-2

STEP3: 下圖應該就是我最想用的功能之一了。我就是用 **Synthesize this...** 的功能從產物去逆推整個反應式。

SciFinder®

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Substance Identifier "Amphetamine" > substances (1) > 300-62-9

Substances

1 Substance 0 Selected

Select All Deselect All Sort by: CAS Registry Number

1. Substance Detail 300-62-9

CAS Registry Number: 300-62-9

Me-CH(NH₂)-CH₂-Ph

C₉H₁₃N

Benzeethanamine, α-methyl-

~10,904 References

Reactions

Commercial Sources

Regulatory Information

Link

Tools

Synthesize this...

View Substance Detail

Explore by Structure

Get Reactions where Substance is a

Get Commercial Sources

Get Regulatory Information

Get References

Export as Image

Send to SciPlanner

Analysis

Analyze by:

Substance Role

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

Analytical Study

Biological Study

Combinatorial Study

Formation, Nonpreparative

Miscellaneous

Occurrence

Preparation

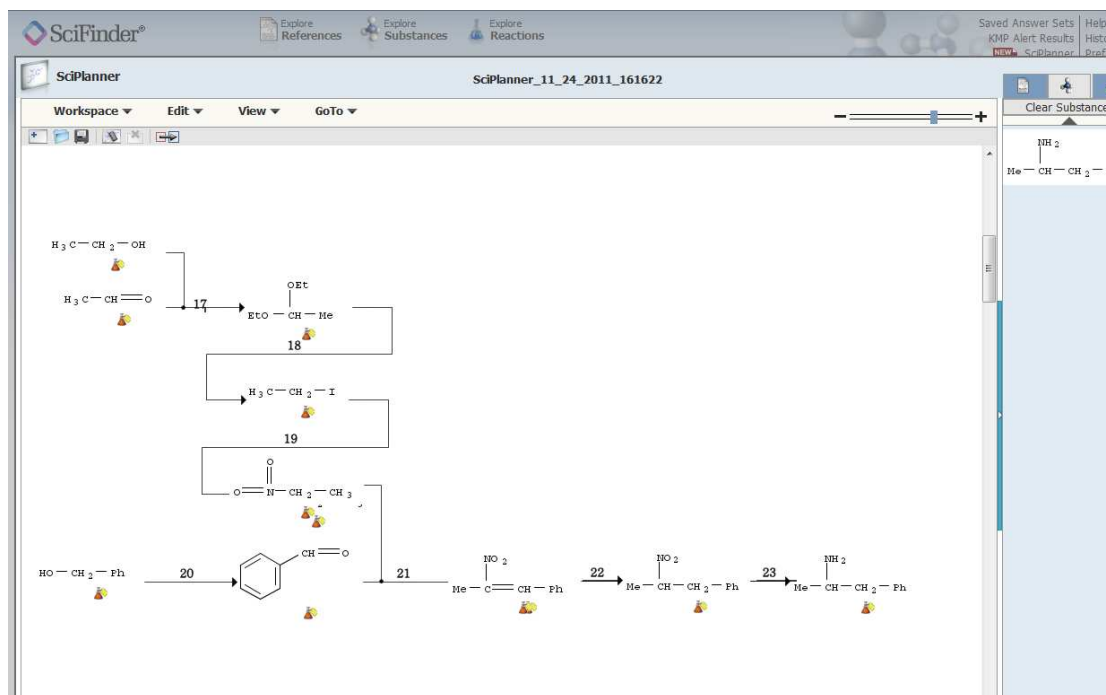
Process

Properties

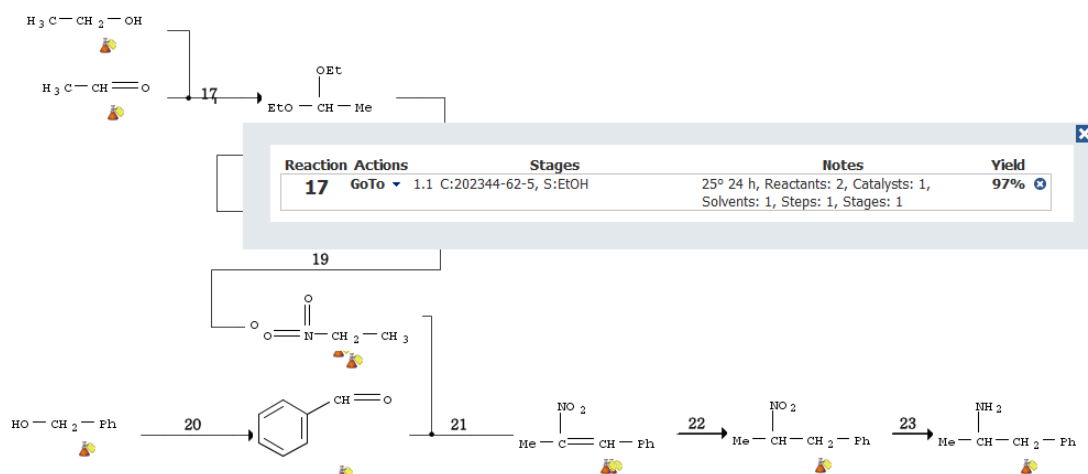
Prophetic in Patents

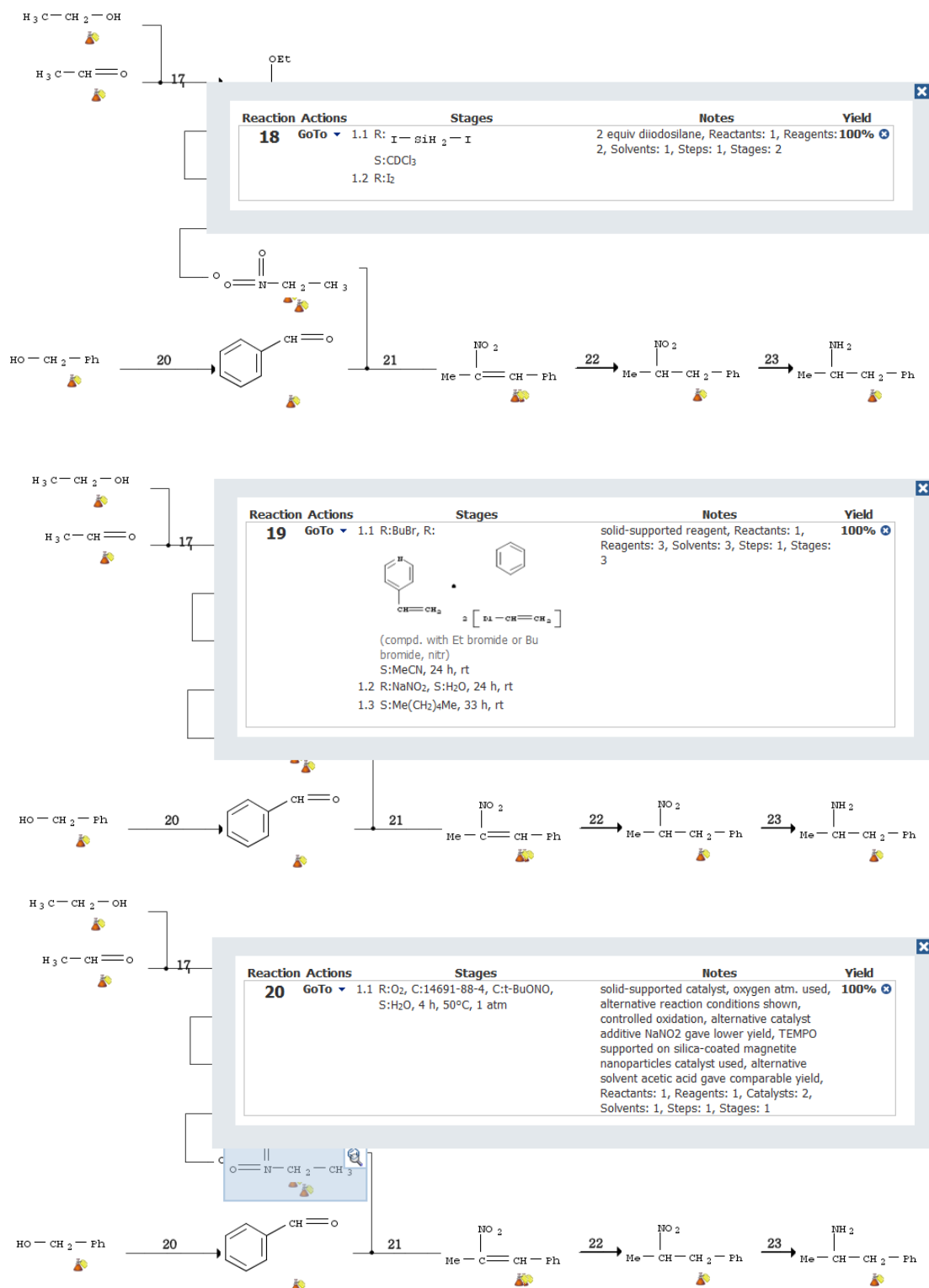
Show More

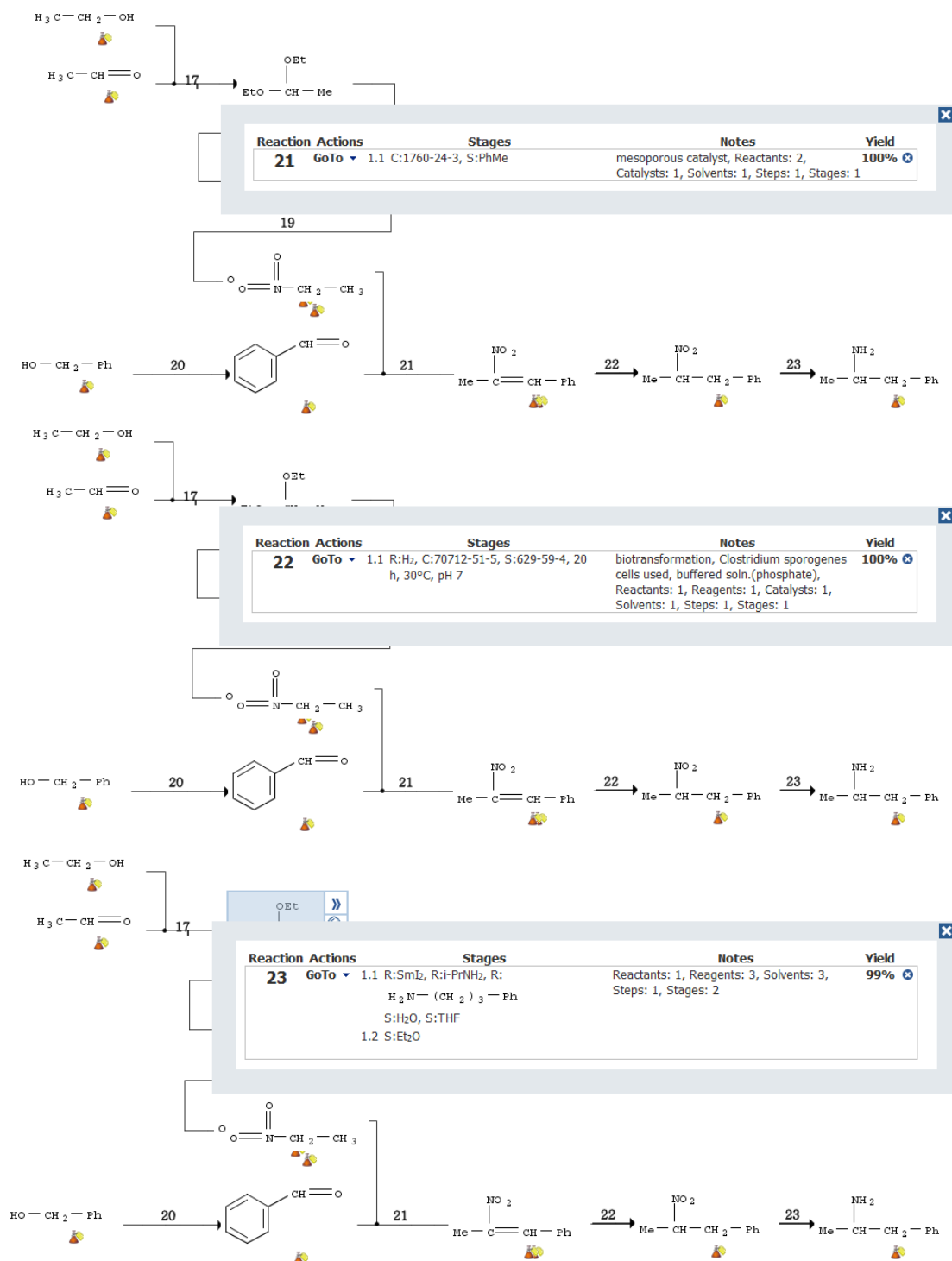
STEP4: 下圖就是我逆推至我認為所能達到最簡單的反應物，用 SciPlanner 畫出屬於我自己的 Amphetamine 合成圖，雖然合成 Amphetamine 不是只有一種方法，但是在 SciFinder 所列出，我所列的這條公式有基本標準是產物產率高達 97% 以上。當然，因為我是以想知道「最簡單反應物」為出發點，所以中間所需製備手續十分複雜，而中間產物在市面上也不是買不到，所以一般人應該不會選擇這麼迂迴的做法吧。



STEP5: 其實 SciFinder 和一般資料庫操作方式我個人覺得挺麻煩的，例如不能開多視窗這一點，常常查到一個反應中有兩個未知物質，就非得先查完其中一個才能再查下一個。不過 SciPlanner 很棒的是不論產物、反應物或是反應方法都能直接按圖片右上角直接就能查，而且反應步驟的出處文獻只要按反應物到產物箭頭上的數字，SciFinder 就會告訴你。

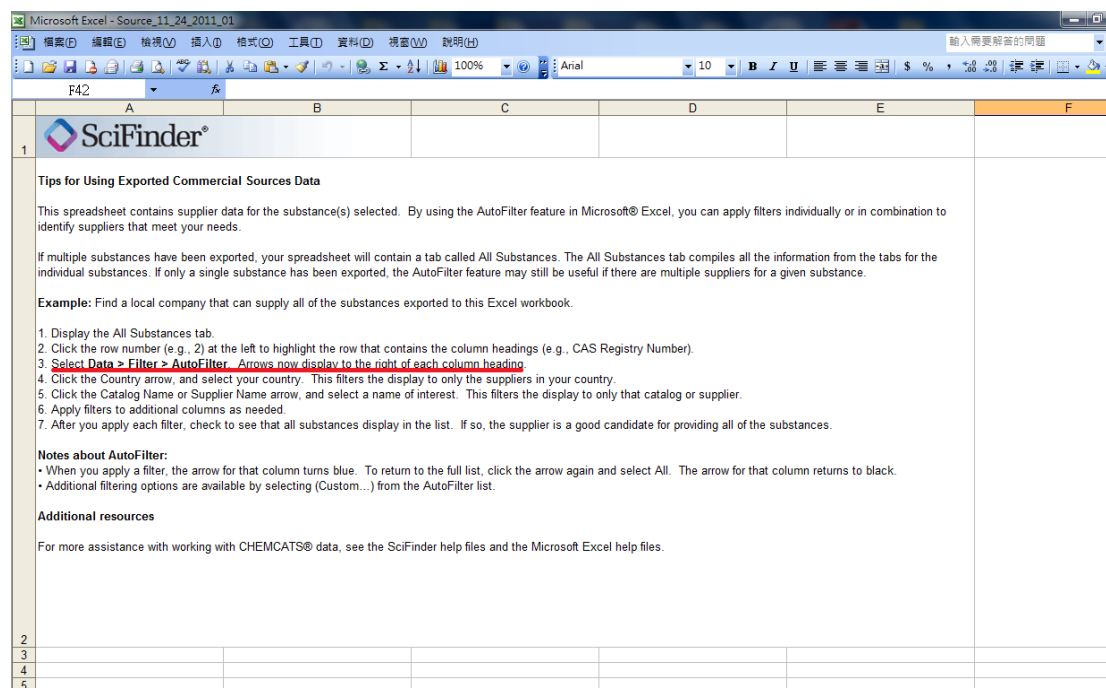






STEP6:知道反應式後如果只是呆呆坐著等可還適合成不了 Amphetamine 的，所以另一 SciFinder 我最喜歡的功能就是它會告訴你所需的原料應該要去哪裡買。只要直接按圖片右上角的 **Commercial Sources** 直接就能查到，而且還可以下載程不同的格式 **Export** 出來，以查資料來說我個人是喜歡存成 Excel。打開存檔的第一頁就是下圖，SciFinder 還會很貼心的告訴你要怎麼「快速的找到適合的供應商」，簡單來說就是使用 Excel 的篩選功能，

多設幾個篩選條件就可以找到最符合需求的供應商了。



Microsoft Excel - Source_11_24_2011_01

SciFinder®

Tips for Using Exported Commercial Sources Data

This spreadsheet contains supplier data for the substance(s) selected. By using the AutoFilter feature in Microsoft® Excel, you can apply filters individually or in combination to identify suppliers that meet your needs.

If multiple substances have been exported, your spreadsheet will contain a tab called All Substances. The All Substances tab compiles all the information from the tabs for the individual substances. If only a single substance has been exported, the AutoFilter feature may still be useful if there are multiple suppliers for a given substance.

Example: Find a local company that can supply all of the substances exported to this Excel workbook.

1. Display the All Substances tab.
2. Click the row number (e.g., 2) at the left to highlight the row that contains the column headings (e.g., CAS Registry Number).
3. Select **Data > Filter > AutoFilter**. Arrows now display to the right of each column heading.
4. Click the Country arrow, and select your country. This filters the display to only the suppliers in your country.
5. Click the Catalog Name or Supplier Name arrow, and select a name of interest. This filters the display to only that catalog or supplier.
6. Apply filters to additional columns as needed.
7. After you apply each filter, check to see that all substances display in the list. If so, the supplier is a good candidate for providing all of the substances.

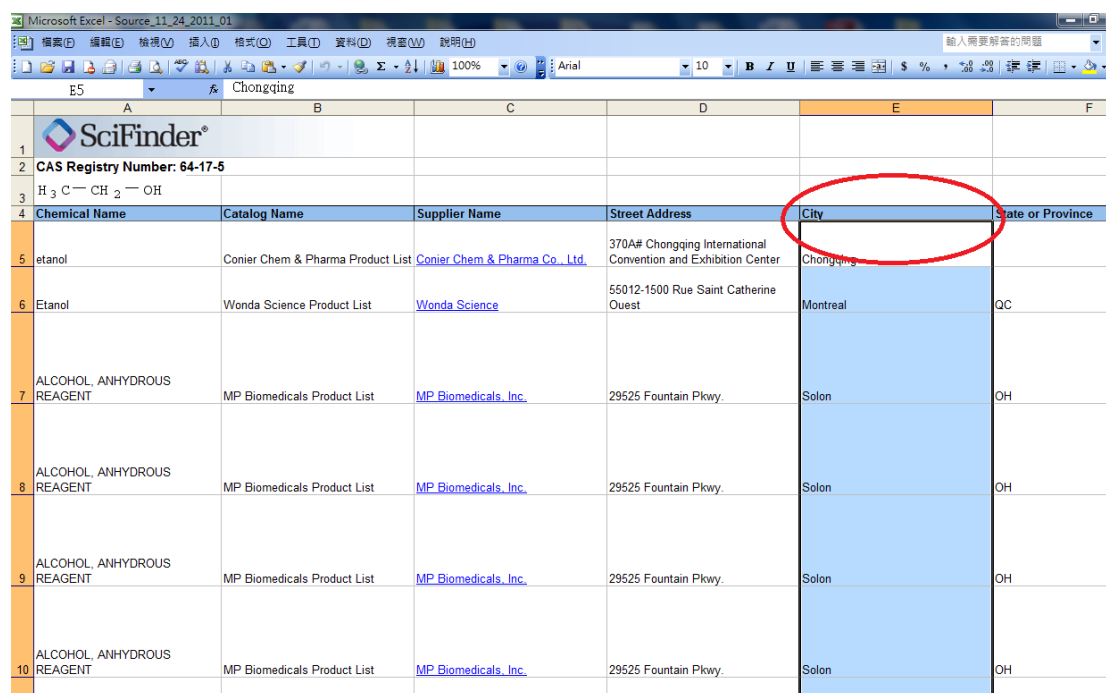
Notes about AutoFilter:

- When you apply a filter, the arrow for that column turns blue. To return to the full list, click the arrow again and select All. The arrow for that column returns to black.
- Additional filtering options are available by selecting (Custom...) from the AutoFilter list.

Additional resources

For more assistance with working with CHEMCATS® data, see the SciFinder help files and the Microsoft Excel help files.

STEP7: 像我 Amphetamine 合成方程式中其中一個最初產物是 Ethanol，所以我想找的是「在台灣 Ethanol 的供應商」，只要點 Excel 的資料→篩選→自動篩選→Taiwan 就能找到。



Microsoft Excel - Source_11_24_2011_01

SciFinder®

CAS Registry Number: 64-17-5

CCO

Chemical Name	Catalog Name	Supplier Name	Street Address	City	State or Province
ethanol	Conier Chem & Pharma Product List	Conier Chem & Pharma Co., Ltd.	370A# Chongqing International Convention and Exhibition Center	Chongqing	
Ethanol	Wonda Science Product List	Wonda Science	55012-1500 Rue Saint Catherine Ouest	Montreal	QC
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH

Microsoft Excel - Source_11_24_2011_01

檔案(F) 編輯(E) 檢視(V) 插入(I) 格式(O) 工具(T) 資料(D) 視窗(W) 說明(H)

SciFinder®

CAS Registry Number: 64-17-5

CCO

Chemical Name	Catalog Name	Supplier Name	Street Address	City	State or Province
etanol	Conier Chem & Pharma	Conier Chem & Pharma Co., Ltd.	370A# Chongqing International Convention and Exhibition Center	Chongqing	
Etanol	Wonda Science Product List	Wonda Science	55012-1500 Rue Saint Catherine Ouest	Montreal	QC
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH

Microsoft Excel - Source_11_24_2011_01

檔案(F) 編輯(E) 檢視(V) 插入(I) 格式(O) 工具(T) 資料(D) 視窗(W) 說明(H)

SciFinder®

CAS Registry Number: 64-17-5

CCO

Chemical Name	Catalog Name	Supplier Name	Street Address	City	State or Province
etanol	Conier Chem & Pharma Product List	Conier Chem & Pharma Co., Ltd.	370A# Chongqing International Convention and Exhibition Center	Chongqing	
Etanol	Wonda Science Product List	Wonda Science	55012-1500 Rue Saint Catherine Ouest	Montreal	QC
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH
ALCOHOL, ANHYDROUS REAGENT	MP Biomedicals Product List	MP Biomedicals, Inc.	29525 Fountain Pkwy.	Solon	OH

Microsoft Excel - Source_11_24_2011_01

檔案(F) 編輯(E) 檢視(V) 插入(I) 格式(O) 工具(T) 資料(D) 視窗(W) 說明(H)

輸入需要解答的問題

10 Arial

Chongqing

	A	B	C	D	E	F
1						
2	CAS Registry Number: 64-17-5					
3	$\text{H}_3\text{C}-\text{CH}_2-\text{OH}$					
4	Chemical Name	Catalog Name	Supplier Name	Street Address	City	State or Province
5	etanol	Conier Chem & Pharma Product List	Conier Chem & Pharma Co., Ltd.	370A# Chongqing International Convention and Exhibition Center	Chongqing	
	Ethanol, anhydrous, denatured, HPLC Grade, 90%, packaged under Argon in resealable ChemSeal t bottles	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
428	Ethanol, denatured, Spectrophotometric Grade, 90%, packaged under Argon in resealable ChemSeal t bottles	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
443	Ethanol, denatured, Spectrophotometric Grade, 90%, packaged under Argon in resealable ChemSeal t bottles	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
458	Ethanol, anhydrous, denatured, 85.8%, 13.3% methanol, 0.9%	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
473	MIBK	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
488	Ethanol, anhydrous, denatured, 85.8%, 13.3% methanol, 0.9%	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
503	MIBK	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
518	Ethanol, anhydrous, denatured, 85.8%, 13.3% methanol, 0.9%	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
533	Ethanol, Alcohol Reagent, anhydrous, denatured, ACS, 94-96%	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	
	Ethanol, Alcohol Reagent, anhydrous, denatured, ACS, 94-96%	Alfa Aesar	Alfa Aesar A Johnson Matthey Company	9F-3, No. 51, Keelung Road Section 2	Taipei	

最後:其實當初聽完 SciFinder 的說明，實在是讓我很驚艷。因為有了 SciFinder 你想要合成什麼東西幾乎都可以找到要怎麼做，而且又不像 innovation 很多功能都不能用、操作又麻煩，SciFinder 對於藥學系的學生真的是一個很實用、功能強大的資料庫呢!能在大學時就接觸到 SciFinder 真的是十分幸運呢。