New Drug Development

(新藥研發)

SciFinder®

CAS Patent Forum

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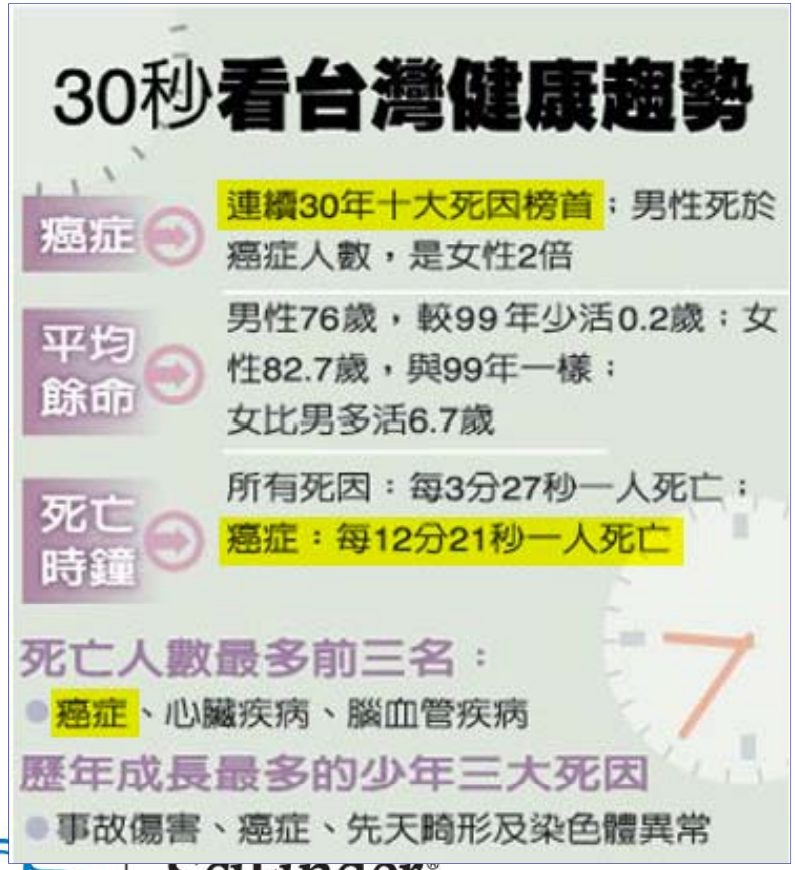
衛生署每年公布國人十大死因，其中惡性腫瘤(俗稱癌症)，連續30年蟬聯十大死因之首，罹癌發作年紀也逐漸降低當中，顯見癌症對國人健康的威脅正逐漸擴大當中。

研發抗癌新藥刻不容緩，如何利用SciFinder加速研發時程呢?



研發－乃最關鍵、最具決定性的步驟

新藥開發過程

* https://scifinder.cas.org

How SciFinder work on it ?

1. 研發

尋找合適的研發項目、文獻檢索與專利追蹤。

2. 臨床前

製備技術、不同劑型、藥物穩定性、藥理學。

3. 臨床

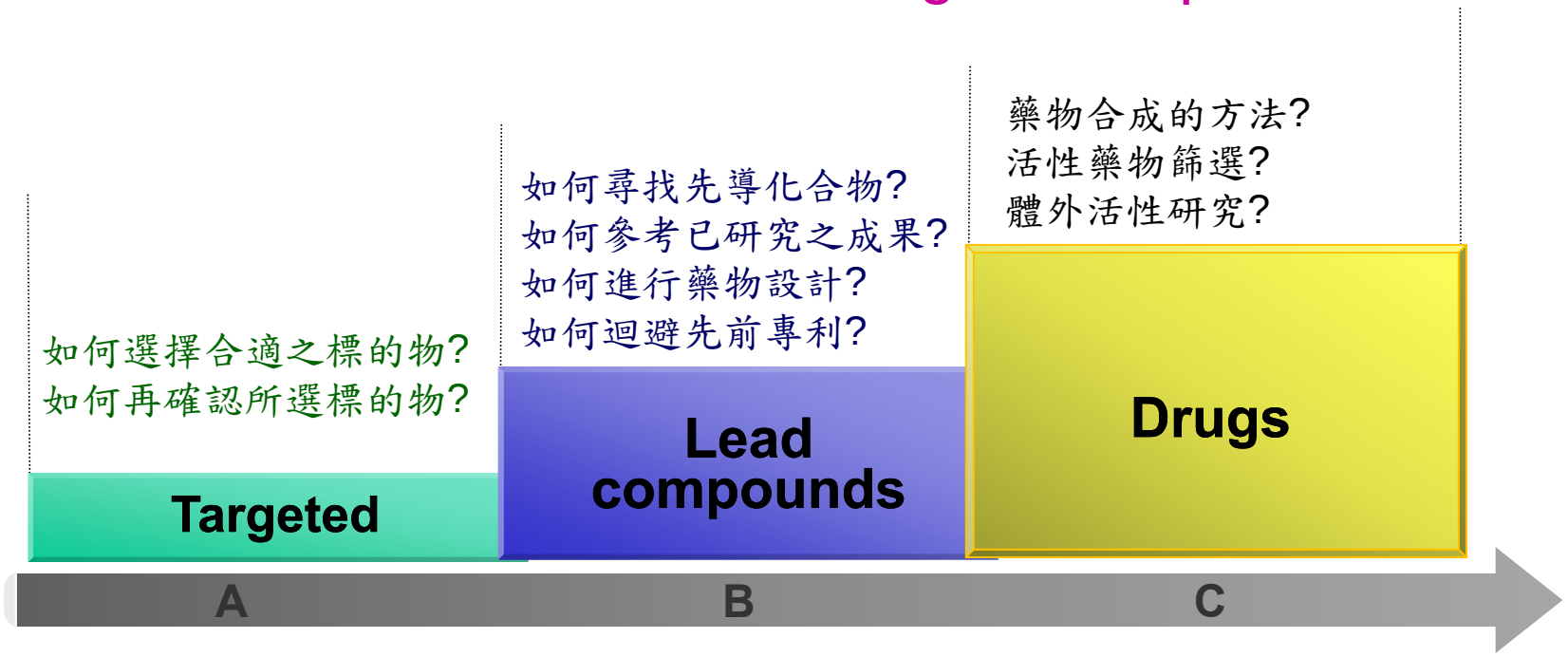
臨床試驗、生物有效性實驗。

4. 上市

不良反應監測。

SciFinder

~Total Solution of New Drug Development~



標的物選擇–
需閱讀大量文獻加以佐證

SciFinder 收錄最豐富之文獻資料，再加上強大的分析功能，省時又省力！

先導化合物的設計&合成

SciFinder可直接串聯物質與合成反應式，並可以**Markush** 結構檢索，進行專利布局與攻防。

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如何選擇合適之標的物?

一疾病之標的物預測與分析系統

儀器、設備等需投入大量資金

針對標的物進行 Random Screening

活性化合物

利用文獻篩選出某些候選標的物

SciFinder®

研究、評估候選標的物 + 文獻佐證

SciFinder®

活性化合物

“抗癌中藥~現代醫學好幫手”

手術、化療、放療是現代醫學治療惡性腫瘤的三大要法，各有所長。中醫辨證論治，綜合患者全身整體表現來分析考量，立方遣藥，而非只侷限於腫瘤，整體觀念較強，可彌補現代醫學的不足。中藥治癌有以下特點：

✓ 1、可以彌補手術治療、放射治療、化學治療的不足：
手術固然能切除腫瘤，但還有殘癌、或區域淋巴轉移等，運用中藥術後長期治療，可以防止復發和轉移。

✓ 2、減輕放、化療對消化道和造血系統之副作用；另，對於癌症末期患者或不能手術和放、化療的病人，中藥治療提供另一救命途徑。

✓ 3、不影響勞動力：癌症患者局部狀況好轉的同時，全身狀況也會改善，甚至能勝任日常的工作。

✓ 4、副作用小：沒有骨髓抑制方面的副作用，對消化道也不會有嚴重的影響。

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本文以中草藥作為抗癌藥物為例，探討：

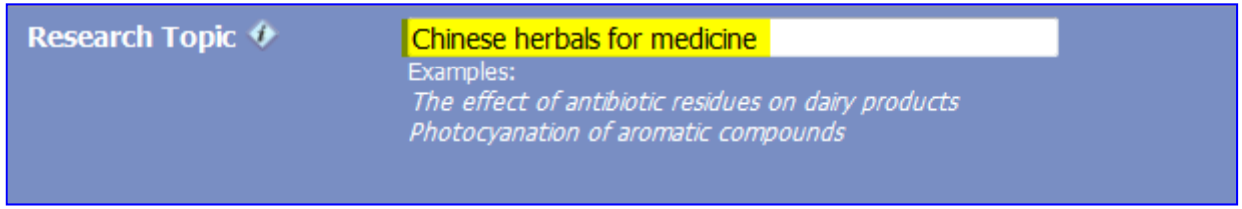
- 所有研發相關文獻。
- 研發情形綜覽。
- 研發標的物搜尋、評估。
- 標的物之物理、化學性質與相關資訊。
- 先導化合物(Lead Compound) 之優化。
- 先導化合物(Lead Compound) 之自行進行藥物設計。
- **Markush** 結構檢索~進行專利布局與迴避設計。
- 黃芩(Baicalein)之最佳合成方式。

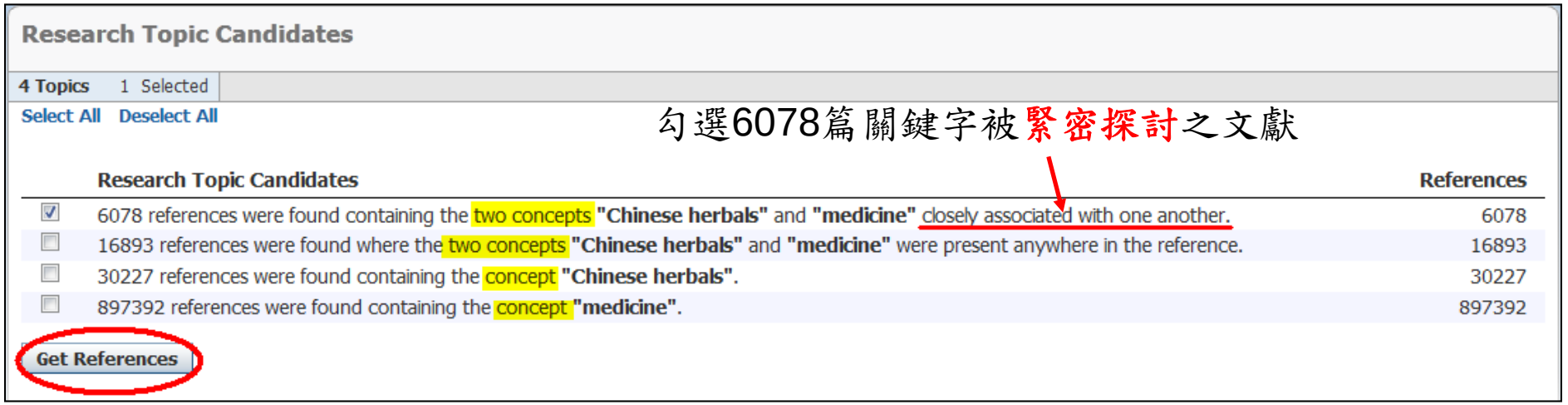
以中草藥作為抗癌藥物之

~所有研發相關文獻~

以中草藥(Chinese herbals for medicine)為主題進行文獻檢索

~ SciFinder幫助使用者獲得最全面、最相關之文獻訊息~



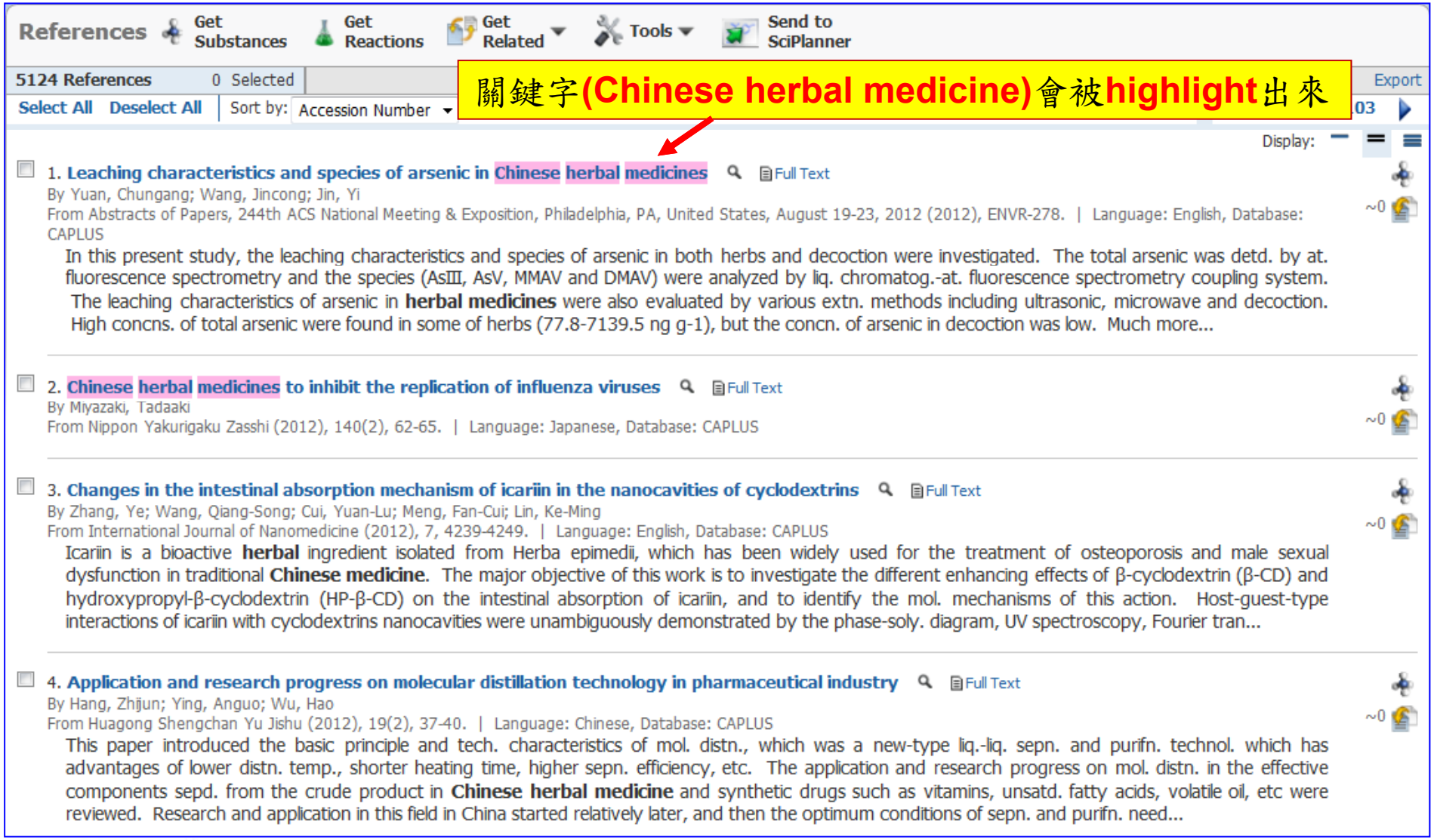


1.最全面：“concept” (概念式比對字詞)

=> SciFinder會同時檢索關鍵字詞之同義字、單複數變化等

2.最相關：“closely associated with one another”

=>表示此二關鍵字詞在文章中是被” 緊密探討” (彼此間隔很近)


References
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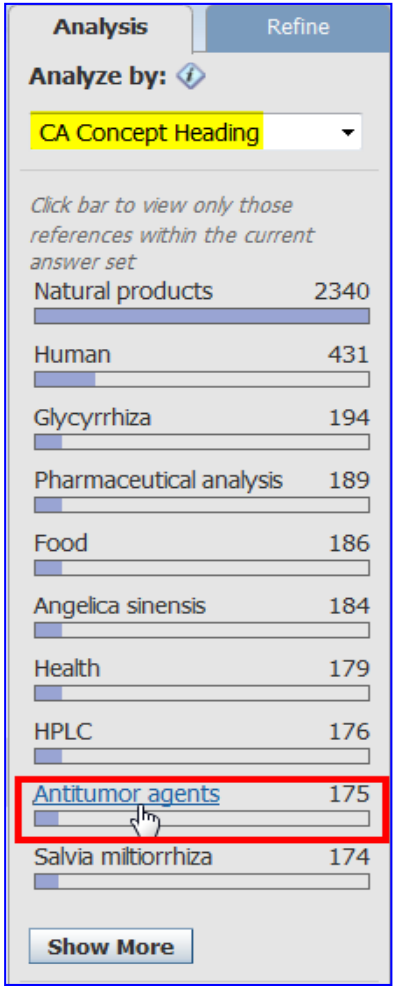
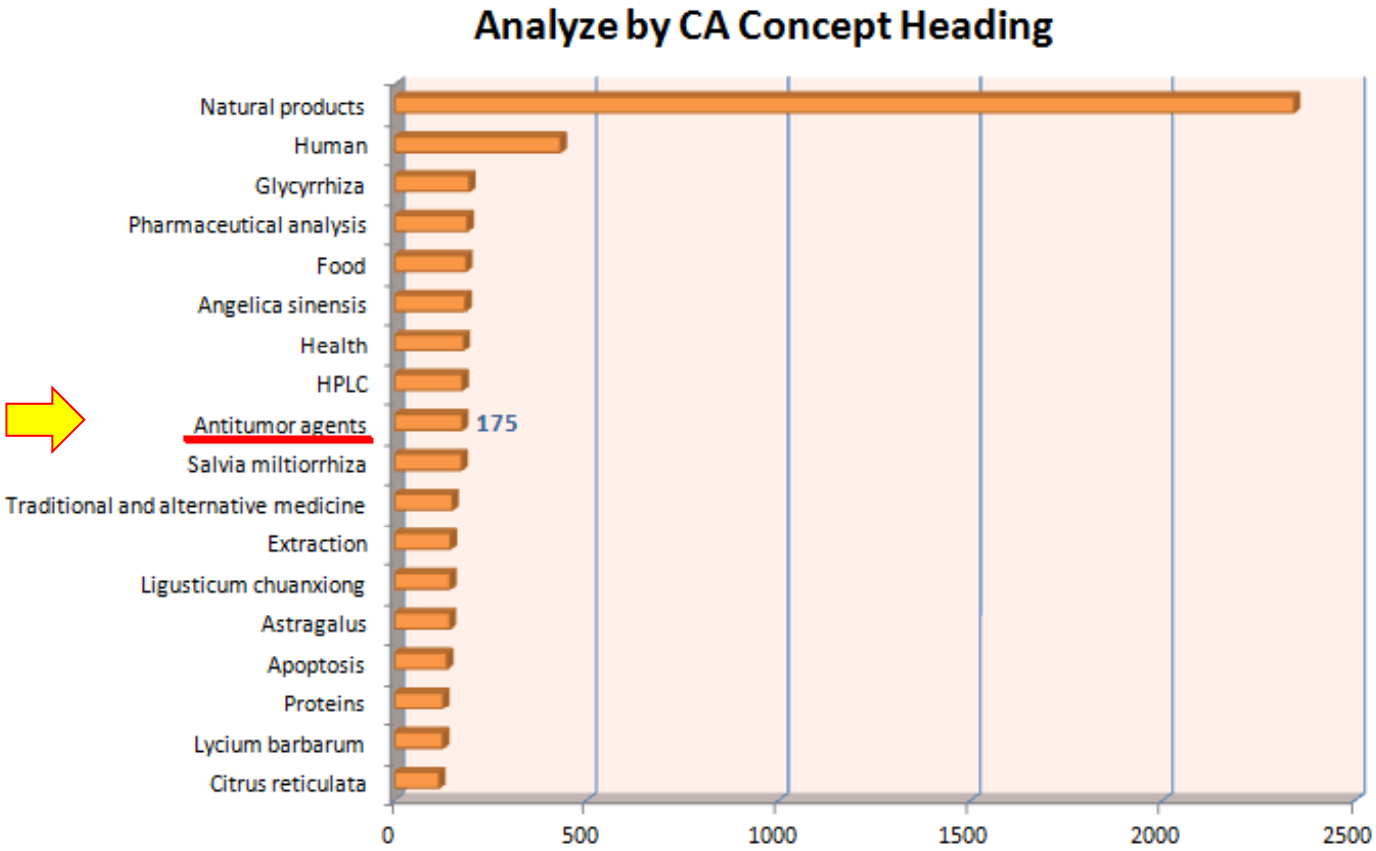
Get Reactions
Get Related
Tools
Send to SciPlanner
5124 References
0 Selected
Export
Select All
Deselect All
Sort by:
Accession Number
關鍵字(Chinese herbal medicine)會被highlight出來
Display:
1. Leaching characteristics and species of arsenic in Chinese herbal medicines
Full Text
By Yuan, Chungang; Wang, Jincong; Jin, Yi
From Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), ENVR-278. | Language: English, Database: CAPLUS
In this present study, the leaching characteristics and species of arsenic in both herbs and decoction were investigated. The total arsenic was detd. by at. fluorescence spectrometry and the species (AsIII, AsV, MMAV and DMAV) were analyzed by liq. chromatog.-at. fluorescence spectrometry coupling system. The leaching characteristics of arsenic in herbal medicines were also evaluated by various extn. methods including ultrasonic, microwave and decoction. High concns. of total arsenic were found in some of herbs (77.8-7139.5 ng g-1), but the concn. of arsenic in decoction was low. Much more...
2. Chinese herbal medicines to inhibit the replication of influenza viruses
Full Text
By Miyazaki, Tadaaki
From Nippon Yakurigaku Zasshi (2012), 140(2), 62-65. | Language: Japanese, Database: CAPLUS
3. Changes in the intestinal absorption mechanism of icariin in the nanocavities of cyclodextrins
Full Text
By Zhang, Ye; Wang, Qiang-Song; Cui, Yuan-Lu; Meng, Fan-Cui; Lin, Ke-Ming
From International Journal of Nanomedicine (2012), 7, 4239-4249. | Language: English, Database: CAPLUS
Icariin is a bioactive herbal ingredient isolated from Herba epimedii, which has been widely used for the treatment of osteoporosis and male sexual dysfunction in traditional Chinese medicine. The major objective of this work is to investigate the different enhancing effects of β-cyclodextrin (β-CD) and hydroxypropyl-β-cyclodextrin (HP-β-CD) on the intestinal absorption of icariin, and to identify the mol. mechanisms of this action. Host-guest-type interactions of icariin with cyclodextrins nanocavities were unambiguously demonstrated by the phase-soly. diagram, UV spectroscopy, Fourier tran...
4. Application and research progress on molecular distillation technology in pharmaceutical industry
Full Text
By Hang, Zhijun; Ying, Anguo; Wu, Hao
From Huagong Shengchan Yu Jishu (2012), 19(2), 37-40. | Language: Chinese, Database: CAPLUS
This paper introduced the basic principle and tech. characteristics of mol. distn., which was a new-type liq.-liq. sepn. and purifn. technol. which has advantages of lower distn. temp., shorter heating time, higher sepn. efficiency, etc. The application and research progress on mol. distn. in the effective components sepd. from the crude product in Chinese herbal medicine and synthetic drugs such as vitamins, unsatd. fatty acids, volatile oil, etc were reviewed. Research and application in this field in China started relatively later, and then the optimum conditions of sepn. and purifn. need...

分析文獻的研究領域(CA Concept Heading)，找"對"研發方向

~ SciFinder 可分析出所有的研發領域，並佐以文獻，幫助使用者取得最完整之資料~



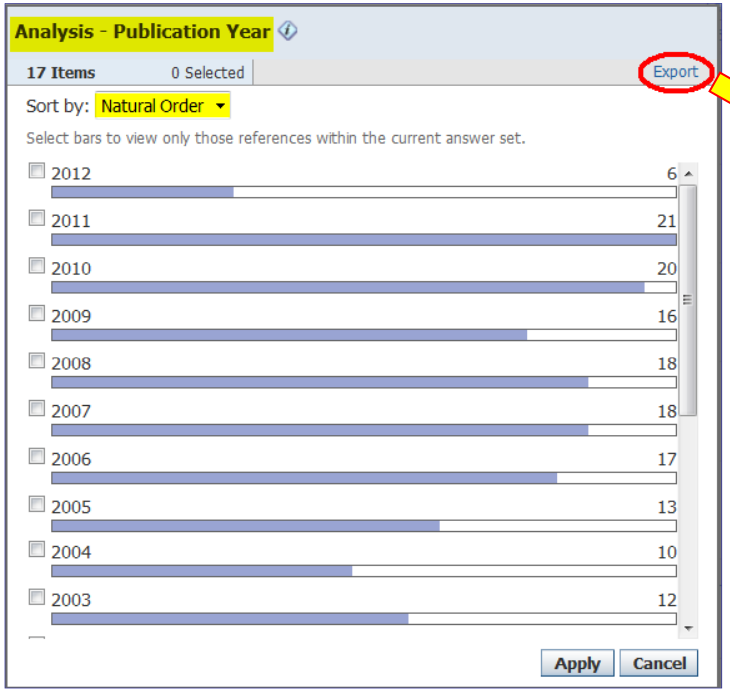


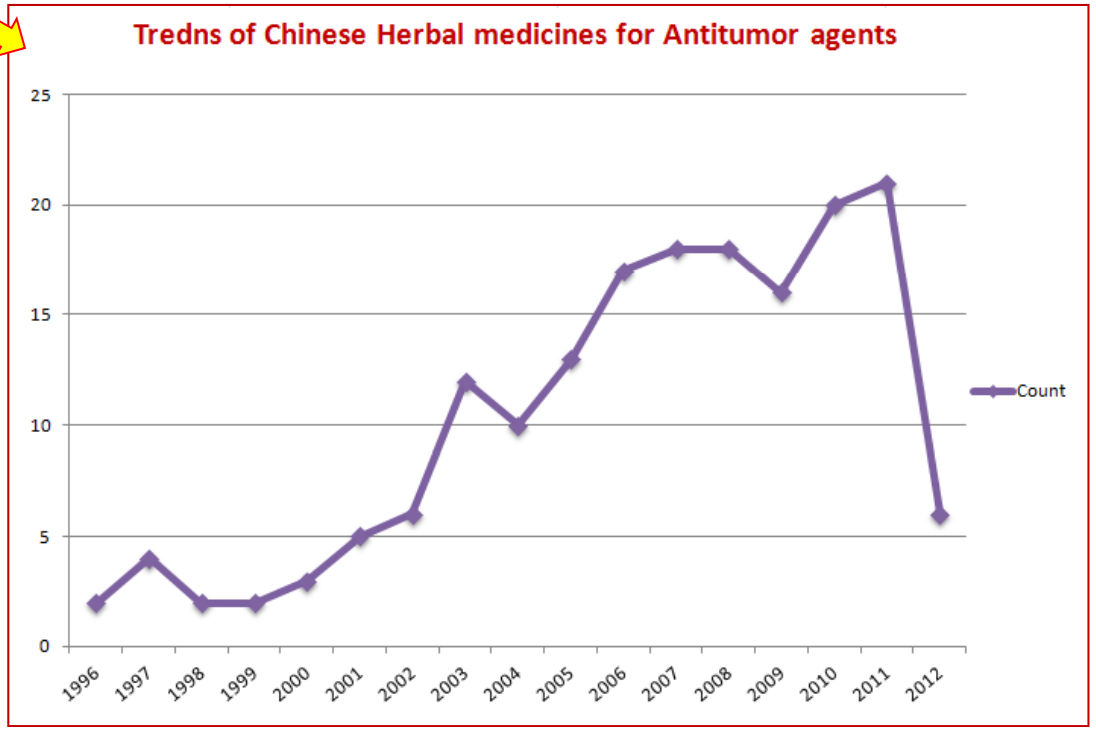
以中草藥作為抗癌藥物之

~研發情形綜覽~

以中草藥作為抗癌藥物：近20年的研究走勢圖

~ 以2010-2011研究能量最高 ~





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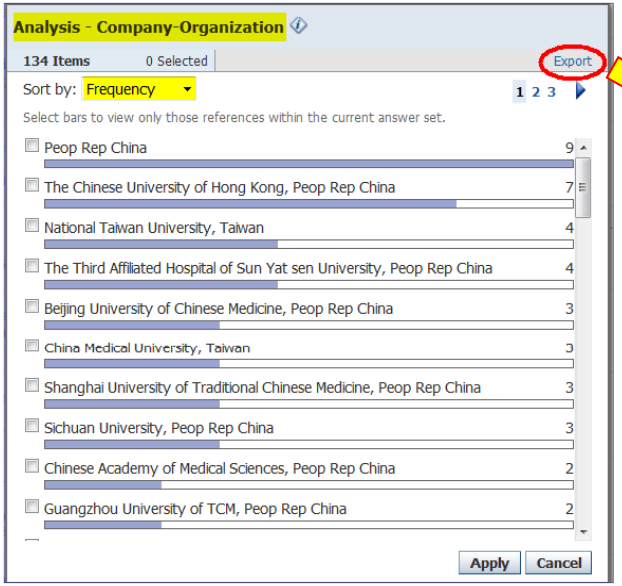
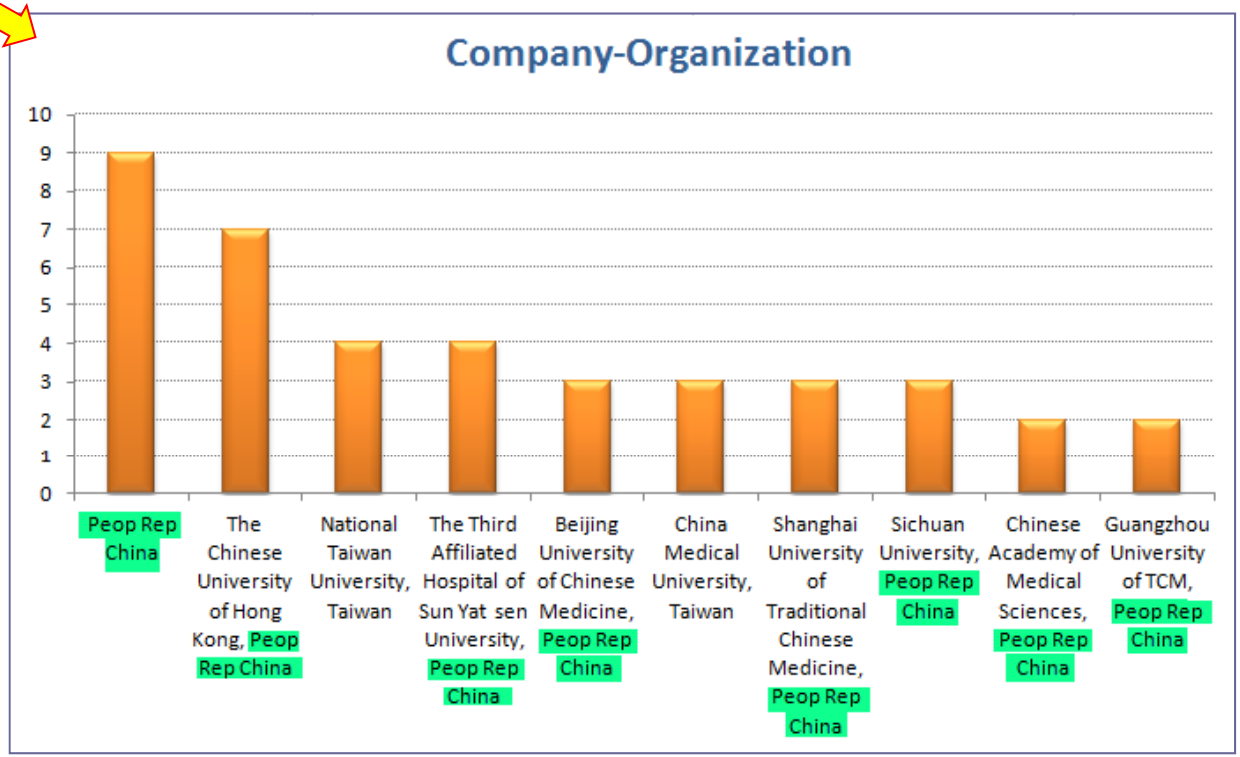
主要的研究公司/機構柱狀圖：追蹤競爭者或尋找合作夥伴

~ 主要研究機構以中國(Peop Rep China) 最多 ~





中國 (Peop Rep China) 在以中草藥作為抗癌藥物之研究領域(CA Concept Heading)分析

~ 針對Reop Rep China： 分析其歷年的文獻研究分布情形，尋找研發可切入的方向~

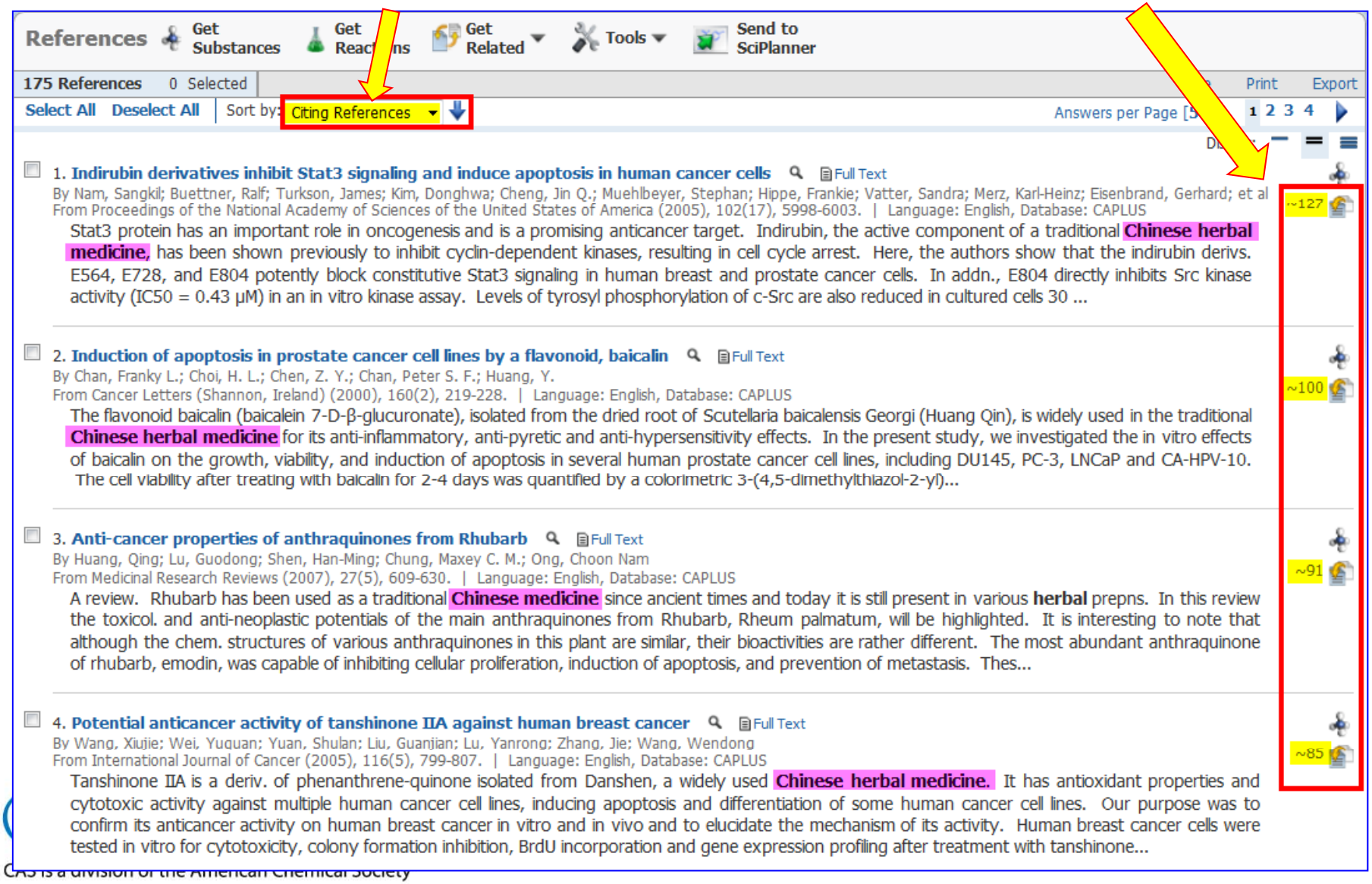
CA Concept Heading	2012	2011	2010	2009	2008
Antitumor agents	4	18	10	15	12
Natural products		11	7	10	7
Cell proliferation	2				
Human		9	7	11	6
Cytokines	2				
Apoptosis		8	2	7	2
Kidney	2				
Signal transduction			4		
Cell proliferation		4			
Traditional & alternative medicine			3		
Proliferation inhibition				4	
Adenocarcinoma	1				
Neoplasm				3	
Antioxidants		3			
Pharmaceutical injections					4
Androgen receptors	1				
Bax proteins		3		2	
Hepatocellular carcinoma				3	
Polysaccharides					3
Antibiotics	1				
Bcl-2 proteins		3		2	
Cell infiltration			2		
Alkaloids					2
Antiviral agents	1				

以中草藥作為抗癌藥物之

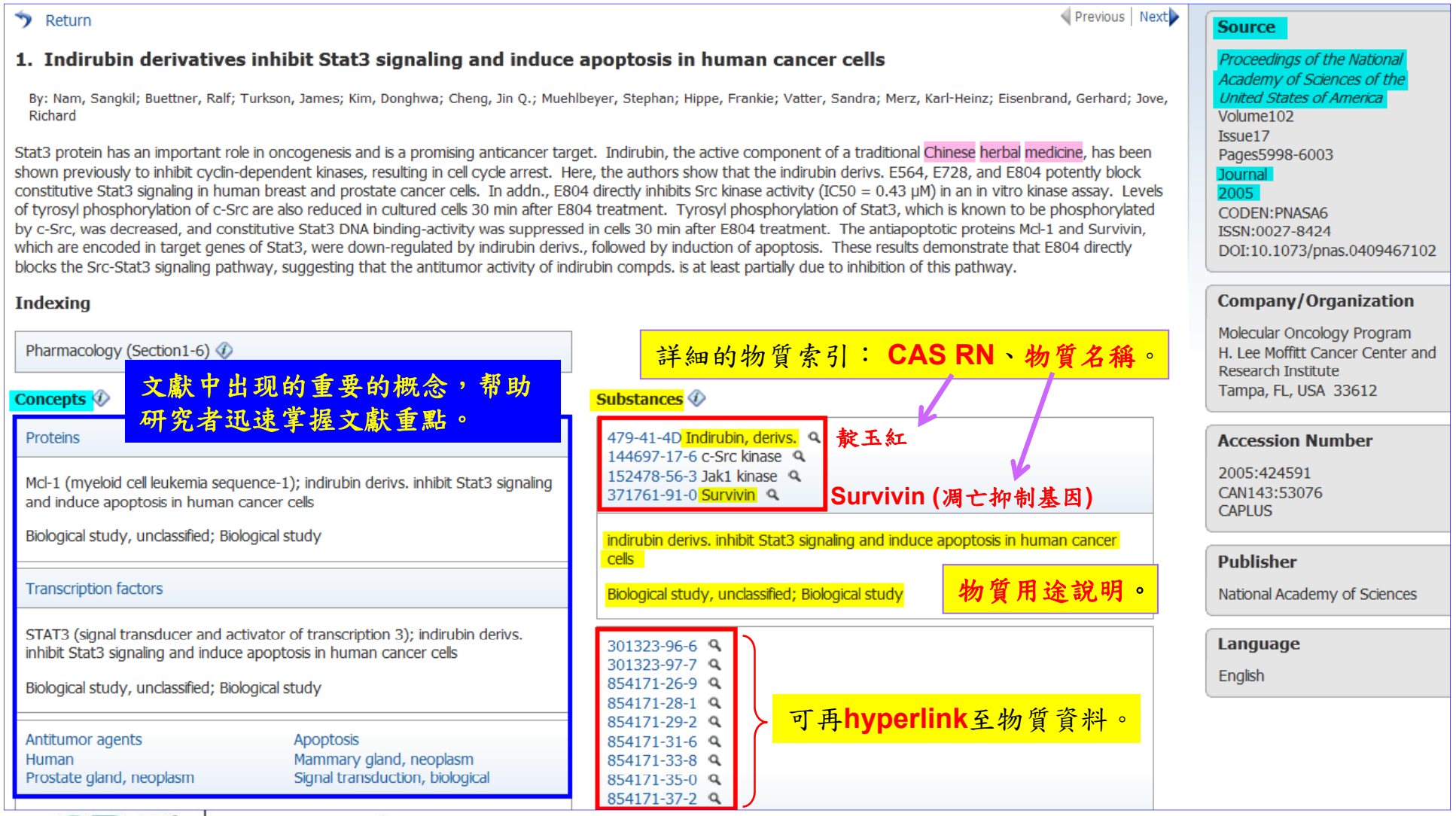
~研發標的物搜尋、 評估~

175篇以中草藥作為抗癌藥物(Antitumor agent)之核心文獻

~依被引用次數(Citing References)排序：直接找到最重要的文獻~



靛玉紅衍生物抑制 Stat 3 訊息傳導並誘發癌症細胞之凋亡



Return

Previous | Next

1. Indirubin derivatives inhibit Stat3 signaling and induce apoptosis in human cancer cells

By: Nam, Sangkil; Buettner, Ralf; Turkson, James; Kim, Donghwa; Cheng, Jin Q.; Muehlbeyer, Stephan; Hippe, Frankie; Vatter, Sandra; Merz, Karl-Heinz; Eisenbrand, Gerhard; Jove, Richard

Stat3 protein has an important role in oncogenesis and is a promising anticancer target. Indirubin, the active component of a traditional Chinese herbal medicine, has been shown previously to inhibit cyclin-dependent kinases, resulting in cell cycle arrest. Here, the authors show that the indirubin derivs. E564, E728, and E804 potently block constitutive Stat3 signaling in human breast and prostate cancer cells. In addn., E804 directly inhibits Src kinase activity (IC50 = 0.43 μM) in an in vitro kinase assay. Levels of tyrosyl phosphorylation of c-Src are also reduced in cultured cells 30 min after E804 treatment. Tyrosyl phosphorylation of Stat3, which is known to be phosphorylated by c-Src, was decreased, and constitutive Stat3 DNA binding-activity was suppressed in cells 30 min after E804 treatment. The antiapoptotic proteins Mcl-1 and Survivin, which are encoded in target genes of Stat3, were down-regulated by indirubin derivs., followed by induction of apoptosis. These results demonstrate that E804 directly blocks the Src-Stat3 signaling pathway, suggesting that the antitumor activity of indirubin compds. is at least partially due to inhibition of this pathway.

Indexing

Pharmacology (Section1-6)

文獻中出現的重要的概念，幫助研究者迅速掌握文獻重點。

Concepts

Proteins

Mcl-1 (myeloid cell leukemia sequence-1); indirubin derivs. inhibit Stat3 signaling and induce apoptosis in human cancer cells

Biological study, unclassified; Biological study

Transcription factors

STAT3 (signal transducer and activator of transcription 3); indirubin derivs. inhibit Stat3 signaling and induce apoptosis in human cancer cells

Biological study, unclassified; Biological study

Antitumor agents
Human
Prostate gland, neoplasm
Apoptosis
Mammary gland, neoplasm
Signal transduction, biological

詳細的物質索引： CAS RN、物質名稱。

Substances

479-41-4D Indirubin, derivs. 靛玉紅
144697-17-6 c-Src kinase
152478-56-3 Jak1 kinase
371761-91-0 Survivin Survivin (凋亡抑制基因)

indirubin derivs. inhibit Stat3 signaling and induce apoptosis in human cancer cells

Biological study, unclassified; Biological study

物質用途說明。

301323-96-6
301323-97-7
854171-26-9
854171-28-1
854171-29-2
854171-31-6
854171-33-8
854171-35-0
854171-37-2

可再hyperlink至物質資料。

Source

Proceedings of the National Academy of Sciences of the United States of America
Volume102
Issue17
Pages5998-6003
Journal
2005
CODEN:PNASA6
ISSN:0027-8424
DOI:10.1073/pnas.0409467102

Company/Organization

Molecular Oncology Program
H. Lee Moffitt Cancer Center and Research Institute
Tampa, FL, USA 33612

Accession Number

2005:424591
CAN143:53076
CAPLUS

Publisher

National Academy of Sciences

Language

English

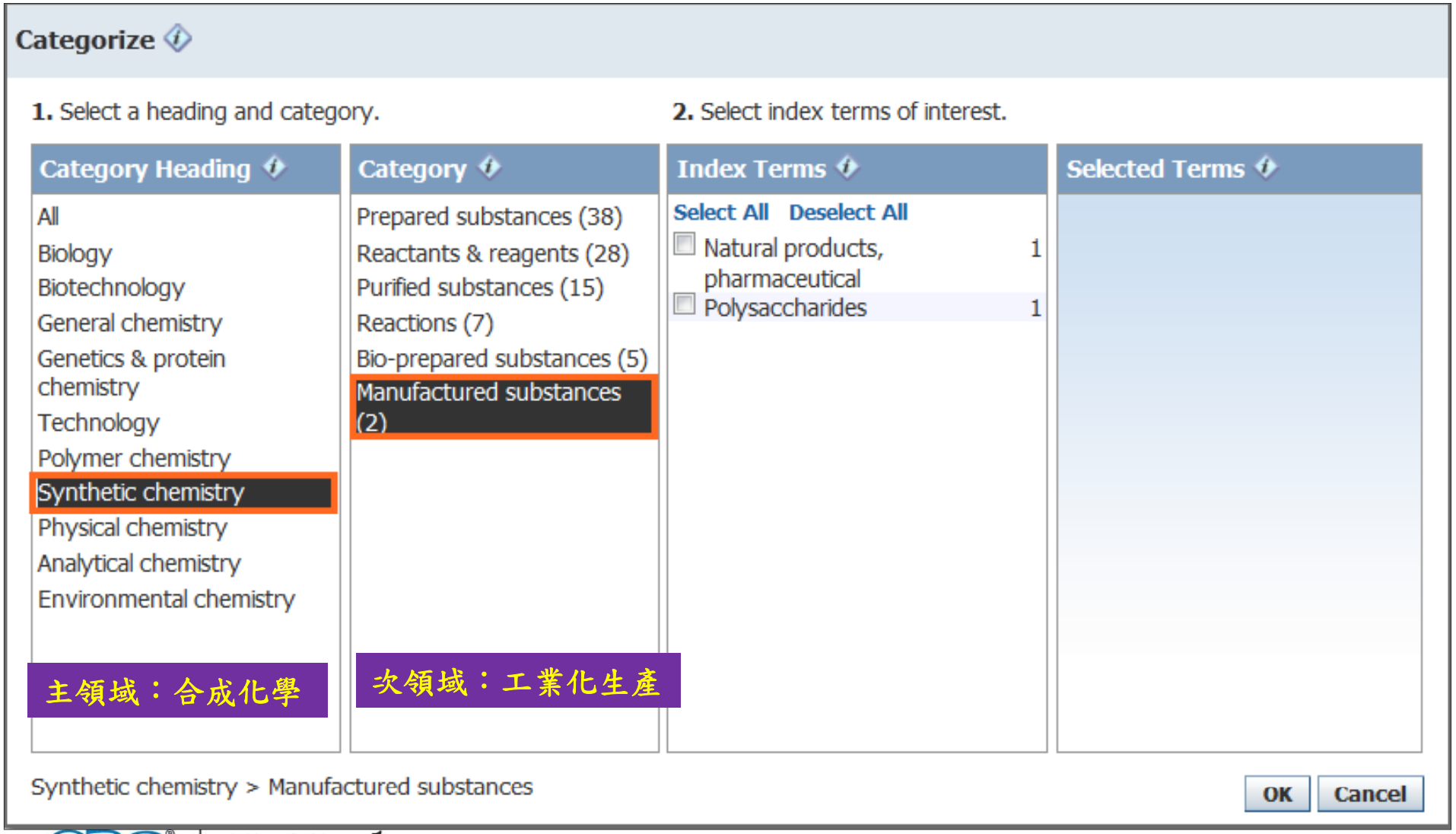
除了靛玉紅，

還有沒有其他標的物可選擇呢?

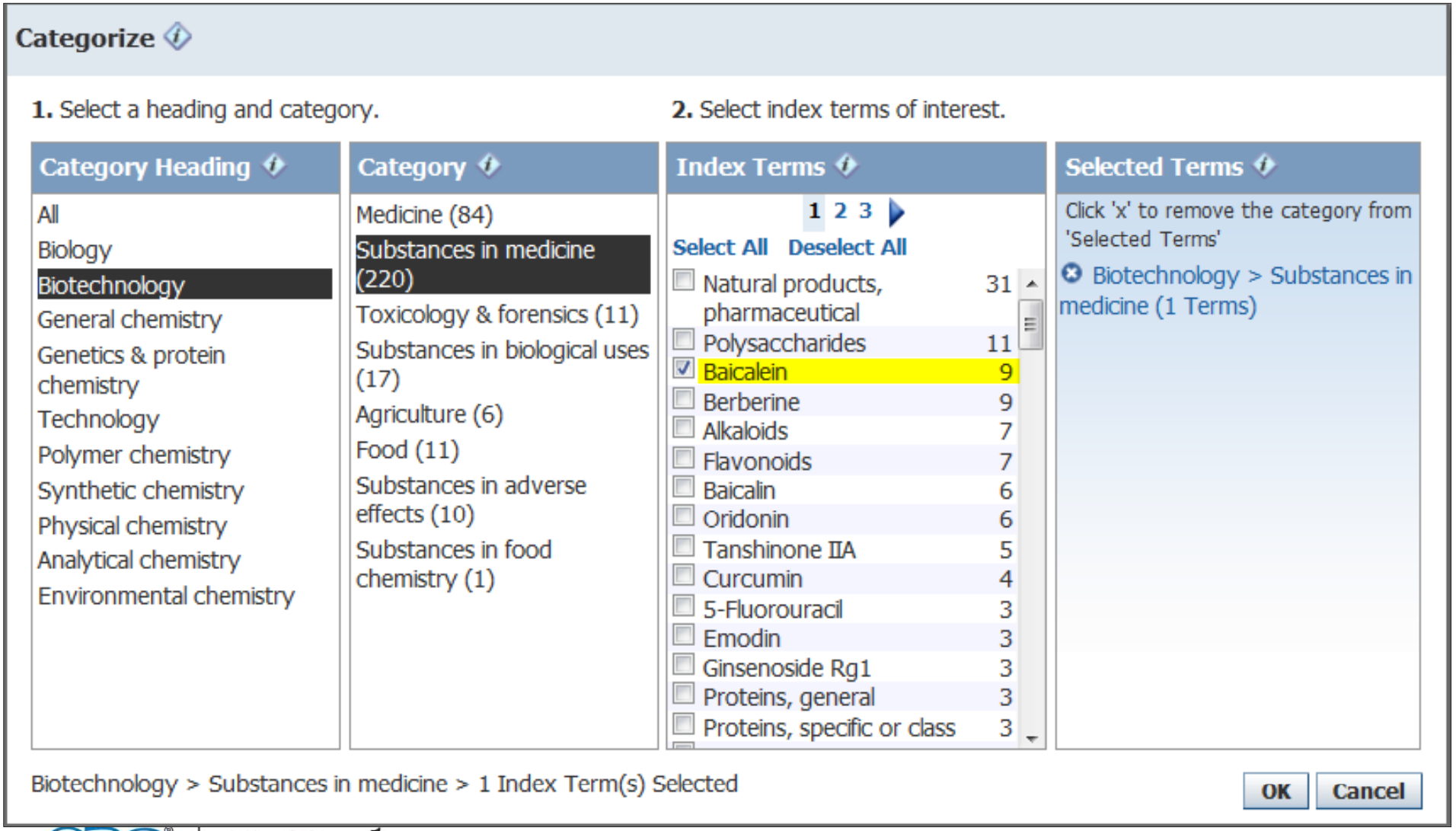
Categorize 功能：針對文獻細分為72個學科領域

~利用Categorize的三階層分類功能，可鉅細靡遺的進行篩選，精準挑選研發標的~

Categorize 功能：分析"可應用於工業生產的物質"



Categorize 功能：挑選"黃芩"作為研發標的



SCIFINDER

利用文獻"再次確認"以黃芩作為研發標的可行性

References | Get Substances | Get Reactions | Get Related | Tools | Send to SciPlanner

9 References | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Accession Number | Answers per Page [50]

Display:

1. **A phase I study of the Chinese herbal medicine PHY906 as a modulator of ironotecan-based chemotherapy in patients with advanced colorectal cancer** Full Text ~1

By Kummar, Shivaani; Gupu, M.; Sitki; Rose, Michal; Wadler, Scott; Stephenson, Joe; O'Rourke, Mark; Brenckman, Wayne; Tilton, Robert; Liu, Shuru Huey; Jiang, Zaoli; et al

From Clinical Colo

晚期大腸癌病人，利用 ironotecan 化療時，以中草藥PHY906作為一調控劑之 phase I 研究。

PHY906 is a [illegible] diarrhea, abdominal cramps, vomiting, fever, and headache. Preclin. and clin. studies were conducted to further investigate the biol. and clin. activities of this **herbal medicine**. To ensure standardization and maintain interbatch reliability of PHY906, high performance liq. chromatog. (HPLC) was used to establish a "chem. fingerprint" of PHY906. In vivo preclin. studies using the murine Colon 39 tumor model showed that PHY906 protected...

2. **Flavonoid baicalein suppresses adhesion, migration and invasion of MDA-MB-231 human breast cancer cells** Full Text ~15

By Wang, Ling; Ling, Yun; Chen, Yan; Li, Cheng-Ling; Feng, Feng; You, Qi-Dong; Lu, Na; Guo, Qing-Long

From Cancer Lett

類黃酮黃芩抑制 MDA-MB-231人類乳癌細胞之附著、移動與入侵。

Baicalein is a [illegible] and anti-cancer therapy. However, the mol. mechanism of its anti-cancer activity remains poorly understood and warrants further investigations. The purpose of this study is to verify the activity of baicalein to inhibit the invasion of MDA-MB-231 human breast cancer cells. The results indicated that baicalein suppressed MDA-MB-231 cell adhesion to fibronectin-coated substrate, wound healing migration and invasion through the Matrigel in a concn.-dependent manner. Western blot and gelatin...

3. **Baicalein, a flavonoid extracted from a methanolic extract of Oroxylum indicum inhibits proliferation of a cancer cell line in vitro via induction of apoptosis** Full Text ~11

By Roy, M. Kumar; Nakahara, K.; Thalang, V. Na; Trakoontivakorn, G.; Takenaka, M.; Isobe, S.; Tsushida, T.

From

黃芩，一取自Oroxylum indicum甲醇粹取物中提煉出的黃酮類化合物，經由誘導細胞凋亡抑制試管內癌細胞增生。

anti-hypersensitivity effects, inhibited in vitro proliferation of HL-60 cells. The flavonoid baicalein was found as an active component in the ext. Anal. of freeze-dried fruits of the plant indicated that this component comprised about 4% of the material by dry wt. In this study, we investigated the in vitro effects of baicalein on the viability and induction of apoptosis in the HL-60 cell line. The cell viability after treating with ...

4. **Role of Baicalein in the regulation of proliferation and apoptosis in human myeloma RPMI8226 cells** Full Text ~9

By Li, Qiu-bai; You, Yong; Chen, Zhi-chao; Lu, Jian; Shao, Jing; Zou, Ping

From C

黃芩在人類骨髓癌 RPMI8226 細胞株中，細胞增生與細胞凋亡的調控過程所扮演的角色。

Baic **Chinese herbal medicine**, which has been utilized in anti-inflammatory therapy. The effects of Baicalein on apoptosis and proliferation of myeloma cells and on the expression of 12-lipoxygenase (12-LOX) in these cells were detd. Baicalein inhibited proliferation and induced apoptosis of the human myeloma cell line RPMI8226 in a time- and dose-dependent manner and caused G0/G1-phase arrest, indicating that cell arrest is involved in inhibiting growth of myeloma cells....

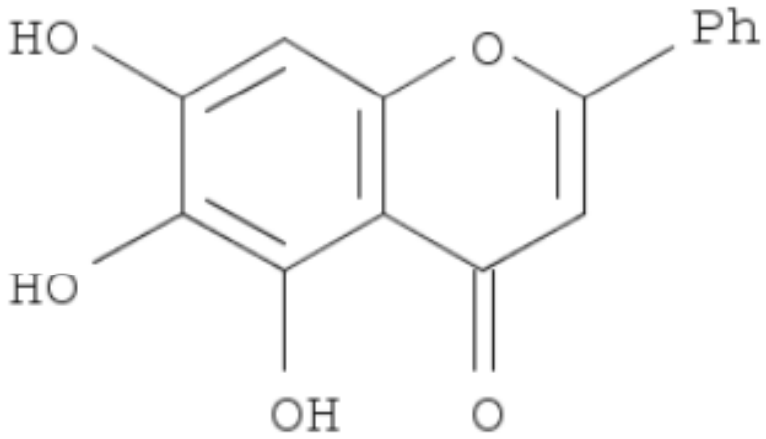
~探討標的物(黃芩)之物理、化學性質與相關資訊~

Get Substances：取得文獻中的相關物質

取得9篇黃芩(Baicalein)文獻中的相關物質

42. **Substance Detail**
491-67-8

Baicalein (黃芩)



~2039 References 相關文獻

Reactions 相關化學反應

Commercial Sources 全球供應商資料

C15 H10 O5

4*H*-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-

Spectra 光譜資料

Experimental Properties 實驗性數據

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Baicalein (黃芩)之詳細物質資訊

CAS 註冊碼

完整化學名稱（包含商品名、俗名）

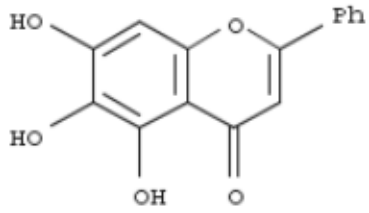
42.

CAS Registry Number: 491-67-8

$C_{15}H_{10}O_5$

4*H*-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-

Baicalein (6CI); Flavone, 5,6,7-trihydroxy- (7CI,8CI); 5,6,7-Trihydroxyflavone; Baikalein; NSC 661431; Noroxylin



化學結構式

~2,039 References

Document Types: Conference, Dissertation, Journal, Patent

CAS Role (物質角色)：
黃芩已被研究的文獻領域

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

▸ **Bioactivity Indicators** NEW

▸ **Target Indicators** NEW

SCIFINDER

詳細化學性質：預測性數據

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

Biological Properties	Value	Condition	Note	Top
Bioconcentration Factor	345	pH 1 Temp: 25 °C	(30)	
Bioconcentration Factor	342	pH 4 Temp: 25 °C	(30)	
Bioconcentration Factor	36.8	pH 7 Temp: 25 °C	(30)	
Bioconcentration Factor	1.0	pH 10 Temp: 25 °C	(30)	

Chemical Properties	Value	Condition	Note	Top
Koc	2280	pH 1 Temp: 25 °C	(30)	
Koc	1320	pH 6 Temp: 25 °C	(30)	
Koc	1.0	pH 9 Temp: 25 °C	(30)	
logD	3.64	pH 2 Temp: 25 °C	(30)	
logD	3.61	pH 5 Temp: 25 °C	(30)	
logD	-0.48	pH 10 Temp: 25 °C	(30)	
Mass Solubility	Sparingly Soluble (0.076 g/L)	pH 1 Temp: 25 °C	(30)	
Mass Solubility	Sparingly Soluble (0.076 g/L)	pH 4 Temp: 25 °C	(30)	
Mass Solubility	Sparingly Soluble (0.70 g/L)	pH 7 Temp: 25 °C	(30)	
Mass Solubility	Soluble (15 g/L)	pH 8 Temp: 25 °C	(30)	
Mass Solubility	Very Soluble (432 g/L)	pH 9 Temp: 25 °C	(30)	
Mass Solubility	Very Soluble (1000 g/L)	pH 10 Temp: 25 °C	(30)	
Molar Solubility	Sparingly Soluble (2.8E-4 mol/L)	pH 1 Temp: 25 °C	(30)	
Molar Solubility	Sparingly Soluble (2.8E-4 mol/L)	pH 4 Temp: 25 °C	(30)	
Molar Solubility	Sparingly Soluble (2.6E-3 mol/L)	pH 7 Temp: 25 °C	(30)	
Molar Solubility	Slightly Soluble (0.054 mol/L)	pH 8 Temp: 25 °C	(30)	
Molar Solubility	Very Soluble (1.60 mol/L)	pH 9 Temp: 25 °C	(30)	
Molar Solubility	Very Soluble (3.70 mol/L)	pH 10 Temp: 25 °C	(30)	
pKa	6.31±0.40	Most Acidic Temp: 25 °C	(30)	
Vapor Pressure	7.27E-14 Torr	Temp: 25 °C	(30)	

在鹼性條件下容易溶解

在鹼性條件下容易溶解

Density Properties	Value	Condition	Note	Top
Density	1.548±0.06 g/cm3	Temp: 20 °C Press: 760 Torr	(30)	
Molar Volume	174.5±3.0 cm3/mol	Temp: 20 °C Press: 760 Torr	(30)	

詳細化學性質：實驗性數據

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

Biological Properties	Value	Condition	Note	Top
ADME (Absorption, Distribution, Metabolism, Excretion)	See full text	1 of 2	(2)CAS	
Half-Life (Biological)	See full text		(8)CAS	
Minimum Inhibitory Concentration	See full text	1 of 2	(25)CAS	
NOAEL/LOAEL	See full text		(27)CAS	

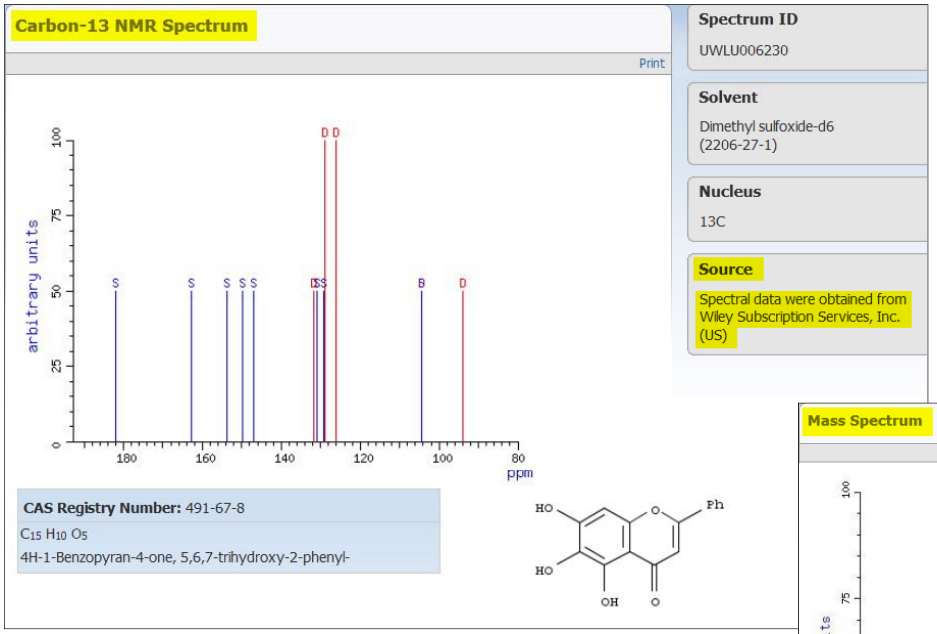
Chemical Properties	Value	Condition	Note	Top
Acid/Base Dissociation Constant (Ka/Kb)	See full text		(1)CAS	
logD	See full text		(11)CAS	
logP	See full text	1 of 2	(12)CAS	
Potential of Electrode Reaction	See full text		(28)CAS	

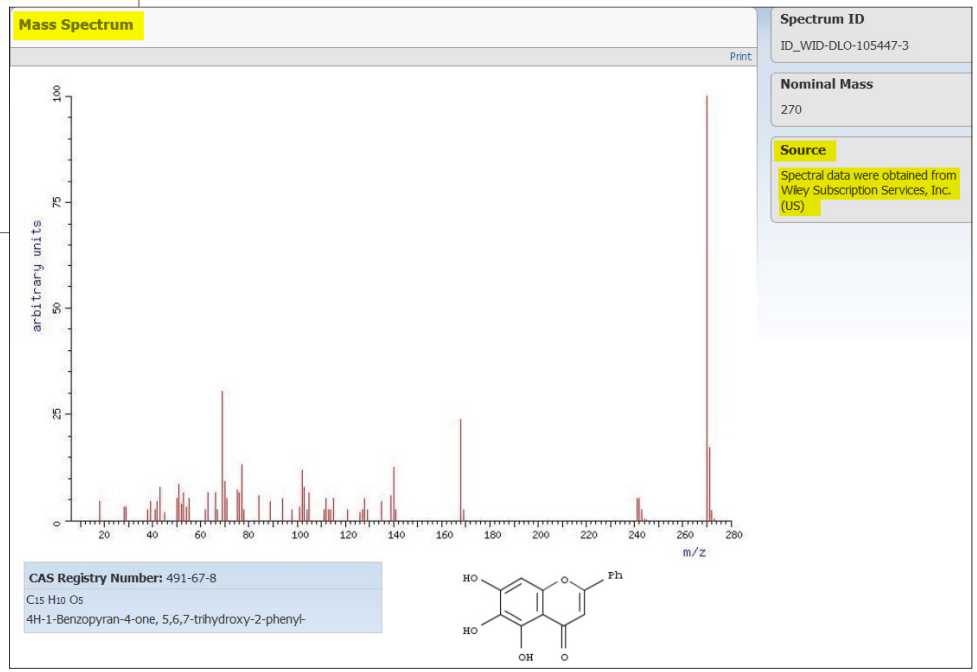
Lipinski and Related Properties	Value	Condition	Note	Top
logP	See full text	1 of 2	(12)CAS	

Spectra Properties	Value	Condition	Note	Top
Carbon-13 NMR Spectrum	See spectrum		(4)WSS	
Carbon-13 NMR Spectrum	See full text	1 of 6	(5)CAS	
Circular Dichroism Spectrum	See full text		(6)CAS	
IR Absorption Spectrum	See full text	1 of 5	(9)CAS	
IR Spectrum	See full text		(10)CAS	
Mass Spectrum	See spectrum		(4)WSS	
Mass Spectrum	See full text	1 of 23	(6)CAS	
Proton NMR Spectrum	See full text	1 of 11	(9)CAS	
Raman Spectrum	See full text		(29)CAS	
Two-Dimensional NMR Spectrum	See full text		(26)CAS	
UV and Visible Absorption Spectrum	See full text	1 of 14	(6)CAS	
UV and Visible Spectrum	See full text	1 of 3	(23)CAS	

Structure-related Properties	Value	Condition	Note	Top
Bond Length	See full text		(3)CAS	
Molecular Structure	See full text		(26)CAS	

各種光譜資料與來源





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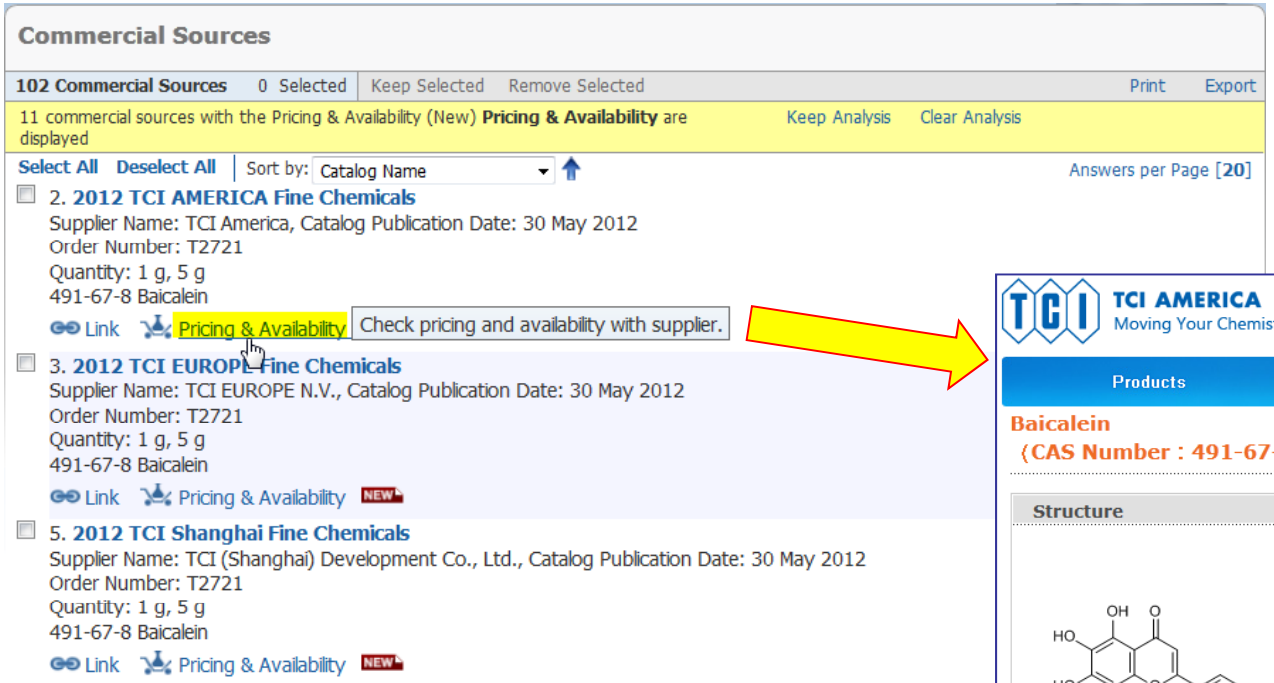
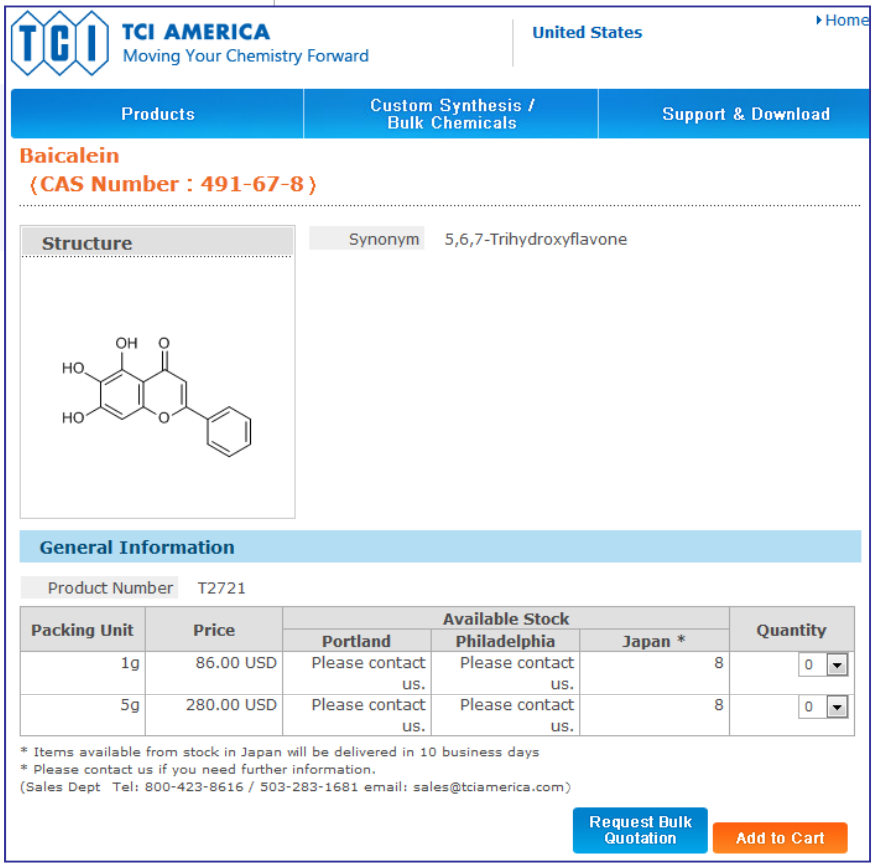
~Pricing & Availability ：可直接連結至供應商網頁，進行線上購物~





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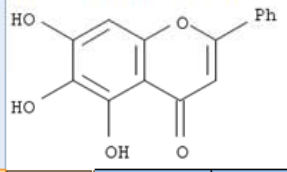
~Export 資料：直接取得包裝規格、報價與供應商資料、~

Microsoft Excel - Baicalein Commercial Source-11_08_24_2012_104052 [相容模式]

SciFinder®

CAS Registry Number:491-67-8

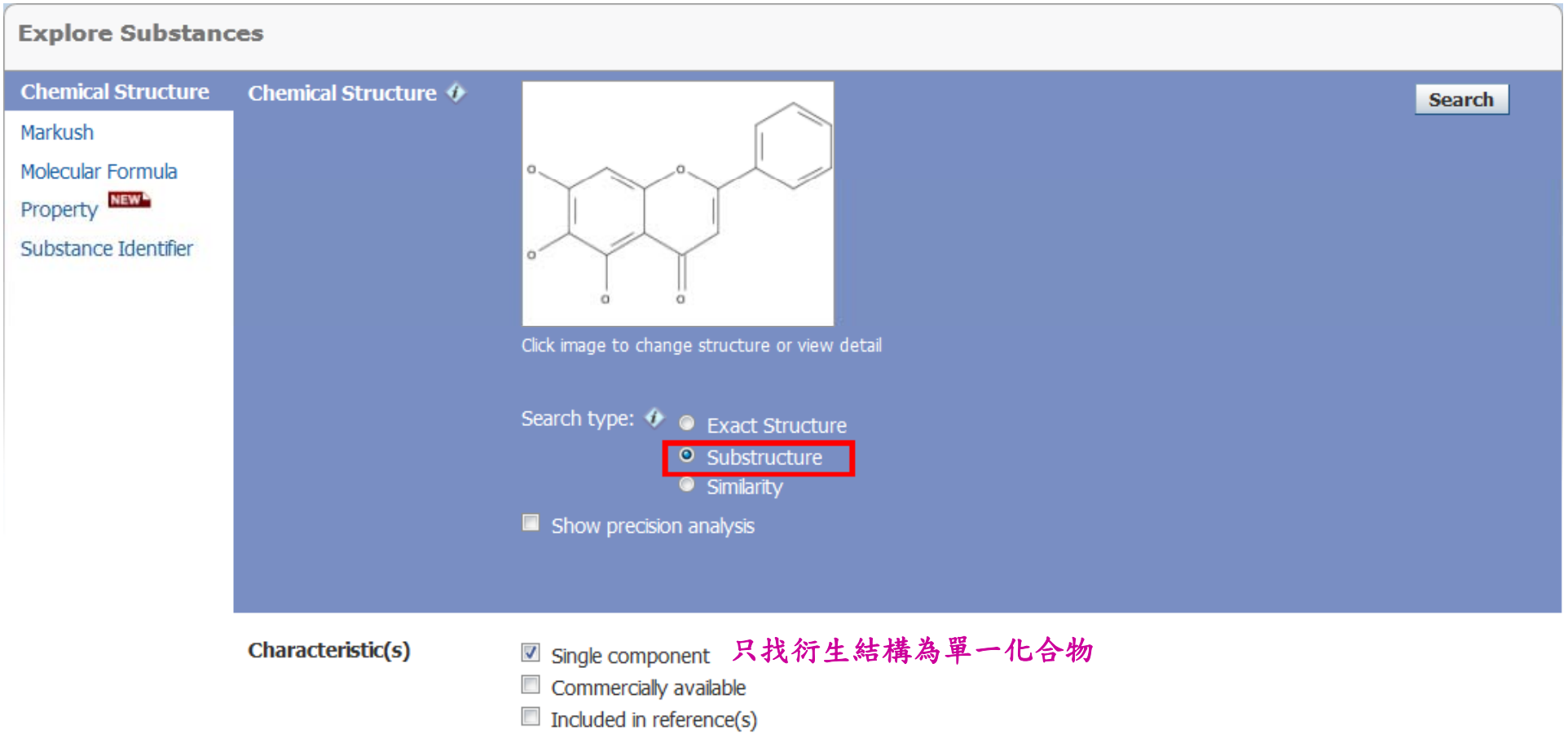


Order N	Chemical N	CAS Index Name	Quantit	Price	Purity	Grac	Catalog Name	Pricing and Availability Info	Supplier Name	Street Address
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI America	9211 N. Harborgate Street
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TOKYO CHEMICAL INDUSTRY CO.	TCI Bldg. 4-10-2, Nihonnbashi-Honcho Chuo-ku
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TOKYO KASEI HAMBAI CO., LTD. (J	3-1-13, Nihonbashi-Honcho Chuo-ku
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TOKYO KASEI Osaka Office	2-6-1, Awaji-Cho Chuo-ku, Osaka-shi
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI EUROPE N.V.	Boerenveldseweg 6 Haven 1063
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI Deutschland GmbH	Mergenthalerallee 79-81
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	Tokyo Chemical Industry UK Ltd.	The Magdalen Centre Robert Robinson Avenue, The Oxford Science Park
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI (Shanghai) Development Co., L	No.96 Pu Gong Road, Shanghai Chemical Industry Park
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	$86.00 $280.00	≥98.0%		2012 TCI AMERICA Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI Chemicals (India) Pvt. Ltd.	Bharanee Subalesh Building, B1, H-71, 5th Main Road Annanagar (East)
T2721	Baicalein	4H-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-	1 g 5 g	EUR64.55 EUR220.00	≥98.0%		2012 TCI EUROPE Fine Chemicals	http://www.tcichemicals.com/eshop/	TCI EUROPE N.V.	Boerenveldseweg 6 Haven 1063

~以黃芩(Baicalein)當先導化合物(Lead Compound)，進行優化~

Substructure Search (基底結構衍生檢索)

~以黃芩 (Baicalein)的結構式為基底，做側鏈或官能基團之衍生 ~



Substructure Search (基底結構衍生檢索)

~共3,586個衍生化合物 => 提供多種藥物設計的選擇~

Substances | Get References | Get Reactions | Tools | Send to SciPlanner

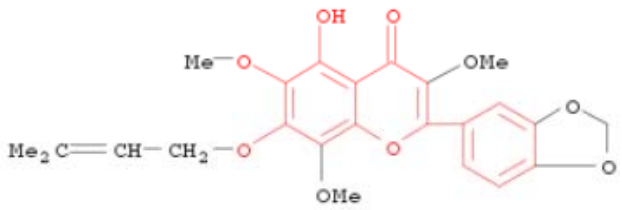
3586 Substances | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: CAS Registry Number | Answers per Page [50] | 1 2 3 4 5 6 ... 72 | View:

直接連結至相關文獻

1. Substance Detail
1388084-65-8

~1 References



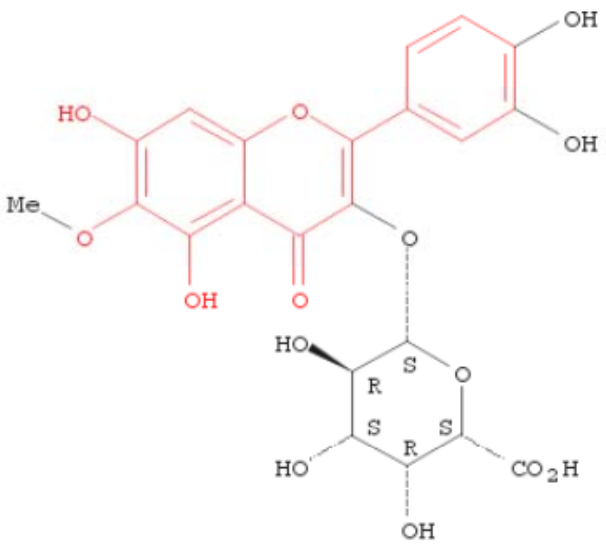
C24 H24 O9

4*H*-1-Benzopyran-4-one, 2-(1,3-benzodioxol-5-yl)-5-hydroxy-3,6,8-trimethoxy-7-[(3-methyl-2-buten-1-yl)oxy]-

直接連結至相關文獻

2. Substance Detail
1386936-78-2

~1 References



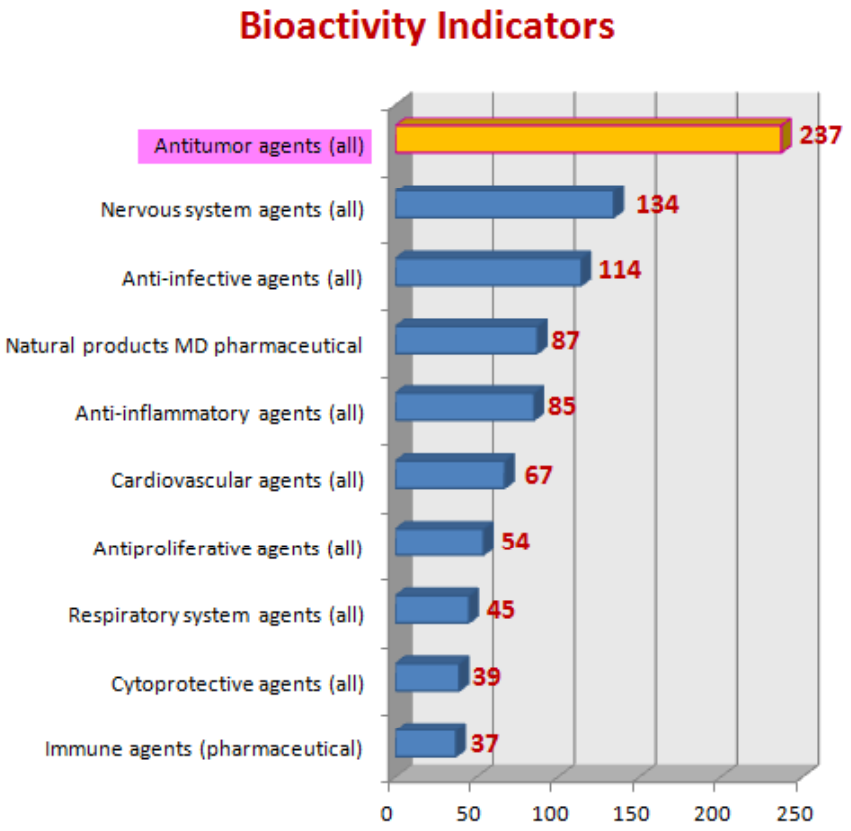
Absolute stereochemistry.

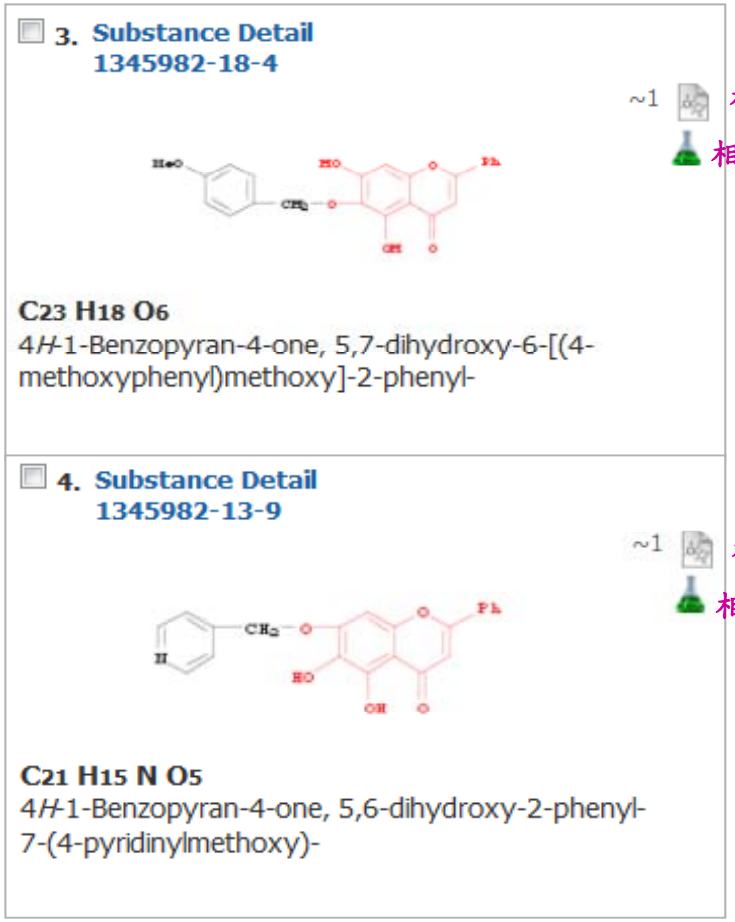
C22 H20 O14

INDEX NAME NOT YET ASSIGNED

3,586 個衍生化合物以活性指標(Bioactivity Indicators)分析

~直接挑出Antitumor agents物質，再串連文獻與反應，節省研發時間~





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3. Substance Detail
1345982-18-4

C23 H18 O6
4*H*-1-Benzopyran-4-one, 5,7-dihydroxy-6-[(4-methoxyphenyl)methoxy]-2-phenyl-

~1 References

具"抗癌"活性指標物質~文獻佐證

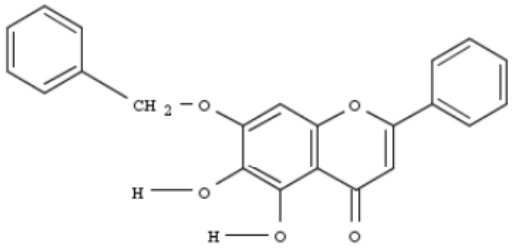
~新合成的黃芩素衍生物造成人類腫瘤細胞之凋亡並活化AMP-activated 蛋白激脢~

Return

Novel synthetic baicalein derivatives caused apoptosis and activated AMP-activated protein kinase in human tumor cells

By: Ding, Derong; Zhang, Baozi; Meng, Tao; Ma, Ying; Wang, Xin; Peng, Hongli; Shen, Jingkang

Studies on the anti-proliferative activities of novel baicalein derivs. demonstrated that compds. 8 (I) and its 4-fluorobenzyl analog 9 were able to activate AMPK by enhancing the levels of phosphorylated AMPKα, and showed more potent anti-proliferative effects than baicalein and AICAR in A431, SK-OV-3, DU 145 and HeLa cells, suggesting an alternative therapeutic approach for benzyl baicalein in cancer therapy.



I

Indexing

Pharmacology (Section1-3)

Section cross-reference(s): 26

Concepts

Substances

Source

Organic & Biomolecular Chemistry
Volume9
Issue21
Pages7287-7291
Journal; Online Computer File
2011
CODEN:OBCRAK
ISSN:1477-0520
DOI:10.1039/c1ob06094e

Company/Organization

State Key Laboratory of Drug Research, Shanghai Institute of Materia Medica
Chinese Academy of Sciences
Shanghai, Peop. Rep. China
201203

Accession Number

2011:1303046
CAN155:605962
CAPLUS

Publisher

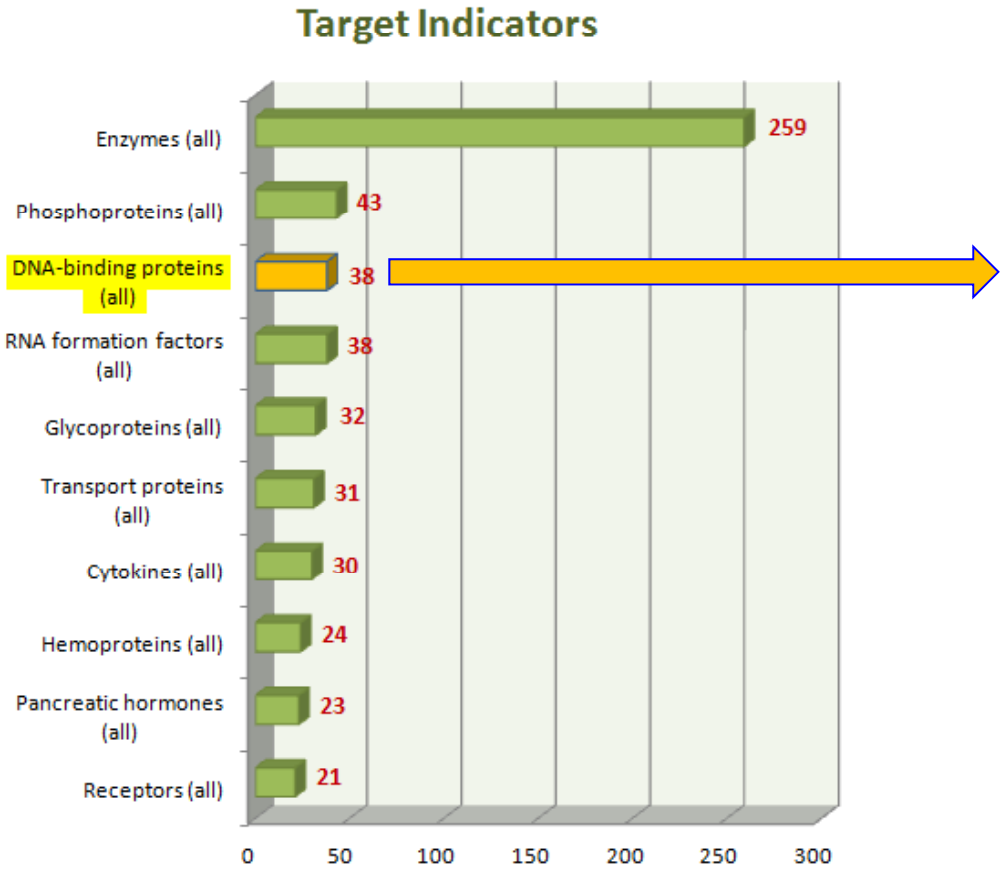
Royal Society of Chemistry

Language

English

以作用指標(Target Indicators)分析：還有哪些可應用對象?

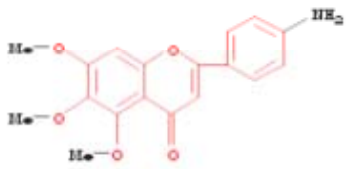
~若以DNA-binding proteins當作用對象，還有哪些可開發或應用的化合物?~



8. Substance Detail
685143-63-9

~3 相關文獻

相關化學反應



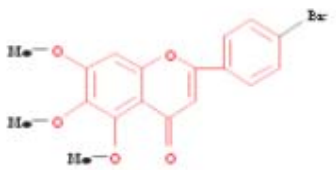
C18 H17 N O5

4*H*-1-Benzopyran-4-one, 2-(4-aminophenyl)-5,6,7-trimethoxy-

9. Substance Detail
1355483-74-7

~1 相關文獻

相關化學反應



C18 H15 Br O5

4*H*-1-Benzopyran-4-one, 2-(4-bromophenyl)-5,6,7-trimethoxy-

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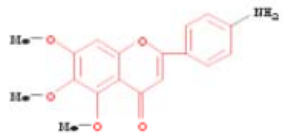
8. Substance Detail
685143-63-9

References ~3



C18 H17 N O5
4*H*-1-Benzopyran-4-one, 2-(4-aminophenyl)-5,6,7-trimethoxy-

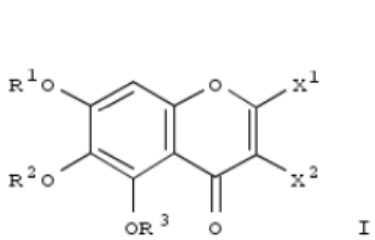
以DNA-binding proteins當作用對象~文獻佐證

~製備chromone衍生物治療敗血性休克、器官損傷與其他疾病~

3. Preparation of chromone derivatives for treatment of septic shock, organ injury, and other disorders

By: Yen, Mao-Hsiung; Wu, Edwin S. C.
Assignee: Jenken Biosciences, Inc., USA

The title compds. I [wherein R1-R3 = independently H, alkyl, alkenyl, alkynyl, SO3H, PO3H2, carbohydrate, etc.; X1 and X2 = independently Ar-X3-T; Ar = none, Ph, furanyl, thienyl, pyridyl, cyclohexyl, or PhCH2; X3 = H, C, N, O, S, etc.; with provisos] or pharmaceutically acceptable salts thereof are prepd. For example, the compd. II was prepd. in a multi-step synthesis. I are useful for the prevention and treatment of septic shock, organ injury, and other disorders (no data).



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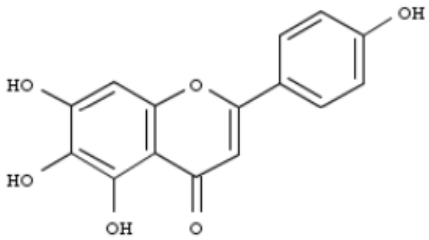
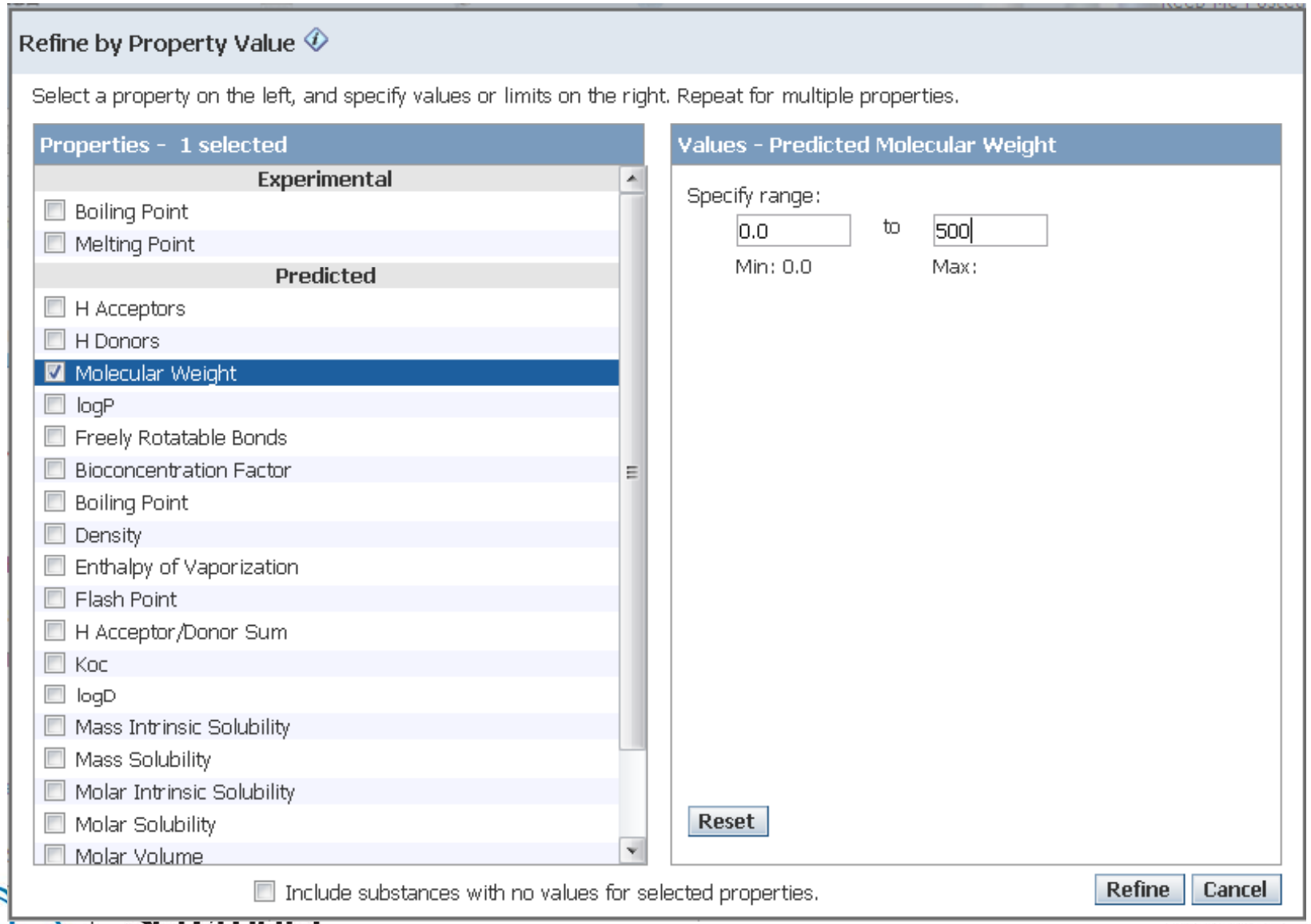


II

Patent Information

Patent No.	Kind	Date	Application No.	Date
WO 2004037193	A2	May 6, 2004	WO 2003-US33578	Oct 22, 2003
WO 2004037193	A3	Feb 17, 2005		
CA 2421887	A1	Apr 22, 2004	CA 2003-2421887	Mar 13, 2003
CA 2502975	A1	May 6, 2004	CA 2003-2502975	Oct 22, 2003

亦可限定分子量、溶點、沸點等參數縮小範圍



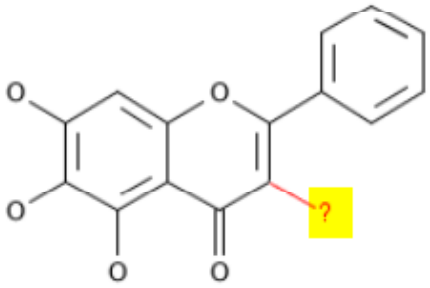
或只探討特定位置的取代情形

Refine by Atom Attachment

1. Click an atom to display the attachments present at that site.

2. Select attachment(s) of interest.

Substructure



Atom Attachments

Select All Deselect All

H or None	2113
O	1407
C	49
Br	5
Cl	4
S	1
N	1
I	1
Other	5
A - Any (not H)	1468
Q - Any (not C,H)	1419
Ak - Alkyl chain	46
X - Halogen	10
Cb - Carbocycle	2
Hy - Heterocycle	1

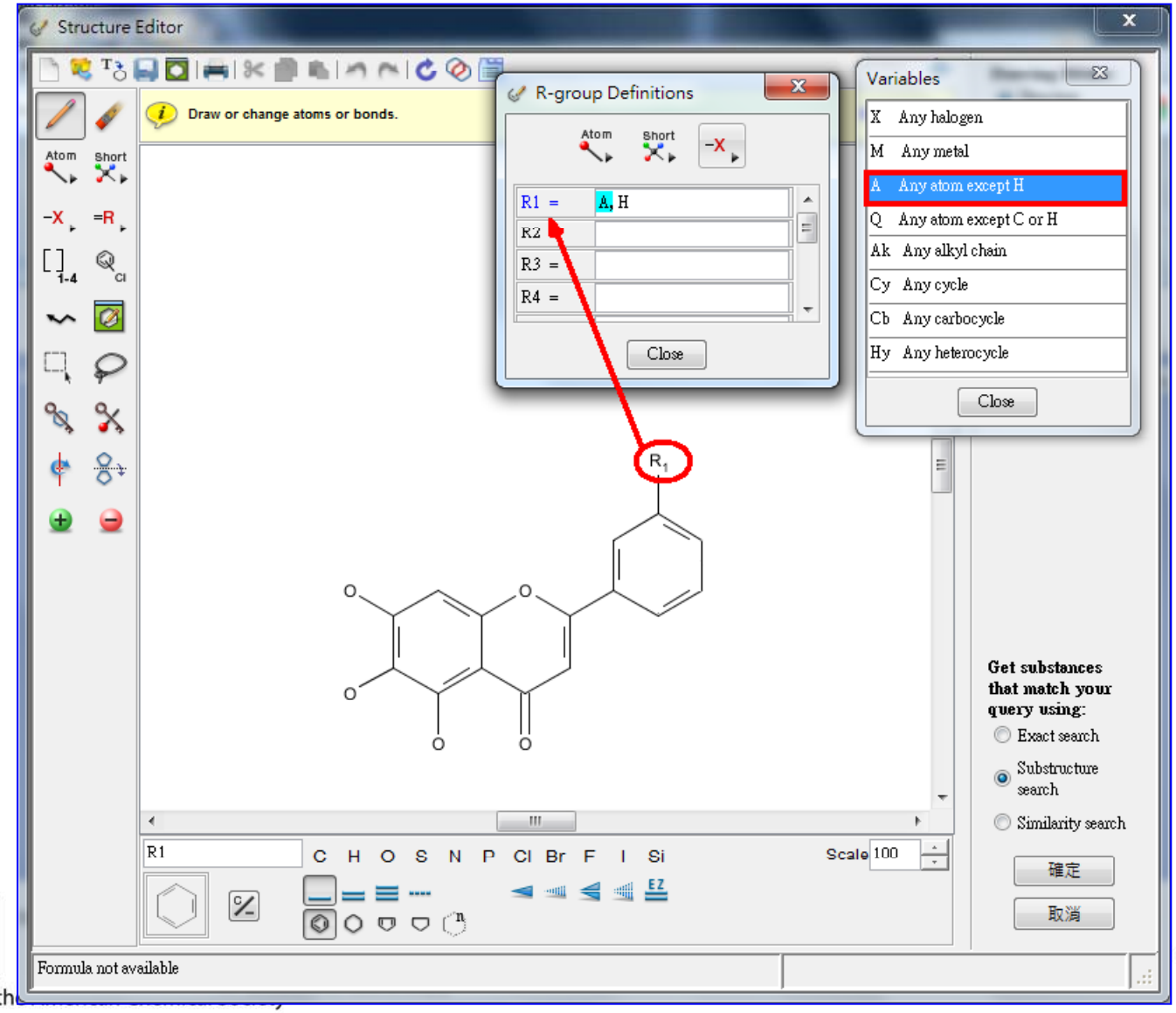
? =

Refine Cancel

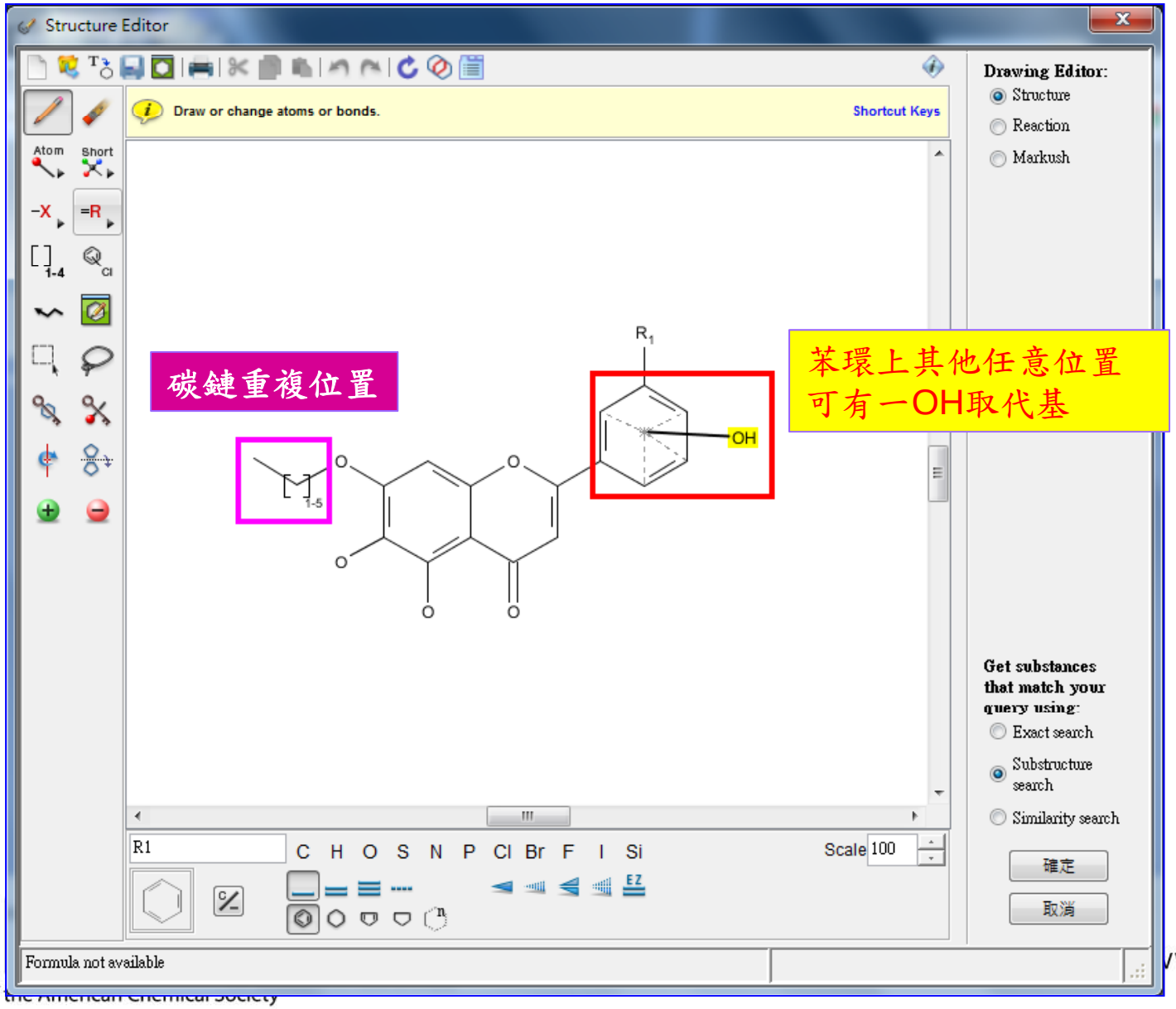
~以黃芩(Baicalein)當先導化合物(Lead Compound)，自行進行藥物設計~

自行設計取代基R1

~例如: R1包含所有原子~



內部結構設計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Structure
Reaction
Markush
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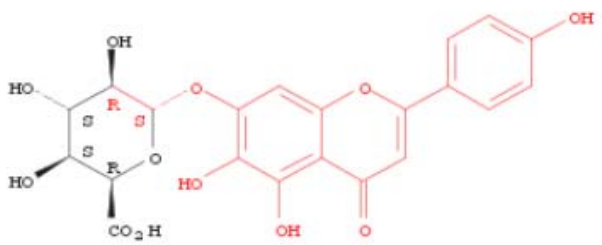
苯環上其他任意位置
可有一OH取代基
R1
OH
1-5
Get substances that match your query using:
Exact search
Substructure search
Similarity search
R1
C H O S N P Cl Br F I Si
Scale 100
確定
取消
Formula not available

獲得符合設計要求的化合物

30. Substance Detail
1258510-15-4

~1

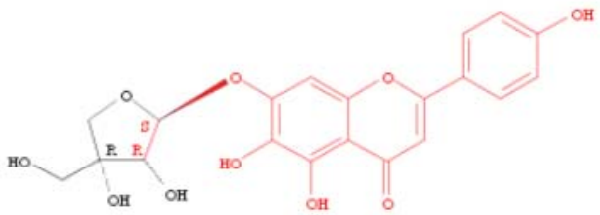


Absolute stereochemistry.

C21 H18 O12
INDEX NAME NOT YET ASSIGNED

36. Substance Detail
1217268-01-3

~1

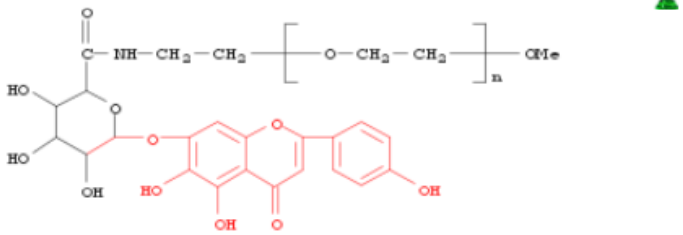


Absolute stereochemistry.,Rotation (-).

C20 H18 O10
4*H*-1-Benzopyran-4-one, 7-(D-apio-β-D-furanosyloxy)-5,6-dihydroxy-2-(4-hydroxyphenyl)-

46. Substance Detail
1180659-38-4

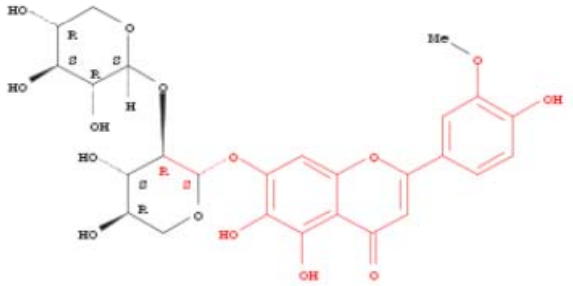
~2



(C2 H4 O)n C24 H25 N O12
Poly(oxy-1,2-ethanediyl), α-[2-[[1-*O*-[5,6-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4*H*-1-benzopyran-7-yl]-β-D-glucopyranuronoyl]amino]ethyl]-ω-methoxy-

105. Substance Detail
847032-40-0

~1



Absolute stereochemistry.

C26 H28 O15
4*H*-1-Benzopyran-4-one, 5,6-dihydroxy-2-(4-hydroxy-3-methoxyphenyl)-7-[(2-*O*-β-D-xylopyranosyl-β-D-xylopyranosyl)oxy]-

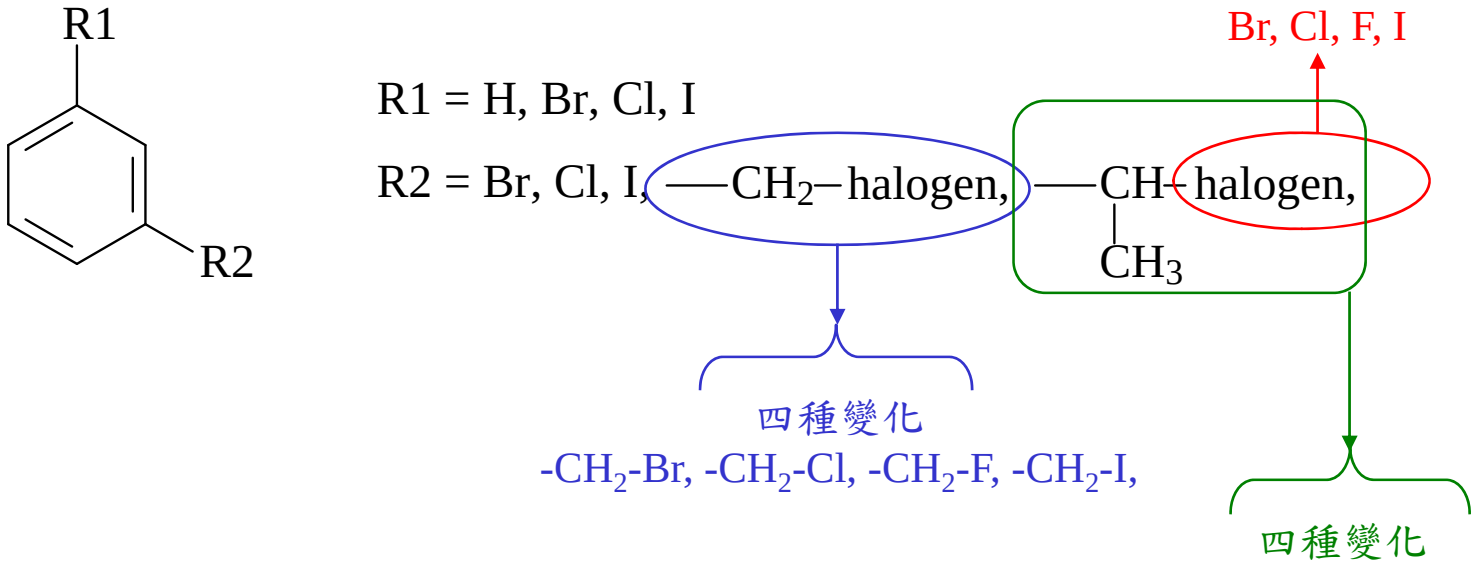
Markush 結構檢索

~進行專利布局與迴避設計~

在專利中描述物質的方式：

- 特定物質[Specific Substance]：
  - 以特定的化學結構所陳述的特定物質，會有CAS RN.
- **預測性物質[Prophetic Substance]：**
  - 使用Markush結構所陳述的預測物質，一個Markush可以陳述上百或上千的化學物質
  - Patent中所陳述的**預測物質**，**不會**被標示CAS RN.
  - Markush 檢索，是Substructure檢索的補充。

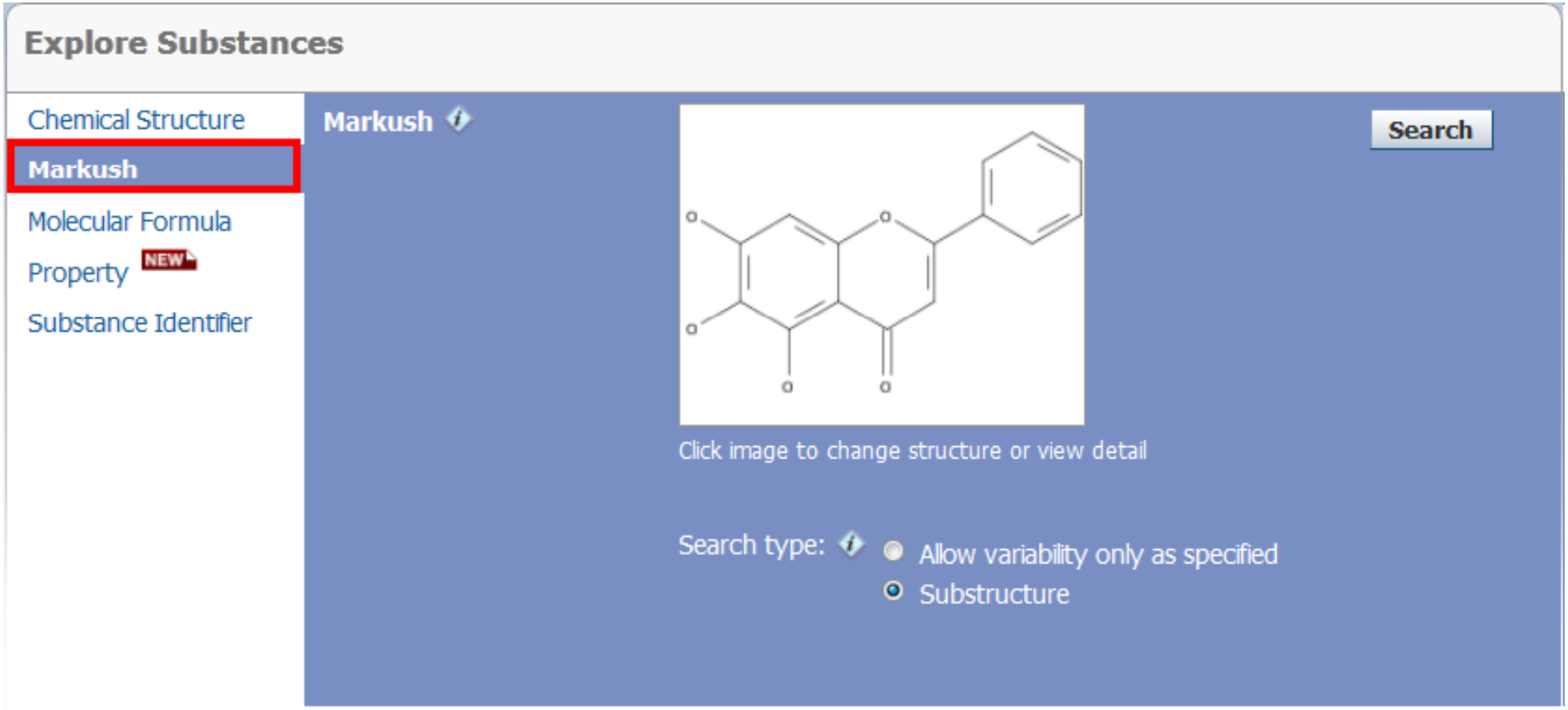
Example of Markush Stucture



- R1有4種變化， R2有11種變化，所以上述的這一個 Markush Structure，就可代表44種 (R1 × R2 = 4 × 11 = 44) 不同的化合物。
- 這一群化合物，我們可稱其為**族性結構**。
- 由此可知，若結構上的可變性稍多一些，**一個 Markush Structure 可代表上千種結構**。

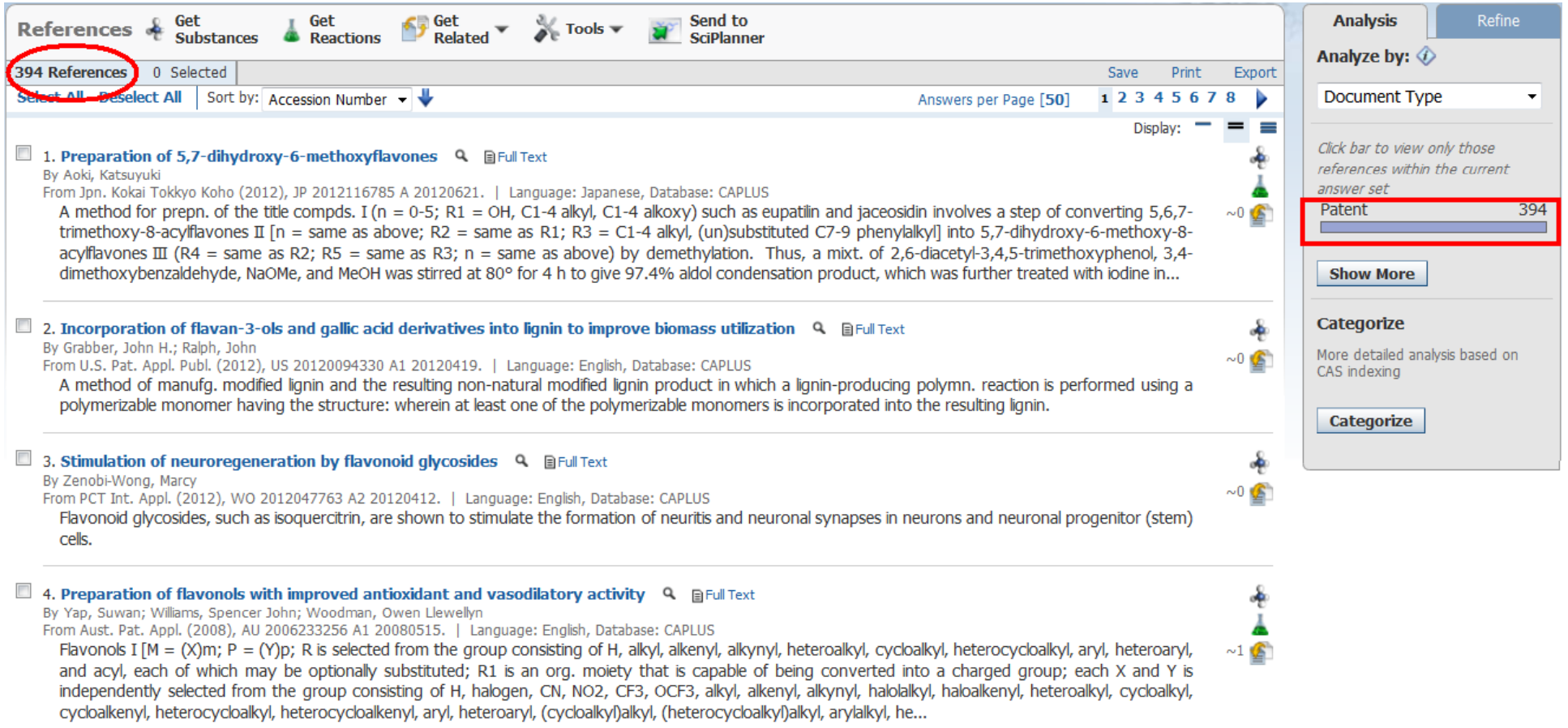
Markush Search (以Markush結構檢索)

~將黃芩 (Baicalein)的結構式拆解，進行檢索 ~



Markush Search Results

~共有394篇專利，裡面有涵蓋被拆解後之黃芩 (Baicalein)結構式~



製備5,7-dihydroxy-6-methoxyflavones

Reference Detail | Get Substances | Get Reactions | Get Cited | Get Citing | Get Full Text | Send to SciPlanner

Link | Save | Print | Export

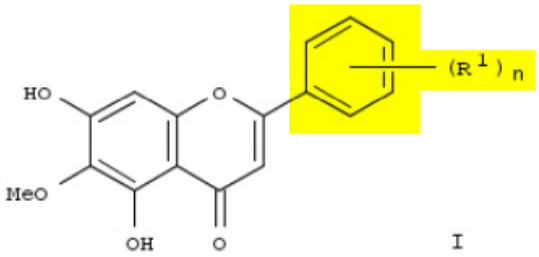
Return | Previous | Next

1. Preparation of 5,7-dihydroxy-6-methoxyflavones

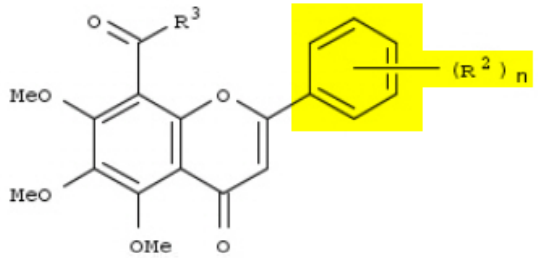
By: Aoki, Katsuyuki

Assignee: Tsumura and Co., Japan

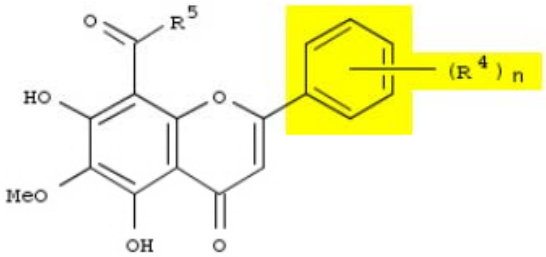
A method for prepn. of the title compds. I (n = 0-5; R1 = OH, C1-4 alkyl, C1-4 alkoxy) such as eupatilin and jaceosidin involves a step of converting 5,6,7-trimethoxy-8-acylflavones II [n = same as above; R2 = same as R1; R3 = C1-4 alkyl, (un)substituted C7-9 phenylalkyl] into 5,7-dihydroxy-6-methoxy-8-acylflavones III (R4 = same as R2; R5 = same as R3; n = same as above) by demethylation. Thus, a mixt. of 2,6-diacetyl-3,4,5-trimethoxyphenol, 3,4-dimethoxybenzaldehyde, NaOMe, and MeOH was stirred at 80° for 4 h to give 97.4% aldol condensation product, which was further treated with iodine in DMSO at 180° for 45 h to give 91.0% II [R3 = CH:CHC6H4(OMe)2-3,4, R3 = (OMe)2-3,4]. The flavone was reduced with H using Pd/C in MeOAc/MeOH at room temp. for 24 h to give II [R3 = CH2CH2C6H4(OMe)2-3,4, R2 = (OMe)2-3,4] (IV). IV and Bu4NI were dissolved in CH2Cl2, treated with BCl3 at -78°, and the reaction mixt. was stirred for 5 h while heating to room temp. and at 0° for 1 h to give 70.9 % III [R5 = CH2CH2C6H4(OMe)2-3,4, R4 = (OMe)2-3,4]. This was treated with Sc(OTf)3 in ClCH2CH2Cl under reflux for 24 h to give 85.6% eupatilin.



I



II

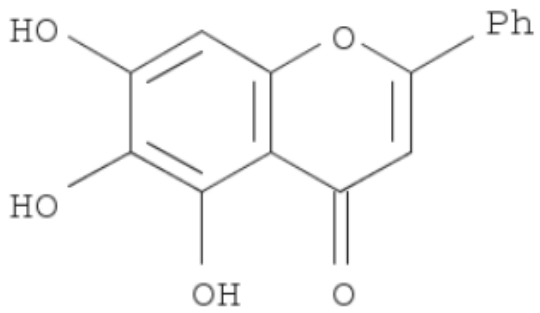


III

~黃芩(Baicalein)之最佳合成方式~

物質直接連結至化學反應式

1. **Substance Detail**
491-67-8



C15 H10 O5
4*H*-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl-

Spectra
Experimental Properties

~2045
Reactions

Get Reactions

Limit results by reaction role:

- (•) Product
- ( ) Reactant
- ( ) Reagent
- ( ) Reactant or reagent
- ( ) Catalyst
- ( ) Solvent
- ( ) Any role

Get | Cancel

SCIFINDER

共63筆化學反應式

~其中16筆有Experimental Procedure (原文中之反應過程)~

Reactions | Get References | Tools | Send to SciPlanner

63 Reactions | 0 Selected | Save | Print | Export

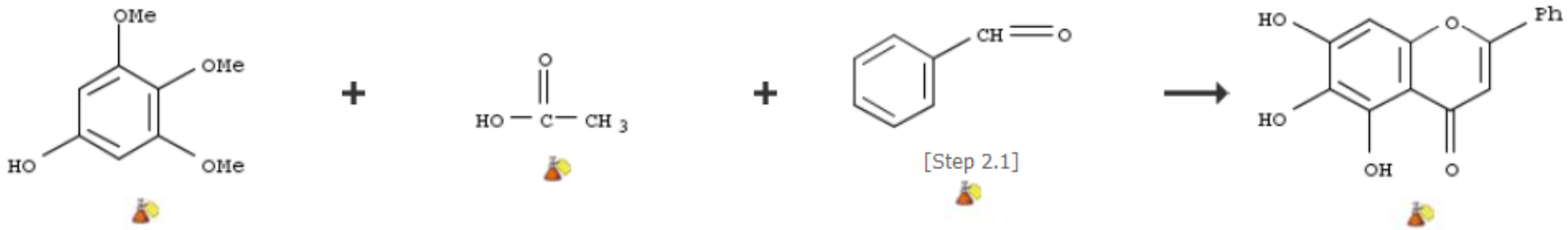
16 reactions with the Experimental Procedure **Experimental Procedures Available** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number | Answers per Page [15] 1 2

Display:

41. **View Reaction Detail Link**

5 Steps *Hover over any structure for more options.*



▾ Overview

Steps/Stages

1.1 R:BF_3-Et_2O, 15 min, reflux
2.1 R:KOH, S:H_2O, S:EtOH, < 15°C; 8 h, rt
2.2 R:H_2O
3.1 2 h, reflux
4.1
5.1 12 h, reflux

Notes

Reactants: 3, Reagents: 3, Solvents: 2, Steps: 5, Stages: 6, Most stages in any one step: 2

References

Methods of synthesizing flavonoids and chalcones | Full Text
By Shaw, Jiajiu et al
From U.S. Pat. Appl. Publ., 20040242907, 02 Dec 2004

▸ Experimental Procedure

利用分析功能~再篩選出產率>80%的反應

Analysis | Refine

Analyze by: Product Yield

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

80-89% 2

Show More

Reactions | Get References | Tools | Send to SciPlanner

16 Reactions 0 Selected | Save | Print | Export

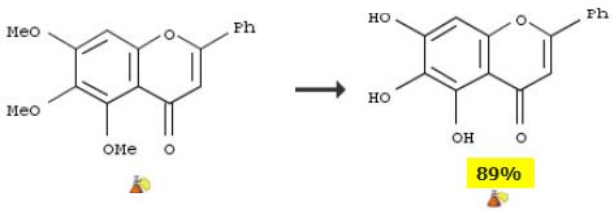
2 reactions with the Product Yields **80-89%** are displayed | Keep Analysis | Clear Analysis

Select All | Deselect All | Sort by: Accession Number | Answers per Page [2]

Display:

15. View Reaction Detail | Link | Similar Reactions

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



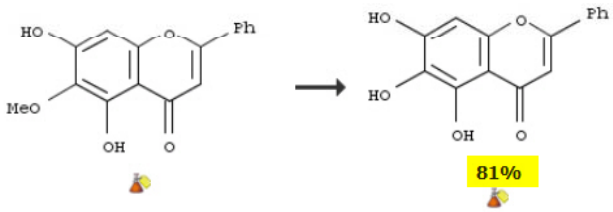
Overview

Experimental Procedure

Baicalein Baicalein was prepared by the modified procedure outlined above either from flavone 2 (reflux, 18 h) in 89% yield. mp 258-260° C. (lit. 263-264° C.). Rf (CH_2Cl_2:EtOAc=5:1) 0.4. ^{1}H-NMR (DMSO-d_6) δ: 6.61 (1 H, s), 6.92 (1 H, s), 7.56 (3 H, m), 8.05 (2 H, d, J=8.1 Hz), 8.81 (1 H, s), 10.57 (1 H, s), 12.65 (1 H, s). IR (KBr) cm^{-1}: 3411, 1654. UV λ_{max} (EtOH) nm (log ε): 326 (4.17), 276 (4.42), 215 (4.49). MS m/z: 270 (M^+).

16. View Reaction Detail | Link | Similar Reactions

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



Overview

Experimental Procedure

Baicalein Baicalein was prepared by the modified procedure outlined above either from oroxylin A (reflux, 12 h) in 81% yield. mp 258-260° C. (lit. 263-264° C.). Rf (CH_2Cl_2:EtOAc=5:1) 0.4. ^{1}H-NMR (DMSO-d_6) δ: 6.61 (1 H, s), 6.92 (1 H, s), 7.56 (3 H, m), 8.05 (2 H, d, J=8.1 Hz), 8.81 (1 H, s), 10.57 (1 H, s), 12.65 (1 H, s). IR (KBr) cm^{-1}: 3411, 1654. UV λ_{max} (EtOH) nm (log ε): 326 (4.17), 276 (4.42), 215 (4.49). MS m/z: 270 (M^+).

SCIFINDER

黃芩(Baicalein)之合成方式：Overview 、Experiment Procedure

Reactions | Get References | Tools | Send to SciPlanner

16 Reactions 1 Selected | Save Print Export

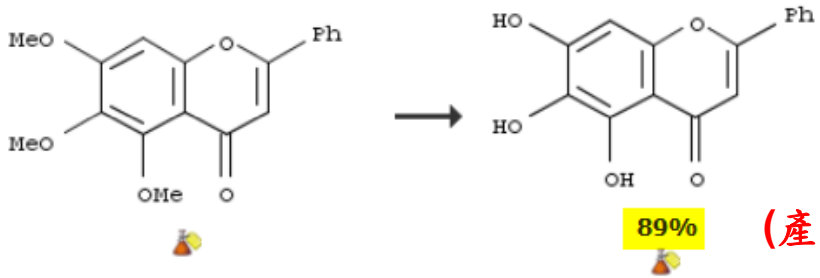
2 reactions with the Product Yields **80-89%** are displayed | Keep Analysis Clear Analysis

Select All Deselect All | Sort by: Accession Number | Answers per Page [2]

Display:

15. View Reaction Detail Link Similar Reactions

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



黃芩
(產率: 89%)

▾ Overview

Steps/Stages

1.1 18 h, reflux

Notes

Reactants: 1, Steps: 1, Stages: 1, Most stages in any one step: 1

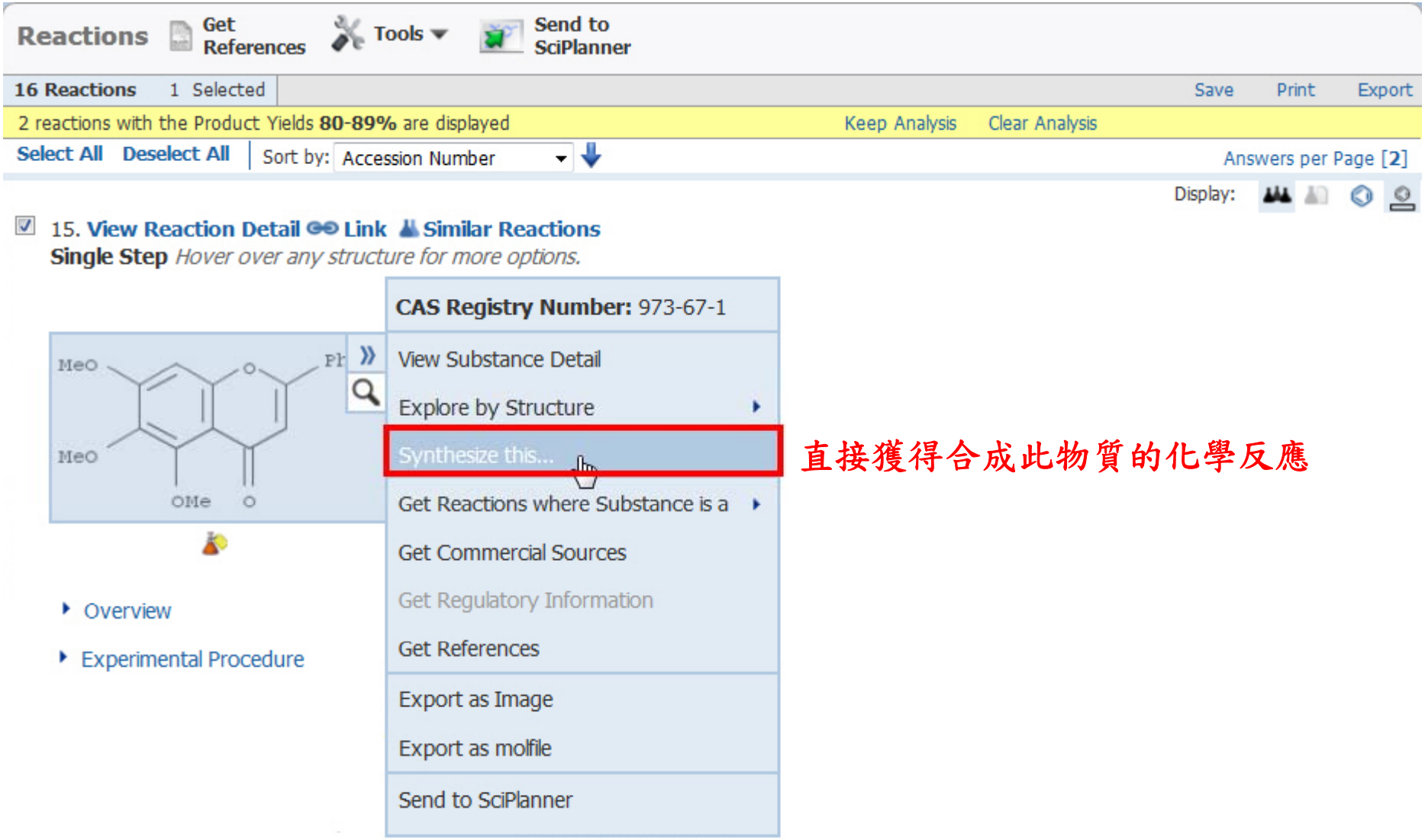
References 可直接連結至出處文獻

Methods of synthesizing flavonoids and chalcones | Full Text
By Shaw, Jiajiu et al
From U.S. Pat. Appl. Publ., 20040242907, 02 Dec 2004

▾ Experimental Procedure

Baicalein Baicalein was prepared by the modified procedure outlined above either from flavone 2 (reflux, 18 h) in 89% yield. mp 258-260° C. (lit. 263-264° C.). Rf (CH_2Cl_2:EtOAc=5:1) 0.4. ^{1}H-NMR (DMSO-d_6) δ: 6.61 (1 H, s), 6.92 (1 H, s), 7.56 (3 H, m), 8.05 (2 H, d, J=8.1 Hz), 8.81 (1 H, s), 10.57 (1 H, s), 12.65 (1 H, s). IR (KBr) cm^{-1}: 3411, 1654. UV λ_{max} (EtOH) nm (log ε): 326 (4.17), 276 (4.42), 215 (4.49). MS m/z: 270 (M^+).

利用反應物再往前延伸， 找出最合適、最簡單之起始原料



直接獲得合成此物質的化學反應

SCIFINDER

產率>80 %，共9筆反應式

~反應物仍然太複雜，須繼續往前搜尋，看是否有更簡單的起始物?~

Reactions | Get References | Tools | Send to SciPlanner

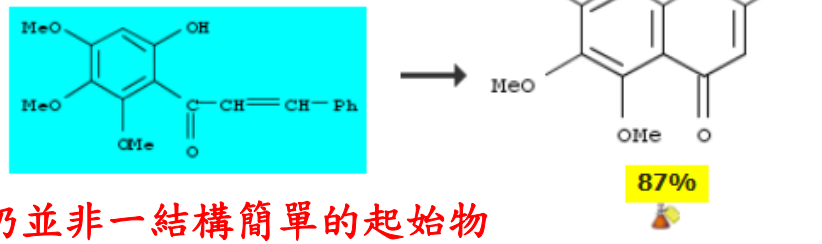
9 Reactions | 0 Selected | Save | Print | Export

Select All | Deselect All | Sort by: Product Yield | Answers per Page [9]

Display:

1. View Reaction Detail | Link | Similar Reactions

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



仍並非一結構簡單的起始物

Overview

Steps/Stages

1.1 R:I_2, S:DMSO, 2 h, reflux
1.2 S:H_2O

Notes

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

References

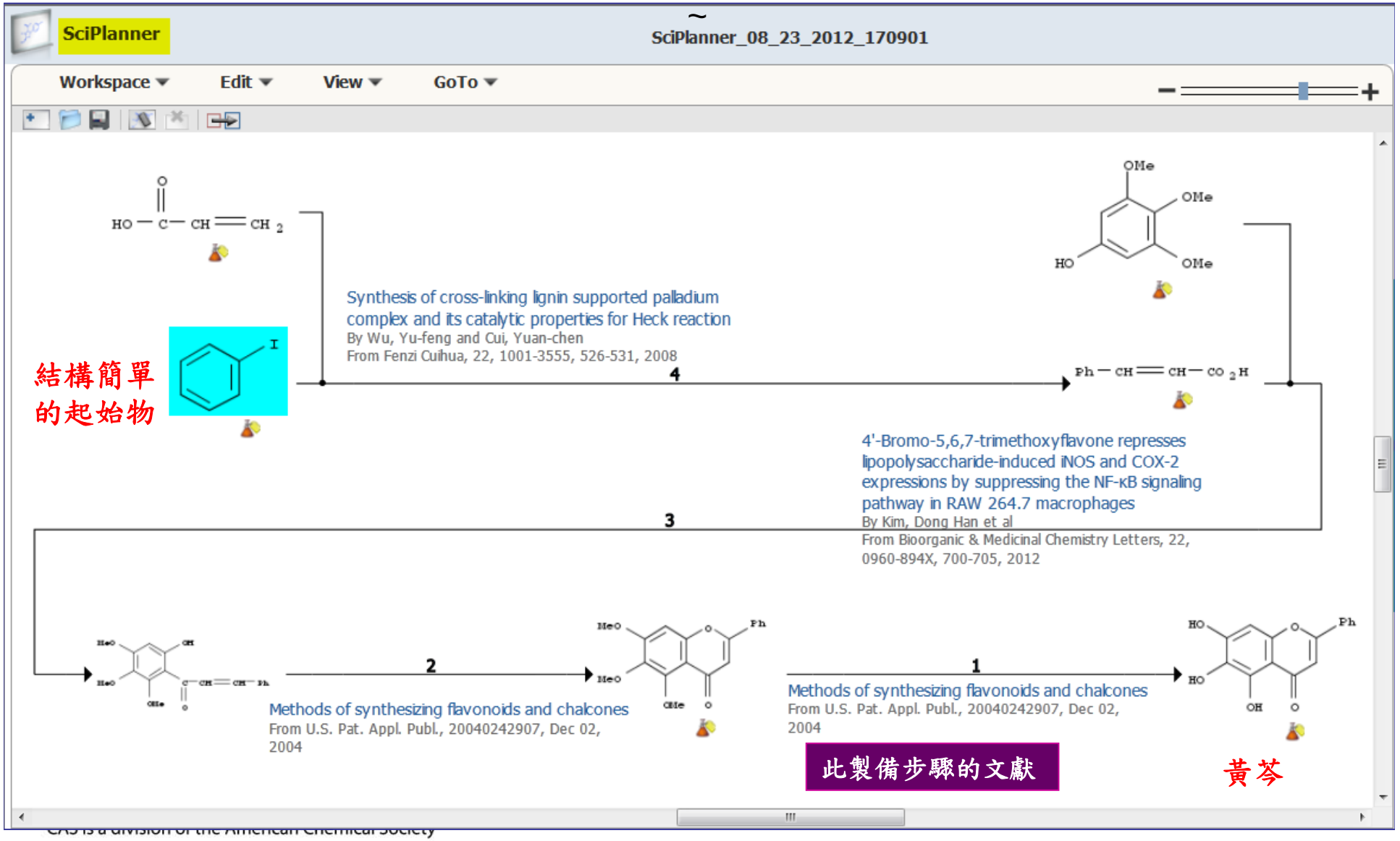
Methods of synthesizing flavonoids and chalcones | Full Text
By Shaw, Jiajiu et al
From U.S. Pat. Appl. Publ., 20040242907, 02 Dec 2004

Experimental Procedure

5,6,7-Trimethoxyflavone (Flavone 2) A mixture of chalcone 1 (7.2 g, 23 mmol) and iodine (200 mg) in DMSO (25 ml) was refluxed for 2 h, and then carefully poured onto crushed ice (200 g). The precipitate was filtered and washed with 20% Na_2SO_3. Purification by flash column chromatography (SiO_2, hexane:EtOAc=3:1) yielded 6.3 g (87%) of flavone 2 and 0.8 g (2.5%) of recovered chalcone 1. mp 146-147° C. (lit. 164-165° C.). ^{1}H-NMR (DMSO-d_6) δ: 3.93 (3 H, s), 3.97 (3 H, s), 3.99 (3 H, s), 6.72 (1 H, s), 6.83 (1 H, s), 7.50 (3 H, m), 7.88 (2 H, d, J=8.7 Hz). IR (KBr) cm^{-1}: 1633. MS m/z: 313 (MH^+).

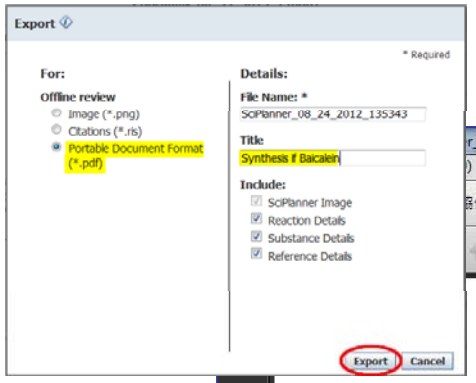
利用SciPlanner(實驗管理平台)，編寫&整合所有製備過程與文獻

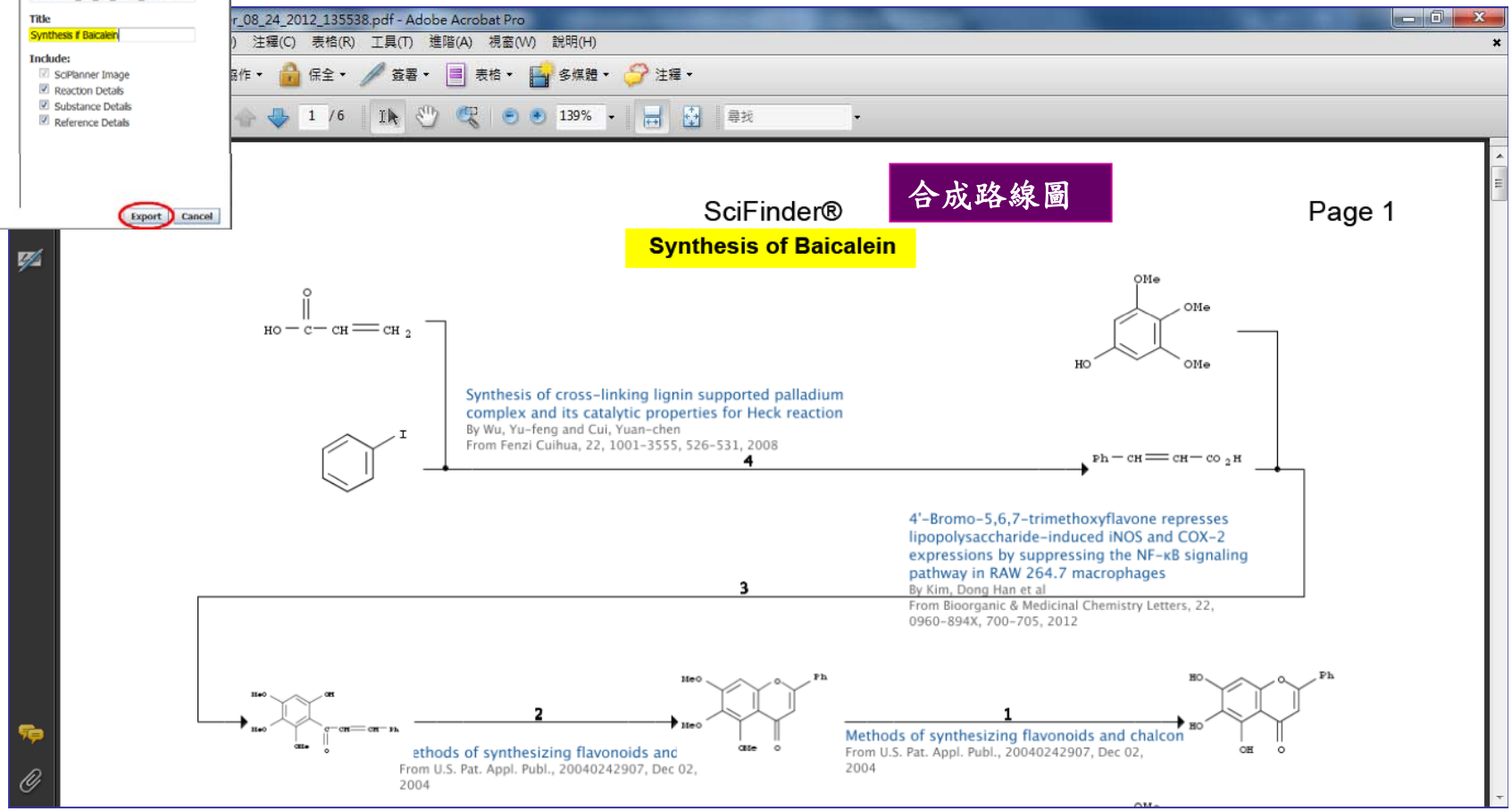
~將所有製程的反應式、參考文獻，彙整於同一平台，亦可轉出此檔案。



利用SciPlanner(實驗管理平台）：匯出成pdf檔案

~合成路徑圖~





利用SciPlanner(實驗管理平台）：匯出成pdf檔案

~每一步驟的反應條件、詳細操作步驟與物質資訊~

Synthesis of Baicalein_SciPlanner_08_24_2012_135538.pdf - Adobe Acrobat Pro

檔案(F) 編輯(E) 檢視(V) 文件(D) 注釋(C) 表格(R) 工具(T) 進階(A) 視窗(W) 說明(H)

SciFinder® Page 2

Reaction Information

Reaction	Stages	Notes	Yield
1	1.1 18 h, reflux	Reactants: 1, Steps: 1, Stages: 1	89%

References

Methods of synthesizing flavonoids and chalcones

By Shaw, Jiajiu et al

From U.S. Pat. Appl. Publ., 20040242907, 02 Dec 2004

Experimental Procedure

Baicalein Baicalein was prepared by the modified procedure outlined above either from flavone 2 (reflux, 18 h) in 89% yield. mp 258-260° C. (lit. 263-264° C.). R_f (CH_2Cl_2:EtOAc=5:1) 0.4. ^{1}H-NMR (DMSO-d_6) δ: 6.61 (1 H, s), 6.92 (1 H, s), 7.56 (3 H, m), 8.05 (2 H, d, J=8.1 Hz), 8.81 (1 H, s), 10.57 (1 H, s), 12.65 (1 H, s). IR (KBr) cm-1: 3411, 1654. UV λ_{max} (EtOH) nm (log ε): 326 (4.17), 276 (4.42), 215 (4.49). MS m/z: 270 (M+).

反應條件、操作步驟

Reaction	Stages	Notes	Yield
2	1.1 R:I_2, S:DMSO, 2 h, reflux 1.2 S:H_2O	Reactants: 1, Reagents: 1, Solvents: 2, Steps: 1, Stages: 2	87%

References

Methods of synthesizing flavonoids and chalcones

By Shaw, Jiajiu et al

From U.S. Pat. Appl. Publ., 20040242907, 02 Dec 2004

Experimental Procedure

5,6,7-Trimethoxyflavone (Flavone 2) A mixture of chalcone 1 (7.2 g, 23 mmol) and iodine (200 mg) in DMSO (25 ml) was refluxed for 2 h, and then carefully poured onto crushed ice (200 g). The precipitate was filtered and washed with 20% Na_2SO_3. Purification by flash column chromatography (SiO_2, hexane:EtOAc=3:1) yielded 6.3 g (87%) of flavone 2 and 0.8 g (2.5%) of recovered chalcone 1. mp 146-147° C. (lit. 164-165° C.). ^{1}H-NMR (DMSO-d_6) δ: 3.93 (3 H, s), 3.97 (3 H, s), 3.99 (3 H, s), 6.72 (1 H, s), 6.83 (1 H, s), 7.50 (3 H, m), 7.88 (2 H, d, J=8.7 Hz). IR (KBr) cm-1: 1633. MS m/z: 313 (MH+).

Reaction	Stages	Notes	Yield
3	1.1 R:$SOCl_2$, S:Benzene, reflux 1.2 R:BF_3-Et_2O, S:PhMe	Reactants: 2, Reagents: 2, Solvents: 2, Steps: 1, Stages: 2	98%

References

4'-Bromo-5,6,7-trimethoxyflavone represses lipopolysaccharide-induced iNOS and COX-2 expressions by suppressing the NF-κB signaling pathway in RAW 264.7 macrophages

By Kim, Dong Han et al

SciFinder® Page 4

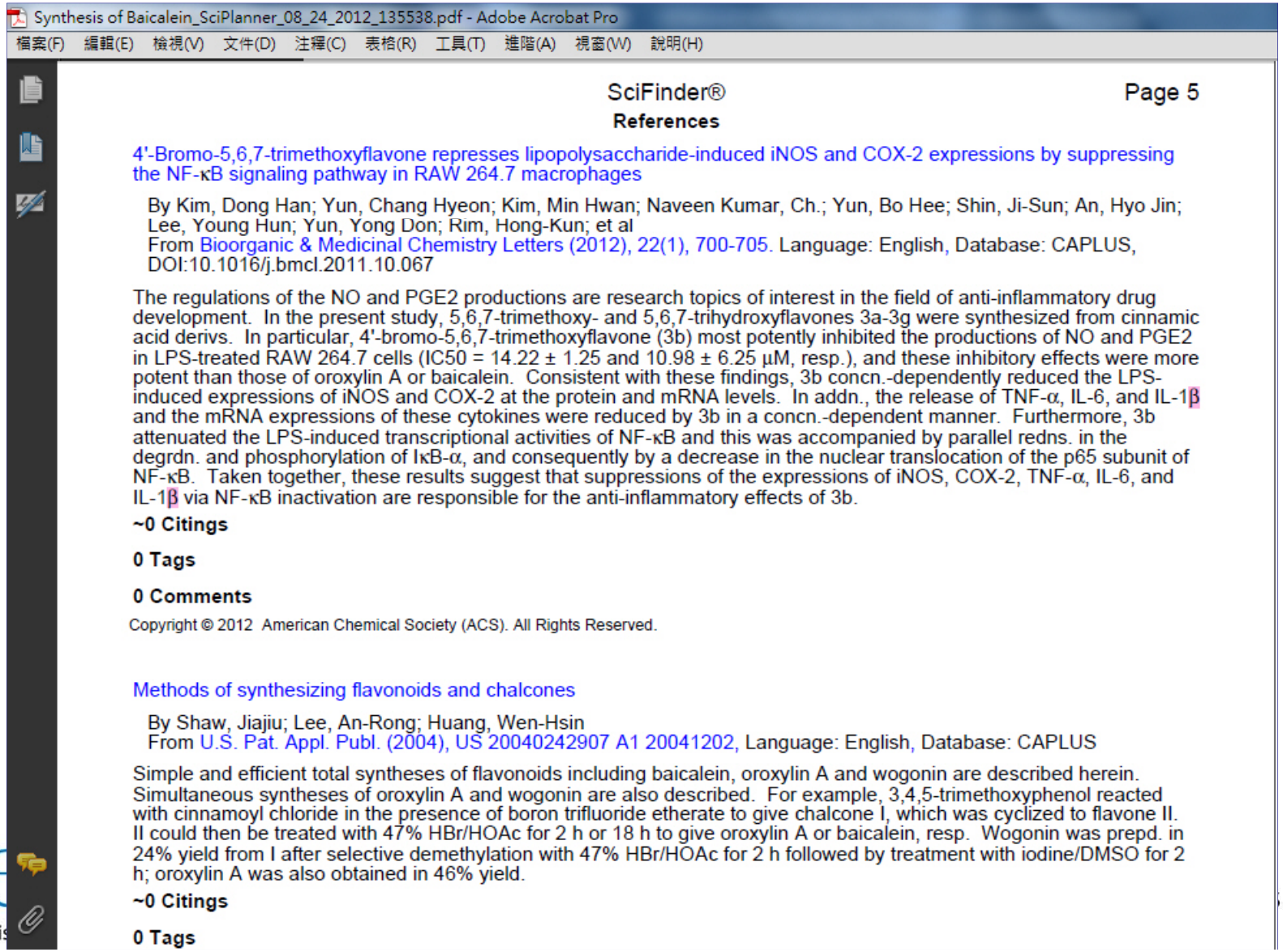
Substance Information

491-67-8 $C_{15}H_{10}O_5$ 4*H*-1-Benzopyran-4-one, 5,6,7-trihydroxy-2-phenyl- Related Info: ~ 2045 References, Reactions, Commercial Sources	531-50-4 C_6H_5I Benzene, Iodo- Related Info: ~ 12005 References, Reactions, Commercial Sources, Regulatory Information	621-82-9 $C_9H_8O_2$ 2-Propenoic acid, 3-phenyl- Related Info: ~ 9927 References, Reactions, Commercial Sources, Regulatory Information
642-71-7 $C_9H_{12}O_4$ Phenol, 3,4,5-trimethoxy- Related Info: ~ 392 References, Reactions, Commercial Sources, Regulatory Information	74064-14-5 $C_{18}H_{18}O_5$ 2-Propen-1-one, 1-(6-hydroxy-2,3,4-trimethoxyphenyl)-3-phenyl- Related Info: ~ 24 References, Reactions	79-10-7 $C_3H_4O_2$ 2-Propenoic acid Related Info: ~ 64103 References, Reactions, Commercial Sources, Regulatory Information
973-67-1 $C_{18}H_{16}O_5$ 4*H*-1-Benzopyran-4-one, 5,6,7-trimethoxy-2-phenyl- Related Info: ~ 99 References, Reactions, Commercial Sources		

反應式中所涉及的物質資訊

利用SciPlanner(實驗管理平台）：匯出成pdf檔案

~每一步驟中之相關文獻~



Synthesis of Baicalein_SciPlanner_08_24_2012_135538.pdf - Adobe Acrobat Pro

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References

4'-Bromo-5,6,7-trimethoxyflavone represses lipopolysaccharide-induced iNOS and COX-2 expressions by suppressing the NF-κB signaling pathway in RAW 264.7 macrophages

By Kim, Dong Han; Yun, Chang Hyeon; Kim, Min Hwan; Naveen Kumar, Ch.; Yun, Bo Hee; Shin, Ji-Sun; An, Hyo Jin; Lee, Young Hun; Yun, Yong Don; Rim, Hong-Kun; et al
From Bioorganic & Medicinal Chemistry Letters (2012), 22(1), 700-705. Language: English, Database: CAPLUS, DOI:10.1016/j.bmcl.2011.10.067

The regulations of the NO and PGE2 productions are research topics of interest in the field of anti-inflammatory drug development. In the present study, 5,6,7-trimethoxy- and 5,6,7-trihydroxyflavones 3a-3g were synthesized from cinnamic acid derivs. In particular, 4'-bromo-5,6,7-trimethoxyflavone (3b) most potently inhibited the productions of NO and PGE2 in LPS-treated RAW 264.7 cells (IC50 = 14.22 ± 1.25 and 10.98 ± 6.25 μM, resp.), and these inhibitory effects were more potent than those of oroxylin A or baicalein. Consistent with these findings, 3b concn.-dependently reduced the LPS-induced expressions of iNOS and COX-2 at the protein and mRNA levels. In addn., the release of TNF-α, IL-6, and IL-1β and the mRNA expressions of these cytokines were reduced by 3b in a concn.-dependent manner. Furthermore, 3b attenuated the LPS-induced transcriptional activities of NF-κB and this was accompanied by parallel redns. in the degrdn. and phosphorylation of IκB-α, and consequently by a decrease in the nuclear translocation of the p65 subunit of NF-κB. Taken together, these results suggest that suppressions of the expressions of iNOS, COX-2, TNF-α, IL-6, and IL-1β via NF-κB inactivation are responsible for the anti-inflammatory effects of 3b.

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Methods of synthesizing flavonoids and chalcones

By Shaw, Jiajiu; Lee, An-Rong; Huang, Wen-Hsin
From U.S. Pat. Appl. Publ. (2004), US 20040242907 A1 20041202, Language: English, Database: CAPLUS

Simple and efficient total syntheses of flavonoids including baicalein, oroxylin A and wogonin are described herein. Simultaneous syntheses of oroxylin A and wogonin are also described. For example, 3,4,5-trimethoxyphenol reacted with cinnamoyl chloride in the presence of boron trifluoride etherate to give chalcone I, which was cyclized to flavone II. II could then be treated with 47% HBr/HOAc for 2 h or 18 h to give oroxylin A or baicalein, resp. Wogonin was prepd. in 24% yield from I after selective demethylation with 47% HBr/HOAc for 2 h followed by treatment with iodine/DMSO for 2 h; oroxylin A was also obtained in 46% yield.

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鄭淮辰 陳劍鵬 許傳奇 蘇甯茱
Tel ：(02) 2571 3369# 221, 226~228
Fax：(02) 2571 3119
email：cas.tw@igrouptaiwan.com