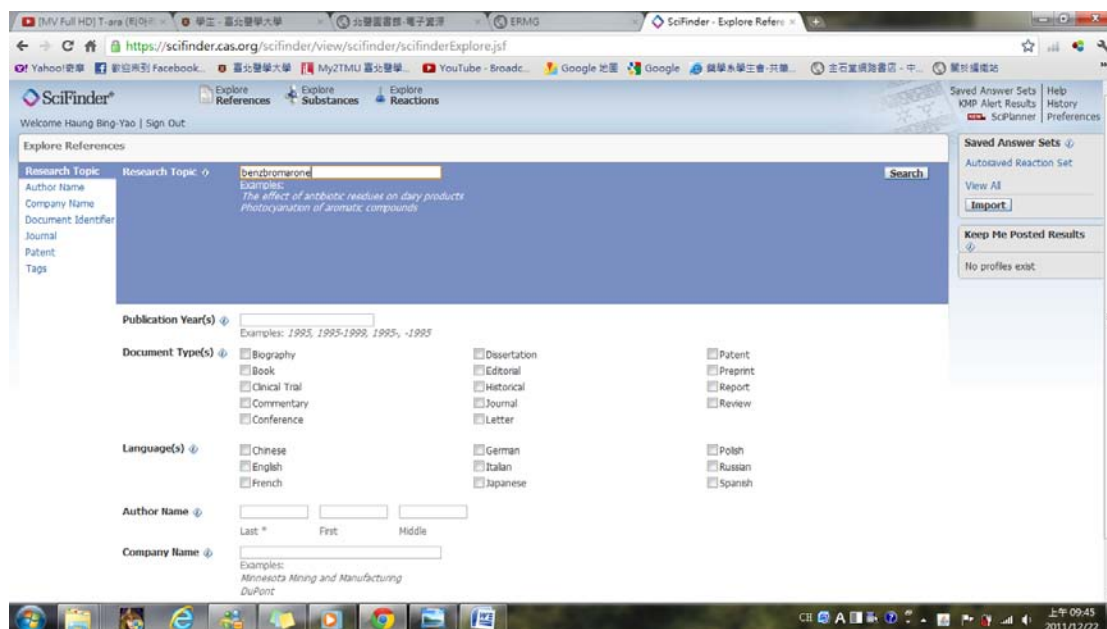


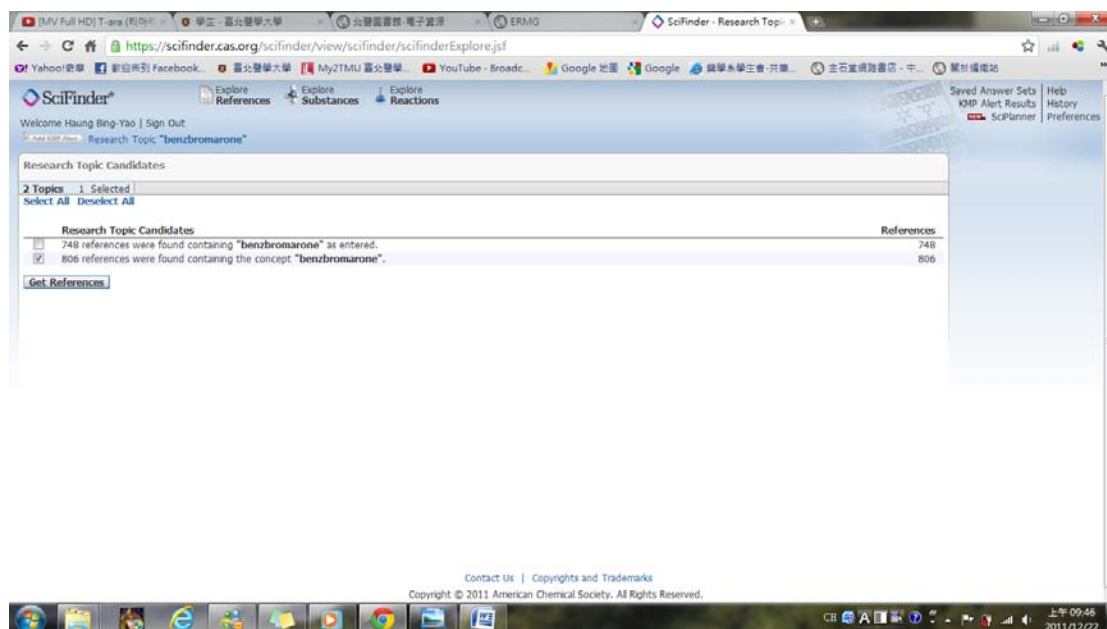
藥學科技(二) Scifinder

B303098194 黃炳堯

1. 從北醫圖書館網站→電子資源→Scifinder→在 Research Topic 上搜尋 Benzbromarone



2. 選取 806 references were found containing the concept "benzbromarone".



3. 點選第一篇文章

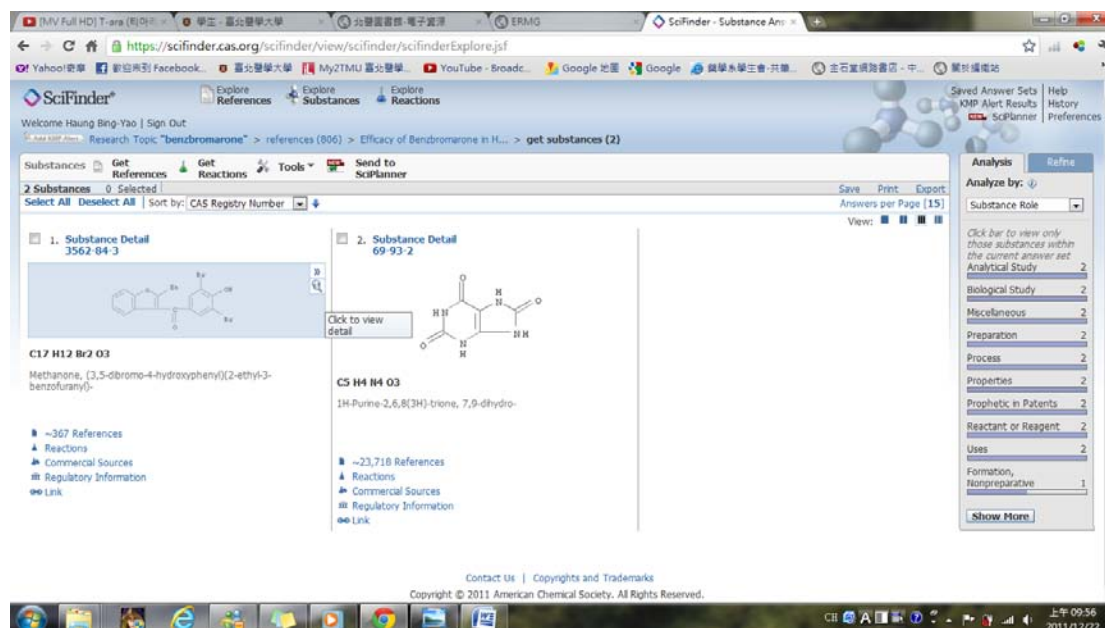
The screenshot shows the SciFinder web interface. The search results for "benzbromarone" are displayed. The first article is selected, and its details are shown. The article title is "1. Efficacy of Benzbromarone in Hyperuricemic Patients Associated with Chronic Kidney Disease". The authors are Fujimori, S.; Ooyama, K.; Ooyama, H.; Morimoto, H. The abstract describes a retrospective evaluation of the uric acid control status and renal function changes over a period of 5-7 years in 35 patients with renal impairment who had stage 3 or higher chronic kidney disease (CKD) stage 3 in 32 patients, stage 4 in 2 patients, and stage 5 in 1 patient. The patients were receiving monotherapy with benzbromarone as an antihyperuricemic drug. Blood serum uric acid levels significantly decreased from 8.5 to 6.1 mg/dL at 6 mo and were subsequently controlled at less than 7.0 mg/dL in most patients. Most patients received benzbromarone at a dose of 25-50 mg/day.

The chemical structure of Benzbromarone is shown, with the SMILES string: Oc1cc(Br)cc(Br)cc1C(=O)Oc2ccccc2.

The article details include:

- Reference Detail:** 1. Efficacy of Benzbromarone in Hyperuricemic Patients Associated with Chronic Kidney Disease. By Fujimori, S.; Ooyama, K.; Ooyama, H.; Morimoto, H.
- Abstract:** We have retrospectively evaluated the uric acid control status and renal function changes over a period of 5-7 years in 35 patients with renal impairment who had stage 3 or higher chronic kidney disease (CKD) stage 3 in 32 patients, stage 4 in 2 patients, and stage 5 in 1 patient. The patients were receiving monotherapy with benzbromarone as an antihyperuricemic drug. Blood serum uric acid levels significantly decreased from 8.5 to 6.1 mg/dL at 6 mo and were subsequently controlled at less than 7.0 mg/dL in most patients. Most patients received benzbromarone at a dose of 25-50 mg/day, whereas 150-200 mg/day was used in some patients with stage 4 or 5 CKD. No significant changes in estimated glomerular filtration rate (eGFR) from the baseline value of 46.2 mL/min/1.73 m² were found after benzbromarone therapy. Although the renal function did not improve by reducing the serum uric acid levels with benzbromarone, the renal function did not deteriorate further on the therapy. These results suggest that benzbromarone is applicable to the management of hyperuricemia associated with renal impairment.
- Indexing:** Pharmacology (Section 1-8).
- Concepts:** Human, benzbromarone in hyperuricemic patients assoc. with chronic kidney disease, Kidney disease, chronic, benzbromarone in hyperuricemic patients assoc. with chronic kidney disease, Cytoprotective agents, renoprotective agents, benzbromarone in hyperuricemic patients assoc. with chronic kidney disease.
- Substances:** 3562-84-3 Benzbromarone. Benzbromarone in hyperuricemic patients assoc. with chronic kidney disease. Pharmacological activity; Therapeutic use; Biological study; Uses.
- Source:** Nucleosides, Nucleotides & Nucleic Acids, Volume 30, Issue 12, Pages 1035-1038, Journal Online Computer File 2011, CODEN: NNNAPY, ISSN: 1525-7770, DOI: 10.1080/15257770.2011.6227.
- Company/Organization:** Department of Internal Medicine, Tokyo University School of Medicine, Tokyo, Japan.
- Accession Number:** 2011:1560852, CAN 155:674538, CAPLUS.
- Publisher:** Taylor & Francis Ltd.
- Language:** English.

4. 點選上方 Get Substances→選取第一個 benzbromarone 結構



SciFinder - Substance Analysis

Welcome Huang Bing-Yao | Sign Out

Research Topic: "benzbromarone" > references (806) > Efficacy of Benzbromarone in H... > get substances (2)

Substances 0 Selected | Sort by: CAS Registry Number

1. Substance Detail 3562-84-3

Click to view detail

2. Substance Detail 69-93-2

Click to view detail

Analysis Refine

Analyze by: Substance Role

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

Analytical Study 2

Biological Study 2

Miscellaneous 2

Preparation 2

Process 2

Properties 2

Prophetic in Patents 2

Reactant or Reagent 2

Uses 2

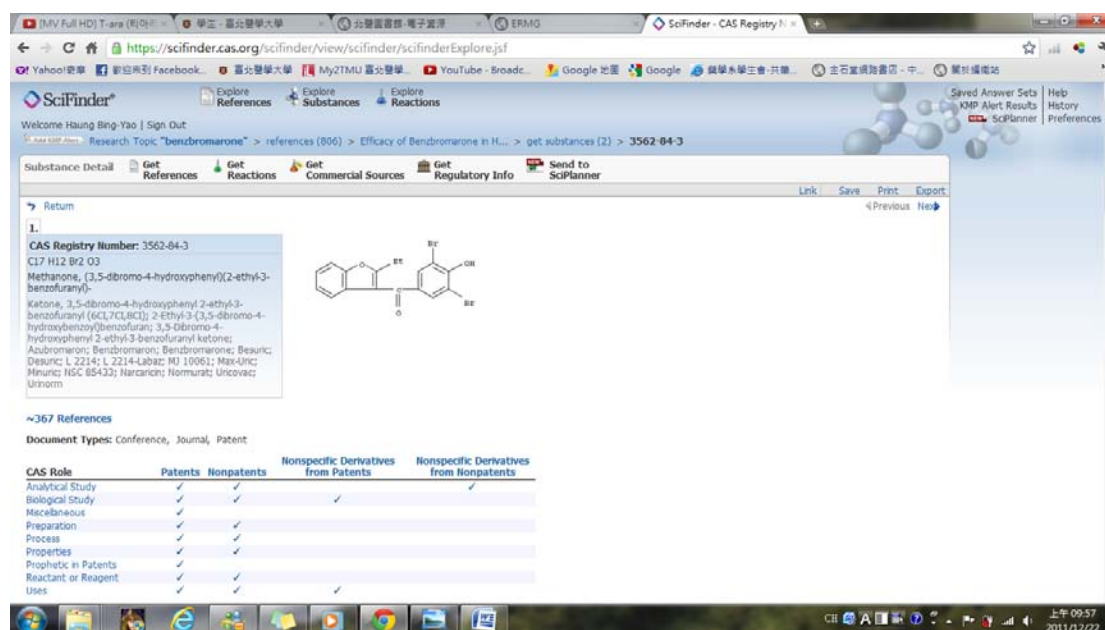
Formation, Nonpreparative 1

Show More

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5. 點選上方 Get Reaction



SciFinder - CAS Registry

Welcome Huang Bing-Yao | Sign Out

Research Topic: "benzbromarone" > references (806) > Efficacy of Benzbromarone in H... > get substances (2) > 3562-84-3

Substance Detail | Get References | Get Reactions | Get Commercial Sources | Get Regulatory Info | Send to SciPlanner

Return

1.

CAS Registry Number: 3562-84-3

CI7 H12 Br2 O3

Methanone, (3,5-dibromo-4-hydroxyphenyl)(2-ethyl-3-benzofuranyl)-

Ketone, 3,5-dibromo-4-hydroxyphenyl 2-ethyl-3-benzofuranyl (6CL7CL8CL); 2-Ethyl-3-(3,5-dibromo-4-hydroxybenzoyl)benzofuran; 3,5-Dibromo-4-hydroxyphenyl 2-ethyl-3-benzofuranyl ketone; Azobromarone; Benzbromarone; Benzbromarone; Resuric; Desuric; L 2214; L 2214-Labaz; MJ 10061; Max-Unc; Minuric; HSC 85433; Nancarcin; Normurat; Uncovaz; Unnorm

~367 References

Document Types: Conference, Journal, Patent

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

6. 選取第一個反應並且點選 Send To SciPlanner

SciFinder - Reaction Analysis

Research Topic: "benzbromarone" > references (806) > Efficacy of Benzbromarone in H... > get substances (2) > 3562-64-3 > get reactions (18)

10 Reactions 0 Selected

1. View Reaction Detail [Link](#)

5 Steps Hover over any structure for more options.

Overview

Steps/Stages:

- 1.1 R:K2CO₃, S:Me₂CO, 2-3 min, rt
- 1.2 2-3 min, rt, 6 h, rt → reflux
- 2.1 S:(HOOCCH₂CH₂)₂O, rt → 130°C
- 2.2 R:NH₄H₂O, 15-20 min, 120-130°C, 10 min, 180-190°C, 190°C → 130°C
- 2.3 R:KOH, 120-130°C, 6 h, 120-130°C
- 3.1 S:CS₂, 3-4 min, 5°C
- 3.2 R:SnCl₄, 5-7 min, 5°C; 3 h, 5°C, 5°C → rt
- 4.1 R:NaSEt, S:DMF, 1 h, 125-130°C
- 4.2 R:NH₄Cl, S:H₂O
- 5.1 R:Bz₂, S:AcOH, 15 min, rt
- 5.2 R:H₂O

Notes

2) Wolff-Kishner reduction; 3) regioselective, sealed tube used; 5) alternative preparation shown; Reactants: 3; Reagents: 6; Solvents: 6; Steps: 5; Stages: 11; Most stages in any one step: 3

References

Developing Potent Human Uric Acid Transporter 1 (URAT1) Inhibitors
By Wempe, Michael F. et al
From Journal of Medicinal Chemistry, 54(8), 2701-2713; 2011
D Full Text

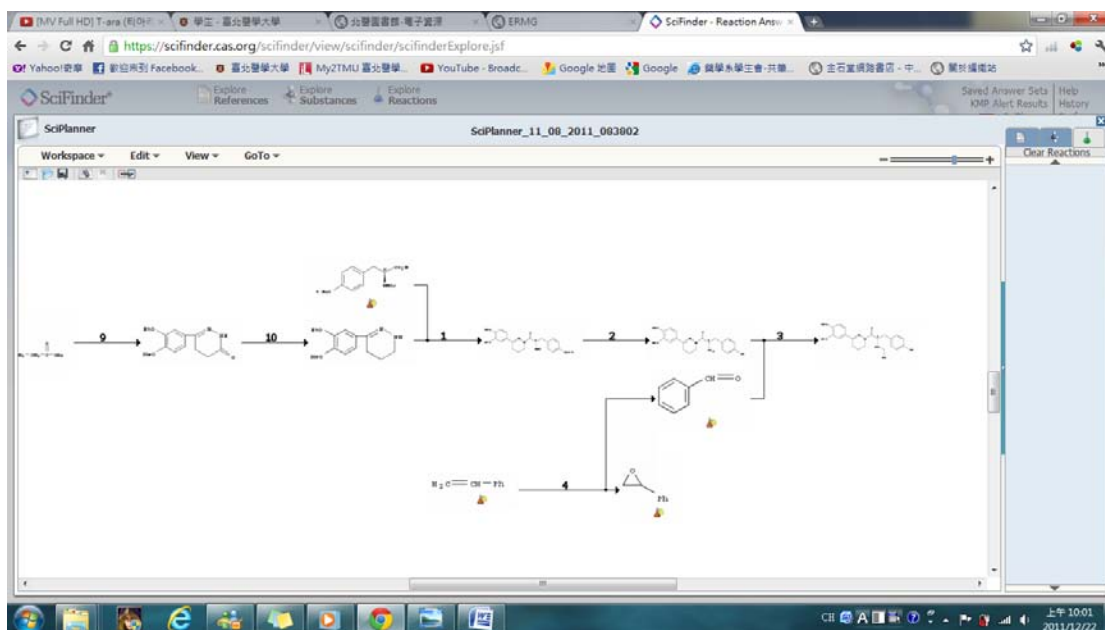
7. 再以相同的方式將其他反應物合成出來，並且在 SciPlanner 裡整理成反應圖

SciPlanner

SciPlanner_11_00_2011_083902

Workspace Edit View GoTo

Reaction scheme showing the synthesis of benzbromarone from 3,4-dihydroxybenzoic acid, acetic anhydride, and 2-bromo-4-chlorobenzoyl chloride.



心得：第一次接觸這個網站的時候覺得相當的新鮮，以往要找某一個藥品或反應的時候總要花相當多的時間在網路上搜尋，自從上過這堂課之後，可以相當輕鬆的找尋到自己想到的反應亦或者是自行編寫反應式，想必以後在撰寫報告的時候會相當依賴這個網站的功能，這次會查詢個藥品 **benzbromarone** 是因為自己本身有在服用這個藥品，之前也有在網路上搜尋一些有關的資訊，大是找來找去東西大多數都是一樣的，而在 **SciFinder** 上面讓我更加認識這個藥品的由來，以及一些有關於它的資訊，真的相當受惠！