



WIPO

WORLD
INTELLECTUAL PROPERTY
ORGANIZATION

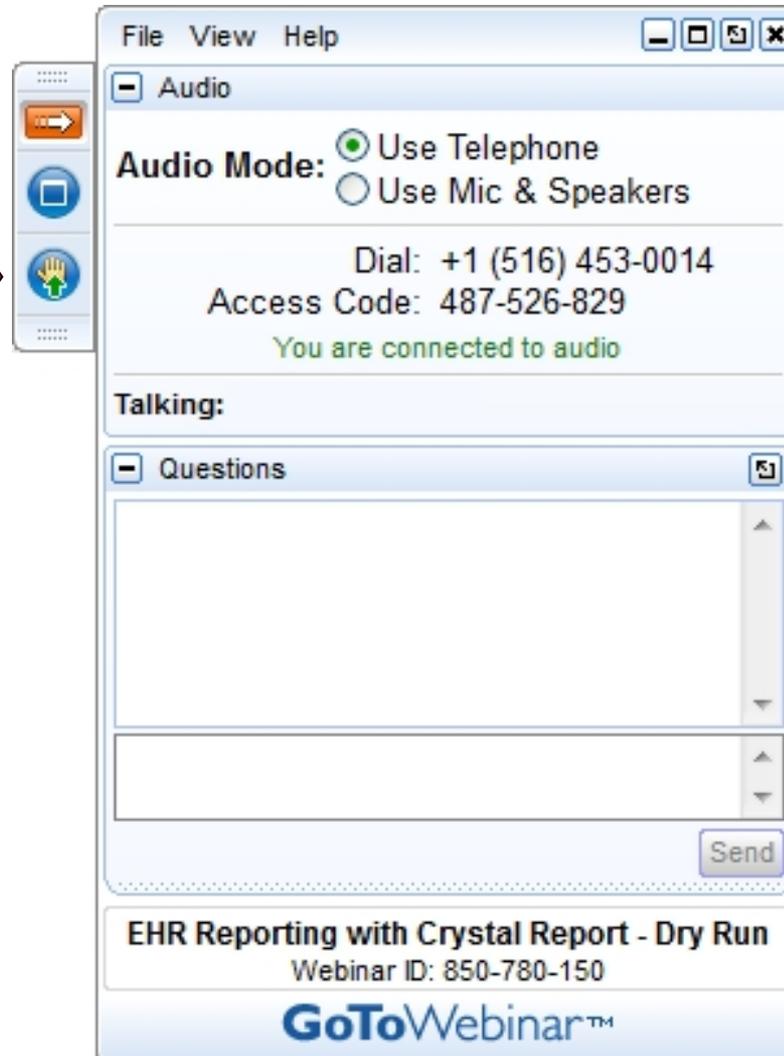
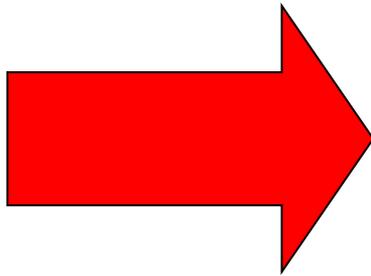


Chemical searches in PATENTSCOPE for and by Experts

Online
24 September
2020



Click this button if you can hear my voice and see my screen



File View Help

Audio

Audio Mode: Use Telephone
 Use Mic & Speakers

Dial: +1 (516) 453-0014
Access Code: 487-526-829
You are connected to audio

Talking:

Questions

Send

EHR Reporting with Crystal Report - Dry Run
Webinar ID: 850-780-150

GoToWebinar™

Agenda

- Introduction
- Indexation process
- Coverage
- Exact compound search
- Substructure search
- Covid-19 searches
- PATENTSCOPE & PubChem
- Conclusion/recommendations
- Q&A - improvement suggestions

To ask questions

The screenshot displays the GoToWebinar control panel. On the left, a vertical toolbar contains several icons: a microphone, a hand, and a question mark. A large red arrow points from the left towards the hand icon, which is also enclosed in a red box. The main window has a menu bar with 'File', 'View', and 'Help'. Below the menu bar, there are two expandable sections: 'Audio' and 'Questions'. The 'Audio' section is expanded, showing options for 'Telephone' and 'Mic & Speakers (test)'. Below these options, a 'MUTED' status is displayed in red text next to a speaker icon and a volume slider. The 'Questions' section is also expanded, showing a text input field with the placeholder text '[Enter a question for staff]' and a 'Send' button. A red box highlights the entire 'Questions' section. At the bottom of the window, there is a 'Webinar Now' section with a 'Webinar ID' field and the 'GoToWebinar' logo. A red arrow points from the bottom towards the 'Send' button.

Experts

- Fanny Irlinger, PhD – InfoChem
- Joseph Eiblmaier, PhD - InfoChem
- Christopher Southan, PhD - TW2Informatics
- Yun Yun Yang, - Bristol-Myers Squibb

WIPO

- Christophe Mazenc - Director of the Global Databases Division WIPO
- Sandrine Ammann, Marketing & Communications Officer, Global Databases Division, WIPO

On the technical side

- Description of the workflow
- Architecture of the solution
- Details on the indexation process
- Recognition accuracy
- CAS numbers indexation

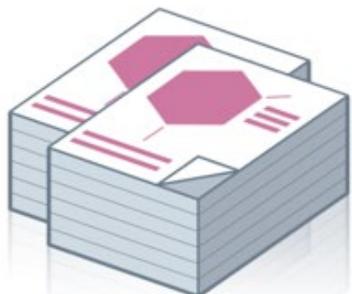
The Concept

(...) At the moment the surgical procedure starts, benzodiazepin, e.g. **diazepam**, is administered in a dose of no more than 5 mg. (...)



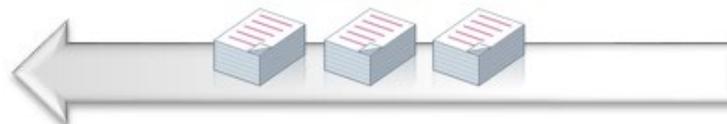
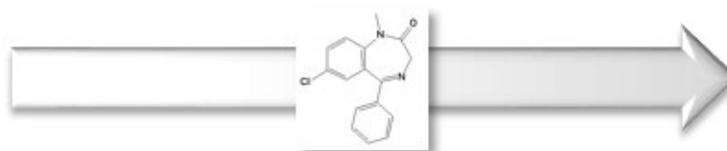
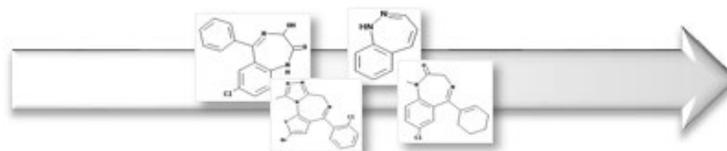
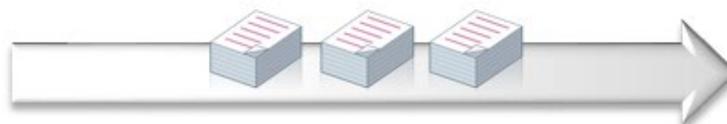
(...) At the moment the surgical procedure starts, benzodiazepin, e.g. **@AAOVKJBEBIDNHE-UHFFFAOYSA-N@**, is administered in a dose of no more than 5 mg. (...)

The workflow



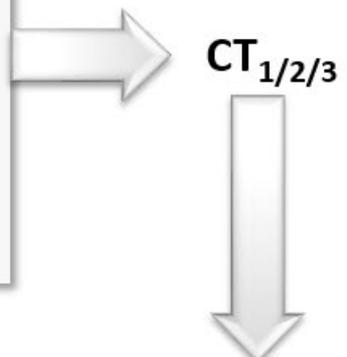
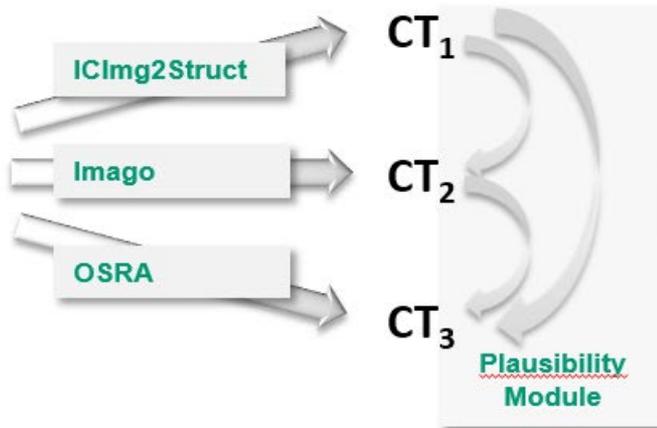
Enriched *PATENTSCOPE* Documents

(...) At the moment the surgical procedure starts, benzodiazepin, e.g. @AAOVKJBEBIDNHE-UHFFFAOYSA-N@, is administered in a dose of no more than 5 mg. (...)

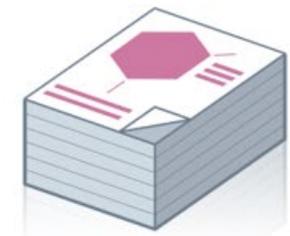
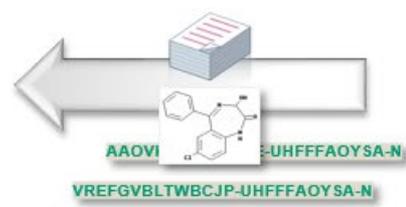


PATENTSCOPE





(...) At the moment the surgical procedure starts, benzodiazepin, e.g. @AAOVKJBEBIDNHE-UHFFFAOYSA-N@, is administered in a dose of no more than 5 mg. (...)



Enriched PATENTSCOPE Documents

Russian patents

- Development a proprietary Russian chemical annotator for ,Rospatent'

Asian patents

- Annotation of Korean, Chinese and Japanese documents:
 - *ChemNameTranslate* by NextMove Software for the initial translation of systematic names
 - Proprietary dictionaries for trade, brand and trivial names including WIPO machine translated names
 - Various filters to reduce the number of false positive annotations

Example in Chinese

尿酸 (uric acid): annotated



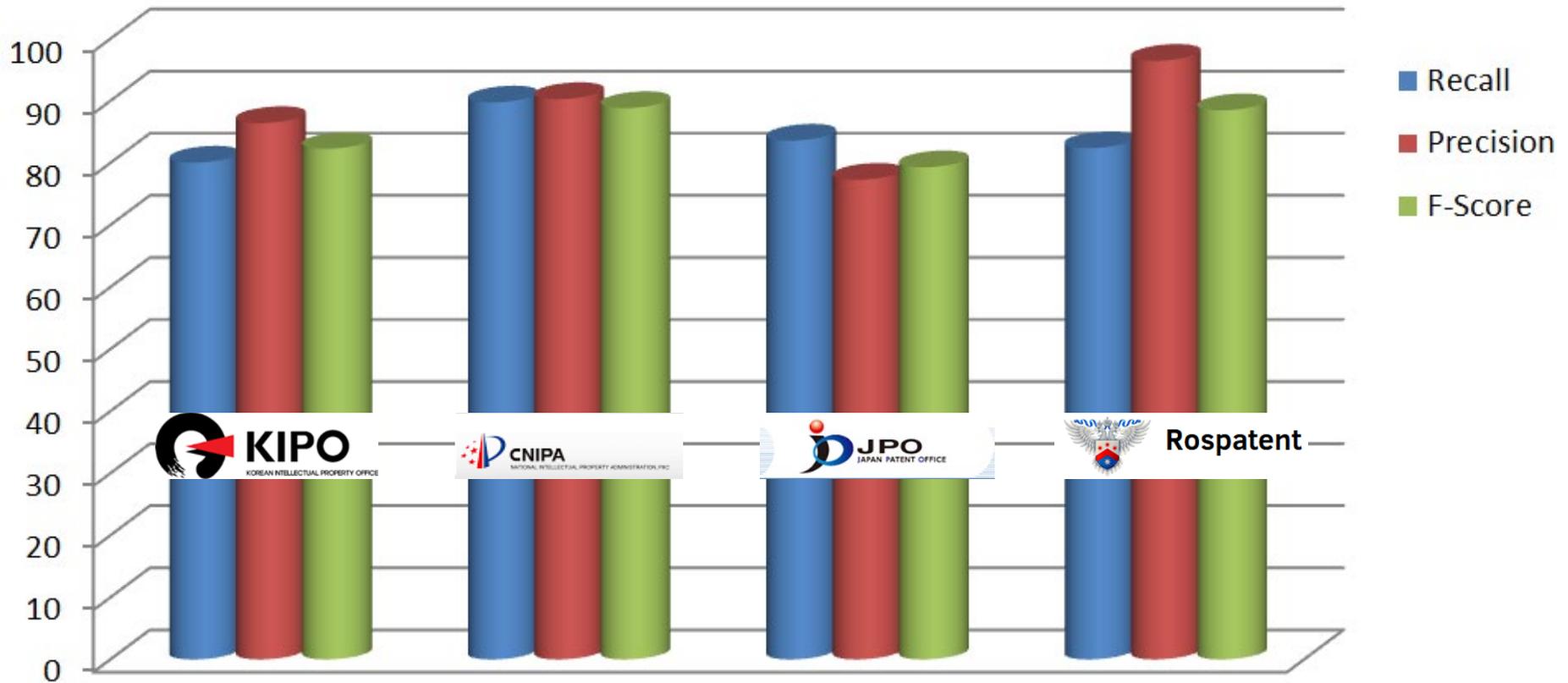
高尿酸血症 (hyperuricemia): not annotated



Quantitative analysis

- Chemists (native speakers): analysis of FP and FN annotations:
 - KO: 14 patents, 2,941 annotations
 - CN: 15 patents, 3,916 annotations
 - JP: 13 patents, 4,352 annotations
 - RU: 12 patents, 18,237 annotations

Quantitative analysis



Coverage - languages

- China [1996 -2020]
- European Patent Office [1978 -2020]
- Eurasian Patent Office [1998 -2020]
- Japan [1993 -2020]
- Republic of Korea [1980 -2020]
- PCT [1979 -2020]
- Russia [1995 -2020]
- United States [1979 -2020]

Updates

- Exact search:
 - 1 to 2 weeks after publication depending on how long it takes to process and index.
- Substructure search:
 - Once every 2 months

IPC codes covered

- A01N
- A01P
- A23J
- A61K
- A61L
- A61P
- A61Q
- B01J
- B01S
- C01B
- C01C
- C01D
- C01F
- C01G
- C06B
- C07B
- C07C
- C07D
- C07F
- C07H
- C07J
- C07K
- C08F
- C08G
- C08J
- C08K
- C08L
- C09B
- C09C
- C09D
- C09J
- C09K
- C10H
- C10L
- C10M
- C10N
- C11D
- C12C
- C12H
- C12M
- C12N
- C12P
- C12Q
- C13B
- C13K
- C14C
- C23C
- C25B
- C40B
- H05B
- G01N
- G03C

Fields searched

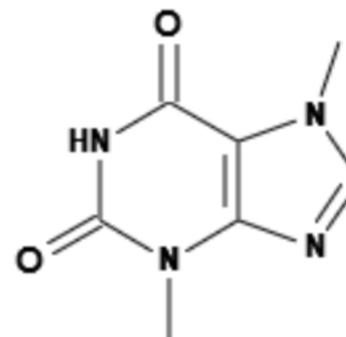
- Title
- Abstract
- Description
- Claim

Exact structure search

- Case study: Theobromine
 - 3 ways to search:
 - structure editor (ICEdit)
 - upload structure
 - convert structure
- Result list
- Patent document
- Tips & tricks
- Scaffold search

Case study: theobromine

- Structure editor (ICEdit)



live demo



Case study: theobromine

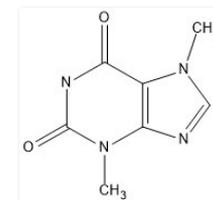
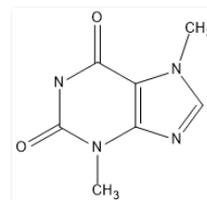
■ Upload structure

CHEMICAL COMPOUNDS SEARCH ▾

Convert structure Structure editor SubStructure **Upload structure**

Select a structure file [MOL] or image file [PNG, GIF, TIFF, JPEG] and upload it. 

- Theobromine.gif
- Theobromine.jpg
- Theobromine.mol**
- Theobromine.png
- Theobromine.tif



Case study: theobromine

■ Convert structure

Convert structure | Structure editor | SubStru

Search type
Compound name

Compound name

INN

InChI

SMILES



IUPAC name	3,7-dimethylpurine-2,6-dione	Ok
CAS names	Xanthine, 3,7-dimethyl-1H-Purine-2,6-dione, 3,7-dihydro-3,7-dimethyl-	Ok Ok
Synonyms	3,7-Dimethylxanthine Diurobromine 3,7-Dimethyl-3,7-dihydro-1H-purine-2,6-dione	Ok not in dictionary Ok
InChI	1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)	Ok
InChI Key	YAPQBXQYLJRXSA-UHFFFAOYSA-N	Ok
SMILES	CN1C=NC2=C1C(=O)NC(=O)N2C	Ok

Results

CHEM:(YAPQBQYLJRXSA-UHFFFAOYSA-N)

31,513 results Offices all Languages all Stemming true Single Family Member false

Sort: Relevance Per page: 100 View: All+Image

1 / 316

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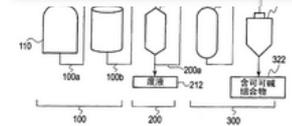
1. [101939321](#) PRODUCTION METHOD AND PRODUCTION DEVICE FOR COMPOSITION HAVING HIGH CONTENT OF THEOBROMINE

Int.Class [C07D 473/10](#) Appl.No 200980104250.7 Applicant Meiji Seika Kaisha Inventor Satoshi Hanamura

Provided is a method for efficiently producing a composition having a high content of theobromine with a simple method. A method for producing a composition containing theobromine is characterized by comprising the steps of: [a] obtaining a crude theobromine extraction liquid through extraction from a plant body containing theobromine or a processed material thereof with a solvent; [b] bringing the crude theobromine extraction liquid into contact with a cation exchange resin which have been replaced with hydrogen ions in advance thereby adsorbing the theobromine onto the cation exchange resin; and subsequently, [c] passing a solvent which does not containing ionic substances through the cation exchange resin thereby obtaining a theobromine extraction liquid.

WIPO Translate

Google Translate

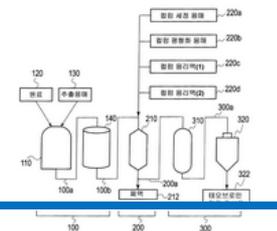


2. [1020100112613](#) METHOD AND APPARATUS FOR PRODUCING THEOBROMINE SOLID-CONTAINING COMPOSITION

Int.Class [C07D 473/10](#) Appl.No 1020107017537 Applicant 메이지 세이카 가부시키가이샤 Inventor 하나무라 사토시

The purpose of the present invention is to provide a method for efficiently preparing a theobromine-containing composition by a simple method. A method for preparing a theobromine-containing composition comprises the steps of: [a] extracting a plant or a processed product containing theobromine as a solvent to obtain a theobromine crude extract; [b] contacting the theobromine crude extract with a hydrogen ion-substituted cation exchange resin to adsorb the theobromine to the cation exchange resin; and [c] passing a solvent which does not include an ionic substance to the cation exchange resin to obtain a theobromine extract.

KR - 19.10.2010



2. KR1020100112613 - 테오브로민 고함유 조성물의 제조 방법 및 제조 장치



National Biblio. Data **Description** Claims Drawings Compounds Documents

PermaLink **Machine translation** ▾

Office
Republic of Korea

Application Number
1020107017537

Application Date
06.02.2009

Publication Number
1020100112613

Publication Date
19.10.2010

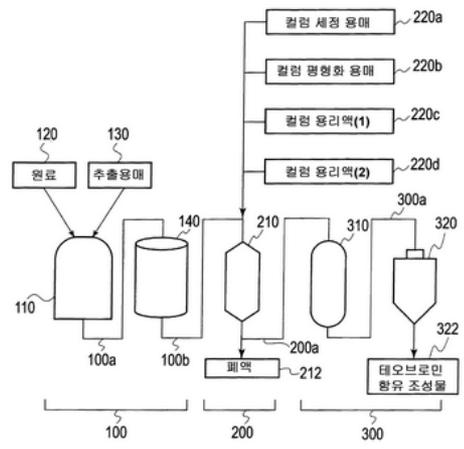
Publication Kind
A

IPC
C07D 473/10 A61K 31/522 A61P 9/08
A61P 25/26

CPC
C07D 473/10

Title
[KO] METHOD AND APPARATUS FOR PRODUCING THEOBROMINE SOLID-CONTAINING COMPOSITION

xxen1



Applicants
메이지 세이카 가부시카이가이샤

Inventors
하나무라 사토시
지카우치 겐
가나자와 시게루
나가 지이치로

Abstract
[KO]
The purpose of the present invention is to provide a method for efficiently preparing a theobromine-containing composition by a simple method. A method for preparing a theobromine-containing composition comprises the steps of: [a] extracting a plant or a processed product containing theobromine as a solvent to obtain a theobromine crude extract; [b] contacting the theobromine crude extract with a hydrogen ion-substituted cation exchange resin to adsorb the theobromine to the cation exchange resin; and [c] passing a solvent which does not include an ionic substance to the cation exchange resin to obtain a theobromine extract.

Also published as
CN101939321 EP2248813 IN3283/KOLNP/2010 JPW02009099221 US20110003834 WO/2009/099221

2. KR1020100112613 - 테오브로민 고함유 조성물의 제조 방법 및 제조 장치

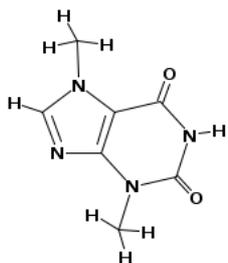


National Biblio. Data Description Claims Drawings **Compounds** Documents

PermaLink

Title Abstract Description Claims

Theobromine



2. KR1020100112613 - 테오브로민 고함유 조성물의 제조 방법 및 제조 장치

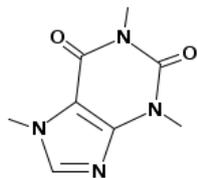
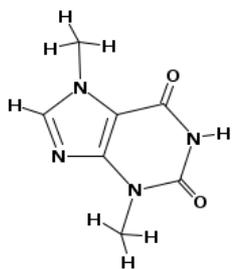


National Biblio. Data Description Claims Drawings Compounds Documents

PermaLink

Title Abstract **Description** Claims

Theobromine



Cl

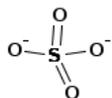
Na⁺

H-O⁻



Na⁺ Cl⁻

Zn²⁺



Highlighting

Result sorting

CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N)



31,613 results Offices all Languages all Stemming true Single Family Member false



Sort: Relevance Per page: 100 View: All+Image

1 / 316

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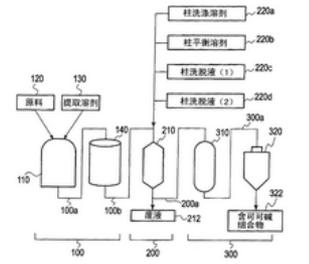
- Relevance
- Pub Date Desc
- Pub Date Asc
- App Date Desc
- App Date Asc

EXTRACTION METHOD AND PRODUCTION DEVICE FOR COMPOSITION HAVING HIGH CONTENT OF THEOBROMINE

Appl.No 200980104250.7 Applicant Meiji Seika Kaisha Inventor Satoshi Hanamura

Efficiently producing a composition having a high content of theobromine with a simple method. A method for producing a composition containing theobromine by comprising the steps of: (a) obtaining a crude theobromine extraction liquid through extraction from a plant body containing theobromine or a plant body containing theobromine with a solvent; (b) bringing the crude theobromine extraction liquid into contact with a cation exchange resin which have been replaced with hydrogen ions in advance with theobromine onto the cation exchange resin; and subsequently, (c) passing a solvent which does not containing ionic substances through the cation exchange resin to obtain a theobromine extraction liquid.

CN - 05.01.2011

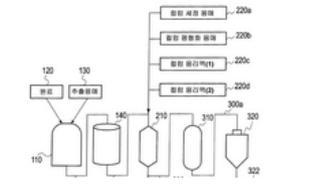


2. 1020100112613 테오브로민 고함유 조성물의 제조 방법 및 제조 장치

Int.Class C07D 473/10 Appl.No 1020107017537 Applicant 메이지 세이카 가부시카가이샤 Inventor 하나무라 사토시

본 발명은, 테오브로민 고함유 조성물을 간편한 방법으로 효율적으로 제조하는 방법의 제공을 목적으로 한다. 테오브로민 함유 조성물의 제조 방법에 있어서, [a] 테오브로민을 함유하는 식물체 또는 그 가공품을 용매로 추출하여, 테오브로민 조추출액을 얻는 공정과, [b] 상기 테오브로민 조추출액, 미리 수소 이온 치환 처리한 양이온 교환 수지에 접촉시켜, 상기 테오브로민을 상기 양이온 교환 수지에 흡착시키는 공정과, [c] 상기 양이온 교환 수지에, 이온성 물질을 포함하지 않는 용매를 통과시켜, 테오브로민 추출액을 얻는 공정을 포함하는 것을 특징으로 한다.

KR - 19.10.2010



Analysis

CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N)



31,513 results Offices all Languages all Stemming true Single Family Member false

Sort: Relevance ▼ Per page: 100 ▼ View: All+Image ▼

< 1/316 >

1. 101939321 PRODUCTION METHOD AND PRODUCTION DEVICE FOR COMPOSITION HAVING HIGH CONTENT OF THEOBROMINE

Int.Class C07D 473/10 ⓘ Appl.No 200980104250.7 Applicant Meiji Seika Kaisha Inventor Satoshi Hanamura

Provided is a method for efficiently producing a composition having a high content of theobromine with a simple method. A method for producing theobromine is characterized by comprising the steps of: [a] obtaining a crude theobromine extraction liquid through extraction from a plant body or processed material thereof with a solvent; [b] bringing the crude theobromine extraction liquid into contact with a cation exchange resin which have been advanced thereby adsorbing the theobromine onto the cation exchange resin; and subsequently, [c] passing a solvent which does not contain ionic exchange resin thereby obtaining a theobromine extraction liquid.

2. 1020100112613 테오브로민 고함유 조성물의 제조 방법 및 제조 장치

Int.Class C07D 473/10 ⓘ Appl.No 1020107017537 Applicant 메이지 세이카 가부시키키가이샤 Inventor 하나무라 사토시

본 발명은, 테오브로민 고함유 조성물을 간편한 방법으로 효율적으로 제조하는 방법의 제공을 목적으로 한다. 테오브로민 함유 조성물의 제조 방법에 하는 식물체 또는 그 가공품을 용매로 추출하여, 테오브로민 조추출액을 얻는 공정과, [b] 상기 테오브로민 조추출액을, 미리 수소 이온 치환 처리한 양

Analysis

ANALYSIS

Close

Filters Charts Timeseries

Countries		Offices		Applicants		Inventors		IPC code		Publication Dates		Filing Dates	
United States of America	10,461	United States of America	13,290	MERCK SHARP & DOHME CORP.	1,362	ZABLOCKI JEFF	170	A61K	25,506	2011	1,829	2011	1,525
PCT	7,443	PCT	7,438	MERCK & CO., INC.	806	MAMMEN MATHAI	132	C07D	15,483	2012	1,636	2012	1,809
Japan	5,617	Japan	5,896	MERCK PATENT GMBH	723	DORSCH DIETER	128	A61P	13,496	2013	1,699	2013	1,634
China	3,430	China	5,310	GENENTECH, INC.	528	KAMBOJ RAJENDER	112	C07C	2,269	2014	1,821	2014	1,553
European Patent Office	2,156	Republic of Korea	3,192	THERAVANCE, INC.	323	ELZEIN ELFATIH	110	A61Q	2,125	2015	1,598	2015	1,571
Republic of Korea	1,674	European Patent Office	2,693	MERCK SHARP & DOHME	295	SUN SHAOYI	105	C07K	1,853	2016	1,655	2016	1,547
Eurasian Patent Organization	468	Canada	1,500	THE PROCTER & GAMBLE COMPANY	291	ZHANG ZAIHUI	102	C12N	1,410	2017	1,691	2017	1,654
Russian Federation	264	India	1,240	TAKEDA PHARMACEUTICAL COMPANY LIMITED	267	LIU SHIFENG	96	A01N	1,203	2018	1,764	2018	1,403
		Eurasian Patent Organization	1,036	HENKEL AG & CO. KGAA	254	KODUMURU VISHNUMURTHY	95	G01N	1,187	2019	1,717	2019	903
		Russian Federation	1,019	F. HOFFMANN-LA ROCHE AG	246	SVIRIDOV SERGUEI	90	A23L	901	2020	1,098	2020	161

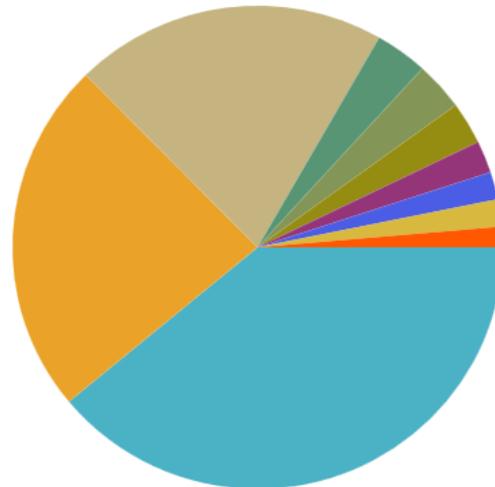
Analysis

ANALYSIS

Close

Filters Charts Timeseries

Countries Offices Applicants Inventors **IPC code** Publication Dates Filing Dates



- A61K
- C07D
- A61P
- C07C
- A61Q
- C07K
- C12N
- A01N
- G01N
- A23L

Customize

Feedback Goto Search ▾ Browse ▾ Tools ▾ **Settings**

SETTINGS

Reset

Close

Save

Query **Office** **Result** Interface Others

Result List Language
Query Language

Result List View
All+Image

Analysis tab open

Analysis type
Table

Analysis graph
Pie

No of Items/Group
10

Group by *

- Countries
- Offices
- Applicants
- Inventors
- IPC code
- CPC codes
- Publication Dates
- Filing Dates

Search by CAS number

■ CAS83-88-5

ADVANCED SEARCH ▾

✓
CHEM:(CAS83x88x5)

Query Assistant [Query Examples](#)

本发明还进一步所述洗手液在日化用品中的应用。

优选的，所述日化用品为洗手巾，所述洗手液吸附于所述洗手巾上。

优选的，所述洗手液通过喷涂或浸泡的方法吸附至所述洗手巾上。

进一步的，所述洗手巾为棉浆纸、木浆纸或无纺布中的一种制成。

本发明中各组分的性质如下：

维生素B1，化学式 $C_{12}H_{16}N_4OS \cdot HCl$ ，为白色晶体，在有氧化剂存在时容易被氧化产生脱氢硫胺素，后者在有紫外光照射时呈现蓝色荧光。

维生素B2，化学式： $C_{17}H_{20}N_4O_6$ ，又叫核黄素，微溶于水，CAS号：83-88-5；为体内黄酶类辅基的组成部分，当缺乏时，就影响机体的生物氧化，使代谢发生障碍。

维生素C，化学式 $C_6H_8O_6$ ，又称L-抗坏血酸，为酸性己糖衍生物，是稀醇式己糖酸内酯，是高等灵长类动物与其他少数生物的必需营养素。

十二烷基硫酸钠，白色或淡黄色粉状，溶于水，对碱和硬水不敏感，CAS号：83-88-5，在日化行业用作乳化剂、灭火剂、发泡剂及纺织助剂，主要用作牙膏和膏状、粉状、洗发香波的发泡剂。

丙三醇，俗称甘油，是无色味甜澄明黏稠液体，无臭、有暖甜味，CAS号：56-81-5，在日化行业可用作软化剂、润滑剂或塑化剂。可与水以任何比例互溶，低浓度丙三醇溶液可做润滑油对皮肤进行滋润。

羧甲基纤维素钠，又名羧甲基纤维素钠盐，为白色纤维状或颗粒状粉末。无臭、无味、无味、有吸湿性，不溶于有机溶剂。CAS号：9004-32-4，在日用化学工业中用作黏结剂、抗再沉凝剂。

羊毛脂，是附着在羊毛上的一种分泌油脂，为淡黄色或棕黄色的软膏状物；有黏性而滑腻；臭微弱而特异。CAS号：8006-54-0，羊毛脂在氯仿或乙醚中易溶，在热乙醇中溶解，在乙醇中极微溶解。日用化学工业制造防裂膏、冷霜、高级香皂，对保护皮肤防止裂口具有特殊的效能。

硬脂酸钠，又名十八酸钠，为白色细微粉末或块状固体，CAS号：822-16-2，有滑腻感，有脂肪味，在空气中有吸水性。微溶于冷水，溶于热水或醇溶液，水溶液因水解而呈碱性。在日用化学工业中用作洗涤剂，用于控制漂洗过程中的泡沫。

本发明的有益效果为：

Combine with applicant

ADVANCED SEARCH ▼

☑ Please enter a valid field... [for use UP/DOWN keys, and TAB or ENTER to select]

CHEM:(BSYNYRMUTXBXSQ-UHFFFAOYSA-N) AND app

Applicant Address

Applicant Address Country

Applicant All Data

Applicant Name

Applicant Nationality

Applicant Residence

Application Date

Application Number

Main Applicant Name

National Phase Application Number

ADVANCED SEARCH ▾



CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND PA:novartis

Query Assistant [Query Examples](#)

1. WO2003033001 - COMBINATIONS COMPRISING COX-2 INHIBITORS AND ASPIRIN

PCT Biblio. Data	Description	Claims	National Phase	Notices	Compounds	Documents
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Latest bibliographic data on file with the International Bureau

[PermaLink](#) [Machin](#)

Publication Number

WO/2003/033001

Publication Date

24.04.2003

International Application No.

PCT/EP2002/011380

International Filing Date

10.10.2002

Chapter 2 Demand Filed

13.03.2003

IPC

[A61K 31/365 \[2006.01\]](#)

[A61K 31/415 \[2006.01\]](#)

[A61K 31/60 \[2006.01\]](#)

[A61K 45/06 \[2006.01\]](#)

[View more classifications](#)

Applicants

NOVARTIS AG [CH/CH]; Lichtstasse 35 CH-4056
Basel, CH [AE, AG, AL, AM, AU, AZ, BA, BB, BE, BG,
BR, BY, BZ, CA, CH, CN, CO, CR, CU, CY, CZ, DE, DK,
DM, DZ, EC, EE, ES, FI, FR, GB, GD, GE, GH, GR, HR,
HU, ID, IE, IL, IN, IS, IT, JP, KE, KG, KP, KR, KZ, LC,
LK, LT, LU, LV, MA, MC, MD, MK, MN, MX, NL, NO, NZ,
OM, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN,

Title

[EN] COMBINATIONS COMPRISING COX-2 INHIBITORS AND ASPIRIN

[FR] COMBINAISONS CONTENANT UN INHIBITEUR DE COX-2 ET DE L'ASPIRINE

Abstract

[EN]

A pharmaceutical composition is provided for treatment of conditions in mammals which are responsive to COX-2 inhibition which comprises COX-2 inhibitor and low-dose aspirin for simultaneous, sequential or separate use.

[FR]

L'invention se rapporte à une composition pharmaceutique utile dans le traitement d'états chez les mammifères qui sont réceptifs à l'inhibition de la COX-2, comprenant à la fois un inhibiteur de COX-2 et de l'aspirine faiblement dosée pour une utilisation simultanée, séquentielle ou séparée.

Also published as

[N020041432](#) [MXPA/a/2004/003365](#) [KR1020040044891](#) [VN9290](#) [ZA2004/01302](#) [IL160620](#) [EP1435968](#) [JP2005505606](#) [US20040235802](#) [US20040235802](#) [US20040235802](#) [CN1625405](#) [CA2458981](#) [NZ532158](#) [AU2002342814](#) [AU2006249254](#) [ID039.128](#)

It has been proposed to treat a condition selected from the group consisting of acute coronary ischemic syndrome, thrombosis, thromboembolism, thrombotic and first or subsequent thrombotic stroke, in a patient having the condition, comprising administering to the patient a therapeutically effective amount of an antiplatelet agent and a therapeutically effective amount of a COX-2 inhibitor [US Patent No. 6,136,804; Merck]. This combination therapy is stated to provide enhanced treatment options as compared to administering the antiplatelet agent alone. Aspirin is identified as an antiplatelet agent that may be used in this combination therapy and recommended for use at dosages generally in the range of 75 to 325 mg per day. It is found, in accordance with the present invention, that diseases involving platelet aggregation, such as those identified above, may be treated or avoided during treatment with a COX-2 inhibitor administered in combination with aspirin at dosages as described above and furthermore that particular advantageous results are obtained if a 5-alkyl-2-substituted salicylic acid is used in combination with aspirin as antiplatelet inhibitor.

Accordingly the present invention provides a pharmaceutical composition comprising a COX-2 inhibitor and low-dose aspirin, for simultaneous or sequential administration. Further the invention provides the use of a COX-2 inhibitor for the treatment of conditions in mammals which are responsive to COX-2 inhibition.

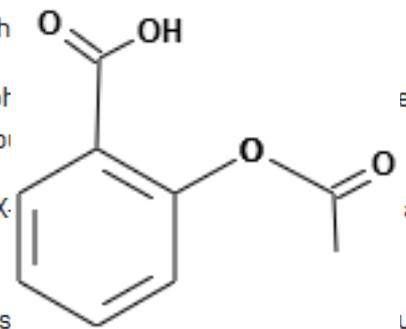
In a further embodiment the invention provides the use of a COX-2 inhibitor in combination with low-dose aspirin.

Yet further the invention provides use of low-dose aspirin to treat acute coronary ischemic syndrome, thrombosis, thromboembolism, thrombotic occlusion and myocardial infarction, and first or subsequent thrombotic stroke, in a patient having the condition, when the low-dose aspirin is administered in combination with an effective amount of a COX-2 inhibitor. Aspirin is administered together with the COX-2 inhibitor for cardio-protection, e.g. in view of the anti-platelet aggregation activity of aspirin.

In the present description the term "treatment" includes both prophylactic or preventative treatment as well as curative or disease modifying treatment, including treatment of patients suspected to have contracted the disease as well as ill patients. In preferred embodiments of the invention "treatment" comprises primary or secondary prevention.

The invention is generally applicable to the treatment of conditions in mammals which are responsive to COX-2 inhibition. For instance, for the treatment of cyclooxygenase-2 mediated inflammation, pyresis, pain, osteoarthritis, rheumatoid arthritis, migraine headache, neurodegenerative diseases [such as multiple sclerosis], Alzheimer's disease, and cancer. COX-2 inhibitors are further useful for the treatment of neoplasia particularly neoplasia that produce prostaglandins or express cyclooxygenase, including both benign and cancerous tumors, growths and polyps. COX-2 inhibitors may be employed for the treatment of any neoplasia as for example in US Patent Publication No. WO 98/16227, published 23 April 1998, in particular epithelium cell-derived neoplasia. COX-2 inhibitors are in particular useful for the treatment of breast cancer and, especially gastrointestinal cancer, for example cancer of the colon, and skin cancer, for example squamous cell or basal cell cancers and melanoma.

The compositions, uses and methods of the present invention represent an improvement to existing therapy of conditions in mammals which are responsive to COX-2 inhibition.



Accordingly the present invention provides a pharmaceutical composition comprising a COX-2 inhibitor and low-dose aspirin, for simultaneous or sequential administration. Further the invention provides the use of a COX-2 inhibitor for the treatment of conditions in mammals which are responsive to COX-2 inhibition. In a further embodiment the invention provides the use of a COX-2 inhibitor in combination with low-dose aspirin. Yet further the invention provides use of low-dose aspirin to treat acute coronary ischemic syndrome, thrombosis, thromboembolism, thrombotic occlusion and myocardial infarction, and first or subsequent thrombotic stroke, in a patient having the condition, when the low-dose aspirin is administered in combination with an effective amount of a COX-2 inhibitor. Aspirin is administered together with the COX-2 inhibitor for cardio-protection, e.g. in view of the anti-platelet aggregation activity of aspirin.

Combine with keyword/dates/IPC

✓
CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND EN_ALL: antipyretic

✓
CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND EN_ALL:(antipyre* OR analg*)

✓
CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND (AD:2018 OR PD:2018)

✓
CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND DP: [2018 TO 2019]

✓
CHEM:(BSYNRYMUTXBXSQ-UHFFFAOYSA-N) AND IC:C01

Combine with a country

REFINE OPTIONS

Close

Search

Offices

All

- All
- PCT
- Africa
 - African Regional Intellectual Property Organization [ARIPO]
- ARABPAT
 - Egypt
 - Saudi Arabia
- Americas
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- LATIPAT
 - Argentina
 - Colombia
 - Dominican Republic
- Kenya
- Jordan
- Tunisia
- United States of America
- Brazil
- Costa Rica
- Ecuador
- South Africa
- Morocco
- Chile
- Cuba
- El Salvador

Combine 2 compounds

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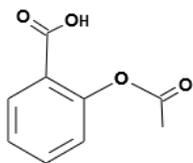
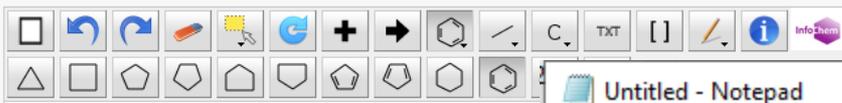
Structure editor

SubStructure

Upload structure

Search type
Compound name

Type an accepted name, commercial name, CAS name, IUPAC name
aspirin|



Untitled - Notepad

File Edit Format View Help

BSYNRYMUTXBXSQ-UHFFFAOYSA-N |

InChI: InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h

InChIKey: BSYNRYMUTXBXSQ-UHFFFAOYSA-N

Molecular Formula: C9H8O4

Molecular Weight: 180.1598 G/mol

Search for scaffold

Offices

All

The present invention relates to orally disintegrating tablets, useful in particular for the treatment of pain, comprising a fixed dose combination of acetylsalicylic acid, acetaminophen, caffeine and corresponding manufacturing processes.

In an effort to develop more convenient dosage forms with an increased likelihood of improved compliance for certain product indications and patient populations, solid dosage forms are developed that can be ingested simply by placing them in the oral cavity, e.g. on the tongue. The products are designed to disintegrate rapidly on contact with saliva, thus eliminating the need to chew the tablet, swallow an intact tablet, or take the tablet with any liquids [7, 8, 9].

A fixed dose combination is a pharmaceutical preparation which contains one or more active pharmaceutical ingredients combined in a single dosage form presented in certain fixed doses. Typically, these fixed dose combination drug products offer benefits over the individually dosed single dose preparations, e.g. efficacy, dose reduction, ease of administration, safety, convenience, compliance.

A known fixed dose combination for the treatment of pain is the triple combination of acetylsalicylic acid, acetaminophen and caffeine. A triple combination of the above ingredients is also listed as a drug product with specifications within USP 31; the monograph is entitled "Acetaminophen, Aspirin and Caffeine Tablets"

[1]-

Acetylsalicylic acid, also known as aspirin (USAN), is 2[acetoxy]benzoic acid, C₉H₈O₄, with a molecular mass of 180.157. Acetylsalicylic acid is slightly soluble in water, freely soluble in alcohol and soluble in chloroform and ether in air but hydrolyses in contact with moisture to acetic and salicylic acids. Its pK_a-value is 3.49. Acetylsalicylic acid exhibits:

Acetylsalicylic acid has a slightly bitter and pronounced acidic taste. Acetylsalicylic acid is used as an analgesic to relieve pain and inflammation. Due to its anti-clotting effect, acetylsalicylic acid (aspirin) is also indicated in long-term

Acetaminophen (USAN), also termed paracetamol, is N-[4-hydroxyphenyl]acetamide, C₈H₉NO₂, with a molecular mass of 151.15. Acetaminophen is sparingly soluble in water, soluble 1 in 20 of boiling water, and in 1 in 10 of alcohol. The compound is very slightly soluble in ether and in methylene chloride. Its pK_a-value is 9.38. The compound has a pronounced bitter taste. The drug substance is widely used as analgesic compound and antipyretic medication. In combination with non-steroidal anti-inflammatory drugs or opioid analgesics, acetaminophen is used also in the management of more severe pain [2].

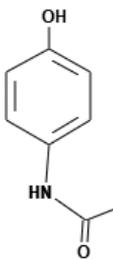
Caffeine, which is 1,3,7-trimethyl-1H-purine-2,6[3H,7H]-dione, C₈H₁₀N₄O₂, with a molecular mass of 194.19 g/mol. Caffeine, CAS 58-08-2, appears as odourless, white needles or powder, which sublime readily. Caffeine is sparingly soluble in water and freely soluble in boiling water and in chloroform. Caffeine is slightly soluble in dehydrated alcohol and in ether. Its pK_a-value is in the order of 0.6. The compound has a pronounced, long lasting, distinct bitter taste [2].

Drug products comprising these active ingredients in a certain ratio are known for decades, e.g. in 1946 Germany's Dr. Karl Thomae GmbH developed Thomapyrin[®] and Bristol-Myers Squibb introduced its Excedrin[®] Extra Strength within the United States within the early 60ties. Both products are non-prescription, over-the-counter pain relievers [3, 4].

The current German Thomapyrin[®] drug product (Thomapyrin[®] classic) comprises 250 mg acetylsalicylic acid, 200 mg acetaminophen and 50 mg caffeine. The current marketed drug product is formulated as an immediate release tablet.

Immediate release Excedrin Extra Strength for the US market comprises 250 mg acetylsalicylic acid, 250 mg acetaminophen and 65 mg caffeine. In contrast to the European product, the US preparation contains slightly higher drug substance loads for acetaminophen and caffeine, i.e. 50 mg and 15 mg, respectively. In addition, the US product is formulated as film-coated tablet instead of a plain tablet.

Paracetamol



salicylic acid, CAS 50-78-2, appears as colourless or white crystals or white powder. Salicylic acid should be stored in airtight containers. The compound is stable in air but hydrolyses in contact with moisture to acetic and salicylic acids. Its pK_a-value is 3.49. Acetylsalicylic acid exhibits:

Acetylsalicylic acid has a slightly bitter and pronounced acidic taste. Acetylsalicylic acid is used as an analgesic to relieve pain and inflammation. Due to its anti-clotting effect, acetylsalicylic acid (aspirin) is also indicated in long-term

Acetaminophen (USAN), also termed paracetamol, is N-[4-hydroxyphenyl]acetamide, C₈H₉NO₂, with a molecular mass of 151.15. Acetaminophen is sparingly soluble in water, soluble 1 in 20 of boiling water, and in 1 in 10 of alcohol. The compound is very slightly soluble in ether and in methylene chloride. Its pK_a-value is 9.38. The compound has a pronounced bitter taste. The drug substance is widely used as analgesic compound and antipyretic medication. In combination with non-steroidal anti-inflammatory drugs or opioid analgesics, acetaminophen is used also in the management of more severe pain [2].

Restrict to the *claims* field

- CHEM:((BSYNRYMUTXBXSQ-UHFFFAOYSA-N BEFORE1000 description) AND (claims BEFORE1000 BSYNRYMUTXBXSQ-UHFFFAOYSA-N))

Sub-structure search

1. Search from a structure

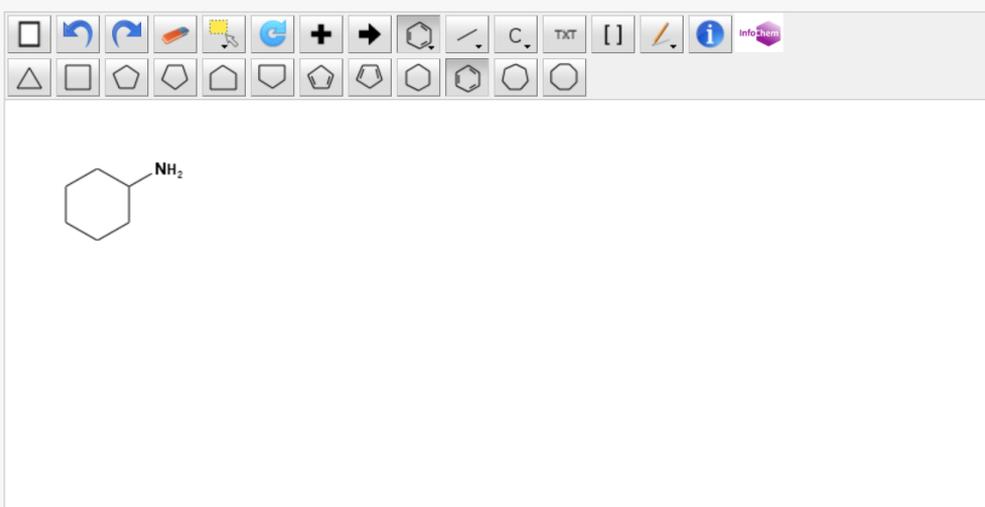
- ✓ Draw the structure in the editor (ICEdit) or
- ✓ Upload the structure from a MOL file or from an image in format PNG, GIF, TIFF or JPEG

✓ E.

- Choose „Exact Structure Search“ or „Substructure Search“

CHEMICAL COMPOUNDS SEARCH ▾

Convert structure Structure editor SubStructure Upload structure



The screenshot shows the IChemTools chemical editor interface. The main window is titled "CHEMICAL COMPOUNDS SEARCH" with a dropdown arrow. Below the title are four tabs: "Convert structure", "Structure editor" (which is selected and highlighted in blue), "SubStructure", and "Upload structure". The "Structure editor" tab contains a toolbar with various icons for drawing and editing. Below the toolbar is a large white canvas where the chemical structure of cyclohexylamine is displayed. The structure consists of a six-membered carbon ring (cyclohexane) with an amino group (-NH₂) attached to one of the carbons.

By Exact Structure Search:

CHEM:(PAFZNILMFXTMIY-UHFFFAOYSA-N)

 64,256 results Offices all Languages en Stemming true Single Family Member false

Sort: Relevance ▼ Per page: 10 ▼ View: All ▼ < 1 / 6,426 >

By substructure Search:

CHEMICAL COMPOUNDS SEARCH ▼

[Convert structure](#) [Structure editor](#) [SubStructure](#) [Upload structure](#)

Substructure search results [35417 + 8%]

[1 of 1476] << < < 1 2 3 4 5 6 7 8 9 10 > >> 24 ▼

Substructure Search: advanced chemistry using Editor

✓ List/not list of atoms

- Edit Atom
- Delete Atom
- Expand Superatom
- Contract Superatom



Dialog box: Edit Atom Properties

Atom properties | Query atom

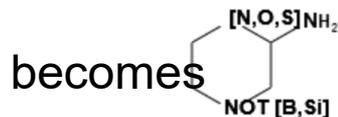
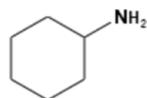
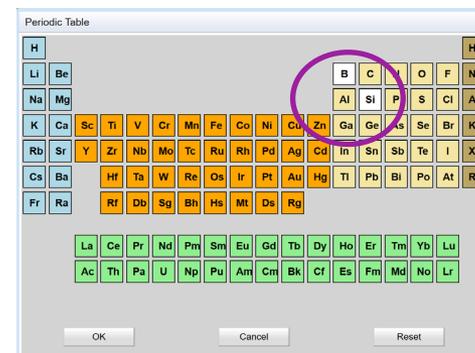
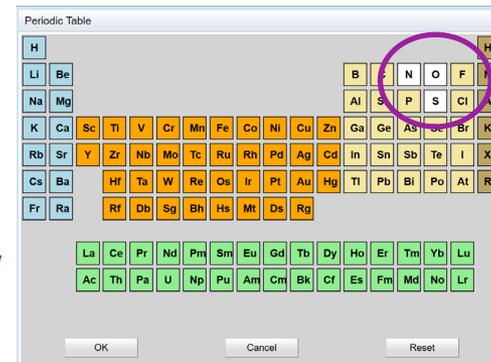
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Reaction Stereo: off | Reaction center: off | NOTList

No Implicit Hydrogens Unsaturated atom Exact change Chain atom

Exact valence Aromatic atom Ring atom

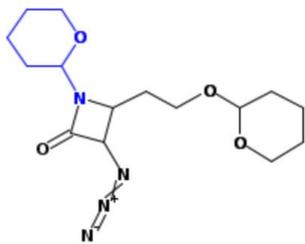
OK Cancel



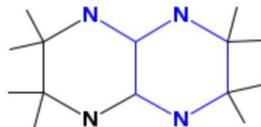
Results:

Substructure search results [2096 + 7%]

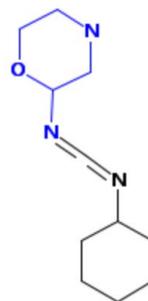
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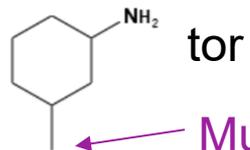


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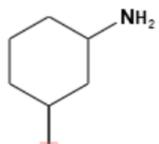


Substructure Search: advanced chemistry

✓ Query atom: atom in a ring



for **Must be a part of a ring**

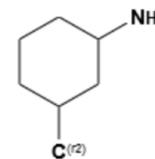


- Edit Atom
- Delete Atom
- Expand Superatom
- Contract Superatom

Edit Atom Properties

Atom properties		Query atom	
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<input type="checkbox"/> Exact valence	<input type="checkbox"/> Aromatic atom	<input type="checkbox"/> Ring atom	

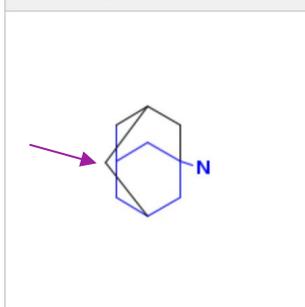
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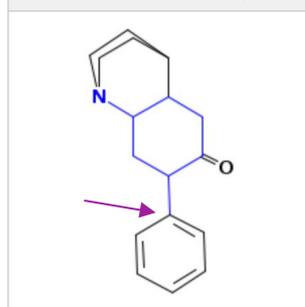
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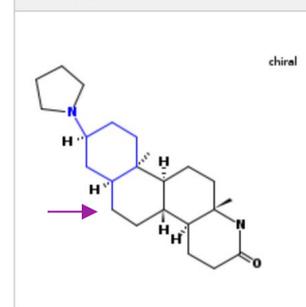
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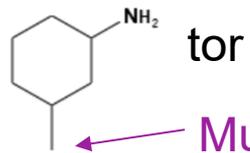


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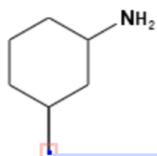


Substructure Search: advanced chemistry

✓ Query atom: atom not in a ring



Must not be a part of a ring

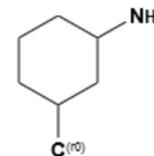


- Edit Atom
- Delete Atom
- Expand Superatom
- Contract Superatom

Edit Atom Properties

Atom properties		Query atom	
Substitution count: off	Ring bond count: 0	List	
Reaction Stereo: off	Reaction center: off	NOTList	
<input type="checkbox"/> No Implicit Hydrogens	<input type="checkbox"/> Unsaturated atom	<input type="checkbox"/> Exact change	<input type="checkbox"/> Chain atom
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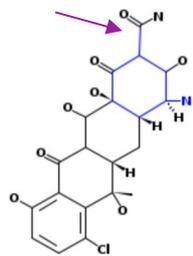
OK Cancel



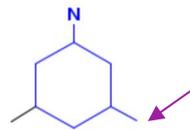
Results:

Substructure search results [3645 + 9%]

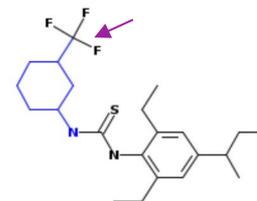
AEWBTXVSKVPUJW-CFMKLNKWSA-N



AUVPFHDQSZJPSZ-UHFFFAOYSA-N

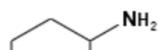


AVHQPCVKVHJRIT-UHFFFAOYSA-N



Substructure Search: advanced chemistry using Editor

✓ Query atom: number of substituents (non-H)

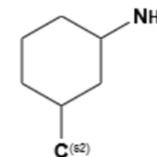


Edit Atom
Delete Atom
Expand Superatom
Contract Superatom

Edit Atom Properties

Atom properties		Query atom		
Substitution count:	2	Ring bond count:	off	List
Reaction Stereo:	off	Reaction center:	off	NOTList
<input type="checkbox"/> No Implicit Hydrogens	<input type="checkbox"/> Unsaturated atom	<input type="checkbox"/> Exact change	<input type="checkbox"/> Chain atom	
<input type="checkbox"/> Exact valence	<input type="checkbox"/> Aromatic atom	<input type="checkbox"/> Ring atom		

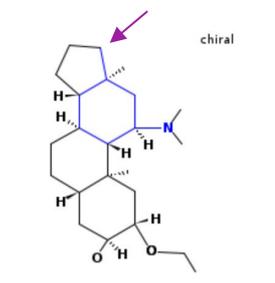
OK Cancel



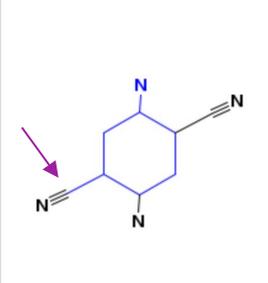
Results:

Substructure search results [7554 + 8%]

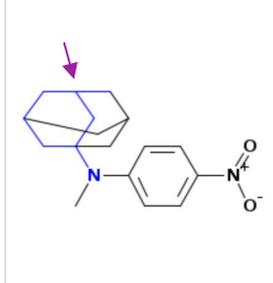
AWMMUVLEYJPGHQ-YGDUABNKSA-N



BENDKXSZMBYLJ-UHFFFAOYSA-N



BOXZZWSXGSWNCV-UHFFFAOYSA-N



Substructure Search: advanced chemistry using Editor

✓ Query atom: specific ring bond attachment and specific number of substituents (

Edit Atom Properties

Atom properties | Query atom

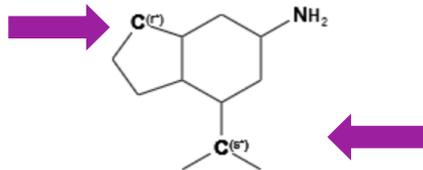
Substitution count: off | Ring bond count: * | List

Reaction Stereo: off | Reaction center: off | NOTList

No Implicit Hydrogens Unsaturated atom Exact change Chain atom

Exact valence Aromatic atom Ring atom

OK Cancel



Edit Atom Properties

Atom properties | Query atom

Substitution count: * | Ring bond count: off | List

Reaction Stereo: off | Reaction center: off | NOTList

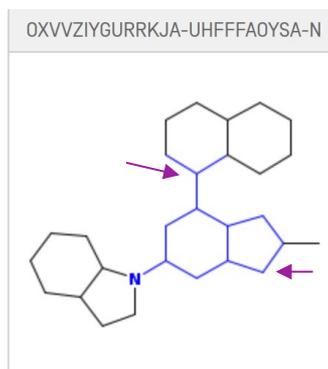
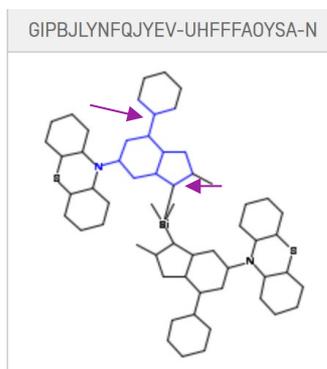
No Implicit Hydrogens Unsaturated atom Exact change Chain atom

Exact valence Aromatic atom Ring atom

OK Cancel

Results:

Substructure search results [2 + 29%]

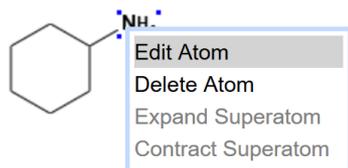


Substructure Search: advanced chemistry using Editor

✓ Query atom: other options

❖ Specific isotope

❖ Explicit valence



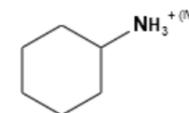
c charge



Dialog box: Edit Atom Properties

Atom properties		Query atom	
Charge:	+1	Radical:	off
Isotope:	off	Valence:	4

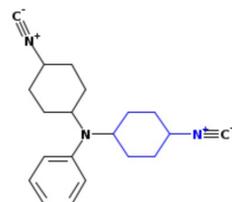
Buttons: OK, Cancel, P-Table



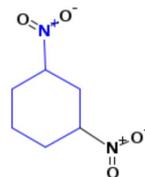
Results:

Substructure search results [2514 + 11%]

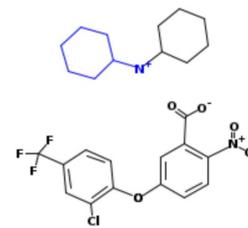
AZJMFK0BJHJPMU-UHFFFAOYSA-N



BFIIVLA0DBYZJC-UHFFFAOYSA-N



BQEUDM0PQTVVGG-UHFFFAOYSA-N



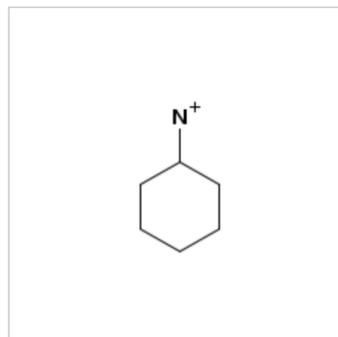
Results: Exact Structure Search

CHEM:(PAFZNILMFXTMIY-UHFFFAOYSA-O)

 60 results Offices all Languages en Stemming true Single Family Member false

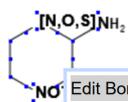
Sort: Relevance ▼ Per page: 10 ▼ View: All ▼

Title Abstract Description



Substructure Search: advanced chemistry using Editor

✓ Bonds: single/double (or other available options)



- Edit Bonds
- Edit Atoms
- Duplicate Object(s)
- Copy
- Paste
- Create Superatom
- Create Chiral Flag
- Group
- Ungroup
- Create No-Structure
- Expand Superatoms
- Contract Superatoms



Edit Bond Properties

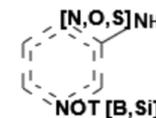
Bond Type:
Triple
Coordinative
Up
Down
Either
Double Either
Aromatic
Any
Single/Double
Single/Aromatic

Reacting Center: None

Topology: None

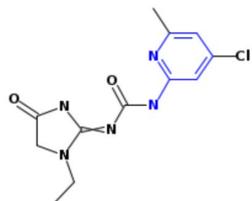
Thickness: 1

OK Cancel

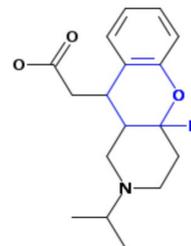


Substructure search results [23763 + 5%]

ACWXZXPINVYDGH-UHFFFA0YSA-N



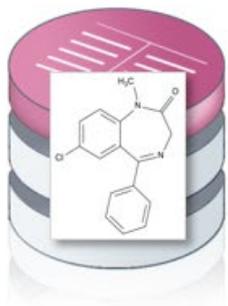
ADCSTDFXGTUKJQ-UHFFFA0YSA-N



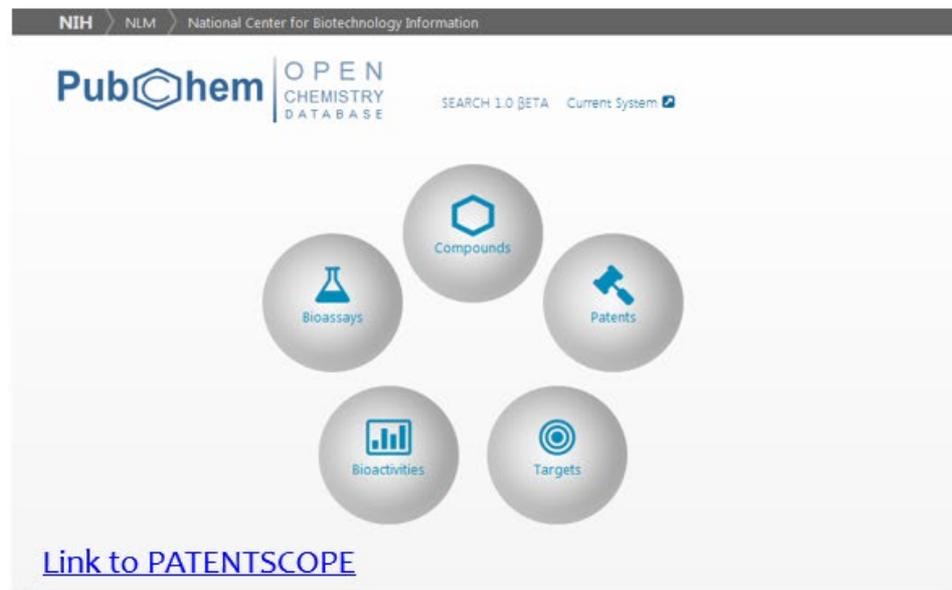
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