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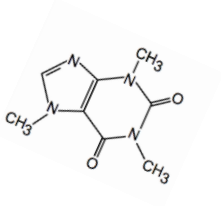
Chemical Compound Search in PATENTSCOPE

SCP, December 13, 2016

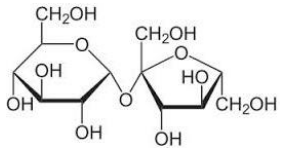
Paul Halfpenny
Senior Administrator, Office of the Assistant Director General

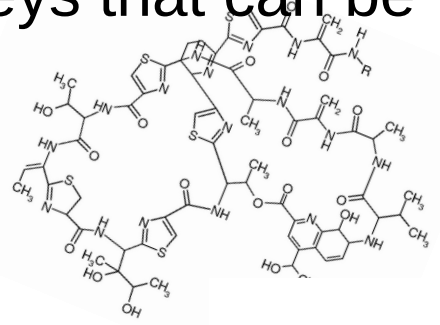
Search chemical compounds

Principle:



- Recognize chemical compounds in patent texts and from embedded drawings included in patent texts
- Standardize all the different representations of chemical structures into Inchikeys and annotate the document
- Implement search functions for Inchikeys that can be used by non chemists

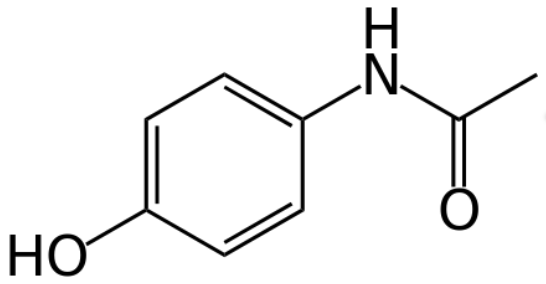




Common Search Phrases

IUPAC name

N-(4-hydroxyphenyl)acetamide



RZVAJINKPMORJF-UHFFFAOYSA-N

INN

paracetamol

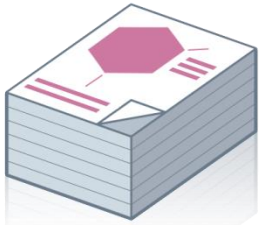
Other names

Acetaminophen, panadol, tylenol, …

Addition of InchiKey Annotation

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

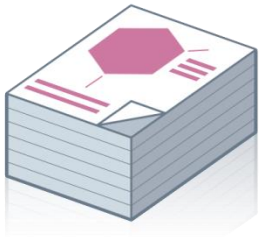
(…) At the moment the surgical procedure starts, benzodiazepin, e.g. @AAOVKJBEBIDNHE-UHFFFAOYSA-N@, is administered in a dose of no more than 5 mg. (…)



PATENTSCOPE Documents

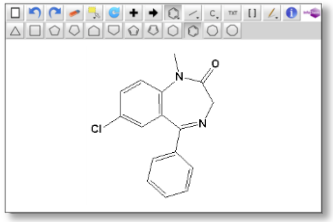
(…) At the moment the surgical procedure starts, benzodiazepin, e.g. diazepam, is administered in a dose of no more than 5 mg. (…)

IC ANNOTATOR



Enriched PATENTSCOPE Documents

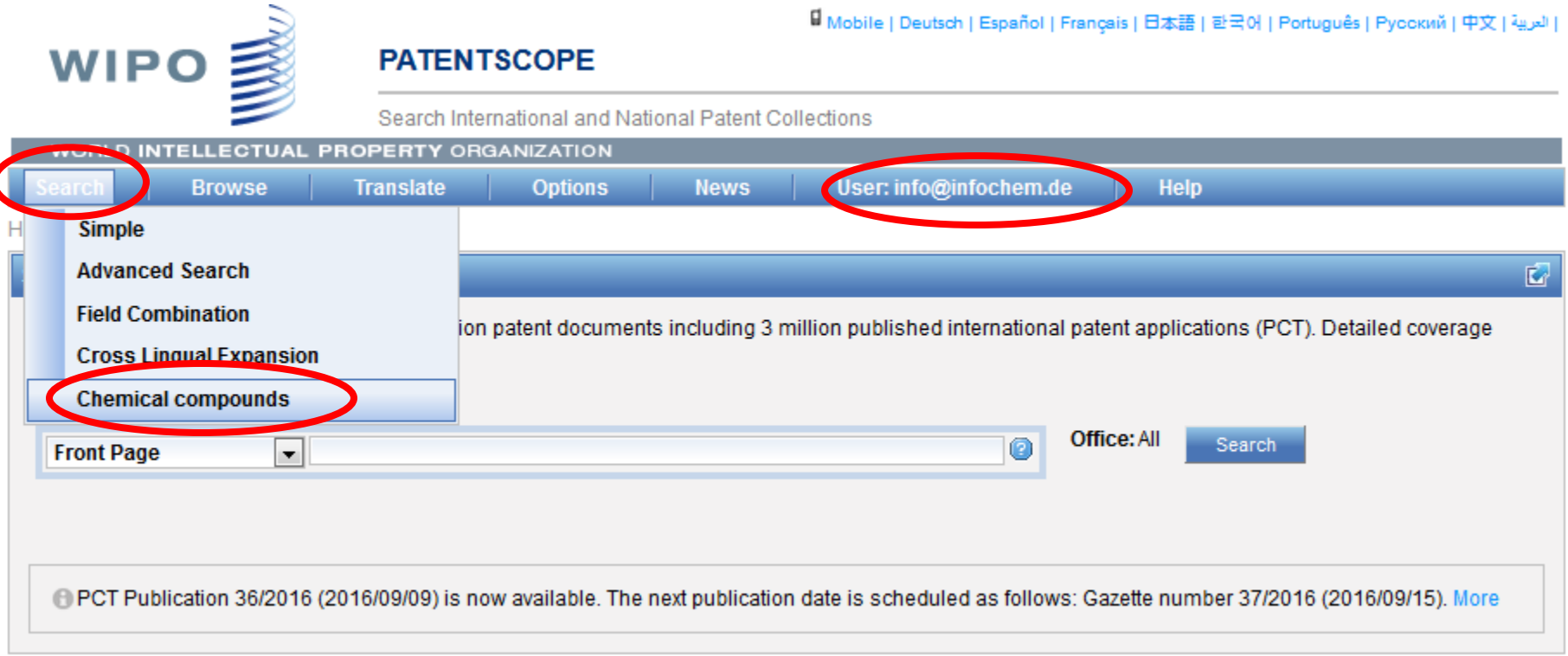
(…) At the moment the surgical procedure starts, benzodiazepin, e.g. @AAOVKJBEBIDNHE-UHFFFAOYSA-N@, is administered in a dose of no more than 5 mg. (…)



AAOVKJBEBIDNH
E-UHFFFAOYSA-N

Access only with a PATENTSCOPE account

How does it work?



How does it work?

Example 1: Theobromine

- Its chemical formula is $C_7H_8N_4O_2$ and IUPAC name:

3,7-dimethyl-1*H*-purine-2,6-dione

- Theobromine is found in the seeds of the plant *Theobroma Cacao*, which is the well-known source of chocolate and cocoa.

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PATENTSCOPE

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Chemical compounds search

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Structure editor | **Convert structure** | Upload structure

Compound name: Theobromine

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Search for scaffold: ☐ **Office:** All Specify ⇨

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Chemical compounds search

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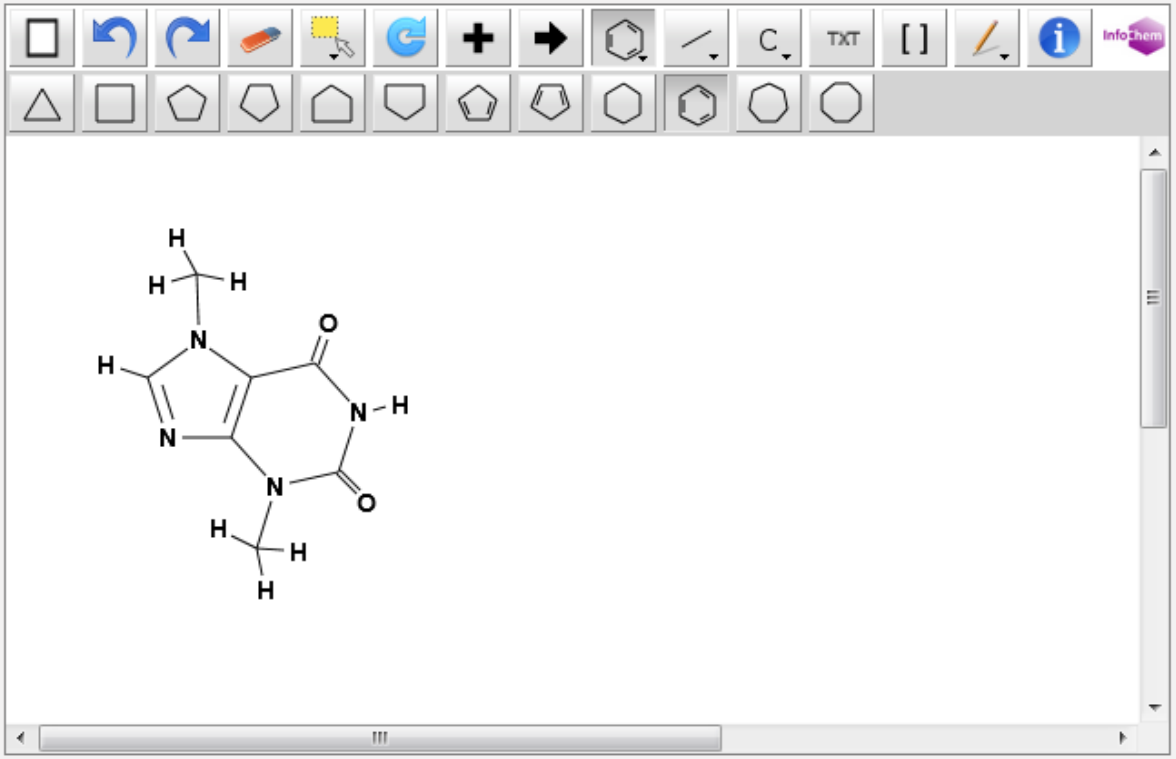

InChI: InChI=1S/C7H8N4O2/c1-10-3-8-5-4(10)6(12)9-7(13)11(5)2/h3H,1-2H3,(H,9,12,13)
InChiKey: YAPQBXQYLJRXSA-UHFFFAOYSA-N
Molecular Formula: C7H8N4O2
Molecular Weight: 180.167 g/mol

Search | Reset

Search for scaffold:

Office: All Specify ⇨

Tooltip Help

Results **1-10** of **5,978** for Criteria:**CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N)** Office(s):**all** Language:**EN** Stemming: **true**

prev 1 2 3 4 5 6 7 8 9 10 next Page: 1 / 598 Go >

Refine Search CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N) Search RSS 10k

Analysis

Sort by: Pub Date Desc View All **List Length** 10 Machine translation

Title			Ctr	PubDate
Int.Class	Appl.No	Applicant	Inventor	
1. WO/2016/141458 **BISPHENOL ETHER DERIVATIVES AND METHODS FOR USING THE SAME**			WO	15.09.2016
C07C 69/21	PCT/CA2016/000070	BRITISH COLUMBIA CANCER AGENCY BRANCH	ANDERSEN, Raymond John	
Compounds having a structure of Formula I, or a pharmaceutically acceptable salt, tautomer or stereoisomer thereof, wherein R1, R2, L1, L2, L3, X, a, b, c, n, and m are as defined herein, are provided. Uses of such compounds for modulating androgen receptor activity and uses as therapeutics as well as methods for treatment of subjects in need thereof, including prostate cancer are also provided.				
2. WO/2016/142250 **BENZAZEPINE DICARBOXAMIDE COMPOUNDS**			WO	15.09.2016
C07D 403/12	PCT/EP2016/054487	F. HOFFMANN-LA ROCHE AG	HOVES, Sabine	
This invention relates to novel benzazepine dicarboxamide compounds of the formula (I), wherein R1 to R4 are as defined in the description and in the claims, as well as pharmaceutically acceptable salts thereof. These compounds are TLR agonists and may therefore be useful as medicaments for the treatment of diseases such as cancer, autoimmune diseases, inflammation, sepsis, allergy, asthma, graft rejection, graft- versus-host disease, immunodeficiencies, and infectious diseases.				
3. WO/2016/142310 **TRICYCLIC DLK INHIBITORS AND USES THEREOF**			WO	15.09.2016
C07D 491/14	PCT/EP2016/054725	F. HOFFMANN-LA ROCHE AG	ESTRADA, Anthony	
The invention relates to compounds of formula (I) and salts thereof, wherein ring A and R1-R2 have any of the values defined in the specification. The compounds and salts are useful for treating DLK mediated disorders. The invention also provides pharmaceutical compositions comprising a compound of formula (I), or a pharmaceutically acceptable salt thereof, as well as methods of using said compounds, salts, or compositions as DLK inhibitors and for treating neurodegeneration diseases and disorders.				

1. (WO2016141458) BISPHENOL ETHER DERIVATIVES AND METHODS FOR USING THE SAME

Latest bibliographic data on file with the International Bureau | Submit observation | PermaLink

Pub. No.: WO/2016/141458 **International Application No.:** PCT/CA2016/000070
Publication Date: 15.09.2016 **International Filing Date:** 11.03.2016

IPC: ***C07C 69/21*** (2006.01), ***A61K 31/05*** (2006.01), ***A61P 35/00*** (2006.01), ***C07C 43/23*** (2006.01), ***C07F 9/40*** (2006.01)

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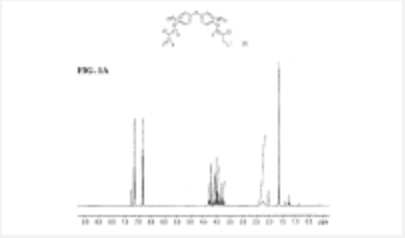
Priority Data: 62/131,969 12.03.2015 US

Title
(EN) BISPHENOL ETHER DERIVATIVES AND METHODS FOR USING THE SAME
(FR) DÉRIVÉS D'ÉTHER DE BISPHÉNOL ET LEURS PROCÉDÉS D'UTILISATION

Abstract:
(EN) Compounds having a structure of Formula I, or a pharmaceutically acceptable salt, tautomer or stereoisomer thereof, wherein R^1, R^2, L^1, L^2, L^3, X, a, b, c, n, and m are as defined herein, are provided. Uses of such compounds for modulating androgen receptor activity and uses as therapeutics as well as methods for treatment of subjects in need thereof, including prostate cancer are also provided.
(FR) Cette invention concerne des composés ayant une structure de formule I : ou un sel , un tautomère ou un stéréoisomère pharmaceutiquement acceptable de ceux-ci, où R^1, R^2, L^1, L^2, L^3, X, a, b, c, n et m étant tels que définis dans la présente. L'invention concerne également les utilisations de ces composés pour moduler l'activité du récepteur des androgènes et leurs utilisations comme substances thérapeutiques, ainsi que des méthodes destinées à traiter des sujets en ayant besoin, dont des sujets atteints de cancer de la prostate.

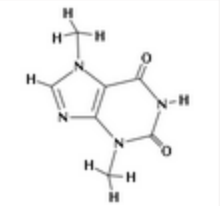


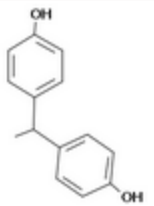
Designated States: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JP, KE, KG, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.
African Regional Intellectual Property Organization (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ, UG, ZM, ZW)
Eurasian Patent Organization (AM, AZ, BY, KG, KZ, RU, TJ, TM)
European Patent Office (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR)

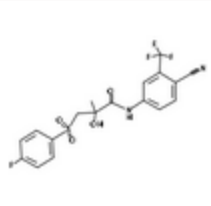
1. (WO2016141458) BISPHENOL ETHER DERIVATIVES AND METHODS FOR USING THE SAME

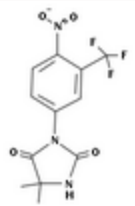
PCT Biblio. Data | Description | Claims | National Phase | Notices | Compounds | Drawings | Documents

Title | Abstract | Description | Claims


Theobromine




Bicalutamide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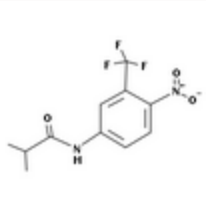
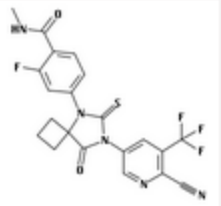
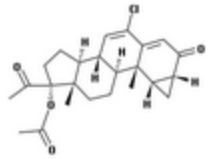
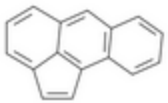
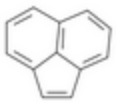
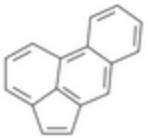

Flutamide

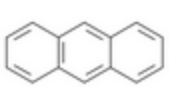


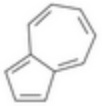


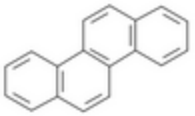


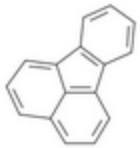


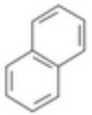


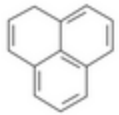


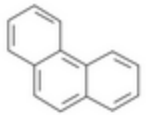






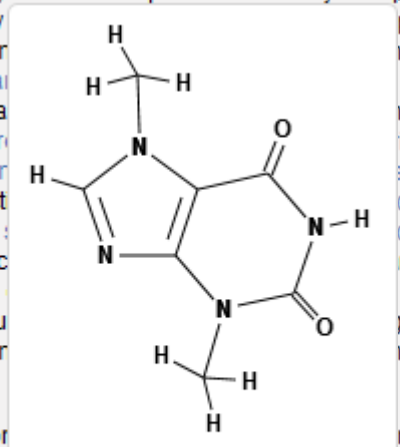




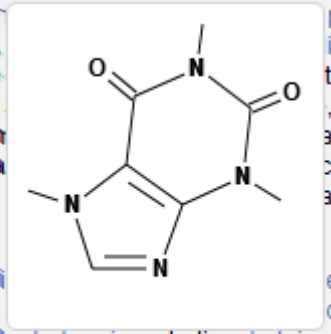


« « « 1 2 3 4 5 6 7 8 9 » » » » » »

Compounds as described herein may be in the free form or in the form of a salt thereof. In some embodiments, compounds as described herein may be in the form of a pharmaceutically acceptable salt, which are known in the art (Berge et al., J. Pharm. Sci. 1977, 66, 1). Pharmaceutically acceptable salt as used herein includes, for example, salts that have the desired pharmacological activity of the parent compound (salts which retain the biological effectiveness and/or properties of the parent compound and which are not biologically and/or otherwise undesirable). Compounds as described herein having one or more functional groups capable of forming a salt may be, for example, formed as a pharmaceutically acceptable salt. Compounds containing one or more basic functional groups may be capable of forming a pharmaceutically pharmaceutically acceptable organic or inorganic acid. Pharmaceutically acceptable salts may be derived fror , acetic acid, adipic acid, alginic acid, aspartic acid, ascorbic acid, benzoic acid, benzenesulfonic acid, butyric acid, cinnar camphorsulfonie acid, cyclopentanepropionic acid, diethylacetic acid, digluconic acid, dodecylsulfonic acid, cthanesulfonic a eptanoic acid, gluconic acid, glycerophosphoric acid, glycolic acid, hemisulfonic acid, heptanoic acid, hexanoic acid, hydr iodic acid, 2-hydroxyethanesulfonic acid, isomcotinic acid, lactic acid, malic acid, maieic acid, malonic acid, mandeiic acid, r sulfonic acid, r p-toluenesulfonic acid, nicotinic acid, nitric acid, oxalic acid, pamoic acid, pect osphoric acid, ic acid, propionic acid, pyruvic acid, salicylic acid, succinic acid, sulfuric acid, c acid or unde taining one or more acidic functional groups may be capable of forming pharmac rmaceutically , and without limitation, inorganic bases based on alkaline metals or alkaline as primary an amine compounds, tertiary amine compounds, quaternary amine compounds, su substituted a ion-exchange resins. Pharmaceutically acceptable salts may be derived fror , a hydroxide, a pharmaceutically acceptable metal cation such as ammonium,



Theobromine



sodium, potassium, lithium, calcium, magnesium, iror num, ammoni ethylamine, dimethylamine, trimethylamine, ethylamine, m^mylami ipropylamine, dethanolamine, 2-drmethylarninoethanol, 2-diethylaruinoethanol, dicyc line, caffeine, hydrabamine, choline, betaine, ethylenediamine, glucosamine, glucamine, memylglucamine, theobromine, procaine, N- etliylpiperidine, theobromine, tetrame ylammonium compounds, tetraethylammonium compounds, p e, N,N-dimemylaniline, N-methylpiperidine, n ohne, N-methylmorpholine, N-ethylmorpholine, dicyclohexylamine, dibenzylamine, N,N- dibenzylp ethylaniine, 1-ephenamine, N^-m¾enzylemylenediamine or polyamine resins. In some embodiments, compounds as described herein may contain both acidic and basic groups and may be in the form of inner salts or zwitterions, for example, and without limitation, betaines. Salts as described herein may be prepared by conventional processes known to a person slcilled in the art, for example, and without limitation, by reacting the free form with an organic acid or inorganic acid or base, or by anion exchange or cation exchange from other salts. Those skilled in the art will appreciate that preparation of salts may occur in situ during isolation and purification of the compounds or preparation of salts may occur by separately reacting an isolated and purified compound.

In some embodiments, compounds and all different forms thereof (e.g. free forms, salts, polymorphs, isomeric forms) as described herein may be in the solvent addition form, for example, solvates. Solvates contain either stoichiometric or non-stoicbiometric amounts of a solvent in physical association the compound or salt thereof. The solvent may be, for example, and without limitation, a pharmaceutically acceptable solvent. For example, hydrates are formed when the solvent is water or alcoholates are formed when the solvent is an alcohol.

In some embodiments, compounds and all different forms thereof (e.g. free forms, salts, solvates, isomeric forms) as described herein may include crystalline and amorphous forms, for example, polymorphs, pseudopolymorphs, conformational polymorphs, amorphous forms, or a combination thereof. Polymorphs include different crystal packing arrangements of the same elemental composition of a compound. Polymorphs usually have different X-ray diffraction patterns, infrared spectra, melting points, density, hardness, crystal shape, optical and electrical properties, stability and/or solubility. Those skilled in the art will appreciate that various factors including recrystallization solvent, rate of crystallization and storage temperature may cause a single crystal form to dominate.

In some embodiments, compounds and all different forms thereof (e.g. free forms, salts, solvates, polymorphs) as described herein include isomers such as geometrical isomers, optical isomers based on asymmetric carbon, stereoisomers, tautomers, individual enantiomers, individual diastereomers, racemates, diastereomeric mixtures and combinations thereof, and are not limited by the description of the formula illustrated for the sake of convenience.

III. Methods

The present compounds find use in any number of methods. For example, in some embodiments the compounds can be useful in methods for modulating

Results **1-10** of **9** for Criteria:**(CTR:WO AND CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N)) AND EN_AB:chocolate** Office(s):**wo** Language:**All** Stemming: **true**

prev 1 next Page: 1 / 1 Go >

Refine Search (CTR:WO AND CHEM:(YAPQBXQYLJRXSA-UHFFFAOYSA-N)) AND EN_AB:chocolate Search

Analysis

Sort by: Pub Date Asc View All **List Length** 10 **Machine translation**

Title	Ctr	PubDate
Int.Class	Appl.No	Applicant	Inventor

1. WO/2002/074321 **COMPOSITION COMPRISING COCOA AND A DOPAMINE D2 RECEPTOR AGONIST** — WO — 26.09.2002

A23L 1/30 — PCT/NL2002/000184 — N.V. NUTRICIA — TER LAAK, Wies

The invention pertains to a composition and a method for the treatment of mood disorders, in particular of treating, preventing or alleviating depression, mood disorders or insufficient mood, obesity, overweight, premenstrual syndrome, craving, carbohydrate craving, chocolate craving, menopausal complaints, erectile dysfunction and/or reduced libido. The composition contains cocoa or one or more if its pharmacologically active components, and a dopamine D2 receptor agonist.

2. WO/2002/078746 **NOVEL CHOCOLATE COMPOSITION AS DELIVERY SYSTEM FOR NUTRIENTS AND MEDICATIONS** — WO — 10.10.2002

A23G 1/00 — PCT/US2002/009597 — ALTAFFER, Paulo — HUGHES, Kerry

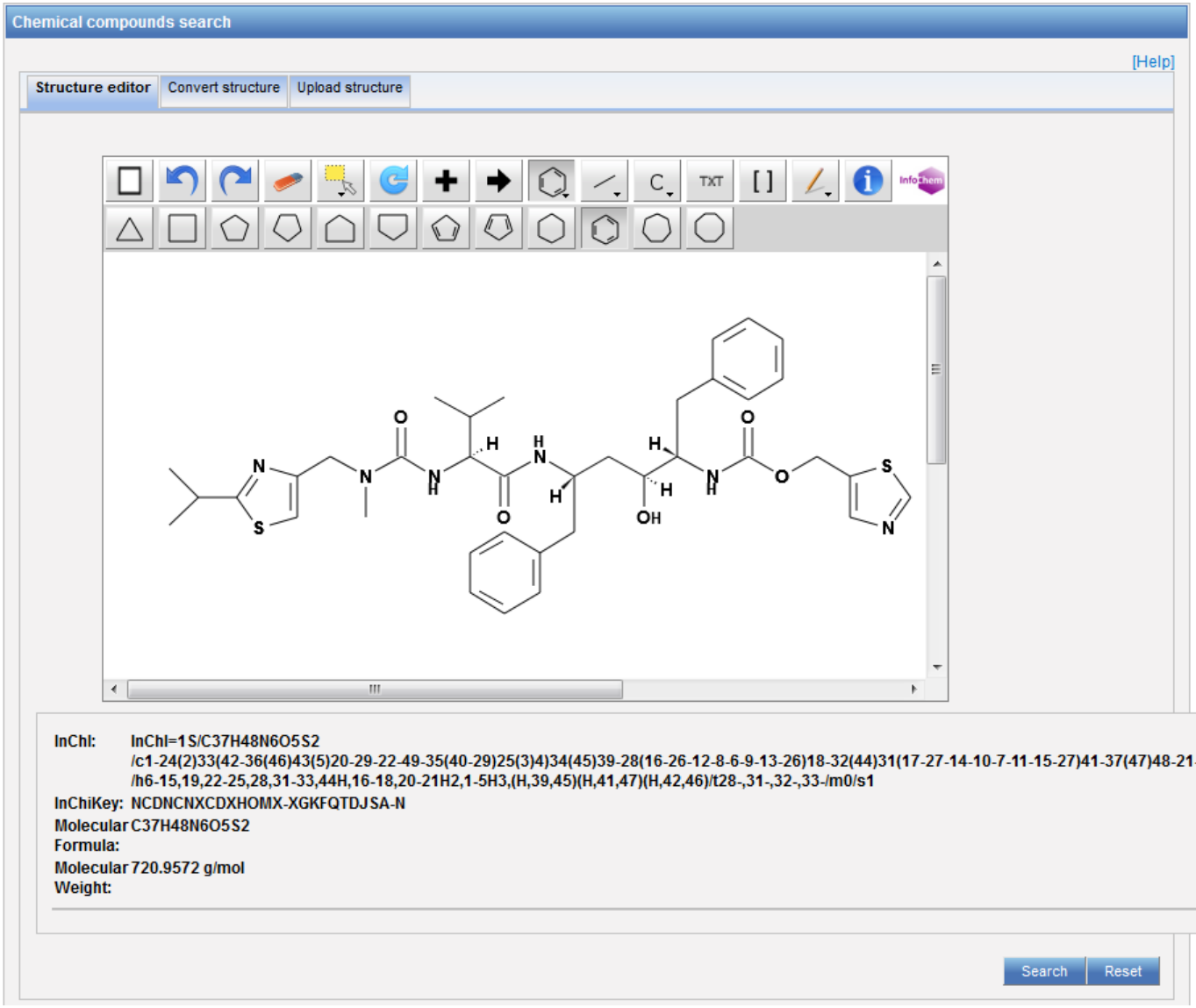
A novel chocolate product for use in delivering medicaments and/or nutrients to animals, particularly humans, specially formulated so that the craving for such product by animals, particularly humans, is significantly greater than the craving for chocolate conventionally used in pharmaceutical compositions and the concentration, optimization, and the addition of endogenous and exogenous ingredients to increase such craving as well as to treat specific indications. The chocolate product contains: from about 0.5 to about 200 milligrams, more preferably from about 5 to about 20 milligrams, of one or more biogenic amines per 1 gram of the chocolate product; from about 10 to about 500 milligrams, more preferably form about 20 to about 200 milligrams, of one or more amino acids per 1

International Non proprietary Names

WIKIPEDIA:

- INNs are official generic and non proprietary names given to a pharmaceutical drug or active ingredients issued by the World Health Organization (WHO).
- Growing need to be able to search INNs in patent texts
- PATENTSCOPE supports the search of 6917 INNs by Inchikey

Example 2: Ritonavir



Results **1-10** of **5,738** for Criteria:**CTR:WO AND CHEM:(NCDNCNXCDXHOMX-XGKFQTDJSA-N)** Office(s):**wo** Language:**All** Stemming: **true**

prev 1 2 3 4 5 6 7 8 9 10 next Page: 1 / 574 Go >

Refine Search CTR:WO AND CHEM:(NCDNCNXCDXHOMX-XGKFQTDJSA-N) Search RSS 10k

Analysis

Sort by: Pub Date Asc View All **List Length** 10 **Machine translation**

Int.Class	Appl.No	Applicant	Ctr	PubDate
1. WO/1994/014436 **RETROVIRAL PROTEASE INHIBITING COMPOUNDS**			WO	07.07.1994
A61K 31/425	PCT/US1993/012326	ABBOTT LABORATORIES	KEMPF, Dale, J.	

A retroviral protease inhibiting compound of formula (A) is disclosed.

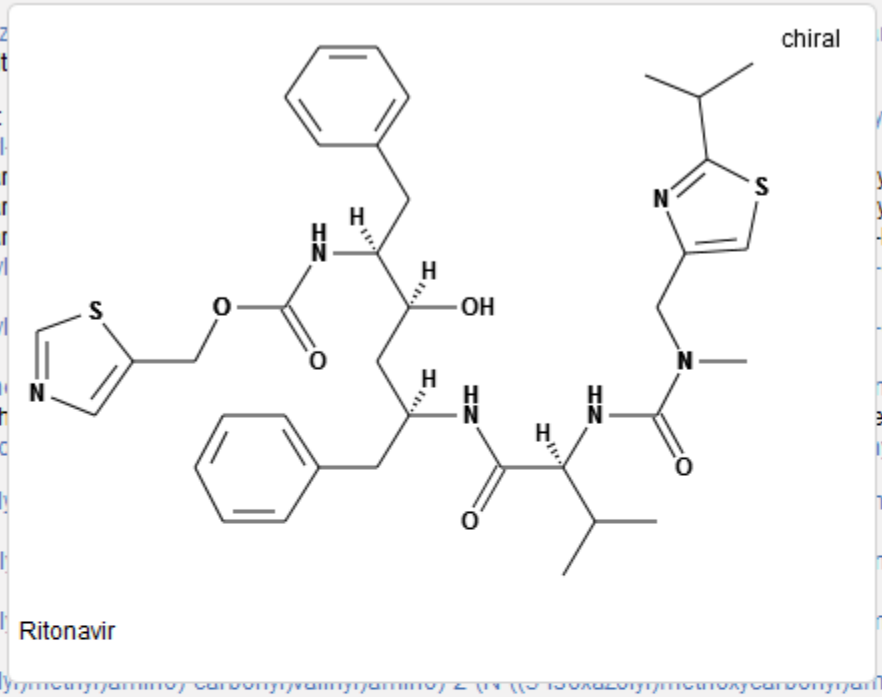
Int.Class	Appl.No	Applicant	Ctr	PubDate
2. WO/1995/007696 **PHARMACEUTICAL COMPOSITION OF HIV-PROTEASE INHIBITORS**			WO	23.03.1995
A61K 9/48	PCT/US1994/009788	ABBOTT LABORATORIES	AL-RAZZAK, Laman, A.	

A pharmaceutical composition is disclosed which comprises a solution of an HIV protease inhibiting compound in a pharmaceutically acceptable organic solvent comprising a pharmaceutically acceptable alcohol. The composition can optionally comprise a pharmaceutically acceptable acid or a combination of pharmaceutically acceptable acids. The solution can optionally be encapsulated in hard gelating capsule or soft elastic gelating capsules. The solution can optionally be granulated with a pharmaceutically acceptable granulating agent.

Int.Class	Appl.No	Applicant	Ctr	PubDate
3. WO/1995/009614 **PHARMACEUTICAL COMPOSITION**			WO	13.04.1995
A61K 9/14	PCT/US1994/010096	ABBOTT LABORATORIES	AL-RAZZAK, Laman, A.	

A solid pharmaceutical composition is disclosed which comprises a pharmaceutically acceptable adsorbent or a mixture of pharmaceutically acceptable adsorbents to which is adsorbed a mixture of (1) a pharmaceutically acceptable organic solvent or a mixture of pharmaceutically accpetable organic solvents, (2) an HIV protease inhibiting compound and (3) one or more pharmaceutically acceptable acids. The solid composition can optionally be encapsulated in a hard gelatin capsule.

8. (2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-thiazolyl)methyl)-amino)carbonyl)valinyl)amino)-2-(N-((5-thiazolyl)methoxycarbonyl)amino)- 1,6-diphenyl-3-hydroxyhexane; or a pharmaceutically acceptable salt, ester or prodrug thereof.

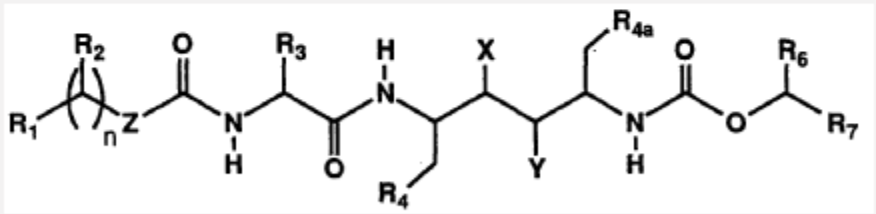


9. (2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-oxaz…mino)-1,6-diphenyl-3-hydroxyhexane; or a pharmaceutically acceptable salt

10. A compound selected from the group consisting of: …yl)alaninyl)amino)-2-(N-((5-thiazolyl)methoxycarbonyl)amino)-1,6-diphenyl-
(2S,3S,5S)-5-(N-(N-((2-Isopropyl-4-thiazolyl)methoxycar…ydroxyhexane;
(2S,3S,5S)-2-(N-(N-((2-Isopropyl-4-thiazolyl)methoxycar…ydroxyhexane;
(2S,3S,5S)-5-(N-(N-((2-Isopropyl-4-thiazolyl)methoxycar…-hydroxyhexane;
(2S,3S,5S)-5-(N-(N-((2-(N,N-Dimethylamino)-4-thiazolyl…-diphenyl-3-hydroxyhexane;
(2S,3S,5S)-2-(N-(N-((2-(N,N-Dimethylamino)-4-thiazolyl…-diphenyl-3-hydroxyhexane;
(2S,3S,5S)-5-(N-(N-((2-(4-Morpholinyl)-4-thiazolyl)meth…nyl-3-hydroxyhexane;
(2S,3S,5S)-2-(N-(N-((2-(4-Morpholinyl)-4-thiazolyl)-meth…enyl-3-hydroxyhexane;
(2S,3S,5S)-5-(N-(N-((2-(1-Pyrrolidinyl)-4-thiazolyl)metho…yl-3-hydroxyhexane;

(2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-oxazoly…no)-1,6-diphenyl-3-hydroxyhexane;
(2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-thiazol…no)-1,6-diphenyl-3-hydroxyhexane;
(2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-thiazol…nino)-1,6-diphenyl-3-hydroxyhexane; and
(2S,3S,5S)-5-(N-(N-((N-Methyl-N-((2-isopropyl-4-oxazoly…nino)-1,6-diphenyl-3-hydroxyhexane; or a pharmaceutically acceptable salt, ester or prodrug thereof.

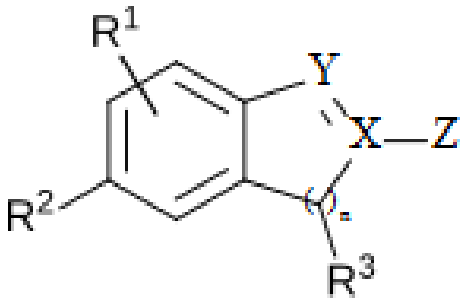
11. A compound of the formula:



wherein R_1 is monosubstituted thiazolyl, monosubstituted oxazolyl, monosubstituted isoxazolyl or monosubstituted isothiazolyl wherein the substituent is selected from (i) loweralkyl, (ii) loweralkenyl, (iii) cycloalkyl, (iv) cycloalkylalkyl, (v) cycloalkenyl, (vi)cycloalkenylalkyl, (vii) heterocyclic wherein the heterocyclic is selected from aziridinyl, azetidinyl, pyrrolidinyl, piperidinyl, piperazinyl, morpholinyl, thiomorpholinyl, thiazolyl, oxazolyl, isoxazolyl, isothiazolyl, pyridinyl, pyrimidinyl, pyridazinyl and pyrazinyl and wherein the heterocyclic is unsubstituted or substituted with a substituent selected from halo, loweralkyl, hydroxy, alkoxy and thioalkoxy, (viii)
(heterocyclic)alkyl wherein heterocyclic is defined as above, (ix) alkoxyalkyl, (x) thioalkoxyalkyl, (xi) alkylamino, (xii) dialkylamino, (xiii) phenyl wherein the phenyl ring is unsubstituted or substituted with a substituent selected from halo, loweralkyl, hydroxy, alkoxy and thioalkoxy, (xiv) phenylalkyl wherein the phenyl ring is unsubstituted or substituted as defined above, (xv) dialkylaminoalkyl, (xvi) alkoxy and (xvii) thioalkoxy;

Scope

- Works on **complete exact formulas** ≠ Markush structures (-R) that are chemical symbols used to indicate a collection of chemicals with similar structures.



- Chemical elements, short names (less than 4 characters), common solvents and polymers are not annotated by design
- PCT and US national collections with IPC codes related to chemistry
- Languages: English and German

Limitations

- Based on state of the art fully automated chemical recognition algorithms
- The technology is NOT 100% accurate

- OCR errors in the available patent full texts make the recognition of chemical compounds even more challenging

Suggested Approach

Use the tool as a guide

- positive identification is a good result
- negative identification is not authoritative