Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1617srh

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'MEDLINE, CAPLUS, BIOSIS, USPATFULL'
AT 11:15:32 ON 05 JAN 2009
FILE 'MEDLINE' ENTERED AT 11:15:32 ON 05 JAN 2009
FILE 'CAPLUS' ENTERED AT 11:15:32 ON 05 JAN 2009
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)
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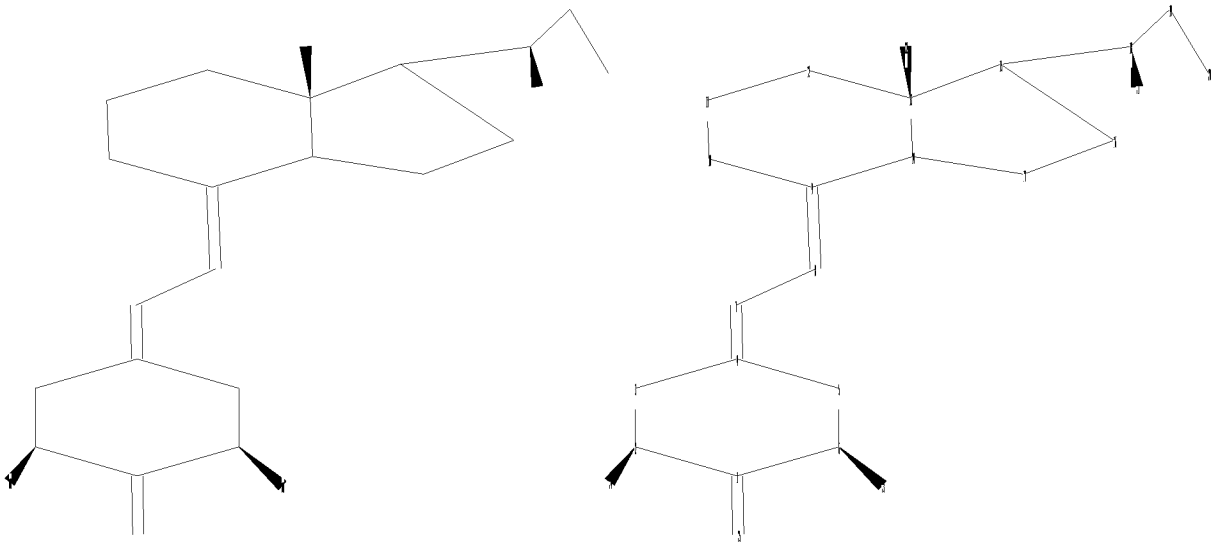
Copyright (c) 2009 The Thomson Corporation
FILE 'USPATFULL' ENTERED AT 11:15:32 ON 05 JAN 2009
CA INDEXING COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	143.88	152.34

=>
Uploading C:\Program Files\Stnexp\Queries\11-944150.str



chain nodes :
7 8 18 19 20 21 22 23 24 25
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 14 15 16 17
chain bonds :

1-25 2-24 4-7 6-23 7-8 8-9 13-22 15-18 18-19 18-21 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-14 10-11 11-12 12-13 13-14 13-15 14-17
15-16 16-17
exact/norm bonds :
1-2 1-6 2-3 2-24 3-4 4-5 5-6 6-23 9-10 9-14 10-11 11-12 12-13 13-14
13-15 14-17 15-16 16-17
exact bonds :
1-25 4-7 7-8 8-9 13-22 15-18 18-19 18-21 19-20

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

Stereo Bonds:

21-18 (Single Wedge).
22-13 (Single Wedge).
23-6 (Single Wedge).
24-2 (Single Hash).

Stereo Chiral Centers:

2   (Parity=Even)
6   (Parity=Even)
13   (Parity=Even)
18   (Parity=Even)

Stereo RSS Sets:

Type=Relative (Default). 4 Nodes= 2 6 13 18

L6   STRUCTURE UPLOADED

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   147.25   155.71

FILE 'REGISTRY' ENTERED AT 11:16:47 ON 05 JAN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JAN 2009 HIGHEST RN 1092523-63-1
DICTIONARY FILE UPDATES: 4 JAN 2009 HIGHEST RN 1092523-63-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of

experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l6
SAMPLE SEARCH INITIATED 11:16:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 405 TO ITERATE

100.0% PROCESSED 405 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 6893 TO 9307
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> d l6
L6 HAS NO ANSWERS
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l6 full
FULL SEARCH INITIATED 11:17:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 8592 TO ITERATE

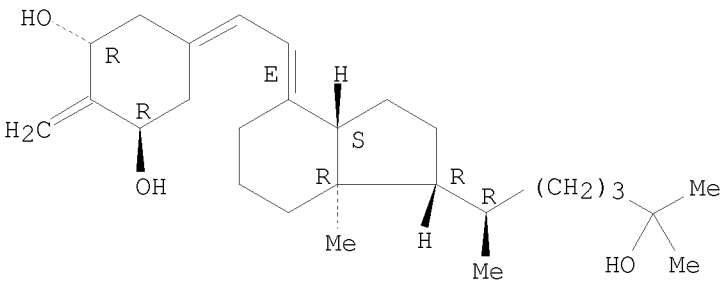
100.0% PROCESSED 8592 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L8 13 SEA SSS FUL L6

=> d scan

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C27 H44 O3

Absolute stereochemistry.
Double bond geometry as shown.

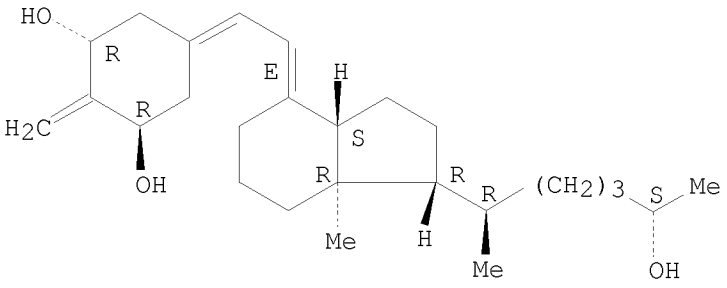


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):12

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R,5S)-5-hydroxy-1-methylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C26 H42 O3

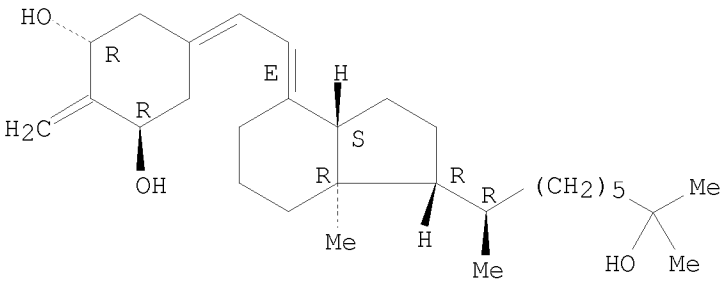
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R)-7-hydroxy-1,7-dimethyloctyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C29 H48 O3

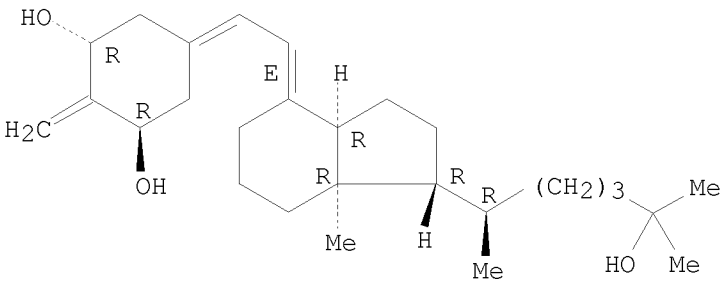
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aR,7aR)-octahydro-1-[(1R)-5-hydroxy-1,5-dimethylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C27 H44 O3

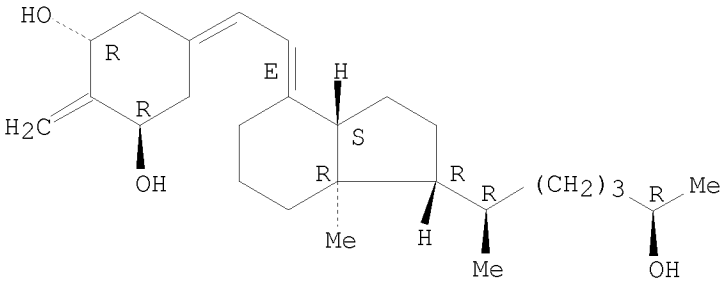
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R,5R)-5-hydroxy-1-methylhexyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C26 H42 O3

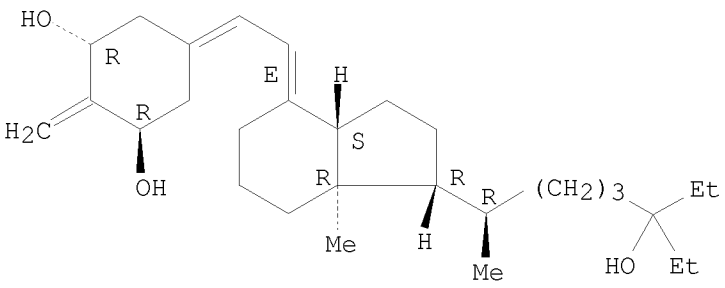
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-5-ethyl-5-hydroxy-1-methylheptyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-methylene-, (1R,3R)-
MF C29 H48 O3

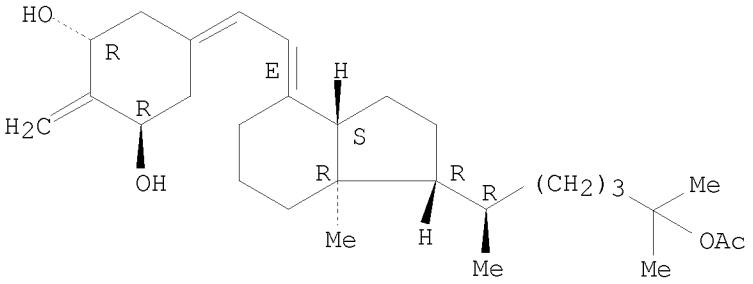
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-5-(acetyloxy)-1,5-dimethylhexyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-methylene-, (1R,3R)-
MF C29 H46 O4

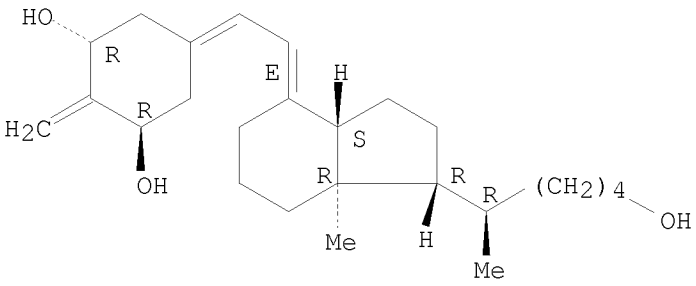
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R)-5-hydroxy-1-methylpentyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C25 H40 O3

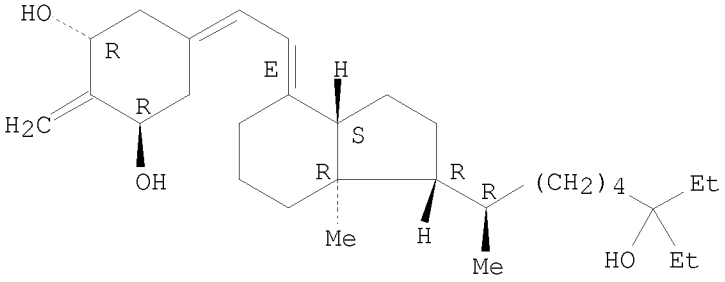
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-6-ethyl-6-hydroxy-1-methyloctyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-methylene-, (1R,3R)-
MF C30 H50 O3

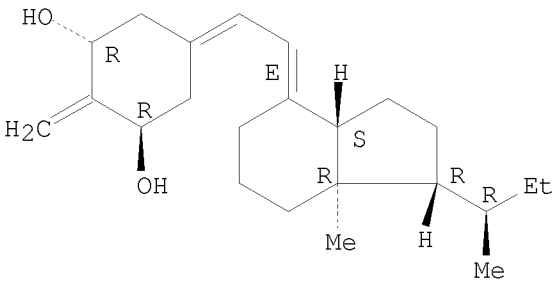
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-7a-methyl-1-[(1R)-1-methylpropyl]-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C23 H36 O2

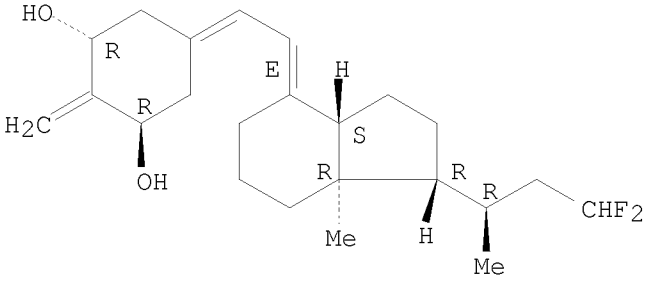
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-3,3-difluoro-1-methylpropyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-methylene-, (1R,3R)-
MF C23 H34 F2 O2

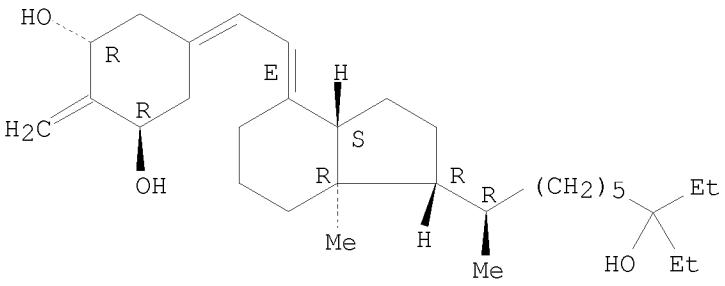
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 5-[(2E)-2-[(1R,3aS,7aR)-1-[(1R)-7-ethyl-7-hydroxy-1-methylnonyl]octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-2-methylene-, (1R,3R)-
MF C31 H52 O3

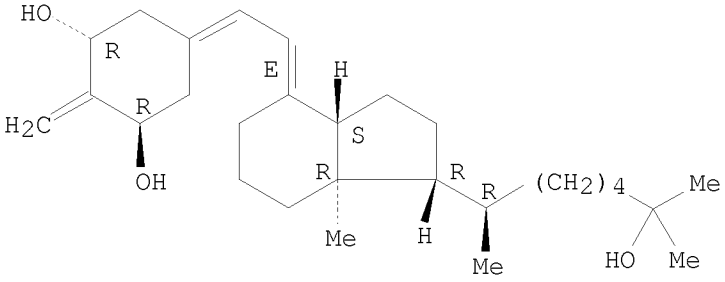
Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L8 13 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-1-[(1R)-6-hydroxy-1,6-dimethylheptyl]-7a-methyl-4H-inden-4-ylidene]ethylidene]-, (1R,3R)-
MF C28 H46 O3

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

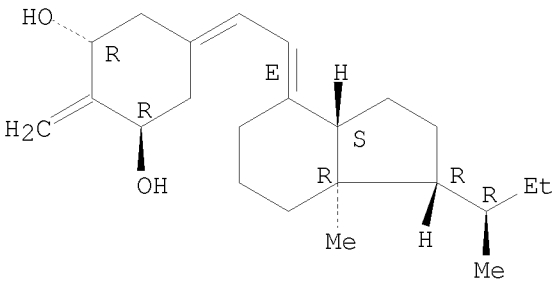
=> s l8 and C23 H36 O2/mf
794 C23 H36 O2/MF
L9 1 L8 AND C23 H36 O2/MF

=> d

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2009 ACS on STN
RN 852658-44-7 REGISTRY
ED Entered STN: 22 Jun 2005
CN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-2-[(1R,3aS,7aR)-octahydro-7a-methyl-1-[(1R)-1-methylpropyl]-4H-inden-4-ylidene]ethylidene]-, (1R,3R)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,3-Cyclohexanediol, 2-methylene-5-[(2E)-[(1R,3aS,7aR)-octahydro-7a-methyl-1-[(1R)-1-methylpropyl]-4H-inden-4-ylidene]ethylidene]-, (1R,3R)- (9CI)

OTHER NAMES:
CN 2-Methylene-19-nor-(20R)-1α-hydroxybishomopregnacalciferol
FS STEREOSEARCH
MF C23 H36 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPAT2, USPATFULL

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil capl
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 194.24 349.95

FILE 'CAPLUS' ENTERED AT 11:18:29 ON 05 JAN 2009

FILE COVERS 1907 - 5 Jan 2009 VOL 150 ISS 2
FILE LAST UPDATED: 4 Jan 2009 (20090104/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s l8

L10 44 L8

=> s l9
L11 7 L9

=> d ibib abs

L11 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1274436 CAPLUS
DOCUMENT NUMBER: 149:455398
TITLE: Oral or topical compositions comprising a 19-norvitamin D with or without a retinoid
INVENTOR(S): Clagett-Dame, Margaret; Deluca, Hector F.; Nieves, Nirca J.; Plum, Lori A.; Kaiser, Mary E.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 46pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20080261925	A1	20081023	US 2007-966504	20071228
WO 2008083370	A2	20080710	WO 2007-US89193	20071231

W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, 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, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:		
US 2006-882705P	P	20061229
US 2007-17217P	P	20071228
US 2007-17219P	P	20071228
US 2007-966504	A	20071228

AB Oral and topical pharmaceutical compns., kits and methods of treatment thereof for treating various skin disorder including acne, psoriasis, ichthyosis, photoaging, photodamaged skin, and, skin cancer. Exemplary vitamin D analogs as active pharmaceutical ingredients are 2-methylene-19-nor-20(S)-1α-hydroxy-bishomopregnacalciferol, 19-nor-26,27-dimethylene-20(S)-2-methylene-1α,25-dihydroxyvitamin D3, 2-methylene-1α,25-dihydroxy-(17E)-17(20)-dehydro-19-nor-vitamin D3, or 2-methylene-19-nor-(24R)-1α,25-dihydroxyvitamin D2, a stereoisomer, a prodrug or a salt thereof, in oral compns. Compds. that activate retinoic acid receptors, are, e.g, all-trans-retinoic acid, (2E,4E,6Z,8E)-3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexeneyl)nona-2,4,6,8-tetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-2,4,6 8-tetraenoic acid, 6-[3-(1-adamantyl)-4-methoxyphenyl]-2-naphthoic acid, or Et 6-[2-(4,4-dimethylthiochroman-6-yl)ethynyl]pyridine-3-carboxylate, an isomer, a prodrug, an ester, or a a salt thereof in oral compns. Combinations of such active ingredients demonstrate synergistic efficacy.

=> d ibib abs 2-7

L11 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1072054 CAPLUS
DOCUMENT NUMBER: 149:463448
TITLE: 2-Methylene-19-nor-20(S)-1α-hydroxy-bishomopregnacalciferol [20(S)-2MbisP], an analog of vitamin D3 [1,25(OH)2D3], does not stimulate intestinal phosphate absorption at levels previously shown to suppress parathyroid hormone
AUTHOR(S): Williams, Katie B.; DeLuca, Hector F.
CORPORATE SOURCE: Department of Biochemistry, College of Agricultural and Life Sciences, University of Wisconsin-Madison, Madison, WI, 53706, USA
SOURCE: Steroids (2008), 73(12), 1277-1284
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Chronic kidney disease results in a reduction in 1,25-dihydroxyvitamin D3 (1,25(OH)2D3) synthesis and an accumulation of phosphorus in the blood, leading to secondary hyperparathyroidism and renal osteodystrophy. Vitamin D analogs that retain the ability to suppress PTH but that are less calcemic and phosphatemic than the native hormone are preferred therapies for secondary hyperparathyroidism. However, even the most favored analog currently approved for the treatment of chronic kidney disease patients, i.e., 1,25-dihydroxy-19-nor-vitamin D2 (19-nor-D2, Zemplar), still retains some ability to stimulate intestinal absorption of calcium and phosphate. A recently described analog of vitamin D3, 2-methylene-19-nor-20(S)-1α-hydroxy-bishomopregnacalciferol [20(S)-2MbisP], suppresses PTH levels, but is unable to stimulate intestinal calcium absorption or bone resorption in rats. The present study shows that 20(S)-2MbisP is unable to stimulate intestinal phosphate absorption at levels known to suppress PTH secretion. Further, 19-nor-vitamin D2 under the same circumstances does stimulate phosphate absorption. Thus, 2MbisP has significant potential in the management of secondary hyperparathyroidism of renal failure.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:832914 CAPLUS
DOCUMENT NUMBER: 149:160587
TITLE: Oral or topical compositions comprising a 19-norvitamin D with or without a retinoid
INVENTOR(S): Clagett-Dame, Margaret; Deluca, Hector F.; Nieves, Nirca J.; Plum, Lori A.; Kaiser, Mary E.; Barycki, Rafal
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: PCT Int. Appl., 117 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008083370	A2	20080710	WO 2007-US89193	20071231
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, 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, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD,				

ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH,
PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM,
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BY, KG, KZ, MD, RU, TJ, TM

US 20080261925 A1 20081023 US 2007-966504 20071228
PRIORITY APPLN. INFO.: US 2006-882705P P 20061229
US 2007-17217P P 20071228
US 2007-17219P P 20071228
US 2007-966504 A 20071228

AB Oral and topical pharmaceutical compns., kits and methods of treatment thereof for treating various skin disorder including acne, psoriasis, ichthyosis, photoaging, photodamaged skin, and, skin cancer. Exemplary vitamin D analogs as active pharmaceutical ingredients are 2-methylene-19-nor-20(S)-1α-hydroxy-bishomopregnacalciferol, 19-nor-26,27-dimethylene-20(S)-2-methylene-1α,25-dihydroxyvitamin D3, 2-methylene-1α,25-dihydroxy-(17E)-17(20)-dehydro-19-nor-vitamin D3, or 2-methylene-19-nor-(24R)-1α,25-dihydroxyvitamin D2, a stereoisomer, a prodrug or a salt thereof, in oral compns. Compds. that activate retinoic acid receptors, are, e.g, all-trans-retinoic acid, (2E,4E,6Z,8E)-3,7-dimethyl-9-(2,6,6-trimethyl-1-cyclohexeneyl)nona-2,4,6,8-tetraenoic acid, 9-(4-methoxy-2,3,6-trimethylphenyl)-3,7-dimethylnona-2,4,6 8-tetraenoic acid, 6-[3-(1-adamantyl)-4-methoxyphenyl]-2-naphthoic acid, or Et 6-[2-(4,4-dimethylthiochroman-6-yl)ethynyl]pyridine-3-carboxylate, an isomer, a prodrug, an ester, or a a salt thereof in oral compns. Combinations of such active ingredients demonstrate synergistic efficacy.

L11 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:1015495 CAPLUS
DOCUMENT NUMBER: 147:420173
TITLE: Differential recruitment of coactivators to the vitamin D receptor transcriptional complex by 1α,25-dihydroxyvitamin D3 analogs
AUTHOR(S): Schwinn, Marie K.; DeLuca, Hector F.
CORPORATE SOURCE: Department of Biochemistry, University of Wisconsin-Madison, Madison, WI, 53706, USA
SOURCE: Archives of Biochemistry and Biophysics (2007), 465(2), 443-451
CODEN: ABBIA4; ISSN: 0003-9861
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To clarify the mol. mechanism for analog potency and selectivity, we investigated the ability of 1,25(OH)2D3 analogs to recruit coactivators to the vitamin D receptor (VDR) transcriptional complex. Using a modified version of the avidin-biotin complex DNA binding assay, we discovered that 20S-analogs enhance the binding of specific coactivators to the transcriptional complex relative to natural hormone and that the enhanced binding occurs independently of vitamin D response element and cell type. With the exception of two of these coactivators, DRIP205 and DRIP240, all proteins were recruited to the transcriptional complex in a dose-dependent manner. While the results do not provide an explanation for tissue selectivity of 2-methylene-19-nor-(20S)-1,25-dihydroxyvitamin D3 (2MD), they provide evidence that in the presence of a full-length side chain, the 20S configuration improves binding of specific proteins to the VDR transcriptional complex while modifications at carbon 2 do not.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2007:321374 CAPLUS
DOCUMENT NUMBER: 146:514986
TITLE: Computational analysis of the active sites in binary and ternary complexes of the vitamin D receptor
AUTHOR(S): Sicinska, Wanda; Rotkiewicz, Piotr
CORPORATE SOURCE: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, 01-224, Pol.
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (2007), 103(3-5), 305-309
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A review. We have developed a program CCOMP that compares overlapping fragments of two protein complexes and identifies differently oriented amino acids. CCOMP initially performs a sequence alignment of the analyzed receptors, then superimposes the corresponding aligned residues, and finally calcs. the root mean square deviation (RMSD) of individual atoms, every amino acid and the entire complex. Thus, amino acids important for functional differences between both complexes can be detected. Application of CCOMP to 1α,25-(OH)2D3-hVDR (1DB1) [Proc. Natl. Acad. Sci. U.S.A. 98 (2001) 5491] and 1α,25-(OH)2D3-rVDR-peptide (1RK3) [Biochem. 43 (2004) 4101] complexes revealed that the peptide (KNHPMLMNLLKDN) mimicking a co-activator sequence significantly changes the side chain conformation of 35 amino acids. Four of these residues (K242, I256, K260, E416) actually contact the peptide, but all of them are essential for biol. activity. Only two (L309 and L400) of the 35 differently oriented amino acids contact the ligand. Interestingly, when the peptide is present (1RK3) leucine 400 shifts closer (0.7 Å) to the vitamin D 26-Me group. Applying the CCOMP and DSSP programs to binary and ternary VDR complexes also resulted in establishing that seven amino acids (I238, S252, I256, L413, L415, E416, V417) exhibit significant differences in solvent accessibility and are capable of interacting with co-activators.
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:510421 CAPLUS
DOCUMENT NUMBER: 145:8315
TITLE: Preparation of 2-methylene-19-nor-(20R)-1α-hydroxybishomopregqnacalciferol for use in pharmaceutical compositions
INVENTOR(S): Deluca, Hector F.; Plum, Lori A.; Clagett-Dame, Margaret
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006057913	A2	20060601	WO 2005-US41886	20051118
WO 2006057913	A3	20061005		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

AU 2005309818	A1	20060601	AU 2005-309818	20051118
CA 2588038	A1	20060601	CA 2005-2588038	20051118
US 20060135799	A1	20060622	US 2005-282972	20051118
EP 1831161	A2	20070912	EP 2005-848203	20051118
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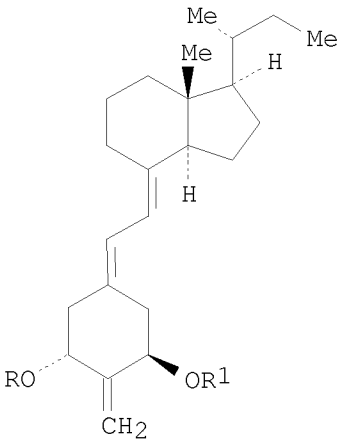
JP 2008520708	T	20080619	JP 2007-543289	20051118
MX 200706090	A	20070711	MX 2007-6090	20070521

PRIORITY APPLN. INFO.:	US 2004-629954P	P	20041122
	WO 2005-US41886	W	20051118

OTHER SOURCE(S): CASREACT 145:8315; MARPAT 145:8315

GI



I

AB The title compound I (R = R1 = H) and its derivs., such as I [R, R1 = hydroxyl protecting group], were prepared for therapeutic use in the treatment of diseases and conditions involving vitamin D receptor (VDR) activity. These pregnacalciferol derivs. were claimed for use in the treatment of cancer, as well as in the treatment autoimmune, inflammatory, bone and skin diseases and conditions. The diseases and conditions that may be treated using these compds. include leukemia, colon cancer, breast cancer, prostate cancer, psoriasis, multiple sclerosis, lupus, diabetes mellitus, host vs. graft reaction, rejection of organ transplants, rheumatoid arthritis, asthma, inflammatory bowel diseases, such as celiac disease, ulcerative colitis and Crohn's disease, renal osteodystrophy, osteoporosis, skin wrinkles, lack of adequate skin firmness, lack of adequate dermal hydration, or insufficient sebum secretion. Thus, I (R = R1 = H) was prepared via a synthetic sequence starting from (αS,1R,3aR,7aR)-octahydro-α,7a-dimethyl-4-oxo-1H-indene-1-acetaldehyde and [2-[(3R,5R)-3,5-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-4-methylenecyclohexylidene]ethyl]diphenylphosphine oxide. The prepared compds. were assayed for VDR binding activity, for effect on HL-60 cell

differentiation, 24-hydroxylase transcription, bone calcium mobilization, intestinal calcium transport, hypercalcemia and parathyroid hormone suppression.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:474934 CAPLUS
DOCUMENT NUMBER: 143:20385
TITLE: Vitamin d analogs for obesity prevention and treatment
INVENTOR(S): Deluca, Hector F.; Clagett-Dame, Margaret; Ahrens, Jamie M.; Ntambi, James M.; Thomson, Brian
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 102 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050119242	A1	20050602	US 2004-997698	20041124
AU 2004293092	A1	20050609	AU 2004-293092	20041124
CA 2544502	A1	20050609	CA 2004-2544502	20041124
WO 2005051396	A2	20050609	WO 2004-US39524	20041124
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WO 2005051323	A2	20050609	WO 2004-US39625	20041124
WO 2005051323	A3	20050707		
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US 20050143358	A1	20050630	US 2004-996642	20041124
US 7053075	B2	20060530		
EP 1689412	A2	20060816	EP 2004-812196	20041124
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EP 1694333	A2	20060830	EP 2004-812109	20041124
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				
JP 2007512371	T	20070517	JP 2006-541701	20041124
JP 2007512376	T	20070517	JP 2006-541728	20041124
MX 2006PA05887	A	20060627	MX 2006-PA5887	20060524
PRIORITY APPLN. INFO.:			US 2003-524798P P	20031125

	US 2003-524813P	P	20031125
	WO 2004-US39524	W	20041124
	WO 2004-US39625	W	20041124

OTHER SOURCE(S): MARPAT 143:20385

AB Methods for treating and preventing obesity, inhibiting adipocyte differentiation, inhibiting increased SCD-1 gene transcription, and/or reducing body fat in a subject include administering at least one analog of 1α,25-dihydroxyvitamin D3, 1α,25-dihydroxyvitamin D2, or 19-nor vitamin D or a pharmaceutical composition that includes such an analog to a subject in need thereof are disclosed.

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---Logging off of STN---

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Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	34.00	383.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.74	-5.74

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