Compound Summary for CID 71406

Tocophersolan

Cite this Record

STRUCTURE VENDORS DRUG INFO PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	71406
Chemical Names:	Tocophersolan; TPGS; Vitamin E TPGS; Tocophersolan [USAN]; Tocofersolano; Tocofersolanum More...
Molecular Formula:	$C_{35}H_{58}O_6$
Molecular Weight:	574.843 g/mol
InChI Key:	AOBORMOPSGHCAX-UHFFFAOYSA-N
Drug Information:	Clinical Trials

Tocophersolan is a water-soluble amphipathic formulation of d-alpha-tocopherol succinate coupled, through a succinate linker, to polyethylene glycol (PEG) 1000. Due to its amphipathic property in which it forms its own micelles, tocophersolan is easily taken up into enterocytes, even in the absence of bile salts; fat soluble d-alpha-tocopherol is then released after hydrolysis. This formulation enhances the absorption of d-alpha-tocopherol compared to the administration of free d-alpha-tocopherol. In addition, tocophersolan may enhance the absorption of water-insoluble agents and other fat-soluble vitamins.

Pharmacology from NCIt

Vitamin E supplement, antioxidant Tocofersolan (INN) or tocophersolan is a synthetic water-soluble version of vitamin E. Natural forms of vitamin E are fat soluble, but not water-soluble. Tocofersolan is polyethylene glycol derivative of -tocopherol that enables water solubility

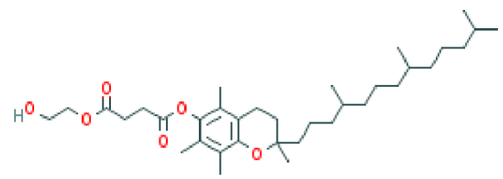
Metabolite Description from Human Metabolome Database (HMDB)

Modify Date: 2018-11-10; Create Date: 2005-08-08

Contents

1 2D Structure

Search Download Get Image



Magnify

from PubChem

2 3D Status

Conformer generation is disallowed since too flexible

from PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

1-O-(2-hydroxyethyl) 4-O-[2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydrochromen-6-yl] butanedioate

from PubChem

3.1.2 InChI

InChI=1S/C35H58O6/c1-24(2)12-9-13-25(3)14-10-15-26(4)16-11-20-35(8)21-19-30-29(7)33(27(5)28(6)34(30)41-35)40-32(38)18-17-31(37)39-23-22-36/h24-26,36H,9-23H2,1-8H3

from PubChem

3.1.3 InChI Key

AOBORMOPSGHCAX-UHFFFAOYSA-N

from PubChem

3.1.4 Canonical SMILES

CC1=C2C(=C(C(=C1C)OC(=O)CCC(=O)OCCO)C)CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C

from PubChem

3.2 Molecular Formula

$C_{35}H_{58}O_6$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

30999-06-5

from Human Metabolome Database (HMDB)

3.4 Synonyms

3.4.1 MeSH Entry Terms

1. (+)-alpha-tocopheryl polyethylene glycol 1000 succinate
2. alpha-D-tocopherol poly(ethylene glycol) 2000 succinate
3. alpha-tocopheryl polyethylene glycol succinate
4. mono-(2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-6-chromanyl) succinate polyethylene glycol monoester
5. poly(oxy-1,2-ethanediyl), alpha-(4-((3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-yl)oxy)-1,4-dioxobutyl-omega-hydroxy-
6. tocofersolan
7. tocopherol poly(ethylene glycol) 2000 succinate
8. tocopherol polyethylene glycol succinate
9. tocophersolan
10. tocophersolan, (2R-(2R*(4R*,8R*)))-isomer
11. tocopheryl poly(ethylene glycol) 1000 succir
12. TPGS
13. TPGS 2K
14. vitamin E-TPGS
15. vitamine E PEG-1000-succinate

from MeSH

3.4.2 Depositor-Supplied Synonyms

1. Tocophersolan
2. TPGS
3. Vitamin E TPGS
4. Tocophersolan [USAN]
11. D 1T
12. alpha-Tocopheryl polyethylene glycol 1000 succinate
13. Tocopheryl polyethylene glycol 1000 succinate
14. 30999-06-5
21. Tocophersolan, USAN
22. Vitamin E PEG succinate
23. alpha-tocopheryl polyethylene gly
24. dl-a-Tocopherol Polyethylene Glyc

5. Tocofersolano
6. Tocofersolanum
7. Tocofersolan (INN)
8. Tocofersolan [INN]
9. Tocophersolan (USAN)
10. (+)-alpha-Tocopheryl polyethylene glycol 1000 succinate
15. UNII-O03S90U1F2
16. d-alpha-Tocopheryl poly(ethylene glycol) 1000 succinate
17. vitamin E-TPGS
18. 2-hydroxyethyl 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-3,4-dihydro-2h-chromen-6-yl succinate
19. Liqui-E
20. Tocofersolan, INN
25. EASTMAN Vitamin E TPGS
26. AC1L2G3T
27. Tocofersolanum [INN-Latin]
28. Tocofersolano [INN-Spanish]
29. Mono-(2,5,7,8-tetramethyl-2-(4,8,1
30. AC1Q685O

from PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value
Molecular Weight	574.843 g/mol
Hydrogen Bond Donor Count	1
Hydrogen Bond Acceptor Count	6
Rotatable Bond Count	20
Complexity	768
CACTVS Substructure Key Fingerprint	AAADcfB8OAAAAAAAAAAAAAAAAAAAAAAAAA0QAAAAAAAAACRAAAAGgAACAAADUSgmAICDoA ABgCIAgDQCAACCAAgIAAAiAEECIgNNjKEMBqCOiCkwBELqAfDwPAOwQADAAAYAACCAAYAADAAAA AAAAAAAA==
Topological Polar Surface Area	82.1 A^2
Monoisotopic Mass	574.423 g/mol
Exact Mass	574.423 g/mol
XLogP3-AA	9.9
Compound Is Canonicalized	true
Formal Charge	0
Heavy Atom Count	41
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	3
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Isotope Atom Count	0
Covalently-Bonded Unit Count	1

from PubChem

4.2 Spectral Properties

4.2.1 Mass Spectrometry

4.2.1.1 GC-MS

1. GC-MS Spectrum 21599 - GC-MS Ei Predicted by CFMID-EI, energy0
2. GC-MS Spectrum 43836 - GC-MS Ei (1 TMS) Predicted by CFMID-EI, Ionization energy 70 eV fully TMS-derivatized (structure: CC1=C(C)C2=C(CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2)C(C)=C1OC(=O)CCC(=O)OCCO[Si](C)(C)C)

from Human Metabolome Database (HMDB)

4.2.1.2 MS-MS

1. MS-MS Spectrum 100473 - 10V Positive Predicted by CFM-ID
2. MS-MS Spectrum 100474 - 20V Positive Predicted by CFM-ID
3. MS-MS Spectrum 100475 - 40V Positive Predicted by CFM-ID
4. MS-MS Spectrum 165810 - 10V Negative Predicted by CFM-ID
5. MS-MS Spectrum 165811 - 20V Negative Predicted by CFM-ID
6. MS-MS Spectrum 165812 - 40V Negative Predicted by CFM-ID

from Human Metabolome Database (HMDB)

5 Related Records

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5.1 Related Compounds with Annotation

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from PubChem

5.2 Related Compounds

Same Connectivity	8 records
Same Parent, Connectivity	10 records

Same Parent, Exact	3 records
Mixtures, Components, and Neutralized Forms	3 records
Similar Compounds	312 records

from PubChem

5.3 Substances

5.3.1 Related Substances

All	35 records
Same	32 records
Mixture	3 records

from PubChem

5.3.2 Substances by Category

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5.4 Entrez Crosslinks

PubMed	7 records
Taxonomy	1 record
Gene	1 record

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6 Chemical Vendors

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7 Drug and Medication Information

7.1 Clinical Trials

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Record ID	Title	Status	Phase
NCT01853475	Healthy Volunteer Study of the Pharmacokinetics of Oral Piperaquine With OZ439 + TPGS Formulation in the Fasted State	Completed	1
NCT01958619	Open Label Pharmacokinetic Study of OZ439 and Piperaquine on Administration of OZ439+TPGS Granules for Oral Suspension Alone or With Either Piperaquine Phosphate Tablets or Granules for Oral Solution in Healthy Volunteers	Completed	1
NCT02387580	Bioavailability Study of Oral OZ439 Prototype Granule Formulations Administered With Piperaquine Phosphate (PQP) Tablets	Completed	1

from ClinicalTrials.gov

8 Pharmacology and Biochemistry

8.1 Pharmacology

Tocophersolan is a water-soluble amphipathic formulation of d-alpha-tocopherol succinate coupled, through a succinate linker, to polyethylene glycol (PEG) 1000. Due to its amphipathic property in which it forms its own micelles, tocophersolan is easily taken up into enterocytes, even in the absence of bile salts; fat soluble d-alpha-tocopherol is then released after hydrolysis. This formulation enhances the absorption of d-alpha-tocopherol compared to the administration of free d-alpha-tocopherol. In addition, tocophersolan may enhance the absorption of water-insoluble agents and other fat-soluble vitamins.

from NCIt

8.2 Human Metabolite Information

8.2.1 Metabolite Description

Description

Vitamin E supplement, antioxidant Tocofersolan (INN) or tocophersolan is a synthetic water-soluble version of vitamin E. Natural forms of vitamin E are fat soluble, but not water-soluble. Tocofersolan is polyethylene glycol derivative of -tocopherol that enables water solubility

from Human Metabolome Database (HMDB)

8.2.2 Cellular Locations

ExtracellularMembrane

from Human Metabolome Database (HMDB)

9 Literature

9.1 Depositor Provided PubMed Citations

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9.2 NLM Curated PubMed Citations

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from PubChem

9.3 Metabolite References

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1 to 5 of 6 View More

PMID	Reference
11413487	Simons K, Toomre D: Lipid rafts and signal transduction. Nat Rev Mol Cell Biol. 2000 Oct;1(1):31-9.
16902246	Watson AD: Thematic review series: systems biology approaches to metabolic and cardiovascular disorders. Lipidomics: a global approach to lipid analysis in biological systems. J Lipid Res. 2006 Oct;47(10):2101-11. Epub 2006 Aug 10.
17374880	Sethi JK, Vidal-Puig AJ: Thematic review series: adipocyte biology. Adipose tissue function and plasticity orchestrate nutritional adaptation. J Lipid Res. 2007 Jun;48(6):1253-62. Epub 2007 Mar 20.
20044567	Lingwood D, Simons K: Lipid rafts as a membrane-organizing principle. Science. 2010 Jan 1;327(5961):46-50. doi: 10.1126/science.1174621.
	Yannai, Shmuel. (2004) Dictionary of food compounds with CD-ROM: Additives, flavors, and ingredients. Boca Raton: Chapman & Hall/CRC.

from Human Metabolome Database (HMDB)

9.4 Springer Nature References

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from Springer Nature

9.5 Chemical Co-Occurrences in Literature

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View More Chemical-Chemical Co-Occurrences and Evidence for Tocophersolan

from PubChem

9.6 Chemical-Disease Co-Occurrences in Literature

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View More Chemical-Disease Co-Occurrences and Evidence for Tocophersolan

from PubChem

9.7 Chemical-Gene Co-Occurrences in Literature

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View More Chemical-Gene Co-Occurrences and Evidence for Tocophersolan

10 Patents

10.1 Depositor-Supplied Patent Identifiers

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11 Biological Test Results

11.1 BioAssay Results

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12 Classification

12.1 Ontologies

12.1.1 MeSH Tree

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from MeSH

12.1.2 KEGG: ATC

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from KEGG

12.1.3 WHO ATC Classification System

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from WHO ATC

12.1.4 WIPO IPC

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from WIPO

12.1.5 ChemIDplus

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▸ *from ChemIDplus*

13 Information Sources

1. ClinicalTrials.gov /source/ClinicalTrials.gov
   Tocophersolan
   https://clinicaltrials.gov/ https://clinicaltrials.gov/
2. Human Metabolome Database (HMDB) /source/Human Metabolome Database (HMDB)
   Tocophersolan
   http://www.hmdb.ca/metabolites/HMDB0034354 http://www.hmdb.ca/metabolites/HMDB0034354
3. NCIt /source/NCIt
   Tocophersolan
   https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C67044 https://ncit.nci.nih.gov/ncitbrowser/ConceptReport.jsp?dictionary=NCI_Thesaurus&ns=NCI_Thesaurus&code=C67044
4. Springer Nature /source/Springer Nature
   Literature references related to scientific contents from Springer Nature journals and books. Read more ... https://link.springer.com/
5. PubChem
   Data deposited in or computed by PubChem
   https://pubchem.ncbi.nlm.nih.gov https://pubchem.ncbi.nlm.nih.gov
6. MeSH /source/MeSH
   tocophersolan
   https://www.ncbi.nlm.nih.gov/mesh/67014225 https://www.ncbi.nlm.nih.gov/mesh/67014225
   MeSH Tree
   http://www.nlm.nih.gov/mesh/meshhome.html http://www.nlm.nih.gov/mesh/meshhome.html
7. KEGG /source/KEGG
   Anatomical Therapeutic Chemical (ATC) classification
   http://www.genome.jp/kegg-bin/get_htext?br08303.keg http://www.genome.jp/kegg-bin/get_htext?br08303.keg
8. WIPO /source/WIPO
   International Patent Classification
   http://www.wipo.int/classifications/ipc/ http://www.wipo.int/classifications/ipc/
9. WHO ATC /source/WHO ATC
   ATC Code
   https://www.whocc.no/atc_ddd_index/ https://www.whocc.no/atc_ddd_index/
10. ChemIDplus /source/ChemIDplus

ChemIDplus Chemical Information Classification
https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp *https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp*

11. NCBI

LinkOut is a service that allows one to link directly from NCBI databases to a wide range of information and services beyond NCBI systems.
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