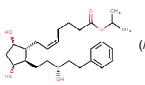
Showing metabocard for Latanoprost (HMDB0014792)

Identification | Taxonomy | Ontology | Physical properties | Spectra | Biological properties | Concentrations | Links | References | XML (/metabolites/HMDB0014792.xml)

enzymes (1) | transporters (1) | Show 2 proteins (/metabolites/HMDB0014792/metabolite_protein_links) | Show Metabolites with Similar Structures

Show more...

Record Information	
Version	4.0
Status	Expected but not Quantified
Creation Date	2012-09-06 15:16:50 UTC
Update Date	2018-05-20 20:10:45 UTC
HMDB ID	HMDB0014792
Secondary Accession Numbers	• HMDB14792
Metabolite Identification	
Common Name	**Latanoprost**
Description	Latanoprost ophthalmic solution is a topical medication used for controlling the progression of glaucoma or ocular hypertension, by reducing intraocular pressure. It is a prostaglandin analogue that works by increasing the outflow of aqueous fluid from the eyes. It is also known by the brand name of Xalatan manufactured by Pfizer.
Structure	 (/structures/HMDB0014792/image.svg) MOL (/structures/metabolites/HMDB0014792.mol) | SDF (/structures/metabolites/HMDB0014792.sdf) | 3D-SDF (/structures/metabolites/HMDB0014792.sdf?dim=3d) PDB (/structures/metabolites/HMDB0014792.pdb) | SMILES (/structures/metabolites/HMDB0014792.smiles) | InChI (/structures/metabolites/HMDB0014792.inchi) View 3D Structure (/structures/metabolites/HMDB0014792)

Synonyms

Value	Source
Isopropyl (Z)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((3R)-3-hydroxy-5-phenylpentyl)cyclopentyl)-5-heptenoate	ChEBI
Latanoprostum	ChEBI
PhXA 41	ChEBI
Propan-2-yl (5Z)-7-{(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl}hept-5-enoate	ChEBI
Xalatan	ChEBI
Isopropyl (Z)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((3R)-3-hydroxy-5-phenylpentyl)cyclopentyl)-5-heptenoic acid	Generator
Propan-2-yl (5Z)-7-{(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl}hept-5-enoic acid	Generator
PHXA41	MeSH
Pfizer brand OF latanoprost	MeSH
PhXA34	MeSH

Chemical Formula	$C_{26}H_{40}O_5$
Average Molecular Weight	432.5928
Monoisotopic Molecular Weight	432.28757439
IUPAC Name	propan-2-yl (5Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl]hept-5-enoate
Traditional Name	latanoprost
CAS Registry Number	130209-82-4
SMILES	CC(C)OC(=O)CCC\C=C/C[C@H]1[C@@H](O)C[C@@H](O)[C@@H]1CC[C@@H](O)CCC1=CC=CC=C1
InChI Identifier	InChI=1S/C26H40O5/c1-19(2)31-26(30)13-9-4-3-8-12-22-23(25(29)18-24(22)28)17-16-21(27)15-14-20-10-6-5-7-11-20/h3,5-8,10-11,19,21-25,27-29H,4,9,12-18H2,1-2H3/b8-3-/t21-,22+,23+,24-,25+/m0/s1
InChI Key	GGXICVAJURFBLW-CEYXHVGTSA-N
Chemical Taxonomy	
Description	This compound belongs to the class of organic compounds known as prostaglandins and related compounds. These are unsaturated carboxylic acids consisting of a 20 carbon skeleton that also contains a five member ring, and are based upon the fatty acid arachidonic acid.
Kingdom	Organic compounds (http://classyfire.wishartlab.com/tax_nodes/C0000000)
Super Class	Lipids and lipid-like molecules (http://classyfire.wishartlab.com/tax_nodes/C0000012)
Class	Fatty Acyls (http://classyfire.wishartlab.com/tax_nodes/C0003909)
Sub Class	Eicosanoids (http://classyfire.wishartlab.com/tax_nodes/C0000513)
Direct Parent	Prostaglandins and related compounds (http://classyfire.wishartlab.com/tax_nodes/C0000514)
Alternative Parents	• Fatty acid esters (http://classyfire.wishartlab.com/tax_nodes/C0000324) • Cyclopentanols (http://classyfire.wishartlab.com/tax_nodes/C0002938) • Benzene and substituted derivatives (http://classyfire.wishartlab.com/tax_nodes/C0002279) • Cyclic alcohols and derivatives (http://classyfire.wishartlab.com/tax_nodes/C0001292) • Carboxylic acid esters (http://classyfire.wishartlab.com/tax_nodes/C0001238) • Monocarboxylic acids and derivatives (http://classyfire.wishartlab.com/tax_nodes/C0001137) • Organic oxides (http://classyfire.wishartlab.com/tax_nodes/C0003940) • Hydrocarbon derivatives (http://classyfire.wishartlab.com/tax_nodes/C0004150) • Carbonyl compounds (http://classyfire.wishartlab.com/tax_nodes/C0001831)

Substituents	• Prostaglandin skeleton • Fatty acid ester • Monocyclic benzene moiety • Cyclopentanol • Benzenoid • Cyclic alcohol • Carboxylic acid ester • Secondary alcohol • Carboxylic acid derivative • Monocarboxylic acid or derivatives • Hydrocarbon derivative • Organic oxide • Alcohol • Carbonyl group • Organic oxygen compound • Organooxygen compound • Aromatic homomonocyclic compound
Molecular Framework	Aromatic homomonocyclic compounds
External Descriptors	• carboxylic ester (CHEBI:6384 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:6384)) • prostaglandins Falpha (CHEBI:6384 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:6384)) • triol (CHEBI:6384 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:6384))
Ontology	
Disposition	Route of exposure: Enteral: ◦ Ingestion (/metabolite_ontology_terms/4903893) Source: ◦ Food (/metabolite_ontology_terms/4903892) Biological location: Biofluid and excreta: ◦ Urine (/metabolite_ontology_terms/3407383) ◦ Blood (/metabolite_ontology_terms/3407384) Cell and elements: ◦ Extracellular (/metabolite_ontology_terms/3240349) Subcellular: ◦ Membrane (/metabolite_ontology_terms/3240350) ◦ Cell membrane (/metabolite_ontology_terms/3674477) ◦ Cytoplasm (/metabolite_ontology_terms/3835947)
Process	Naturally occurring process: Biological process: Biochemical process: ◦ Lipid transport (/metabolite_ontology_terms/4903896) ◦ Lipid metabolism (/metabolite_ontology_terms/4903897) ◦ Fatty acid metabolism (/metabolite_ontology_terms/4903898) Chemical reaction: ◦ Lipid peroxidation (/metabolite_ontology_terms/4903895) Biochemical pathway: ◦ Lipid metabolism pathway (/metabolite_ontology_terms/4903894) Multicellular process: ◦ Inflammatory response (/metabolite_ontology_terms/3835951) ◦ Immune response (/metabolite_ontology_terms/3835952) Cellular process: ◦ Cell signaling (/metabolite_ontology_terms/3449682)
Role	Biological role: ◦ Membrane stabilizer (/metabolite_ontology_terms/3674474) ◦ Energy source (/metabolite_ontology_terms/3674475) ◦ Energy storage (/metabolite_ontology_terms/3674476) ◦ Nutrient (/metabolite_ontology_terms/3835948) ◦ Inflammatory (/metabolite_ontology_terms/3835949) Modulator: ◦ Immunomodulator (/metabolite_ontology_terms/3835950) Industrial application: ◦ Drug (/metabolite_ontology_terms/3449680) ◦ Surfactant (/metabolite_ontology_terms/3674472) ◦ Emulsifier (/metabolite_ontology_terms/3674473) Pharmaceutical industry: ◦ Pharmaceutical (/metabolite_ontology_terms/3602520) Cardiovascular drug: ◦ Antihypertensive (/metabolite_ontology_terms/3449681)
Physical Properties	
State	Liquid

Experimental Properties

Property	Value	Reference
Melting Point	Not Available	Not Available
Boiling Point	Not Available	Not Available
Water Solubility	0.013 g/L	Not Available
LogP	4.4	Not Available

Predicted Properties

Property	Value	Source
Water Solubility	0.013 g/L	ALOGPS (http://www.vcclab.org/lab/alogps/)
logP	4.16	ALOGPS (http://www.vcclab.org/lab/alogps/)
logP	3.98	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#logp_logd)
logS	-4.5	ALOGPS (http://www.vcclab.org/lab/alogps/)
pKa (Strongest Acidic)	14.47	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#pka)
pKa (Strongest Basic)	-2.7	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#pka)
Physiological Charge	0	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#pka)
Hydrogen Acceptor Count	4	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#h_bond)
Hydrogen Donor Count	3	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#h_bond)
Polar Surface Area	86.99 Å²	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topolgical_surface)
Rotatable Bond Count	14	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topology_analysis)
Refractivity	124.34 m³·mol⁻¹	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#refractivity)
Polarizability	50.71 Å³	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)
Number of Rings	2	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topology_analysis)
Bioavailability	1	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)
Rule of Five	Yes	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)
Ghose Filter	Yes	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)
Veber's Rule	Yes	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)
MDDR-like Rule	Yes	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/molecular-modelling/#polarization)

Spectra

Spectra

Spectrum Type	Description	Splash Key (http://splash.fiehnlab.ucdavis.edu/)	
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (Non-derivatized) - 70eV, Positive (/spectra/c_ms/17619)	splash10-00kf-5469500000-3070e3312e2f54422eeb	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-00kf-5469500000-3070e3312e2f54422eeb)
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (3 TMS) - 70eV, Positive (/spectra/c_ms/40446)	splash10-001l-7110196000-109246e3e73496dba6fd	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-001l-7110196000-109246e3e73496dba6fd)

Biological Properties

Cellular Locations

- Extracellular
- Membrane

Biospecimen Locations

- Blood
- Urine

Tissue Locations

Not Available

Pathways

Not Available

Name	SMPDB/Pathwhiz	KEGG

Normal Concentrations

Biospecimen	Status	Value	Age	Sex	Condition	Reference	Details
Blood	Expected but not Quantified		Not Available	Not Available	Taking drug identified by DrugBank entry DB00654	21059682 (http://www.ncbi.nlm.nih.gov/pubmed/21059682)	details (/concentrations/67281)
Urine	Expected but not Quantified		Not Available	Not Available	Taking drug identified by DrugBank entry DB00654	21059682 (http://www.ncbi.nlm.nih.gov/pubmed/21059682)	details (/concentrations/67280)

Abnormal Concentrations	
	Not Available
Associated Disorders and Diseases	
Disease References	None
Associated OMIM IDs	None
External Links	
DrugBank ID	DB00654 (http://www.drugbank.ca/drugs/DB00654)
Phenol Explorer Compound ID	Not Available
FoodDB ID	Not Available
KNApSAcK ID	Not Available
Chemspider ID	4470740 (http://www.chemspider.com/Chemical-Structure.4470740.html)
KEGG Compound ID	Not Available
BioCyc ID	Not Available
BiGG ID	Not Available
Wikipedia Link	Latanoprost (http://en.wikipedia.org/wiki/Latanoprost)
METLIN ID	Not Available
PubChem Compound	5311221 (http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=5311221)
PDB ID	Not Available
ChEBI ID	6384 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=6384)
References	
Synthesis Reference	Not Available
Material Safety Data Sheet (MSDS)	Not Available
General References	1. Hara T: [Increased iris pigmentation after use of latanoprost in Japanese brown eyes]. Nippon Ganka Gakkai Zasshi. 2001 May;105(5):314-21. [PubMed:11406947 (http://www.ncbi.nlm.nih.gov/pubmed/11406947)] 2. Simons K, Toomre D: Lipid rafts and signal transduction. Nat Rev Mol Cell Biol. 2000 Oct;1(1):31-9. [PubMed:11413487 (http://www.ncbi.nlm.nih.gov/pubmed/11413487)] 3. 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. [PubMed:16902246 (http://www.ncbi.nlm.nih.gov/pubmed/16902246)] 4. 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. [PubMed:17374880 (http://www.ncbi.nlm.nih.gov/pubmed/17374880)] 5. Lingwood D, Simons K: Lipid rafts as a membrane-organizing principle. Science. 2010 Jan 1;327(5961):46-50. doi: 10.1126/science.1174621. [PubMed:20044567 (http://www.ncbi.nlm.nih.gov/pubmed/20044567)] 6. Gunstone, Frank D., John L. Harwood, and Albert J. Dijkstra (2007). The lipid handbook with CD-ROM. CRC Press.

Enzymes

1. Prostaglandin F2-alpha receptor (/proteins/HMDBP01950) — Enzyme Details (/proteins/HMDBP01950)

General function: Involved in G-protein coupled receptor protein signaling pathway
Specific function: Receptor for prostaglandin F2-alpha (PGF2-alpha). The activity of this receptor is mediated by G proteins which activate a phosphatidylinositol-calcium second messenger system. Initiates luteolysis in the corpus luteum
Gene Name: PTGFR
Uniprot ID: P43088 (http://www.uniprot.org/uniprot/P43088)
Molecular weight: 40054.1

References

1. Ota T, Aihara M, Narumiya S, Araie M: The effects of prostaglandin analogues on IOP in prostanoid FP-receptor-deficient mice. Invest Ophthalmol Vis Sci. 2005 Nov;46(11):4159-63. [PubMed:16249494 (http://www.ncbi.nlm.nih.gov/pubmed/16249494)]
2. Nakajima T, Matsugi T, Goto W, Kageyama M, Mori N, Matsumura Y, Hara H: New fluoroprostaglandin F(2alpha) derivatives with prostanoid FP-receptor agonistic activity as potent ocular-hypotensive agents. Biol Pharm Bull. 2003 Dec;26(12):1691-5. [PubMed:14646172 (http://www.ncbi.nlm.nih.gov/pubmed/14646172)]
3. Takagi Y, Nakajima T, Shimazaki A, Kageyama M, Matsugi T, Matsumura Y, Gabelt BT, Kaufman PL, Hara H: Pharmacological characteristics of AFP-168 (tafluprost), a new prostanoid FP receptor agonist, as an ocular hypotensive drug. Exp Eye Res. 2004 Apr;78(4):767-76. [PubMed:15037111 (http://www.ncbi.nlm.nih.gov/pubmed/15037111)]
4. Ocklind A: Effect of latanoprost on the extracellular matrix of the ciliary muscle. A study on cultured cells and tissue sections. Exp Eye Res. 1998 Aug;67(2):179-91. [PubMed:9733584 (http://www.ncbi.nlm.nih.gov/pubmed/9733584)]
5. Maxey KM, Johnson JL, LaBrecque J: The hydrolysis of bimatoprost in corneal tissue generates a potent prostanoid FP receptor agonist. Surv Ophthalmol. 2002 Aug;47 Suppl 1:S34-40. [PubMed:12204699 (http://www.ncbi.nlm.nih.gov/pubmed/12204699)]
6. Chen X, Ji ZL, Chen YZ: TTD: Therapeutic Target Database. Nucleic Acids Res. 2002 Jan 1;30(1):412-5. [PubMed:11752352 (http://www.ncbi.nlm.nih.gov/pubmed/11752352)]

Transporters

1. Solute carrier organic anion transporter family member 2B1 (/proteins/HMDBP02021) — Enzyme Details (/proteins/HMDBP02021)

General function: Involved in transporter activity
Specific function: Mediates the Na(+)-independent transport of organic anions such as taurocholate, the prostaglandins PGD2, PGE1, PGE2, leukotriene C4, thromboxane B2 and iloprost
Gene Name: SLCO2B1
Uniprot ID: O94956 (http://www.uniprot.org/uniprot/O94956)

Molecular weight: 76697.9

References

1. Kraft ME, Glaeser H, Mandery K, Konig J, Auge D, Fromm MF, Schlotzer-Schrehardt U, Welge-Lussen U, Kruse FE, Zolk O: The prostaglandin transporter OATP2A1 is expressed in human ocular tissues and transports the antiglaucoma prostanoid latanoprost. Invest Ophthalmol Vis Sci. 2010 May;51(5):2504-11. doi: 10.1167/iovs.09-4290. Epub 2009 Dec 17. [PubMed:20019365 (http://www.ncbi.nlm.nih.gov/pubmed/20019365)]

(http://www.cihr-irsc.gc.ca) The Metabolomics Innovation Centre (http://www.metabolomicscentre.ca) (http://www.aihealthsolutions.ca) (http://genomealberta.ca) (http://genomebc.ca) (http://genomecanada.ca)

This project is supported by the Canadian Institutes of Health Research (http://www.cihr-irsc.gc.ca) (award #111062), Alberta Innovates - Health Solutions (http://www.aihealthsolutions.ca), and by The Metabolomics Innovation Centre (TMIC) (http://www.metabolomicscentre.ca/), a nationally-funded research and core facility that supports a wide range of cutting-edge metabolomic studies. TMIC is funded by Genome Alberta (http://www.genomealberta.ca), Genome British Columbia (http://www.genomebc.ca/), and Genome Canada (http://www.genomecanada.ca), a not-for-profit organization that is leading Canada's national genomics strategy with $900 million in funding from the federal government.