Showing metabocard for Latanoprost (HMDB0014792)

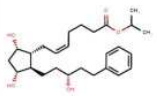
Identification | Taxonomy | Ontology | Physical properties | Spectra | Biological properties | Concentrations | Links | References | XML (/metabolites/HMDB0014792.xml)

Enzymes (1) | Transporters (1) | Show 2 proteins (/metabolites/HMDB0014792/metabolite_protein_links) | Show Metabolites with Similar Structures

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 prostagla 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**	**Sou**
	Isopropyl (Z)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((3R)-3-hydroxy-5-phenylpentyl)cyclopentyl)-5-heptenoate	ChE
	Latanoprostum	ChE
	PhXA 41	ChE
	Propan-2-yl (5Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl]hept-5-enoate	ChE
	Xalatan	ChE
	Isopropyl (Z)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((3R)-3-hydroxy-5-phenylpentyl)cyclopentyl)-5-heptenoic acid	Gen
	Propan-2-yl (5Z)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(3R)-3-hydroxy-5-phenylpentyl]cyclopentyl]hept-5-enoic acid	Gen
	PHXA41	MeS
	Pfizer brand OF latanoprost	MeS
	PhXA34	MeS

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 s 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-prec
pKa (Strongest Basic)	-2.7	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-prec
Physiological Charge	0	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-prec
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 $m^3 \cdot mol^{-1}$	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-5469500000-3070e3312e
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-7110196000-109246e3e7
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-qTof , Positive (/spectra/ms_ms/374384)	splash10-052r-1958000000-c694c9459db45a20b9af	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459c
LC-MS/MS	LC-MS/MS Spectrum - , positive (/spectra/ms_ms/450974)	splash10-052r-1958000000-c694c9459db45a20b9af	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459c
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 10V, Positive (/spectra/ms_ms/63027)	splash10-014j-1019700000-ea3b09b676d18f1597e8	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-014j-1019700000-ea3b09b67
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 20V, Positive (/spectra/ms_ms/63028)	splash10-03di-5119100000-970c5bfecae331f19237	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-5119100000-970c5bfeca
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 40V, Positive (/spectra/ms_ms/63029)	splash10-03dl-9123000000-71493bbb4b5c38c17db2	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03dl-9123000000-71493bbb4
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 10V, Negative (/spectra/ms_ms/119895)	splash10-053r-3002900000-194e702a216b0d2dfe90	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-053r-3002900000-194e702a2
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 20V, Negative (/spectra/ms_ms/119896)	splash10-0a4i-9104400000-d8c800c6e0be22ba0c3b	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9104400000-d8c800c6e
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 40V, Negative (/spectra/ms_ms/119897)	splash10-0a4i-9001000000-d471d19421c5af96709a	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9001000000-d471d19421

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 (/concentr
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 (/concentr

Abnormal Concentrations

Not Available

Associated Disorders and Diseases

Disease References None

Associated OMIM IDs None

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