Showing metabocard for Tafluprost (HMDB0015704)

Identification | Taxonomy | Ontology | Physical properties | Spectra | Biological properties | Concentrations | Links | References | XML (/metabolites/HMDB0015704.xml)

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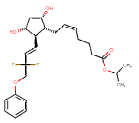
Record Information	
Version	4.0
Status	Expected but not Quantified
Creation Date	2012-09-06 15:16:52 UTC
Update Date	2018-05-20 20:22:11 UTC
HMDB ID	HMDB0015704
Secondary Accession Numbers	• HMDB15704
Metabolite Identification	
Common Name	**Tafluprost**
Description	Tafluprost is only found in individuals that have used or taken this drug. It is a prostaglandin analogue used topically (as eye drops) to control the progression of glaucoma and in the management of ocular hypertension. Tafluprost was approved for use in the U.S. on February 10, 2012.Tafluprost is a prostaglandin F2a analogue. Specifically, Tafluprost is a prostanoid selective FP receptor agonist that is believed to reduce the intraocular pressure (IOP) by increasing the outflow of aqueous humor. Studies in animals and man suggest that the main mechanism of action is increased uveoscleral outflow.
Structure	 (/structures/HMDB0015704/image.svg) MOL (/structures/metabolites/HMDB0015704.mol) SDF (/structures/metabolites/HMDB0015704.sdf) 3D-SDF (/structures/metabolites/HMDB0015704.sdf?dim=3d) PDB (/structures/metabolites/HMDB0015704.pdb) SMILES (/structures/metabolites/HMDB0015704.smiles) InChI (/structures/metabolites/HMDB0015704.inchi) View 3D Structure (/structures/metabolites/HMDB0015704)
Synonyms	**Value** / **Source** Zioptan / ChEBI AFP-168 / HMDB Saflutan / HMDB 1-Methylethyl (5Z)-7-((1R,2R, 3R,5S)-2-((1E)-3,3-difluoro-4-phenoxy -1-butenyl)-3,5-dihydroxycyclopentyl)-5-heptenoate / MeSH
Chemical Formula	$C_{25}H_{34}F_2O_5$
Average Molecular Weight	452.5313
Monoisotopic Molecular Weight	452.237430608
IUPAC Name	propan-2-yl (5Z)-7-[(1R,2R,3R,5S)-2-[(1E)-3,3-difluoro-4-phenoxybut-1-en-1-yl]-3,5-dihydroxycyclopentyl]hept-5-enoate
Traditional Name	tafluprost
CAS Registry Number	209860-87-7
SMILES	CC(C)OC(=O)CCC\C=C/C[C@H]1[C@@H](O)C[C@@H](O)[C@@H]1\C=C\C(F)(F)COC1=CC=CC=C1
InChI Identifier	InChI=1S/C25H34F2O5/c1-18(2)32-24(30)13-9-4-3-8-12-20-21(23(29)16-22(20)28)14-15-25(26,27)17-31-19-10-6-5-7-11-19/h3,5-8,10-11,14-15,18,20-23,28-29H,4,9,12-13,16-17H2,1-2H3/b8-3-,15-14+/t20-,21-,22+,23-/m1/s1
InChI Key	WSNODXPBBALQOF-VEJSHDCNSA-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	• Phenoxy compounds (http://classyfire.wishartlab.com/tax_nodes/C0004742) • Phenol ethers (http://classyfire.wishartlab.com/tax_nodes/C0002341) • Fatty acid esters (http://classyfire.wishartlab.com/tax_nodes/C0000324) • Alkyl aryl ethers (http://classyfire.wishartlab.com/tax_nodes/C0000128) • Cyclopentanols (http://classyfire.wishartlab.com/tax_nodes/C0002938) • 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) • Organofluorides (http://classyfire.wishartlab.com/tax_nodes/C0001517) • 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) • Alkyl fluorides (http://classyfire.wishartlab.com/tax_nodes/C0001027)

Substituents	• Prostaglandin skeleton • Phenoxy compound • Phenol ether • Alkyl aryl ether • Fatty acid ester • Benzenoid • Monocyclic benzene moiety • Cyclopentanol • Cyclic alcohol • Secondary alcohol • Carboxylic acid ester • Carboxylic acid derivative • Monocarboxylic acid or derivatives • Ether • Organooxygen compound • Alkyl fluoride • Alcohol • Organohalogen compound • Organofluoride • Carbonyl group • Hydrocarbon derivative • Alkyl halide • Organic oxygen compound • Organic oxide • Aromatic homomonocyclic compound
Molecular Framework	Aromatic homomonocyclic compounds
External Descriptors	• organofluorine compound (CHEBI:66899 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:66899)) • carboxylic ester (CHEBI:66899 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:66899)) • prostaglandins Falpha (CHEBI:66899 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:66899))
Ontology	
Disposition	Route of exposure: Enteral: ◦ Ingestion (/metabolite_ontology_terms/4858540) Source: ◦ Food (/metabolite_ontology_terms/4858539) Biological location: Subcellular: ◦ Membrane (/metabolite_ontology_terms/3241642) ◦ Cell membrane (/metabolite_ontology_terms/3675827) ◦ Cytoplasm (/metabolite_ontology_terms/3836229) Biofluid and excreta: ◦ Urine (/metabolite_ontology_terms/3395340) ◦ Blood (/metabolite_ontology_terms/3395341)
Process	Naturally occurring process: Biological process: Biochemical process: ◦ Lipid transport (/metabolite_ontology_terms/4858543) ◦ Lipid metabolism (/metabolite_ontology_terms/4858544) ◦ Fatty acid metabolism (/metabolite_ontology_terms/4858545) Chemical reaction: ◦ Lipid peroxidation (/metabolite_ontology_terms/4858542) Biochemical pathway: ◦ Lipid metabolism pathway (/metabolite_ontology_terms/4858541) Multicellular process: ◦ Inflammatory response (/metabolite_ontology_terms/3836233) ◦ Immune response (/metabolite_ontology_terms/3836234) Cellular process: ◦ Cell signaling (/metabolite_ontology_terms/3836235)
Role	Biological role: ◦ Nutrient (/metabolite_ontology_terms/3836230) ◦ Inflammatory (/metabolite_ontology_terms/3836231) ◦ Energy storage (/metabolite_ontology_terms/4858546) ◦ Energy source (/metabolite_ontology_terms/4858547) ◦ Membrane stabilizer (/metabolite_ontology_terms/4858548) Modulator: ◦ Immunomodulator (/metabolite_ontology_terms/3836232) Industrial application: ◦ Drug (/metabolite_ontology_terms/3451451) Pharmaceutical industry: ◦ Pharmaceutical (/metabolite_ontology_terms/3603864) Cardiovascular drug: ◦ Antihypertensive (/metabolite_ontology_terms/3451452)
Physical Properties	

Experimental Properties

Property	Value	Reference
Melting Point	Not Available	Not Available
Boiling Point	Not Available	Not Available
Water Solubility	0.0053 g/L	Not Available
LogP	Not Available	Not Available

Predicted Properties

Property	Value	Source
Water Solubility	0.0053 g/L	ALOGPS (http://www.vcclab.org/lab/alogps/)
logP	4.46	ALOGPS (http://www.vcclab.org/lab/alogps/)
logP	4.29	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#logp_logd)
logS	-4.9	ALOGPS (http://www.vcclab.org/lab/alogps/)
pKa (Strongest Acidic)	14.51	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-predictors/#pka)
pKa (Strongest Basic)	-2.9	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	2	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#h_bond)
Polar Surface Area	75.99 Å²	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topolgical_surface)
Rotatable Bond Count	13	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topology_analysis)
Refractivity	120.59 m³·mol⁻¹	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#refractivity)
Polarizability	48.65 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/17077)	splash10-052f-4439700000-5f902e96f572f76cc593	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052f-4439700000-5f902e96f572f76cc593)
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (2 TMS) - 70eV, Positive (/spectra/c_ms/40772)	splash10-001l-7200690000-8373b0788e1ed396a7fa	View in MoNA (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-001l-7200690000-8373b0788e1ed396a7fa)

Biological Properties

Cellular Locations

- 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 DB08819	21059682 (http://www.ncbi.nlm.nih.gov/pubmed/21059682)	details (/concentrations/69057)
	Urine	Expected but not Quantified		Not Available	Not Available	Taking drug identified by DrugBank entry DB08819	21059682 (http://www.ncbi.nlm.nih.gov/pubmed/21059682)	details (/concentrations/69056)

Abnormal Concentrations	
	Not Available
Associated Disorders and Diseases	
Disease References	None
Associated OMIM IDs	None
External Links	
DrugBank ID	DB08819 (http://www.drugbank.ca/drugs/DB08819)
Phenol Explorer Compound ID	Not Available
FoodDB ID	Not Available
KNApSAcK ID	Not Available
Chemspider ID	8044182 (http://www.chemspider.com/Chemical-Structure.8044182.html)
KEGG Compound ID	Not Available
BioCyc ID	Not Available
BiGG ID	Not Available
Wikipedia Link	Tafluprost (http://en.wikipedia.org/wiki/Tafluprost)
METLIN ID	Not Available
PubChem Compound	9868491 (http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=9868491)
PDB ID	Not Available
ChEBI ID	66899 (http://www.ebi.ac.uk/chebi/searchId.do?chebiId=66899)
References	
Synthesis Reference	Not Available
Material Safety Data Sheet (MSDS)	Not Available
General References	1. 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)] 2. Pantcheva MB, Seibold LK, Awadallah NS, Kahook MY: Tafluprost: a novel prostaglandin analog for treatment of glaucoma. Adv Ther. 2011 Sep;28(9):707-15. doi: 10.1007/s12325-011-0055-8. Epub 2011 Aug 18. [PubMed:21858491 (http://www.ncbi.nlm.nih.gov/pubmed/21858491)] 3. Fukano Y, Kawazu K: Disposition and metabolism of a novel prostanoid antiglaucoma medication, tafluprost, following ocular administration to rats. Drug Metab Dispos. 2009 Aug;37(8):1622-34. doi: 10.1124/dmd.108.024885. Epub 2009 May 28. [PubMed:19477946 (http://www.ncbi.nlm.nih.gov/pubmed/19477946)] 4. Papadia M, Bagnis A, Scotto R, Traverso CE: Tafluprost for glaucoma. Expert Opin Pharmacother. 2011 Oct;12(15):2393-401. doi: 10.1517/14656566.2011.606810. [PubMed:21916788 (http://www.ncbi.nlm.nih.gov/pubmed/21916788)] 5. 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)] 6. 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.

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

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