

http://www.metabolomicscentre.ca?utm_source=hmdb&utm_medium=banner&utm_campaign=tmic-campaign

Showing metabocard for Tafluprost (HMDB0015704)

Identification Taxonomy Ontology Physical properties Spectra Biological properties Concentrations Links References XML (/metabolites/HMDB0015704.xml)											
Show Metabolites with Similar Structures											
Show more... Show more...											
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	<ul style="list-style-type: none"> 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	 <p>(/structures/HMDB0015704/image.svg)</p> <table border="1"> <tr> <td>MOL (/structures/metabolites/HMDB0015704.mol)</td> <td>SDF (/structures/metabolites/HMDB0015704.sdf)</td> <td>3D-SDF (/structures/metabolites/HMDB0015704.sdf?dim=3d)</td> </tr> <tr> <td>PDB (/structures/metabolites/HMDB0015704.pdb)</td> <td>SMILES (/structures/metabolites/HMDB0015704.smiles)</td> <td>InChI (/structures/metabolites/HMDB0015704.inchi)</td> </tr> </table> <p>View 3D Structure (/structures/metabolites/HMDB0015704)</p>	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)				
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)									
Synonyms	<table border="1"> <thead> <tr> <th>Value</th> <th>Source</th> </tr> </thead> <tbody> <tr> <td>Zioptan</td> <td>ChEBI</td> </tr> <tr> <td>AFP-168</td> <td>HMDB</td> </tr> <tr> <td>Saflutan</td> <td>HMDB</td> </tr> <tr> <td>1-Methylethyl (5Z)-7-((1R,2R, 3R,5S)-2-((1E)-3,3-difluoro-4-phenoxy -1-butenyl)-3,5-dihydroxycyclopentyl)-5-heptenoate</td> <td>MeSH</td> </tr> </tbody> </table>	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
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 ₂₈ H ₃₈ F ₂ O 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]1C=C(C(F)F)COC1=CC=CC=C1										
InChI Identifier	InChI=1S/C28H34F2O5/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-/m 1/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://classifyfire.wishartlab.com/tax_nodes/C0000000)										
Super Class	Lipids and lipid-like molecules ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0000012)										
Class	Fatty Acyls ☞ (http://classifyfire.wishartlab.com/tax_nodes/C00003909)										
Sub Class	Eicosanoids ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0000513)										
Direct Parent	Prostaglandins and related compounds ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0000514)										
Alternative Parents	<ul style="list-style-type: none"> Phenoxy compounds ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0004742) Phenol ethers ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0002341) Fatty acid esters ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0000324) Alkyl aryl ethers ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0000128) Cyclopentanols ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0002938) Cyclic alcohols and derivatives ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001292) Carboxylic acid esters ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001238) Monocarboxylic acids and derivatives ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001137) Organofluorides ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001517) Organic oxides ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0003940) Hydrocarbon derivatives ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0004150) Carbonyl compounds ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001831) Alkyl fluorides ☞ (http://classifyfire.wishartlab.com/tax_nodes/C0001027) 										

Docket Alarm

Find authenticated court documents without watermarks at docketalarm.com.

Substituents	<ul style="list-style-type: none"> • 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 • Organoxygen 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	<ul style="list-style-type: none"> • 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	<p>Route of exposure:</p> <p>Enteral:</p> <ul style="list-style-type: none"> ◦ Ingestion (/metabolite_ontology_terms/4858540) <p>Source:</p> <ul style="list-style-type: none"> ◦ Food (/metabolite_ontology_terms/4858539) <p>Biological location:</p> <p>Subcellular:</p> <ul style="list-style-type: none"> ◦ Membrane (/metabolite_ontology_terms/3241642) ◦ Cell membrane (/metabolite_ontology_terms/3675827) ◦ Cytoplasm (/metabolite_ontology_terms/3836229) <p>Biofluid and excreta:</p> <ul style="list-style-type: none"> ◦ Urine (/metabolite_ontology_terms/3395340) ◦ Blood (/metabolite_ontology_terms/3395341)
Process	<p>Naturally occurring process:</p> <p>Biological process:</p> <p>Biochemical process:</p> <ul style="list-style-type: none"> ◦ Lipid transport (/metabolite_ontology_terms/4858543) ◦ Lipid metabolism (/metabolite_ontology_terms/4858544) ◦ Fatty acid metabolism (/metabolite_ontology_terms/4858545) <p>Chemical reaction:</p> <ul style="list-style-type: none"> ◦ Lipid peroxidation (/metabolite_ontology_terms/4858542) <p>Biochemical pathway:</p> <ul style="list-style-type: none"> ◦ Lipid metabolism pathway (/metabolite_ontology_terms/4858541) <p>Multicellular process:</p> <ul style="list-style-type: none"> ◦ Inflammatory response (/metabolite_ontology_terms/3836233) ◦ Immune response (/metabolite_ontology_terms/3836234) <p>Cellular process:</p> <ul style="list-style-type: none"> ◦ Cell signaling (/metabolite_ontology_terms/3836235)
Role	<p>Biological role:</p> <ul style="list-style-type: none"> ◦ 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) <p>Modulator:</p> <ul style="list-style-type: none"> ◦ Immunomodulator (/metabolite_ontology_terms/3836232) <p>Industrial application:</p> <ul style="list-style-type: none"> ◦ Drug (/metabolite_ontology_terms/3451451) <p>Pharmaceutical industry:</p> <ul style="list-style-type: none"> ◦ Pharmaceutical (/metabolite_ontology_terms/3603864) <p>Cardiovascular drug:</p> <ul style="list-style-type: none"> ◦ 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 Å ²	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topoligical_surface)	
		Rotatable Bond Count	13	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#topology_analysis)	
		Refractivity	120.59 m ³ ·mol ⁻¹	ChemAxon (http://www.chemaxon.com/products/calculator-plugins/property-calculations/#refractivity)	
		Polarizability	48.65 Å ³	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)	splash10-0011-7200690000-8373b0788e1ed396a7fa	View in MoNA ☞ (http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0011-7200690000-8373b0788e1ed396a7fa)
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) (http://www.drugbank.ca/drugs/DB08819)

Phenol Explorer Compound ID Not Available

FoodDB ID Not Available

KNApSAck ID Not Available

Chempid ID 8044182 [Ⓞ](http://www.chemspider.com/Chemical-Structure.8044182.html) (http://www.chemspider.com/Chemical-Structure.8044182.html)

KEGG Compound ID Not Available

BioCyc ID Not Available

BIGG ID Not Available

Wikipedia Link [Ⓞ](http://en.wikipedia.org/wiki/Tafuprost) (http://en.wikipedia.org/wiki/Tafuprost)

METLIN ID Not Available

PubChem Compound 9868491 [Ⓞ](http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=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) (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 (tafuprost), a new prostanoïd 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) (http://www.ncbi.nlm.nih.gov/pubmed/15037111)]
2. Pantcheva MB, Seibold LK, Awadallah NS, Kahook MY: Tafuprost: 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) (http://www.ncbi.nlm.nih.gov/pubmed/21858491)]
3. Fukano Y, Kawazu K: Disposition and metabolism of a novel prostanoïd antiglaucoma medication, tafuprost, 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) (http://www.ncbi.nlm.nih.gov/pubmed/19477946)]
4. Papadia M, Bagnis A, Scotto R, Traverso CE: Tafuprost 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) (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(11):31-9. [PubMed:11413487 [Ⓞ](http://www.ncbi.nlm.nih.gov/pubmed/11413487) (http://www.ncbi.nlm.nih.gov/pubmed/11413487)]
6. Watson AD: Thematic review series: systems biology approaches to metabolic and cardiovascular disorders. I. 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>)



(<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.

HMDB Version 4.0 — Contact Us ([/w/contact](#))