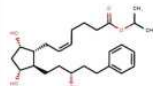


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(http://www.metabolomicscentre.ca?utm\_source=hmdb&amp;utm\_medium=banner&amp;utm\_campaign=tmic-campaign)

## Showing metabocard for Latanoprost (HMDB0014792)

Identification	Taxonomy	Ontology	Physical properties	Species	Biological properties	Concentrations	Links	References	XML (/metabolites/HMDB0014792.xml)									
<a href="#">Synonyms (1)</a> <a href="#">Proteins (1)</a> <a href="#">Show 2 proteins (/metabolites/HMDB0014792/metabolite_protein_links)</a>		<a href="#">Show Metabolites with Similar Structures</a>																
<b>Record Information</b>																		
<b>Version</b>	4.0																	
<b>Status</b>	Expected but not Quantified																	
<b>Creation Date</b>	2012-09-06 15:16:50 UTC																	
<b>Update Date</b>	2018-05-20 20:10:45 UTC																	
<b>HMDB ID</b>	HMDB0014792																	
<b>Secondary Accession Numbers</b>	<ul style="list-style-type: none"> <li>HMDB14792</li> </ul>																	
<b>Metabolite Identification</b>																		
<b>Common Name</b>	Latanoprost																	
<b>Description</b>	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.																	
<b>Structure</b>																		
 (/structures/HMDB0014792/image.svg)																		
<table border="1"> <tr> <td><a href="#">MOL (/structures/metabolites/HMDB0014792.mol)</a></td> <td><a href="#">SDF (/structures/metabolites/HMDB0014792.sdf)</a></td> <td><a href="#">3D-SDF (/structures/metabolites/HMDB0014792.sdf?dim=3d)</a></td> </tr> <tr> <td><a href="#">PDB (/structures/metabolites/HMDB0014792.pdb)</a></td> <td><a href="#">SMILES (/structures/metabolites/HMDB0014792.smiles)</a></td> <td><a href="#">INCHI (/structures/metabolites/HMDB0014792.inchi)</a></td> </tr> <tr> <td colspan="3"><a href="#">View 3D Structure (/structures/metabolites/HMDB0014792)</a></td> </tr> </table>										<a href="#">MOL (/structures/metabolites/HMDB0014792.mol)</a>	<a href="#">SDF (/structures/metabolites/HMDB0014792.sdf)</a>	<a href="#">3D-SDF (/structures/metabolites/HMDB0014792.sdf?dim=3d)</a>	<a href="#">PDB (/structures/metabolites/HMDB0014792.pdb)</a>	<a href="#">SMILES (/structures/metabolites/HMDB0014792.smiles)</a>	<a href="#">INCHI (/structures/metabolites/HMDB0014792.inchi)</a>	<a href="#">View 3D Structure (/structures/metabolites/HMDB0014792)</a>		
<a href="#">MOL (/structures/metabolites/HMDB0014792.mol)</a>	<a href="#">SDF (/structures/metabolites/HMDB0014792.sdf)</a>	<a href="#">3D-SDF (/structures/metabolites/HMDB0014792.sdf?dim=3d)</a>																
<a href="#">PDB (/structures/metabolites/HMDB0014792.pdb)</a>	<a href="#">SMILES (/structures/metabolites/HMDB0014792.smiles)</a>	<a href="#">INCHI (/structures/metabolites/HMDB0014792.inchi)</a>																
<a href="#">View 3D Structure (/structures/metabolites/HMDB0014792)</a>																		
<b>Synonyms</b>																		
<b>Value</b>									<b>Sou</b>									
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									
<b>Chemical Formula</b>																		
<b>Chemical Formula</b>	C <sub>26</sub> H <sub>40</sub> O <sub>5</sub>																	
<b>Average Molecular Weight</b>																		
<b>Average Molecular Weight</b>	432.5928																	
<b>Monoisotopic Molecular Weight</b>																		
<b>Monoisotopic Molecular Weight</b>	432.28757439																	
<b>IUPAC Name</b>																		
<b>IUPAC Name</b>	propan-2-yl (5Z)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((3R)-3-hydroxy-5-phenylpentyl)cyclopentyl)hept-5-enoate																	
<b>Traditional Name</b>																		
<b>Traditional Name</b>	latanoprost																	



**CAS Registry Number** 130209-82-4

**SMILES** CC(C)OC(=O)CCC=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) ([http://classyfire.wishartlab.com/tax\\_nodes/C0000000](http://classyfire.wishartlab.com/tax_nodes/C0000000))

**Super Class** Lipids and lipid-like molecules [☞](http://classyfire.wishartlab.com/tax_nodes/C0000012) ([http://classyfire.wishartlab.com/tax\\_nodes/C0000012](http://classyfire.wishartlab.com/tax_nodes/C0000012))

**Class** Fatty Acyls [☞](http://classyfire.wishartlab.com/tax_nodes/C0003909) ([http://classyfire.wishartlab.com/tax\\_nodes/C0003909](http://classyfire.wishartlab.com/tax_nodes/C0003909))

**Sub Class** Eicosanoids [☞](http://classyfire.wishartlab.com/tax_nodes/C0000513) ([http://classyfire.wishartlab.com/tax\\_nodes/C0000513](http://classyfire.wishartlab.com/tax_nodes/C0000513))

**Direct Parent** Prostaglandins and related compounds [☞](http://classyfire.wishartlab.com/tax_nodes/C0000514) ([http://classyfire.wishartlab.com/tax\\_nodes/C0000514](http://classyfire.wishartlab.com/tax_nodes/C0000514))

**Alternative Parents**

- Fatty acid esters [☞](http://classyfire.wishartlab.com/tax_nodes/C0000324) ([http://classyfire.wishartlab.com/tax\\_nodes/C0000324](http://classyfire.wishartlab.com/tax_nodes/C0000324))
- Cyclopentanols [☞](http://classyfire.wishartlab.com/tax_nodes/C0002938) ([http://classyfire.wishartlab.com/tax\\_nodes/C0002938](http://classyfire.wishartlab.com/tax_nodes/C0002938))
- Benzene and substituted derivatives [☞](http://classyfire.wishartlab.com/tax_nodes/C0002279) ([http://classyfire.wishartlab.com/tax\\_nodes/C0002279](http://classyfire.wishartlab.com/tax_nodes/C0002279))
- Cyclic alcohols and derivatives [☞](http://classyfire.wishartlab.com/tax_nodes/C0001292) ([http://classyfire.wishartlab.com/tax\\_nodes/C0001292](http://classyfire.wishartlab.com/tax_nodes/C0001292))
- Carboxylic acid esters [☞](http://classyfire.wishartlab.com/tax_nodes/C0001238) ([http://classyfire.wishartlab.com/tax\\_nodes/C0001238](http://classyfire.wishartlab.com/tax_nodes/C0001238))
- Monocarboxylic acids and derivatives [☞](http://classyfire.wishartlab.com/tax_nodes/C0001137) ([http://classyfire.wishartlab.com/tax\\_nodes/C0001137](http://classyfire.wishartlab.com/tax_nodes/C0001137))
- Organic oxides [☞](http://classyfire.wishartlab.com/tax_nodes/C0003940) ([http://classyfire.wishartlab.com/tax\\_nodes/C0003940](http://classyfire.wishartlab.com/tax_nodes/C0003940))
- Hydrocarbon derivatives [☞](http://classyfire.wishartlab.com/tax_nodes/C0004150) ([http://classyfire.wishartlab.com/tax\\_nodes/C0004150](http://classyfire.wishartlab.com/tax_nodes/C0004150))
- Carbonyl compounds [☞](http://classyfire.wishartlab.com/tax_nodes/C0001831) ([http://classyfire.wishartlab.com/tax\\_nodes/C0001831](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) (<http://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:6384>))
- prostaglandins FaIpha (CHEBI:6384 [☞](http://www.ebi.ac.uk/chebi/searchId.do?chebiId=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) (<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)

<b>Process</b>	<p>Naturally occurring process:</p> <p>Biological process:</p> <p>Biochemical process:</p> <ul style="list-style-type: none"> <li>◦ Lipid transport (/metabolite_ontology_terms/4903896)</li> <li>◦ Lipid metabolism (/metabolite_ontology_terms/4903897)</li> <li>◦ Fatty acid metabolism (/metabolite_ontology_terms/4903898)</li> </ul> <p>Chemical reaction:</p> <ul style="list-style-type: none"> <li>◦ Lipid peroxidation (/metabolite_ontology_terms/4903895)</li> </ul> <p>Biochemical pathway:</p> <ul style="list-style-type: none"> <li>◦ Lipid metabolism pathway (/metabolite_ontology_terms/4903894)</li> </ul> <p>Multicellular process:</p> <ul style="list-style-type: none"> <li>◦ Inflammatory response (/metabolite_ontology_terms/3835951)</li> <li>◦ Immune response (/metabolite_ontology_terms/3835952)</li> </ul> <p>Cellular process:</p> <ul style="list-style-type: none"> <li>◦ Cell signaling (/metabolite_ontology_terms/3449682)</li> </ul>		
<b>Role</b>	<p>Biological role:</p> <ul style="list-style-type: none"> <li>◦ Membrane stabilizer (/metabolite_ontology_terms/3674474)</li> <li>◦ Energy source (/metabolite_ontology_terms/3674475)</li> <li>◦ Energy storage (/metabolite_ontology_terms/3674476)</li> <li>◦ Nutrient (/metabolite_ontology_terms/3835948)</li> <li>◦ Inflammatory (/metabolite_ontology_terms/3835949)</li> </ul> <p>Modulator:</p> <ul style="list-style-type: none"> <li>◦ Immunomodulator (/metabolite_ontology_terms/3835950)</li> </ul> <p>Industrial application:</p> <ul style="list-style-type: none"> <li>◦ Drug (/metabolite_ontology_terms/3449680)</li> <li>◦ Surfactant (/metabolite_ontology_terms/3674472)</li> <li>◦ Emulsifier (/metabolite_ontology_terms/3674473)</li> </ul> <p>Pharmaceutical industry:</p> <ul style="list-style-type: none"> <li>◦ Pharmaceutical (/metabolite_ontology_terms/3602520)</li> </ul> <p>Cardiovascular drug:</p> <ul style="list-style-type: none"> <li>◦ Antihypertensive (/metabolite_ontology_terms/3449681)</li> </ul>		
<b>Physical Properties</b>			
<b>State</b>	Liquid		
<b>Experimental Properties</b>	<b>Property</b>	<b>Value</b>	<b>Reference</b>
	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

7/9/2018

## Human Metabolome Database: Showing metabocard for Latanoprost (HMDB0014792)

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

Spectra

Spectra		Spectrum Type	Description	Splash Key ( <a href="http://splash.fiehnlab.ucdavis.edu/">http://splash.fiehnlab.ucdavis.edu/</a> )	
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (Non-derivatized) - 70eV, Positive (/spectra/c_ms/17619)	splash10-00kf-5469500000-3070e3312e2f54422e2eb	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-00kf-5469500000-3070e3312e2f54422e2eb">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-00kf-5469500000-3070e3312e2f54422e2eb">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-00kf-5469500000-3070e3312e2f54422e2eb</a>	
Predicted GC-MS	Predicted GC-MS Spectrum - GC-MS (3 TMS) - 70eV, Positive (/spectra/c_ms/40446)	splash10-001f-7110196000-109246e3e73496dba6fd	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-001f-7110196000-109246e3e73496dba6fd">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-001f-7110196000-109246e3e73496dba6fd">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-001f-7110196000-109246e3e73496dba6fd</a>	
LC-MS/MS	LC-MS/MS Spectrum - LC-ESI-qTof, Positive (/spectra/ms_ms/374384)	splash10-052r-1958000000-c694c9459db45a20b9af	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af</a>	
LC-MS/MS	LC-MS/MS Spectrum -, positive (/spectra/ms_ms/450974)	splash10-052r-1958000000-c694c9459db45a20b9af	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-052r-1958000000-c694c9459db45a20b9af</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 10V, Positive (/spectra/ms_ms/63027)	splash10-014j-1019700000-ea3b09b676d18f1597e8	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-014j-1019700000-ea3b09b676d18f1597e8">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-014j-1019700000-ea3b09b676d18f1597e8">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-014j-1019700000-ea3b09b676d18f1597e8</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 20V, Positive (/spectra/ms_ms/63028)	splash10-03di-5119100000-970c5bfecae331f19237	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-5119100000-970c5bfecae331f19237">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-5119100000-970c5bfecae331f19237">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-5119100000-970c5bfecae331f19237</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 40V, Positive (/spectra/ms_ms/63029)	splash10-03di-9123000000-71493bbb4b5c38c17db2	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-9123000000-71493bbb4b5c38c17db2">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-9123000000-71493bbb4b5c38c17db2">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-03di-9123000000-71493bbb4b5c38c17db2</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 10V, Negative (/spectra/ms_ms/119895)	splash10-053r-3002900000-194e702a216b0d2dfe90	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-053r-3002900000-194e702a216b0d2dfe90">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-053r-3002900000-194e702a216b0d2dfe90">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-053r-3002900000-194e702a216b0d2dfe90</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 20V, Negative (/spectra/ms_ms/119896)	splash10-0a4i-9104400000-d8c800c6e0be22ba0c3b	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9104400000-d8c800c6e0be22ba0c3b">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9104400000-d8c800c6e0be22ba0c3b">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9104400000-d8c800c6e0be22ba0c3b</a>	
Predicted LC-MS/MS	Predicted LC-MS/MS Spectrum - 40V, Negative (/spectra/ms_ms/119897)	splash10-0a4i-9001000000-d471d19421c5af96709a	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9001000000-d471d19421c5af96709a">View in MoNA</a>	<a href="http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9001000000-d471d19421c5af96709a">http://mona.fiehnlab.ucdavis.edu/#/spectra/splash/splash10-0a4i-9001000000-d471d19421c5af96709a</a>	

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 <a href="http://www.ncbi.nlm.nih.gov/pubmed/21059682">C</a> ( <a href="http://www.ncbi.nlm.nih.gov/pubmed/21059682">http://www.ncbi.nlm.nih.gov/pubmed/21059682</a> )	<a href="#">View</a> ( <a href="#">/concentr.</a> )
Urine	Expected but not Quantified		Not Available	Not Available	Taking drug identified by DrugBank entry DB00654	21059682 <a href="http://www.ncbi.nlm.nih.gov/pubmed/21059682">C</a> ( <a href="http://www.ncbi.nlm.nih.gov/pubmed/21059682">http://www.ncbi.nlm.nih.gov/pubmed/21059682</a> )	<a href="#">View</a> ( <a href="#">/concentr.</a> )

Abnormal Concentrations

Not Available

Associated Disorders and Diseases

**Disease References** None

**Associated OMIM IDs** None

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