



Product Information

Integrin inhibitor, Lifitegrast, Purity $\geq 98\%$

Cat. No.: X24-08-YM305

Size: 10 mg; 50 mg; 100 mg; 200 mg

MDL: MFCD28502439

CAS Number: 1025967-78-5

Compound CID: 11965427

Synonym: 1025967-78-5; SAR-1118; SAR 1118; SAR1118; Lifitegrast; brand name:

Xiidra.;

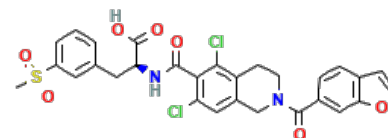
(2S

)-2-[[2-(1-Benzofuran-6-carbonyl)-5,7-dichloro-3,4-dihydro-1H

isoquinoline-6-carbonyl]amino]-3-(3-methylsulfonylphenyl)propanoic acid

-isoquinoline-6-carbonyl]amino]-3-(3-methylsulfonylphenyl)propanoic acid

This product is for research use only and is not intended for diagnostic use.



Product Information

Description	Lifitegrast, soluble in DMSO and ethanol and insoluble in water, is an effective cytoskeleton inhibitor, that has the ability to prevent the pathway of cytoskeletal signaling by inhibiting integrin.
Molecular Weight	615.478
Molecular Formula	C ₂₉ H ₂₄ Cl ₂ N ₂ O ₇ S
IUPAC Name	(2S)-2-[[2-(1-Benzofuran-6-carbonyl)-5,7-dichloro-3,4-dihydro-1H-isoquinoline-6-carbonyl]amino]-3-(3-methylsulfonylphenyl)propanoic acid
InChI	InChI=1S/C29H24Cl2N2O7S/c1-41(38,39)20-4-2-3-16(11-20)12-23(29(36)37)32-27(34)25-22(30)13-19-15-33(9-7-21(19)26(25)31)28(35)18-6-5-17-8-10-40-24(17)14-18/h2-6,8,10-11,13-14,23H,7,9,12,15H2,1H3,(H,32,34)(H,36,37)/t23-m/s1
InChI Key	PMBSPGRUJJNPQ-PSHVLCQKSA-N
Canonical SMILES	CN1C(C(=O)NC(C(=O)NC(CC(=O)NCC(=O)NC(C1=O)CCCN=C(N)N)C(=O)O)C2=CC=CC=C2)CCCN
Isomeric SMILES	CN1[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](CC(=O)NCC(=O)N[C@H](C1=O)CCCN=C(N)N)C(=O)O)C2=CC=CC=C2)CCCCN
Form	Lyophilized powder
Purity	$\geq 98\%$



Titer	Free from inappropriate visible particulates, foreign matter, discoloration, or other defects
Solubility	<i>In vitro</i> : DMSO: 98 mg/mL (159.22 mM); Water: insoluble; Ethanol: 20 mg/mL
Stability	In its lyophilized form, the chemical remains stable for 36 months.
Quality Level	Research grade
Applications	Lifitegrast is a cytoskeletal signaling inhibitor that can be studied extensively for its potential therapeutic applications in the treatment of dry eye disease by blocking the interaction of integrin α L β 2 with its ligand, which reduces inflammation and improves symptoms.
Storage	Store at -20°C, and keep desiccated.