



Sitagliptin

Cat. No.:	OB0225WX-2615
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	25 mg; 50 mg; 100 mg; 1 g; 2 g

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

Product Overview

Description	Sitagliptin is a highly selective, orally bioavailable inhibitor of the dipeptidyl peptidase-4 (DPP-4) enzyme, characterized by an IC50 of 18 nM.
Synonym	MK-0431; 486460-32-6; Xelevia; LEZ763; Tesavel; Sitagliptina; Sitagliptine; Sitaagliptinum; Zituvio; (3R)-3-amino-1-[3-(trifluoromethyl)-6,8-dihydro-5H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]-4-(2,4,5-trifluorophenyl)butan-1-one; Sitagliptin (Metformin, MK-0431); 1,2,4-Triazolo[4,3-a]pyrazine, 7-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-; 7-[(3R)-3-Amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-trifluoromethyl-1,4-triazolo(4,3-a); (3R)-3-amino-1-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl]-4-(2,4,5-trifluorophenyl)butan-1-one; 1,2,4-Triazolo(4,3-a)pyrazine, 7-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-; (3R)-3-amino-1-(3-(trifluoromethyl)-5,6-dihydro(1,2,4)triazolo(4,3-a)pyrazin-7(8H)-yl)-4-(2,4,5-trifluorophenyl)butan-1-one; MFCD09838015; (3R)-3-amino-1-[3-(trifluoromethyl)-5H,6H,7H,8H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]-4-(2,4,5-trifluorophenyl)butan-1-one; (R)-3-amino-1-(3-(trifluoromethyl)-5,6-dihydro-[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl)-4-(2,4,5-trifluorophenyl)butan-1-one; 4-oxo-4-(3-(trifluoromethyl)-5,6-dihydro(1,2,4)triazolo(4,3-a)pyrazin-7(8H)-yl)-1-(2,4,5-trifluorophenyl)butan-2-amine
CAS No.	486460-32-6
Compound CID	4369359



Formula	C ₁₆ H ₁₅ F ₆ N ₅
Formula Weight	407.31

Specification

IUPAC Name	(3R)-3-Amino-1-[3-(trifluoromethyl)-6,8-dihydro-5H-[1,2,4]triazolo [4,3-a]pyrazin-7-yl]-4-(2,4,5-trifluorophenyl)butan-1-one
InChI	InChI=1S/C16H15F6N5O/c17-10-6-12(19)11(18)4-8(10)3-9(23)5-14(28)26-1-2-27-13(7-24)25-15(27)16(20,21)22/h4,6,9H,1-3,5,7,23H2/t9-/m1/s1
InChI Key	MFFMDFFZMYVKS-SECBINFHSA-N
SMILES string	C1CN2C(=NN=C2C(F)(F)F)CN1C(=O)C[C@@H](CC3=CC(=C(C=C3F)F)F)N
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	Sitagliptin is utilized in metabolic pharmacology as a selective DPP-4 inhibitor to examine the regulation of incretin hormones and the improvement of glycemic control through enhanced insulin secretion.

Library Information

Target	DPP
Receptor	DPP4
Pathways	Proteases
Plate Number	L6700-06
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	81 mg/mL; 198.87 mM
Water Max Solubility	5 mg/mL
Ethanol Max Solubility	81 mg/mL
ALogP	1.93
HBA_Count	3
HBD_Count	1
Rotatable Bond	5