

Saxagliptin (BMS-477118)

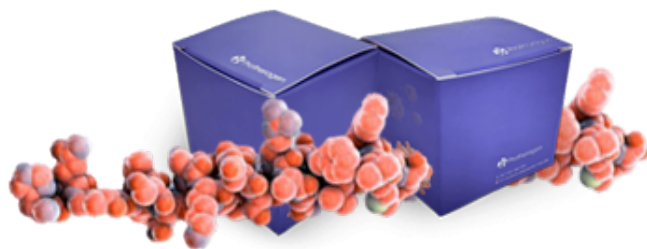
Cat. No.:	OB0225WX-2423
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	10 mg; 25 mg; 100 mg; 1 g

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

Product Overview

Description	Saxagliptin (BMS-477118) is a high-affinity, reversible antagonist of the DPP4 enzyme, exhibiting a half-maximal inhibitory concentration (IC ₅₀) of 26 nM.
Synonym	Onglyza; BMS-477118; 361442-04-8; Saxagliptin; Onglyza; OPC-262; Saxagliptin anhydrous; (1S,3S,5S)-2-((2S)-2-Amino-2-(3-hydroxyadamantan-1-yl)acetyl)-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (1S,3S,5S)-2-((2S)-Amino(3-hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)acetyl)-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (1S,3S,5S)-2-[(2S)-2-amino-2-(3-hydroxy-1-adamantyl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (1S,3S,5S)-2-[(2S)-2-amino-2-(3-hydroxyadamantan-1-yl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (S)-3-Hydroxyadamantylglycine-L-cis-4,5-methanoprolinenitrile TFA salt; (1S,6S)-2-(2-adamantan-1-yl-2-amino-acetyl)-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (1S,3S,5S)-2-[(2S)-2-amino-2-(3-hydroxyadamantan-1-yl)acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile; 2,2,2-trifluoroacetic acid; (1S,3S,5S)-2-[(2S)-2-amino-2-(3-hydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl)-1-oxoethyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile; (1S,3S,5S)-2-[(S)-2-amino-2-(3-hydroxyadamantan-1-yl)-acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile
CAS No.	361442-04-8
Compound CID	11243969
Formula	C ₁₈ H ₂₅ N ₃ O ₂
Formula Weight	315.41

Specification



IUPAC Name	(1S,3S,5S)-2-[(2S)-2-Amino-2-(3-hydroxy-1-adamantyl) acetyl]-2-azabicyclo[3.1.0]hexane-3-carbonitrile
InChI	InChI=1S/C18H25N3O2/c19-8-13-2-12-3-14(12)21(13)16(22)15(20)17-4-10-1-11(5-17)7-18(23,6-10)9-17/h10-15,23H,1-7,9,20H2/t10?,11?,12-,13+,14+,15-,17?,18?/m1/s1
InChI Key	QGJUIPDUBHWZPV-SGTAVMJGSA-N
SMILES string	<chem>C1[C@@H]2C[C@@H]2N([C@@H]1C#N)C(=O)[C@H](C34CC5CC(C3)CC(C5)(C4)O)N</chem>
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	Saxagliptin (BMS-477118) is utilized in metabolic research as a potent and selective DPP-4 inhibitor to investigate the enhancement of incretin hormone levels and the improvement of glucose-dependent insulin secretion.

Library Information

Target	DPP
Receptor	DPP4
Pathways	Proteases
Plate Number	L6700-02
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	63 mg/mL; 199.74 mM
Water Max Solubility	63 mg/mL; 199.74 mM
ALogP	0.275
HBA_Count	1
HBD_Count	1
Rotatable Bond	2