



WS3

Cat. No.:	OB0225WX-2686
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	10 mg; 50 mg; 200 mg

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

Product Overview

Description	WS3 functions as an inducer of beta-cell proliferation by modulating the I-kappa -B kinase pathway and Erb3 binding protein-1 (EBP1).
Synonym	1421227-52-2; WS3; N-(6-(4-(3-(4-((4-methylpiperazin-1-yl)methyl)-3-(trifluoromethyl)phenyl)ureido)phenoxy)pyrimidin-4-yl)cyclopropanecarboxamide; N-(6-{4-[(4-(4-methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl} carbamoyl)amino}phenoxy}pyrimidin-4-yl)cyclopropanecarboxamide; Cyclopropanecarboxamide, N-[6-[4-[[[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-4-pyrimidinyl]-; N-[6-[4-[[4-[(4-methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl]carbamoylamino]phenoxy]pyrimidin-4-yl)cyclopropanecarboxamide; MFCD26142950; N-[6-[4-[[[4-[(4-Methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]-amino]carbonyl]amino]phenoxy]-4-pyrimidinyl]-cyclopropanecarboxamide; Cyclopropanecarboxamide, N-[6-[4-[[[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]phenoxy]-4-pyrimidinyl]-cyclopropanecarboxamide
CAS No.	1421227-52-2
Compound CID	72551586
Formula	C ₂₈ H ₃₀ F ₃ N ₇ O ₃
Formula Weight	569.58

Specification



IUPAC Name	<i>N</i> -[6-[4-[[4-[(4-Methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl]carbamoylamino]phenoxy]pyrimidin-4-yl]cyclopropanecarboxamide
InChI	InChI=1S/C28H30F3N7O3/c1-37-10-12-38(13-11-37)16-19-4-5-21(14-23(19)28(29,30)31)35-27(40)34-20-6-8-22(9-7-20)41-25-15-24(32-17-33-25)36-26(39)18-2-3-18/h4-9,14-15,17-18H,2-3,10-13,16H2,1H3,(H2,34,35,40)(H,32,33,36,39)
InChI Key	KIKOYRNAERIVSJ-UHFFFAOYSA-N
SMILES string	CN1CCN(CC1)CC2=C(C=C(C=C2)NC(=O)NC3=CC=C(C=C3)OC4=NC=NC(=C4)NC(=O)C5CC5)C(F)(F)F
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	WS3 is applied in regenerative medicine research as a potent small molecule to study the promotion of beta-cell proliferation and the potential for increasing functional pancreatic cell mass.

Library Information

Target	IκB/IKK; EBP1
Pathways	NF-κB
Plate Number	L6700-08
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	100 mg/mL; 175.57 mM
Ethanol Max Solubility	80 mg/mL
ALogP	4.234
HBA_Count	5
HBD_Count	3
Rotatable Bond	9