



MK-4101

Cat. No.:	OB0225WX-2733
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	2 mg; 5 mg; 25 mg

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

Product Overview

Description	MK-4101 acts as a potent antagonist of the Hedgehog pathway, exerting its biological effects through the inhibition of cellular proliferation and the induction of apoptosis.
Synonym	935273-79-3; 5-(3,3-Difluorocyclobutyl)-3-[4-[4-methyl-5-[2-(trifluoromethyl)phenyl]-4H-1,2,4-triazol-3-yl]bicyclo[2.2.2]oct-1-yl]-1,2,4-oxadiazole; 5-(3,3-difluorocyclobutyl)-3-(4-(4-methyl-5-(2-(trifluoromethyl)phenyl)-4H-1,2,4-triazol-3-yl)bicyclo[2.2.2]octan-1-yl)-1,2,4-oxadiazole; 5-(3,3-difluorocyclobutyl)-3-[4-[4-methyl-5-[2-(trifluoromethyl)phenyl]-1,2,4-triazol-3-yl]-1-bicyclo[2.2.2]octan-1-yl]-1,2,4-oxadiazole; 5-(3,3-Difluorocyclobutyl)-3-(4-{4-methyl-5-[2-(trifluoromethyl)phenyl]-4H-1,2,4-triazol-3-yl}bicyclo[2.2.2]oct-1-yl)-1,2,4-oxadiazole; 5-(3,3-Difluoro-cyclobutyl)-3-{4-[4-methyl-5-(2-trifluoromethyl-phenyl)-4H-[1,2,4] triazol-3-yl]-bicyclo[2.2.2]oct-1-yl}-[1,2,4]oxadiazole; 5-(3,3-difluorocyclobutyl)-3-(4-{4-methyl-5-[2-(trifluoromethyl)phenyl]-1,2,4-triazol-3-yl}bicyclo[2.2.2]octan-1-yl)-1,2,4-oxadiazole
CAS No.	935273-79-3
Compound CID	16222379
Formula	C ₂₄ H ₂₄ F ₅ N ₅
Formula Weight	493.47

Specification



IUPAC Name	5-(3,3-Difluorocyclobutyl)-3-[4-[4-methyl-5-[2-(trifluoromethyl)phenyl]-1,2,4-triazol-3-yl]-1-bicyclo[2.2.2]octanyl]-1,2,4-oxadiazole
InChI	InChI=1S/C24H24F5N5O/c1-34-17(15-4-2-3-5-16(15)24(27,28)29)31-32-20(34)22-9-6-21(7-10-22,8-11-22)19-30-18(35-33-19)14-12-23(25,26)13-14/h2-5,14H,6-13H2,1H3
InChI Key	HKJOIWLYDJCTQR-UHFFFAOYSA-N
SMILES string	<chem>CN1C(=NN=C1C23CCC(CC2)(CC3)C4=NOC(=N4)C5CC(C5)(F)F)C6=CC=CC=C6C(F)(F)F</chem>
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	MK-4101 is employed in developmental biology and oncology research as a potent Hedgehog signaling antagonist to investigate the inhibition of the Smoothed receptor and the suppression of Hh-driven tumor growth.

Library Information

Target	Hedgehog/Smoothed
Pathways	Stem cells & Wnt
Plate Number	L6700-10
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	98 mg/mL; 198.59 mM
Ethanol Max Solubility	98 mg/mL
ALogP	4.784
HBA_Count	5
HBD_Count	0
Rotatable Bond	5