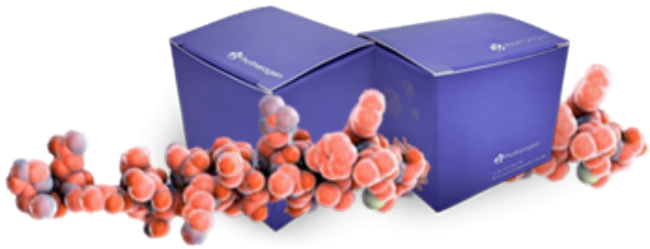
Protheragen
Obesity



PF-5274857

Cat. No.:	OB0225WX-2516
Appearance:	Solid
Purity:	≥99%
Identity:	Confirmed by NMR, and HPLC.
Size:	5 mg; 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	PF-5274857 is a brain-penetrable Smoothened (Smo) antagonist that potently inhib its Hedgehog (Hh) signaling with a Ki of 4.6 nM.
Synonym	1373615-35-0; 1-(4-(5-chloro-4-(3,5-dimethylpyridin-2-yl)pyridin-2-yl)piperazin- 1-yl)-3-(methylsulfonyl)propan-1-one; PF-5274857 freebase; 1-[4-[5-chloro-4-(3,5 -dimethylpyridin-2-yl)pyridin-2-yl]piperazin-1-yl]-3-methylsulfonylpropan-1-one; 1-(4-(5'-chloro-3,5-dimethyl-[2,4'-bipyridin]-2'-yl)piperazin-1-yl)-3-(methylsu lfonyl)propan-1-one; 1-(4-(5'-chloro-3,5-dimethyl-2,4'-bipyridin-2'-yl)piperazin -1-yl)-3-(methylsulfonyl)propan-1-one; 1-[4-(5'-chloro-3,5-dimethyl-2,4'-bipyrid in-2'-yl)piperazin-1-yl]-3-(methylsulfonyl)propan-1-one; 1-[4-(5'-Chloro-3,5-dim ethyl[2,4'-bipyridin]-2'-yl)piperazin-1-yl]-3-(methanesulfonyl)propan-1-one
CAS No.	1373615-35-0
Compound CID	56956240
Formula	$C_{20}H_{25}ClN_4O_3S$
Formula Weight	436.96

Specification

IUPAC Name	1-[4-[5-Chloro-4-(3,5-dimethylpyridin-2-yl)pyridin-2-yl]piperazin-1-yl]-3-methyl sulfonylpropan-1-one
InChI	InChI=1S/C20H25ClN4O3S/c1-14-10-15(2)20(23-12-14)16-11-18(22-13-17(16)21)24-5-7-25(8-6-24)19(26)4-9-29(3,27)28/h10-13H,4-9H2,1-3H3

Address: 101-4 Colin Dr, Holbrook, NY 11741, USA
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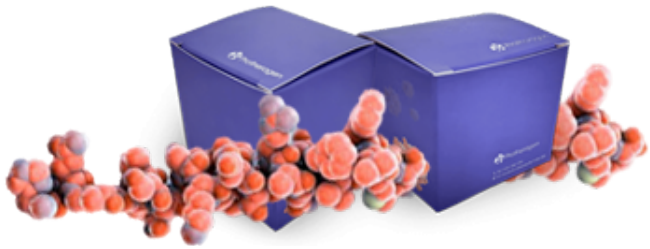

InChI Key	BBVNTTZIOTWDSV-UHFFFAOYSA-N
SMILES string	CC1=CC(=C(N=C1)C2=CC(=NC=C2Cl)N3CCN(CC3)C(=O)CCS(=O)(=O)C)C
Stability	3 years in powder form.
Storage	Storage at -20°C.
Applications	PF-5274857 is employed in developmental biology research as a potent and selecti ve Smoothened (Smo) antagonist to investigate the inhibition of the Hedgehog sig naling pathway in tissue patterning.

Library Information

Target	Hedgehog/Smoothened
Receptor	Smo
Pathways	Stem cells & Wnt
Plate Number	L6700-04
Empty Location	a1-h1; a12-h12
Container	96-well plate
Formulation	10mM DMSO
DMSO Max Solubility	93 mg/mL; 212.83 mM
Water Max Solubility	93 mg/mL; 212.83 mM
ALogP	2.744
HBA_Count	5
HBD_Count	0
Rotatable Bond	5

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