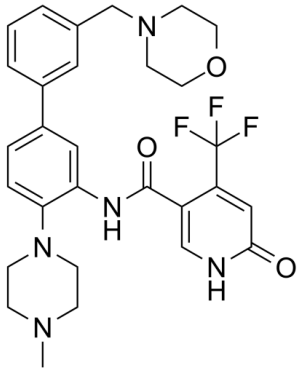
Data Sheet

Product Name:	OICR-9429
Cat. No.:	CS-5776
CAS No.:	1801787-56-3
Molecular Formula:	C29H32F3N5O3
Molecular Weight:	555.59
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : ≥ 32 mg/mL (57.60 mM)



BIOLOGICAL ACTIVITY:

OICR-9429 is a novel small-molecule antagonist of the Wdr5-MLL interaction with IC50 of 5 uM. inhibit proliferation and induce differentiation . target: Wdr5 IC 50: 5 uM In vitro: OICR-9429 inhibit proliferation and induce differentiation in p30-expressing human AML cells. OICR-9429 cause a significant decrease in viability in the majority of patient cells with mutations in the N-terminal part of the CEBPA gene. OICR-9429 displays exquisite cellular selectivity and specificity in disrupting critical protein-protein interactions between WDR5. [1] reduce the viability of primary human AML cells with N-terminal C/EBPα mutations by about 50% (mean value, n = 8) at 5 μM [2] In vivo:The reference for OICR-9429 to mice (female NOD-SCID) is 3 mg/kg.

References:

[1]. Grebien F et al. Pharmacological targeting of the Wdr5-MLL interaction in C/EBPα N-terminal leukemia. Nat Chem Biol. 2015 Aug;11(8):571-8.

[2]. Getlik M et al. Structure-Based Optimization of a Small Molecule Antagonist of the Interaction Between WD Repeat-Containing Protein 5 (WDR5) and Mixed-Lineage Leukemia 1 (MLL1). J Med Chem. 2016 Mar 24;59(6):2478-96.

CAIndexNames:

3-Pyridinecarboxamide, 1,6-dihydro-N-[4-(4-methyl-1-piperazinyl)-3'-(4-morpholinylmethyl)[1,1'-biphenyl]-3-yl]-6-oxo-4-(trifluoromethyl)-

SMILES:

O=C(C1=CNC(C=C1C(F)(F)F)=O)NC2=CC(C3=CC(CN4CCOCC4)=CC=C3)=CC=C2N5CCN(C)CC5

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA