Certificate of Analysis

Product Name: **OICR 9429** **Catalog No.: 5267** **Batch No.: 1**

CAS Number: 1801787-56-3

IUPAC Name: *N*-[2-(4-Methylpiperazin-1-yl)-5-[3-(morpholin-4-ylmethyl)phenyl]phenyl]-6-oxo-4-(trifluoromethyl)-1,6-dihydropyridine-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{32}F_3N_5O_3$

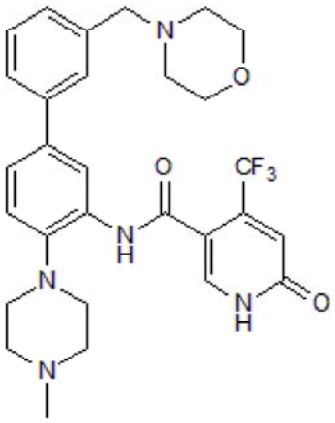
Batch Molecular Weight: 555.59

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.21 (Dichloromethane:Methanol:Ammonia soln. [9:1:0.04])

HPLC: Shows 98.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.69	5.81	12.61
Found	62.44	5.8	12.52

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Product Information

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Description:

High affinity WDR5 antagonist (K_d = 93 nM; IC_{50} = 64 nM); disrupts WDR5-MLL interaction. Exhibits selectivity for WDR5 over 22 methyltransferases and a panel of kinases, GPCRs, ion channels, and transporters. Reduces viability of acute myeloid leukemia cells in vitro. Also disrupts MLL1-RbBP5 interaction. To request the negative control for OICR 9429, please fill out the OICR 0547 request form on the SGC website.

Physical and Chemical Properties:

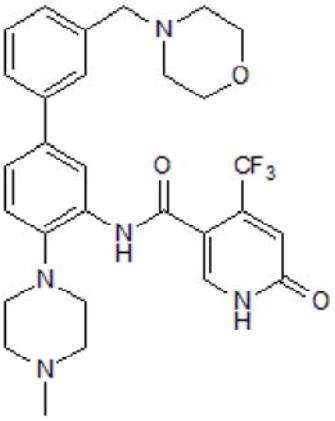
Batch Molecular Formula: $C_{29}H_{32}F_3N_5O_3$

Batch Molecular Weight: 555.59

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the OICR-9429 probe summary on the SGC website.

References:

Getlik *et al* (2016) 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. ***59*** 2478. PMID: 26958703.

Grebien *et al* (2015) Pharmacological targeting of the Wdr5-MLL interaction in C/EBPα N-terminal leukemia. Nat.Chem.Biol. ***11*** 571. PMID: 26167872.