

Product Name: NI 57

Catalog No.: 5546

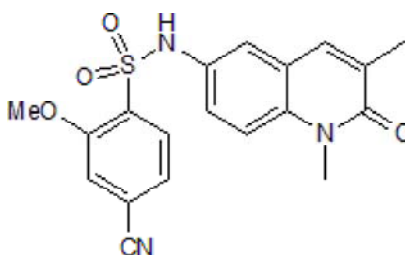
Batch No.: 1

CAS Number: 1883548-89-7

IUPAC Name: 4-Cyano-*N*-(1,3-dimethyl-2-oxo-1,2-dihydroquinolin-6-yl)-2-methoxybenzene-1-sulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₁₇N₃O₄S
Batch Molecular Weight: 383.42
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [95:5])
HPLC: Shows >99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.52	4.47	10.96
Found	59.49	4.41	10.86

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

NI 57 is a potent and selective BRPF bromodomain inhibitor (K_d values are 31, 108 and 408 nM, for BRPF1B, 2 and 3, respectively, which exhibits >32-fold selectivity for BRPFs over BRD9 and other non-Class IV bromodomains. NI 57 inhibits RANKL-induced differentiation of primary murine bone marrow cells and human primary monocytes into osteoclasts.

Physical and Chemical Properties:

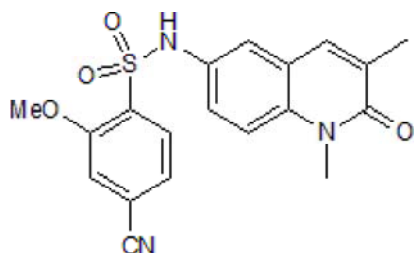
Batch Molecular Formula: C₁₉H₁₇N₃O₄S

Batch Molecular Weight: 383.42

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Igoe et al (2017) Design of a chemical probe for the bromodomain and plant homeodomain finger-containing (BRPF) family of proteins. *J.Med.Chem.* **60** 6998. PMID: 28714688.

Meier et al (2017) Selective targeting of bromodomains of the bromodomain-PHD fingers family impairs osteoclast differentiation. *ACS Chem.Biol.* **12** 2619. PMID: 28849908.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 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 NI 57 probe summary on the SGC website.

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