

Product Name: Ceritinib

Catalog No.: 6905

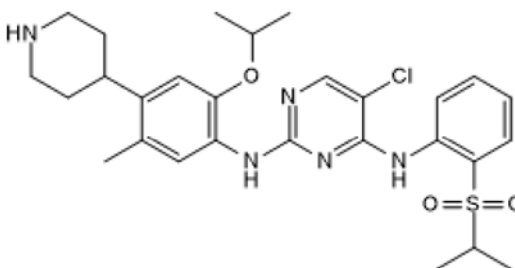
Batch No.: 1

CAS Number: 1032900-25-6

IUPAC Name: 5-Chloro-*N*⁴-[2-[(1-methylethyl)sulfonyl]phenyl]-*N*²-[5-methyl-2-(1-methylethoxy)-4-(4-piperidinyl)phenyl]-2,4-pyrimidinediamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₈ H ₃₆ ClN ₅ O ₃ S
Batch Molecular Weight:	558.14
Physical Appearance:	White solid
Solubility:	DMSO to 5 mM with gentle warming ethanol to 5 mM with gentle warming
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.6% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	60.25	6.5	12.55
Found	60.3	6.48	12.5

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

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Description:

Highly potent anaplastic lymphoma kinase (ALK) inhibitor (IC₅₀ = 0.2 nM). Also displays potent inhibition of insulin receptor (IR), insulin-like growth factor receptor 1 (IGF1R), serine/threonine-protein kinase STK22D and FLT3 (IC₅₀ values are 7, 8, 23 and 60 nM, respectively). Inhibits tumor growth in Karpas299 and H2228 rat xenograft models.

Physical and Chemical Properties:

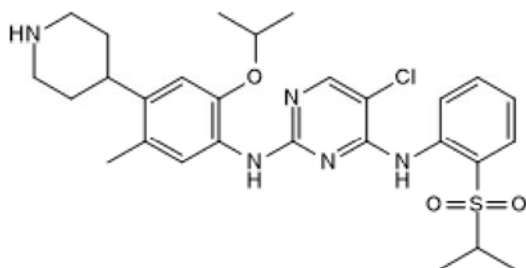
Batch Molecular Formula: C₂₈H₃₆ClN₅O₃S

Batch Molecular Weight: 558.14

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 5 mM with gentle warming
ethanol to 5 mM with gentle warming

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.

References:

Marsilje et al (2013) Synthesis, structure-activity relationships, and *in vivo* efficacy of the novel potent and selective anaplastic lymphoma kinase (ALK) inhibitor 5-chloro-*N*²-(2-isopropoxy-5-methyl-4-(piperidin-4-yl)phenyl)-*N*⁴-(2-(isopropylsulfonyl)phenyl)pyrimidine-2,4-diamine (LDK378) currently in phase 1 and phase 2 clinical trials. *J.Med.Chem.* **56** 5675. PMID: 23742252.

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