TOCRIS
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Print Date: Apr 6th 2020

Certificate of Analysis

www.tocris.com

Product Name: **LDN 193189 dihydrochloride** **Catalog No.: 6053** **Batch No.: 5**

CAS Number: 1435934-00-1

IUPAC Name: 4-[6-[4-(1-Piperazinyl)phenyl]pyrazolo[1,5-*a*]pyrimidin-3-yl]quinoline dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{22}N_6.2HCl.1¼H_2O$

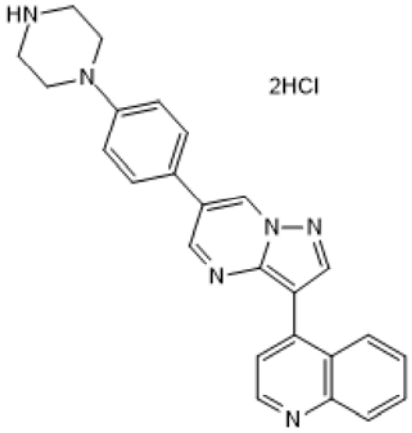
Batch Molecular Weight: 501.92

Physical Appearance: Orange solid

Solubility: water to 50 mM
DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	59.82	5.32	16.74	14.13
Found	59.88	5.33	16.55	14.23

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Description:

Potent and selective ALK2 and ALK3 inhibitor (IC_{50} values are 5 and 30 nM, respectively); inhibits BMP4-mediated Smad1/5/8 activation. Exhibits >200-fold selectivity for BMP signaling over TGF-β signaling. Also exhibits selectivity over AMPK, PDGFR and MAPK signaling. Promotes neural induction of hPSCs in combination with SB 431542 (Cat.No. 1614). Also induces differentiation of hPSCs into nociceptive sensory neurons in combination with SB 431542 (Cat.No. 1614), SU 5402 (Cat.No.3300), CHIR 99021 (Cat.No. 4423) and DAPT (Cat.No. 2634). Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

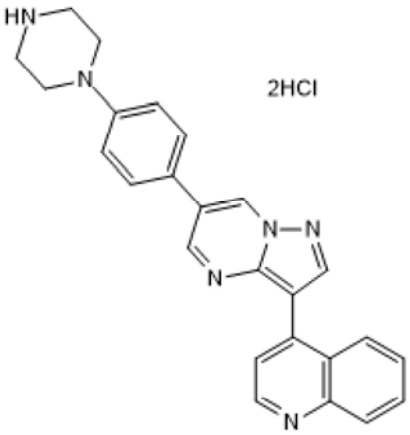
Batch Molecular Formula: $C_{25}H_{22}N_6.2HCl.1¼H_2O$

Batch Molecular Weight: 501.92

Physical Appearance: Orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 50 mM
DMSO to 20 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:

Sold for research purposes under exclusive agreement from The Brigham and Women's Hospital Inc. US patents 8,507,501 and 9,045,484

References:

Wimmer *et al* (2019) Human blood vessel organoids as a model of diabetic vasculopathy. Nature ***565*** 505. PMID: 30651639.

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Li *et al* (2013) Chemical approaches to stem cell biology and therapeutics. Cell Stem Cell ***13*** 270. PMID: 24012368.

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Cuny *et al* (2008) Structure-activity relationship study of bone morphogenetic protein (BMP) signaling inhibitors. Bioorg.Med.Chem.Lett. ***18*** 4388. PMID: 18621530

Yu *et al* (2008) BMP type I receptor inhibition reduces heterotopic ossification. Nat.Med. ***14*** 1363. PMID: 19029982.

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