TOCRIS
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Print Date: Mar 10th 2023

Certificate of Analysis

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Product Name: **GSK 329** **Catalog No.: 7637** **Batch No.: 1**

CAS Number: 1268490-12-5

IUPAC Name: *N*-[3,5-Dichloro-4-[[6-(methylamino)-4-pyrimidinyl]oxy]phenyl]-*N*'-[3-(trifluoromethyl)phenyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{14}Cl_2F_3N_5O_2$

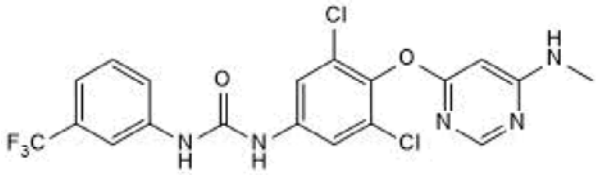
Batch Molecular Weight: 472.25

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	48.32	2.99	14.83
Found	48.08	2.89	14.59

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Description:

GSK 329 is a potent and selective TNNI3K (cardiac troponin I-interacting kinase) inhibitor (IC_{50} = 10 nM). It exhibits selectivity against human VEGFR2 (40-fold), p38α (80-fold), B-Raf (>200-fold) and displays >100-fold selectivity over 80% of 185 kinases tested. In vivo, GSK 329 reduces infarct size, ROS levels, and p38 activation in a mouse model of ischemia/reperfusion cardiac injury. This compound is orally bioavailable.

Physical and Chemical Properties:

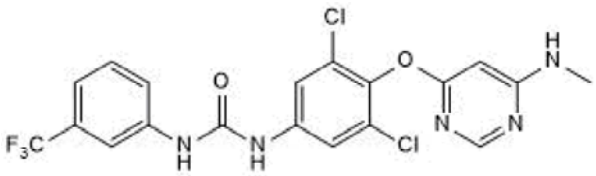
Batch Molecular Formula: $C_{19}H_{14}Cl_2F_3N_5O_2$

Batch Molecular Weight: 472.25

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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.

References:

Patterson *et al* (2021) Identification of diarylurea inhibitors of the cardiac-specific kinase TNNI3K by designing selectivity against VEGFR2, p38a, and B-Raf. J.Med.Chem. ***64*** 15651. PMID: 34699203.

Vagnozzi *et al* (2013) Inhibition of the cardiomyocyte-specific kinase TNNI3K limits oxidative stress, injury, and adverse remodeling in the ischemic heart. Sci.Transl.Med. ***5*** 207ra141. PMID: 24132636.