

Product Name: PFI 653

Catalog No.: 7963

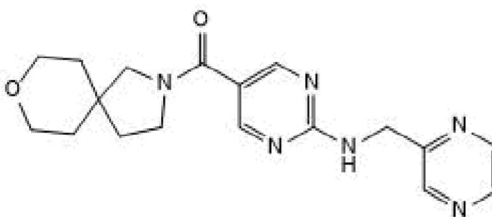
Batch No.: 1

CAS Number: 2173134-00-2

IUPAC Name: 8-Oxa-2-azaspiro[4.5]dec-2-yl[2-[(2-pyrazinylmethyl)amino]-5-pyrimidinyl]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₂N₆O₂.
Batch Molecular Weight: 354.41
Physical Appearance: White solid
Solubility: ethanol to 5 mM
DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61	6.26	23.71
Found	61.14	6.12	23.4

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

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Description:

PFI 653 is a potent and selective vanin 1 inhibitor (IC₅₀ values in the range 6.85 - 24.5 nM). The compound exhibits selectivity over a panel of 40 kinases and a selection of 35 other targets including enzymes, receptors and ion channels (IC₅₀ vs biotinidase > 50 μM). Following administration of a single dose of PFI 653 (2 mg/kg iv) in rats AUC is 1790 ng.h/mL, half-life is 1 h and clearance is 19 mL/min/kg. Following oral administration of PFI 653 in solution, bioavailability is 96%. In mice with DSS-induced inflammatory bowel disease (IBD), oral administration of PFI 653 dose-dependently reduces vanin 1 enzyme activity and disease symp... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

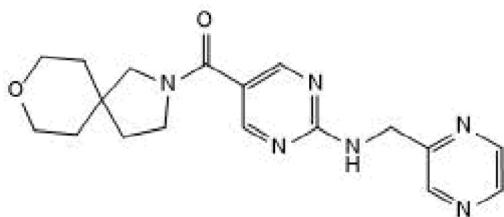
Batch Molecular Formula: C₁₈H₂₂N₆O₂.

Batch Molecular Weight: 354.41

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Casimiro-Garcia et al (2022) Discovery of a series of pyrimidine carboxamides as inhibitors of vanin-1. *J.Med.Chem.* **65** 757. PMID: 34967602.

Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 5 mM

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 compound is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the PFI-653 probe summary on the SGC website.

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