

Product Name: PF 04449613

Catalog No.: 5915

Batch No.: 3

CAS Number: 1236858-52-8

IUPAC Name: 1,5-Dihydro-6-[(1*R*)-1-(3-phenoxy-1-azetidiny)ethyl]-1-(tetrahydro-2*H*-pyran-4-yl)-4*H*-pyrazolo[3,4-*d*]pyrimidin-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₅N₅O₃·¼H₂O

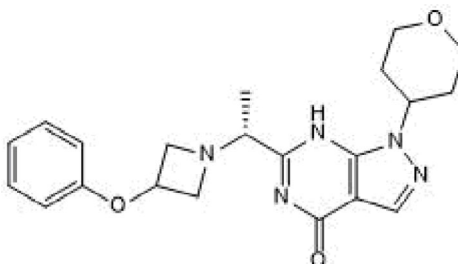
Batch Molecular Weight: 399.95

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

Chiral HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.06	6.43	17.51
Found	62.33	6.35	17.39

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Description:

PF 04449613 is a potent PDE9 inhibitor (IC₅₀ = 22 nM). PF 4449613 shows more than 1000-fold selectivity for PDE9A over most of 79 other non-PDE targets investigated, except for cytochrome P450 2C19 (IC₅₀ = 1600 nM), dopamine transporter (K_i = 110 nM), μ-opioid receptor (K_i = 3500 nM), and sodium channel binding site 2 (K_i = 470 nM). PF 04449613 reduces body fat in mice with diet-induced obesity, stimulating mitochondrial activity in brown and white fat, and improving cardiometabolic syndrome symptoms. Brain penetrant. PF 04449613 increases synaptic calcium activity and learning-dependent synaptic plasticity in mice. Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

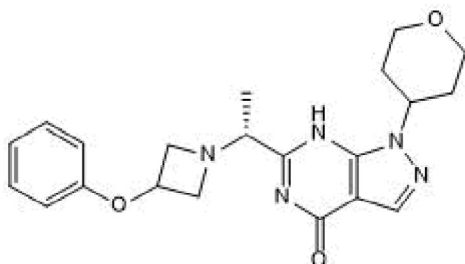
Batch Molecular Formula: C₂₁H₂₅N₅O₃·¼H₂O

Batch Molecular Weight: 399.95

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Mishra et al (2021) Inhibition of phosphodiesterase type 9 reduces obesity and cardiometabolic syndrome in mice. *J.Clin.Invest.* **131** e148798. PMID: 34618683.

Lai et al (2018) The phosphodiesterase 9 inhibitor PF-04449613 promotes dendritic spine formation and performance improvement after motor learning. *Dev.Neurobiol.* **78** 859. PMID: 30022611.

Lee et al (2015) Phosphodiesterase 9A controls nitric-oxide-independent cGMP and hypertrophic heart disease. *Nature* **519** 472. PMID: 25799991.

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. *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:

Sold for research purposes under agreement from Pfizer Inc.

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