Product Name: **PF 04449613** **Catalog No.: 5915** **Batch No.: 2**

CAS Number: 1236858-52-8

IUPAC Name: 1,5-Dihydro-6-[(1*R*)-1-(3-phenoxy-1-azetidinyl)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: $C_{21}H_{25}N_5O_3$

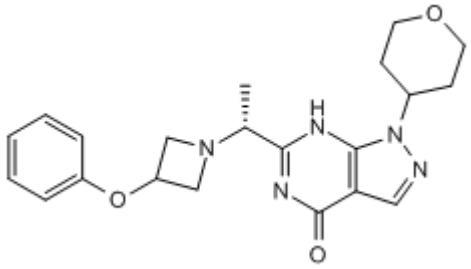
Batch Molecular Weight: 395.45

Physical Appearance: White solid

Solubility: DMSO to 100 mM
1eq. HCl to 10 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Chloroform:Methanol [97:3])

HPLC: Shows >99.1% purity

Chiral HPLC: Shows >99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.78	6.37	17.7
Found	63.61	6.45	17.31

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

Product Information

Product Name: **PF 04449613** **Catalog No.: 5915** **Batch No.: 2**

CAS Number: 1236858-52-8

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

Description:

Potent PDE9 inhibitor (IC_{50} = 22 nM). Also exhibits a high affinity for cGMP (K_m ~170 nM). Brain penetrant.

Physical and Chemical Properties:

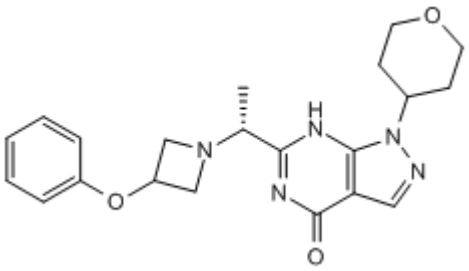
Batch Molecular Formula: $C_{21}H_{25}N_5O_3$

Batch Molecular Weight: 395.45

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
1eq. HCl to 10 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

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

Claffey *et al* (2012) Application of structure-based drug design and parallel chemistry to identify selective, brain penetrant, *in vivo* active phosphodiesterase 9A inhibitors. J.Med.Chem. ***55*** 9055. PMID: 23025719.

Kleiman *et al* (2012) Phosphodiesterase 9A regulates central cGMP and modulates responses to cholinergic and monoaminergic perturbation *in vivo*. J.Pharmacol.Exp.Ther. ***341*** 396. PMID: 22328573.

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956