

Product Name: PH 797804

Catalog No.: 5866

Batch No.: 1

CAS Number: 1358027-80-1

IUPAC Name: (-)-3-[3-Bromo-4-[(2,4-difluorophenyl)methoxy]-6-methyl-2-oxo-1(2H)-pyridinyl]-N,4-dimethylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₁₉BrF₂N₂O₃

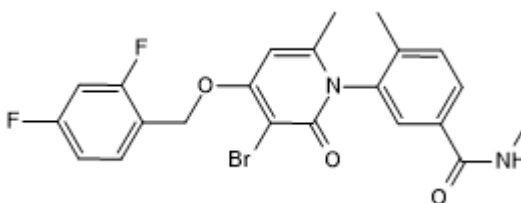
Batch Molecular Weight: 477.3

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.26 (Dichloromethane:Ethanol [95:5])

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -35.3 (Concentration = 0.51, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.36	4.01	5.87
Found	55.19	3.73	6.01

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Description:

Potent and selective p38 α / β inhibitor (IC₅₀ values are 26 and 102 nM, respectively). Exhibits >100-fold selectivity for p38 α / β over 71 other kinases, enzymes and GPCRs, including p38 γ , p38 δ , JNK and ERK2. Inhibits LPS-induced TNF α production in U937 monocytes in vitro. Suppresses acute and chronic inflammatory responses in rat models of arthritis. Orally active.

Physical and Chemical Properties:

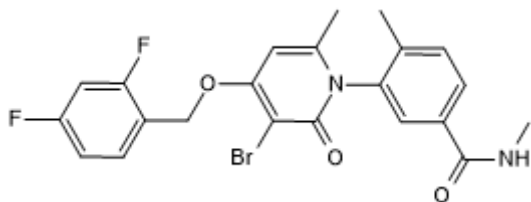
Batch Molecular Formula: C₂₂H₁₉BrF₂N₂O₃

Batch Molecular Weight: 477.3

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Selness et al (2011) Discovery of PH-797804, a highly selective and potent inhibitor of p38 MAP kinase. *Bioorg.Med.Chem.Lett.* **21** 4066. PMID: 21641211.

Hope et al (2009) Anti-inflammatory properties of a novel N-phenyl pyridinone inhibitor of p38 mitogen-activated protein kinase: preclinical-to-clinical translation. *J.Pharmacol.Exp.Ther.* **331** 882. PMID: 19720877.

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