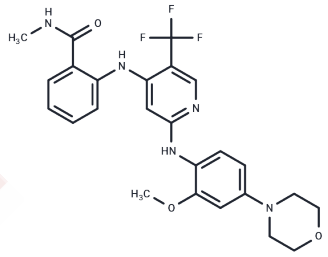
Data Sheet (Cat.No.T1950)

TargetMol

PND-1186

Chemical Properties



CAS No. : 1061353-68-1

Formula: C25H26F3N5O3

Molecular Weight: 501.5

Storage: Store at low temperature
Powder: -20°C for 3 years | In solvent: -80°C for 1 year
Actual storage temperature shall be subject to the COA.

Biological Description

Description	PND-1186 (VS-4718) is a small molecule inhibitor, a highly specific, reversible FAK inhibitor (IC50=1.5 nM) with good selectivity and cell permeability. This compound inhibits FAK phosphorylation, blocking tumor cell survival, proliferation, migration, and angiogenesis, and is primarily used for anti-tumor research on solid tumors.
Targets(IC50)	Apoptosis,FAK
In vitro	**Methods**: In multiple MPM cell lines (MSTO-211H, H28, Ren, 1157, etc.) and non-MPM cells, the AlamarBlue proliferation assay was used to detect the IC50 of gradient concentrations of PND-1186 after 72 h treatment. **Results**: MPM cells with high CDH1 mRNA expression (such as Ren, 1157) were resistant to PND-1186 (IC50 reaching 7.20–24.86 μM), while those with low expression were sensitive (IC50 0.70–1.20 μM); flow cytometry cell cycle analysis confirmed that PND-1186 induced G2/M phase arrest. [1] **Methods**: In high glucose-induced H9c2 and primary cardiomyocytes, the MTT assay was used to determine safe doses of PND-1186 (5, 10 μM), with 1 h pretreatment followed by combined high glucose stimulation for 24–48 h. **Results**: PND-1186 significantly inhibited the expression of fibrosis (Col-1, TGF-β), hypertrophy (β-Myhc), and inflammatory factors (TNF-α, IL-6, IL-1β), and blocked NF-κB activation. [2]
In vivo	**Methods**: In a streptozotocin (STZ)-induced type 1 diabetic mouse model, PND-1186 was dissolved in 0.5% sodium carboxymethyl cellulose buffer at a dose of 50 mg/kg and administered orally every two days, starting from the 9th week after diabetes confirmation for 8 consecutive weeks. **Results**: PND-1186 effectively inhibited cardiac FAK phosphorylation, attenuated myocardial fibrosis and hypertrophy, improved ejection fraction and fractional shortening, and reduced inflammatory factor expression and NF-κB activation. [3]
Kinase Assay	In vitro kinase activity: GST-FAK in vitro kinase activity is measured and compared to His-tagged FAK 411–686 using the K-LISA screening kit and poly(Glu:Tyr) (4:1) copolymer as a substrate immobilized on microtiter plates. IC50 values are determined with various concentrations of test compounds in a buffer containing 50 μM ATP and 10 mM MnCl2, 50 mM HEPES (pH 7.5), 25 mM NaCl, 0.01% BSA, and 0.1 mM Na orthovanadate for 5 min at room temperature. Serial diluted compounds are tested in triplicate. Substrate phosphorylation is measured using horseradish peroxidase-conjugated anti-pTyr

Kinase Assay	antibodies with spetrophotometric color quantitation. IC50 values are determined using the Hill-Slope Model. Kinase selectivity profiling is performed by using the KinaseProfiler service.
Cell Research	For soft agar assays, 48-well plates are coated with a 1:4 mix of 2% agar (EM Science) in 0.2 mL growth media (bottom layer). 5×104 cells are plated per well (in triplicate) in a mixture of 0.3% agar in 0.2 mL growth media (top layer). After agar solidification, 0.2 mL growth media is added containing DMSO or PND-1186 (final concentration for 0.6 mL). In separate experiments, PND-1186 is added after 4 days. After 10 days, colonies are imaged in phase contrast, enumerated by counting 9 fields (3 fields per well), and total area determined using Image J. For all analyses, experimental points are performed in triplicate and repeated at least two times. (Only for Reference)

Solubility Information

Solubility	H2O: < 1 mg/mL (insoluble or slightly soluble), Ethanol: < 1 mg/mL (insoluble or slightly soluble), DMSO: 34 mg/mL (67.8 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (3.99 mM),Sonication is recommended. *Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.994 mL	9.9701 mL	19.9402 mL
5 mM	0.3988 mL	1.994 mL	3.988 mL
10 mM	0.1994 mL	0.997 mL	1.994 mL
50 mM	0.0399 mL	0.1994 mL	0.3988 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Yuen, Man Lee et al. The Role of E-Cadherin and microRNA on FAK Inhibitor Response in Malignant Pleural Mesothelioma (MPM). International journal of molecular sciences vol. 22,19 10225. 23 Sep. 2021.
Jin, Bo et al. Focal adhesion kinase induces cardiac remodeling through NF-κB-mediated inflammatory responses in diabetic cardiomyopathy. International immunopharmacology vol. 120 (2023): 110280.
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