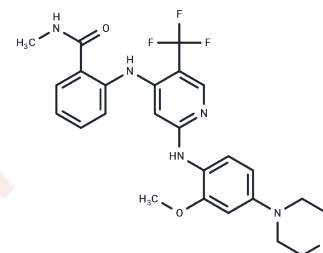


PND-1186

Chemical Properties

CAS No. :	1061353-68-1
Formula:	C ₂₅ H ₂₆ F ₃ N ₅ O ₃
Molecular Weight:	501.5
Storage:	Store at low temperature Powder: -20°C for 3 years In solvent: -80°C for 1 year <small>Actual storage temperature shall be subject to the COA.</small>



Biological Description

Description	PND-1186 (VS-4718) is a specific and reversible FAK inhibitor with an IC ₅₀ of 1.5 nM.
Targets(IC ₅₀)	Apoptosis,FAK
In vitro	In mice implanted with 4T1 tumors, PND-1186 (100 mg/kg, s.c.) induces apoptosis and inhibits the growth of subcutaneous 4T1 tumors. Additionally, in mice carrying ID8 tumors, PND-1186 (0.5 mg/mL, p.o.) suppresses the growth of ovarian cancer tumors.
In vivo	In vitro, PND-1186 demonstrates an inhibitory effect on the motility of 4T1 breast cancer cells, promotes apoptosis in suspended 4T1 cells, and reduces both the number and size of 4T1 soft agar colonies. Additionally, in HEY and OVCAR8 cells, PND-1186 induces G ₀ -G ₁ cell cycle arrest, leading to cell death.
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. IC ₅₀ values are determined with various concentrations of test compounds in a buffer containing 50 μM ATP and 10 mM MnCl ₂ , 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 antibodies with spectrophotometric color quantitation. IC ₅₀ 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). 5×10 ⁴ 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

A DRUG SCREENING EXPERT

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. <i>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.</i>

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

Tanjoni I, et al. Cancer Biol Ther. 2010, 9(10), 764-777.

Tancioni I, et al. Mol Cancer Ther. 2014, 13(8), 2050-2061.

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