PND-1186 hydrochloride

Cat. No.: HY-13917A

CAS No.: 1356154-94-3

Molecular Formula: $C_{25}H_{27}ClF_3N_5O_3$

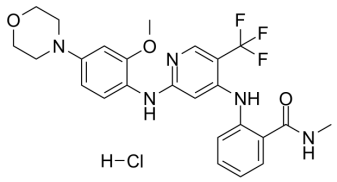
Molecular Weight: 537.96

Target: FAK; Apoptosis

Pathway: Protein Tyrosine Kinase/RTK; Apoptosis

Storage: 4°C, sealed storage, away from moisture

* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 200 mg/mL (371.77 mM; Need ultrasonic)

H_2O : 20 mg/mL (37.18 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8589 mL	9.2944 mL	18.5887 mL
5 mM	0.3718 mL	1.8589 mL	3.7177 mL
10 mM	0.1859 mL	0.9294 mL	1.8589 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 5 mg/mL (9.29 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (9.29 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

PND-1186 hydrochloride (VS-4718 hydrochloride) is a potent, highly-specific and reversible inhibitor of FAK with an IC_{50} of 1.5 nM. PND-1186 hydrochloride selectively promotes tumor cell apoptosis[1].

In Vitro

PND-1186 has an IC_{50} of ~100 nM in breast carcinoma cells as determined by anti-phospho-specific immunoblotting to FAK Tyr-397[1].

In murine 4T1 breast carcinoma cells, FAK is important in promoting an invasive and metastatic cell phenotype. Increasing concentrations of PND-1186 (0.1 to 1.0 μM) added to 4T1 cells inhibits FAK Tyr-397 phosphorylation (pY397) and results in elevated levels of total FAK protein within 1 h[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[1]

Cell Line:	4T1 breast carcinoma cells
Concentration:	0.1, 0.2, 0.4, 0.6 and 1.0 μM
Incubation Time:	1 hour
Result:	Inhibited FAK Tyr-397 phosphorylation (pY397) and resulted in elevated levels of total FAK protein.

In Vivo

PND-1186 (30 mg/kg or 100 mg/kg; subcutaneously; injected subcutaneously in the neck region) inhibits 4T1 subcutaneous tumor growth by induction of apoptosis[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	BALB/c mice[1]
Dosage:	30 mg/kg or 100 mg/kg
Administration:	Injected (100 μL) subcutaneously in the neck region; every 12 h (twice-daily, b.i.d.) for 5 days.
Result:	100 mg/kg treatment significantly reduced final 4T1 tumor weight 2-fold whereas 30 mg/kg treatment slightly reduced final tumor weight but was not significantly different compared to control.

CUSTOMER VALIDATION

- Cancer Cell. 2019 Mar 18;35(3):457-472.e5.
- Cancer Commun (Lond). 2023 May 31.
- Clin Cancer Res. 2019 Jul 15;25(14):4552-4566.
- J Exp Clin Cancer Res. 2022 Jun 3;41(1):193.
- Cancers (Basel). 2023 Apr 13, 15(8), 2280.

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REFERENCES

[1]. Tanjoni I, et al. PND-1186 FAK inhibitor selectively promotes tumor cell apoptosis in three-dimensional environments. Cancer Biol Ther. 2010 May 15;9(10):764-77.

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