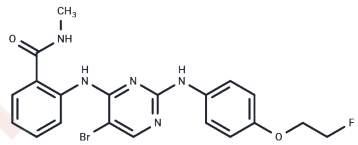
Data Sheet (Cat.No.T207475)

TargetMol

FAK-IN-26

Chemical Properties



CAS No. : 2801785-12-4

Formula: C20H19BrFN5O2

Molecular Weight: 460.30

Storage: 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	FAK-IN-26 is a blood-brain barrier-penetrating inhibitor of Focal Adhesion Kinase (FAK) with an IC50 of 0.87 nM. It significantly reduces tumor cell viability, cancer stem cell activity, and cell migration in A549 and SKOV-3 cell lines. FAK-IN-26 exhibits potent anticancer activity, achieving tumor inhibition rates of 59.15% and 57.9% in A549 and SKOV-3 tumor mouse models, respectively.
Targets(IC50)	FAK
In vitro	FAK-IN-26 (Compound A8) exhibits excellent binding affinity for FAK with a Kd value of 15 μM. At 1 μmol/L, it broadly inhibits various kinases, achieving inhibition rates over 95% for both FAK and FYNα. FAK-IN-26 reduces the viability of A549 and SKOV-3 cells significantly at lower concentrations compared to Defactinib (VS6063) at 0.5-10 μM. It also decreases the cancer stem cell population in A549 and SKOV-3 cells in a dose-dependent manner at 0.2-1.6 μM. Moreover, FAK-IN-26 induces significant G2/M phase arrest in these cell lines at concentrations of 62.5-1000 nM over a period of 72 hours. The compound reduces cell migration and distance traveled by A549 and SKOV-3 cells in a dose-dependent manner within 0.1-10 nM over 6-48 hours, with significant inhibition observed at 1 nM and 10 nM. It effectively inhibits FAK autophosphorylation in a dose-dependent manner in the cell lines at 31.25-62.5 nM over 48 hours, with stronger inhibition noted in A549 cells. Additionally, FAK-IN-26 demonstrates good metabolic stability in human liver microsomes, with CL int of 31.8 μL/min/mg and a half-life (T 1/2) of 43.6 minutes.
In vivo	In the A549 and SKOV-3 tumor mouse models, FAK-IN-26 (Compound A8) [(25-50 mg/kg, oral administration, once or twice daily for 5 days, followed by a 2-day break, over 28 days)] exhibits superior antitumor efficacy compared to Defactinib (VS6063), Erlotinib, and Paclitaxel, with enhanced effects when combined with Paclitaxel in the SKOV-3 model. FAK-IN-26 shows good tolerability in mice up to the highest tested dose of 2000 mg/kg without acute toxicity. Additionally, FAK-IN-26 demonstrates effective tumor uptake and retention, with peak uptake of 4.16 ID/g at 30 minutes in S180 tumor mice and penetrates the BBB, registering brain uptake of 2.63% ID/g at 15 minutes and 1.62% ID/g at 120 minutes.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.1725 mL	10.8625 mL	21.725 mL
5 mM	0.4345 mL	2.1725 mL	4.345 mL
10 mM	0.2172 mL	1.0862 mL	2.1725 mL
50 mM	0.0434 mL	0.2172 mL	0.4345 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.