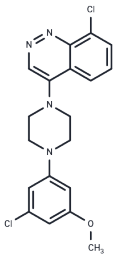
Data Sheet (Cat.No.T61746)

TargetMol

Anticancer agent 82

Chemical Properties



CAS No. : 2319587-80-7

Formula: C19H18Cl2N4O

Molecular Weight: 389.28

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	Anticancer agent 82 is a FiVe1 derivative, an orally active and selective anticancer agent. FiVe1 binds type III intermediate filament protein vimentin (VIM), to induce hyperphosphorylation of Ser56, resulting selective disruption of mitosis and multinucleation in transformed VIM-expressing mesenchymal cancer cells. Anticancer agent 82 shows better oral bioavailability and pharmacokinetic profiles than FiVe1 [1].
Targets(IC50)	Others,Proteasome
In vitro	Anticancer agent 82 (compound 4e) (0-10 mM; 72 h) exhibits an IC50 value of 44 nM against HT-1080 fibrosarcoma, surpassing FiVe1 (IC50 = 1.6 μM, HT-1080) [1]. It induces phosphorylation of VIM at Ser56 (0.1 μM; 24 h) [1] and demonstrates poor stability, with 0.0% remaining after 60 minutes in mouse liver microsomes (100 μM; sampled at 0, 5, 15, 30, 45, and 60 min) [1]. Cell viability assays show inhibition of HT-1080, RD, and MCF-7 cells, with IC50 values of 44 nM, 61 nM, and 49 nM, respectively (0-10 mM; 72 hours) [1].
In vivo	Anticancer agent 82 (compound 4e), administered orally at a dose of 10 mg/kg, demonstrated superior oral pharmacokinetic properties compared to Five1 [1]. Detailed pharmacokinetic analysis in mice [1] revealed that when given orally, compound 4e resulted in an area under the curve (AUC) from time zero to the last measurable concentration (0-last) of 371.33 ng·h/mL, an AUC from time zero to infinity (0-inf) of 534.33 ng·h/mL, a half-life (T 1/2) of 4.68 hours, time to maximum concentration (T max) of 0.67 hours, time of the last measurable concentration (T last) of 8 hours, and a maximum concentration (C max) of 154.67 ng/mL. In comparison, Five1, also given orally but at a 25 mg/kg dose, showed an AUC (0-last) of 309.78 ng·h/mL, AUC (0-inf) of 339.21 ng·h/mL, T 1/2 of 4.57 hours, T max of 0.5 hours, T last of 18 hours, and C max of 110.43 ng/mL.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.5688 mL	12.8442 mL	25.6885 mL
5 mM	0.5138 mL	2.5688 mL	5.1377 mL
10 mM	0.2569 mL	1.2844 mL	2.5688 mL
50 mM	0.0514 mL	0.2569 mL	0.5138 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.

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