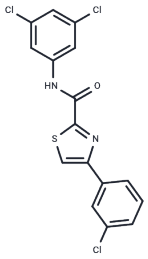
Data Sheet (Cat.No.T211184)

TargetMol

CYP1B1-IN-9

Chemical Properties



CAS No. : 3077254-39-5

Formula: C16H9Cl3N2OS

Molecular Weight: 383.68

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	CYP1B1-IN-9 is a highly selective and competitive CYP1B1 inhibitor, with IC50 values of 1.48 nM for CYP1B1, and greater than 100 μM and 80 μM for CYP1A1 and CYP1A2, respectively. This compound effectively inhibits the migration and invasion of A549/T cells, offers the potential to resensitize paclitaxel-resistant cells, and exhibits good metabolic stability and safety, as well as favorable pharmacokinetic properties. CYP1B1-IN-9 is applicable in research on tumor resistance.
Targets(IC50)	Cytochromes P450
In vitro	CYP1B1-IN-9 (Compound B20) exhibits an IC50 greater than 100 and 80 against CYP1A1 and CYP1A2, respectively, while inhibiting CYP2C8, CYP2C9, CYP2C19, CYP2D6, and CYP3A4 by 15.7%, 2.21%, 7.73%, 0.0%, and 0.94%. At concentrations of 0-8 nM over 30 minutes, it competitively binds to the CYP1B1 active site. At 20 and 40 μM over 48 hours, it shows low cytotoxicity with IC50 values greater than 40 μM for HUVEC and greater than 20 μM for BEAS-2B but is sensitive to A549/T cells with an IC50 of 7.5 μM. Additionally, CYP1B1-IN-9 (2.5 μM, 48 h) synergizes strongly with paclitaxel (0.025 μM, CI = 0.08), demonstrating its potential to reverse multidrug resistance by inhibiting CYP1B1. The compound (2.5-10 μM, 24 h) also inhibits A549/T cell migration in a concentration-dependent manner. Furthermore, CYP1B1-IN-9 shows excellent metabolic stability in extrahepatic microsomes with a half-life (T1/2) exceeding 60 minutes and an intrinsic clearance (CLint) of 1.1 mL/min/kg. In human plasma, at 100 μM over 5-120 minutes, it maintains good stability with a half-life (T1/2) over 2 hours.

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.6063 mL	13.0317 mL	26.0634 mL
5 mM	0.5213 mL	2.6063 mL	5.2127 mL
10 mM	0.2606 mL	1.3032 mL	2.6063 mL
50 mM	0.0521 mL	0.2606 mL	0.5213 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.