

S19-1035

Chemical Properties

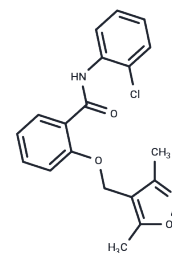
CAS No. :

Formula: C₁₉H₁₇ClN₂O₃

Molecular Weight: 356.80

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	S19-1035 is a potent and specific inhibitor of aldo-keto reductase 1C3 (AKR1C3), displaying an inhibitory concentration (IC ₅₀) of 3.04 nM. It is primarily utilized in tumor research.
Targets(IC ₅₀)	Others,NADPH
In vitro	S19-1035 demonstrates low cytotoxicity (0-100 μM ; 72 h or 96 h) and limited antitumor efficacy when used alone.[1] S19-1035 significantly reverses the resistance of doxorubicin-resistant breast cancer cell lines when administered at 10 μM for 8 days.[1]
In vivo	Setrobuvir (200, 400, and 800 mg) BID were -2.1, -2.2, and -2.9 log ₁₀ IU/mL, respectively (vs ≤0.1 log ₁₀ IU/mL with placebo).[3]

Solubility Information

Solubility	DMSO: 112.5 mg/mL (315.3 mM),Sonication and heating to 60°C are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+90% Corn Oil: 3.3 mg/mL (9.25 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	2.8027 mL	14.0135 mL	28.0269 mL
5 mM	0.5605 mL	2.8027 mL	5.6054 mL
10 mM	0.2803 mL	1.4013 mL	2.8027 mL
50 mM	0.0561 mL	0.2803 mL	0.5605 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

Liu Y, et al. Development of highly potent and specific AKR1C3 inhibitors to restore the chemosensitivity of drug-resistant breast cancer. *Eur J Med Chem.* 2023;247:115013.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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