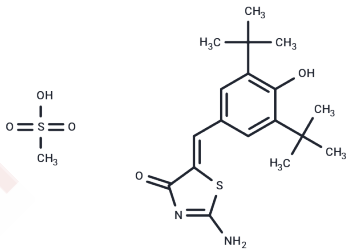
Data Sheet (Cat.No.T10960L)

TargetMol

Darbufelone mesylate

Chemical Properties



CAS No. :	139340-56-0
Formula:	C19H28N2O5S2
Molecular Weight:	428.57
Storage:	Store at low temperature 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	Darbufelone mesylate (CI-1004 mesylate) inhibited PGF2α and LTB4 in cells and demonstrated IC50 values of 0.19 μM for PGHS-2 and 20 μM for PGHS-1.
Targets(IC50)	LTR,Leukotriene Receptor,Prostaglandin Receptor
In vitro	Darbufelone, a noncompetitive inhibitor of PGHS-2 with a Ki value of 10±5 μM, exhibits fluorescence quenching of PGHS-2 at 325 nm (λex=280 nm) with a Kd of 0.98±0.03 μM[2]. To assess the putative anti-proliferative effect of Darbufelone, A549, H520, and H460 cell lines derived from three distinct pathological subtypes of non-small cell lung cancer (NSCLC) (adenocarcinoma, squamous, and large cell lung cancer, respectively) are utilized. The cell lines are treated with increasing concentrations of Darbufelone, ranging from 5 to 60 μM, for a duration of 72 hours. The growth inhibition of these three cell lines gradually increases with higher concentrations of the drug. The IC50 values for A549 and H520 are 20±3.6 and 21±1.8 μM, respectively, while H460 exhibits a lower IC50 of 15±2.7 μM[1].
In vivo	Darbufelone, a dual inhibitor of cellular PGF2R and LTB4 production, exhibits oral activity in animal models of inflammation and arthritis without causing ulcers. When mice were treated with bufafenone at a dose of 80 mg/kg/day, the tumor volume decreased in a time-dependent manner. In contrast, lower doses of bufafenone (20 or 40 mg/kg/day) did not significantly inhibit tumor weight. At necropsy, the tumor weight of mice treated with bufafenone (80 mg/kg/day) was reduced by 30.2% compared to the control group.

Solubility Information

Solubility	DMSO: 100 mg/mL (233.33 mM),Sonication is recommended. H2O: <0.1 mg/mL (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.3333 mL	11.6667 mL	23.3334 mL
5 mM	0.4667 mL	2.3333 mL	4.6667 mL
10 mM	0.2333 mL	1.1667 mL	2.3333 mL
50 mM	0.0467 mL	0.2333 mL	0.4667 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

Ye X, et al. Darbufelone, a novel anti-inflammatory drug, induces growth inhibition of lung cancer cells both in vitro and in vivo. Cancer Chemother Pharmacol. 2010 Jul;66(2):277-85.
Johnson AR, et al. Slow-binding inhibition of human prostaglandin endoperoxide synthase-2 with darbufelone, an isoform-selective antiinflammatory di-tert-butyl phenol. Biochemistry. 2001 Jun 26;40(25):7736-45.