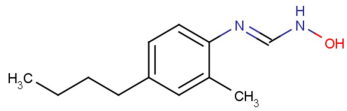
Data Sheet (Cat.No.T11556)

HET0016

Chemical Properties



CAS No.:	339068-25-6
Formula:	C12H18N2O
Molecular Weight:	206.28
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	HET0016 is a potent and selective 20-HETE synthase inhibitor (IC50s: 17.7 nM, 12.1 nM, and 20.6 nM for recombinant CYP4A1-, CYP4A2- and CYP4A3-catalyzed 20-HETE synthesis). HET0016 also is a selective CYP450 inhibitor, which has been shown to inhibit angiogenesis and tumor growth.
Targets(IC_{50})	CYP4A1: 17.7 nM CYP4A2: 12.1 nM CYP4A3: 20.6 nM
In vitro	HET0016 (100 μM; 24 hours, 48 hours) decreases migration and invasion of breast cancer metastatic cells [2]. HET0016 is a non-competitive and irreversible inhibitor of CYP4A [1].
In vivo	HET0016 reduces the metalloproteinases' levels in the lungs via PI3K/AKT pathway in mice. HET0016 (10 mg/kg/day; i.v.; for 3 weeks) reduces tumor volume and lung metastasis in an immunocompetent breast cancer mouse model. HET0016 decreases the expression of pro-inflammatory and growth factors and granulocytic MDSCs population in the lung microenvironment [2]. HET0016 protects BBB dysfunction after I/R by regulating the expression of MMP-9 and tight junction proteins [3].

Solubility Information

Solubility	DCM: 12.5 mg/mL (60.60 mM) DMSO: 5 mg/mL (24.24 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	4.848 mL	24.239 mL	48.478 mL
5 mM	0.97 mL	4.848 mL	9.696 mL
10 mM	0.485 mL	2.424 mL	4.848 mL
50 mM	0.097 mL	0.485 mL	0.97 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Seki T, et al. Cytochrome P450 4A isoform inhibitory profile of N-hydroxy-N'-(4-butyl-2-methylphenyl)-formamidine (HET0016), a selective inhibitor of 20-HETE synthesis. Biol Pharm Bull. 2005 Sep;28(9):1651-4.

2. Borin TF, et al. HET0016 decreases lung metastasis from breast cancer in immune-competent mouse model. PLoS One. 2017 Jun 13;12(6):e0178830.

3. Liu Y, et al. The protective effect of HET0016 on brain edema and blood-brain barrier dysfunction after cerebral ischemia/reperfusion. Brain Res. 2014 Jan 28;1544:45-53.

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