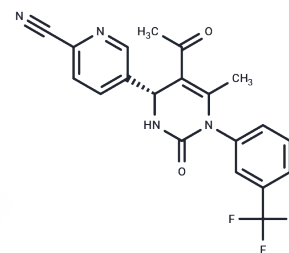


BAY-678

Chemical Properties

CAS No. : 675103-36-3
 Formula: C₂₀H₁₅F₃N₄O₂
 Molecular Weight: 400.35
 Appearance: no data available
 Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year



Biological Description

Description	BAY-678 is a human neutrophil elastase (HNE; IC ₅₀ : 20 nM) inhibitor with oral bioactivity, potency and selectivity. BAY-678 is a chemical probe recommended by the Structural Genomics Consortium (SGC).
Targets(IC ₅₀)	Others
In vitro	BAY-678 is also nominated as a chemical probe to the public via the Structural Genomics Consortium.[2] The K _i value of BAY-678 for MNE is 700 nM. BAY-678 is the 4th generation inhibitor of HNE.[1]
In vivo	BAY-678 reveals significant efficacy in preclinical models of ALI and lung emphysema. Additionally, BAY-678 has shown significant beneficial pulmonary hemodynamic and vascular effects in models of PAH in rats and mice.[2]

Solubility Information

Solubility	DMSO: 90 mg/mL (224.8 mM), Sonication is recommended. Ethanol: 4.3 mg/mL (10.74 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.4978 mL	12.4891 mL	24.9781 mL
5 mM	0.4996 mL	2.4978 mL	4.9956 mL
10 mM	0.2498 mL	1.2489 mL	2.4978 mL
50 mM	0.050 mL	0.2498 mL	0.4996 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.

Reference

- von Nussbaum F, et al. Freezing the Bioactive Conformation to Boost Potency: The Identification of BAY 85-8501, a Selective and Potent Inhibitor of Human Neutrophil Elastase for Pulmonary Diseases. *ChemMedChem*. 2015 Jul;10 (7):1163-73.
- von Nussbaum F, et al. Neutrophil elastase inhibitors for the treatment of (cardio)pulmonary diseases: Into clinical testing with pre-adaptive pharmacophores. *Bioorg Med Chem Lett*. 2015 Oct 15;25(20):4370-81.
- BAY-678 Selective chemical probe for Human Neutrophil Elastase.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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