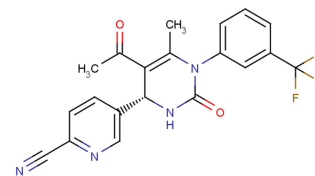


BAY-678

Chemical Properties

CAS No.:	675103-36-3
Formula:	C ₂₀ H ₁₅ F ₃ N ₄ O ₂
Molecular Weight:	400.35
Appearance:	N/A
Storage:	0-4°C for short term (days to weeks), or -20°C for long term (months).



Biological Description

Description	BAY-678 is an orally bioavailable, selective and cell-permeable inhibitor of human neutrophil elastase (HNE; IC ₅₀ : 20 nM).
Targets(IC ₅₀)	HNE: 20 nM
In vitro	The K _i value of BAY-678 for MNE is 700 nM. BAY-678 is the 4th generation inhibitor of HNE [1]. BAY-678 is also nominated as a chemical probe to the public via the Structural Genomics Consortium [2]. BAY-678 has more than 2,000-fold selectivity in a panel of 21 serine proteases [3].
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: 100 mg/mL (249.78 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)
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Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.498 mL	12.489 mL	24.978 mL
5 mM	0.5 mL	2.498 mL	4.996 mL
10 mM	0.25 mL	1.249 mL	2.498 mL
50 mM	0.05 mL	0.25 mL	0.5 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 °C for 6 months; - 20 °C for 1 month. Please use it as soon as possible.

Reference

1. 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.
2. 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.
3. BAY-678 Selective chemical probe for Human Neutrophil Elastase.

Inhibitors · Natural Compounds · Compound Libraries

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