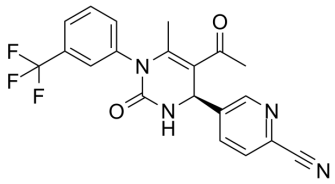
BAY-678

Cat. No.:	HY-111457A
CAS No.:	675103-36-3
Molecular Formula:	$C_{20}H_{15}F_3N_4O_2$
Molecular Weight:	400.35
Target:	Elastase
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (249.78 mM)
Ethanol : ≥ 4.76 mg/mL (11.89 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
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

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.24 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.24 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BAY-678 is an orally bioavailable, highly potent, selective and cell-permeable inhibitor of human neutrophil elastase (HNE), with an IC_{50} of 20 nM. BAY-678 is also nominated as a chemical probe to the public via the Structural Genomics Consortium (SGC).

IC_{50} & Target

IC50: 20 nM (HNE)[1].

In Vitro

BAY-678 is an orally bioavailable, highly potent, selective and cell-permeable inhibitor of human neutrophil elastase (HNE), with an IC_{50} of 20 nM. The Ki 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 (SGC)[2]. BAY-678 has more than 2,000-fold selectivity in a panel of 21 serine proteases[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	BAY-678 (17) reveals significant efficacy in preclinical models of ALI and lung emphysema, demonstrating their anti-inflammatory and anti-remodeling mode of action. Additionally, BAY-678 (17) has shown significant beneficial pulmonary hemodynamic and vascular effects in models of PAH in rats and mice[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[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.

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