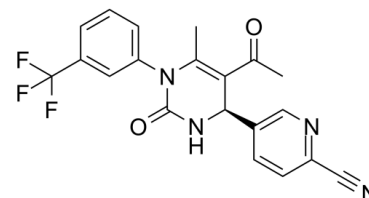


Data Sheet

Product Name:	BAY-678
Cat. No.:	CS-0041053
CAS No.:	675103-36-3
Molecular Formula:	C ₂₀ H ₁₅ F ₃ N ₄ O ₂
Molecular Weight:	400.35
Target:	Elastase
Pathway:	Metabolic Enzyme/Protease
Solubility:	Ethanol : ≥ 4.76 mg/mL (11.89 mM); DMSO : ≥ 100 mg/mL (249.78 mM)



BIOLOGICAL ACTIVITY:

BAY-678 is an orally bioavailable, highly potent, selective and cell-permeable inhibitor of human neutrophil elastase (**HNE**), with an **IC₅₀** of 20 nM. BAY-678 is also nominated as a chemical probe to the public via the Structural Genomics Consortium (SGC). **IC₅₀ & 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 IC₅₀ 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]. **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].

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.

CAIndexNames:

2-Pyridinecarbonitrile, 5-[(4R)-5-acetyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]-

SMILES:

N#CC1=NC=C([C@H](C(C(C)=O)=C(C)N2C3=CC=CC(C(F)(F)F)=C3)NC2=O)C=C1

Caution: Product has not been fully validated for medical applications. For research use only.

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