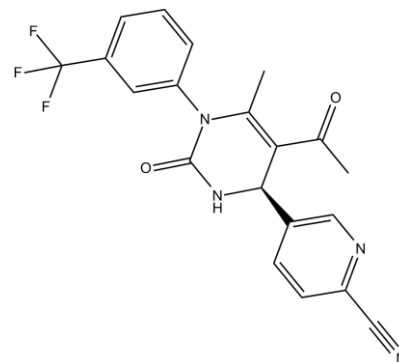


Product Data Sheet

Chemical Properties

Product Name:	BAY-678
Cas No.:	675103-36-3
M.Wt:	400.4
Formula:	C ₂₀ H ₁₅ F ₃ N ₄ O ₂



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

Canonical SMILES: O=C1N(C2=CC(C(F)(F)F)=CC=C2)C(C)=C(C(C)=O)[C@@H](C3=CN=C(C#N)C=C3)N1

Solubility: ≤30mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide

Storage: Store at 2-8°C

General tips: For obtaining a higher solubility , please warm the tube at 37° C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20° C for several months.

Shopping Condition: Evaluation sample solution : ship with blue ice
All other available size: ship with RT , or blue ice upon request

Biological Activity

Targets : Proteases

Pathways: Elastase

Description:

BAY-678 is an orally active, potent and selective inhibitor of human neutrophil elastase (HNE) [1][2].

Human neutrophil elastase (HNE) is a member of the chymotrypsin-like family of serine proteases

and is stored in the neutrophil cytoplasm. HNE is a key protease for matrix degradation and high HNE activity is occurred in inflammatory diseases. So HNE is a potential target for the treatment of pulmonary diseases such as acute lung injury (ALI), acute respiratory distress syndrome (ARDS), chronic obstructive pulmonary disease (COPD), bronchiectasis (BE), and pulmonary hypertension (PH) [1].

BAY-678 is an orally active, potent and selective inhibitor of human neutrophil elastase (HNE). BAY-678 inhibited HNE reversibly with IC50 value of 20 nM and Ki value of 15 nM. BAY-678 showed no inhibition against 21 related serine proteases, up to a concentration of 30 μ M [1].

In rats, BAY-678 showed medium clearance with t1/2 of 1.3h [1].

Reference:

[1]. von Nussbaum F, Li VM, Allerheiligen S, 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, Li VM, Meibom D, et al. Potent and Selective Human Neutrophil Elastase Inhibitors with Novel Equatorial Ring Topology: in vivo Efficacy of the Polar Pyrimidopyridazine BAY-8040 in a Pulmonary Arterial Hypertension Rat Model. *ChemMedChem*. 2016 Jan 19;11(2):199-206.

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

ApexBio Technology

www.apexbt.com

7505 Fannin street, Suite 410, Houston, TX 77054.

Tel: +1-832-696-8203 | Fax: +1-832-641-3177 | Email: info@apexbt.com