

**Product Name:** BAY 678

**Catalog No.:** 5706

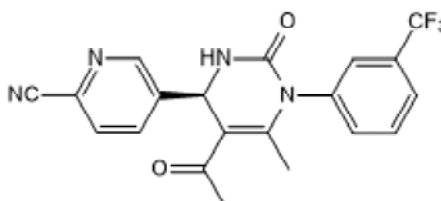
**Batch No.:** 1

CAS Number: 675103-36-3

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

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>20</sub>H<sub>15</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 400.35  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.35 (Dichloromethane:Methanol [95:5])  
**HPLC:** Shows 98.9% purity  
**Chiral HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = +23.8 (Concentration = 0.505, Solvent = Methanol)  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60	3.78	13.99
Found	59.74	3.82	13.75

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Potent and selective cell-permeable human neutrophil elastase (HNE) inhibitor ( $IC_{50}$  = 20 nM). Exhibits around 2000-fold selectivity for NHE against a panel of 21 other serine proteases. Effective in an acute lung injury model in vivo. Orally bioavailable. Inactive S-enantiomer (Cat.No.6389) also available.

**Physical and Chemical Properties:**

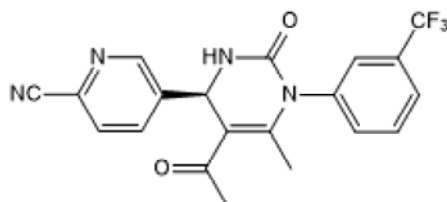
Batch Molecular Formula:  $C_{20}H_{15}F_3N_4O_2$

Batch Molecular Weight: 400.35

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**Licensing Information:**

This compound is supplied in conjunction with the Structural Genomics Consortium For further characterization details, please visit the BAY 678 probe summary on the SGC website.

**References:**

von Nussbaum *et al* (2015) 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*. **10** 1163. PMID: 26083237.

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