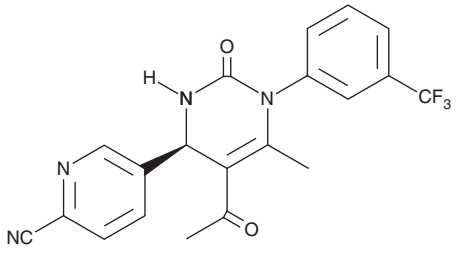
PRODUCT INFORMATION

BAY-678

Item No. 18615

CAS Registry No.: 675103-36-3
Formal Name: 5-[(4R)-5-acetyl-1,2,3,4-tetrahydro-6-methyl-2-oxo-1-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]-2-pyridinecarbonitrile
MF: $C_{20}H_{15}F_3N_4O_2$
FW: 400.4
Purity: ≥98%
UV/Vis.: λ_{max}: 228, 277 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

BAY-678 is supplied as a crystalline solid. A stock solution may be made by dissolving the BAY-678 in the solvent of choice. BAY-678 is soluble in organic solvents such as DMSO and dimethyl formamide, which should be purged with an inert gas. The solubility of BAY-678 in these solvents is approximately 30 mg/ml.

BAY-678 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, BAY-678 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. BAY-678 has a solubility of approximately 0.33 mg/ml in a 1:2 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

BAY-678 is a cell permeable inhibitor of human neutrophil elastase. This product, the (R) isomer, inhibits human neutrophil elastase with an *in vitro* IC_{50} value of 20 nM.[1,2] BAY-678 displays greater than 2,000-fold selectivity for neutrophil elastase over a panel of 21 serine proteases, and there is no significant inhibition against 7 serine/threonine kinases and 64 pharmacologically relevant proteins.[1,2] It has a favorable pharmacokinetic profile and demonstrates efficacy in acute *in vivo* models, including protease-induced acute lung injury in mice.[1,2] See the Structural Genomics Consortium (SGC) website for more information.

References

1. von Nussbaum, F., and Li, V.M.J. Neutrophil elastase inhibitors for the treatment of (cardio) pulmonary diseases: Into clinical testing with pre-adaptive pharmacophores. *Bioorg. Med. Chem. Lett.* **25(20)**, 4370-4381 (2015).
2. von Nussbaum, F., Li, V.M.-J., 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.* **10(7)**, 1163-1173 (2015).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM