

PRODUCT INFORMATION

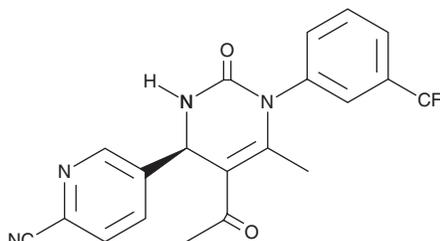


BAY-678

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: C₂₀H₁₅F₃N₄O₂
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* IC₅₀ 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).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

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