

Product Name: BAY 677

Catalog No.: 6389

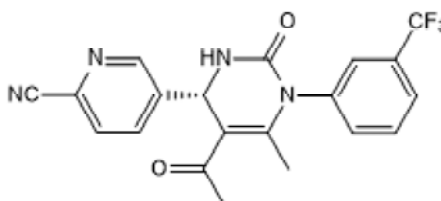
Batch No.: 1

CAS Number: 2117404-84-7

IUPAC Name: 5-[(4S)-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: C₂₀H₁₅F₃N₄O₂
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_f = 0.35 (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.3% purity
Chiral HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = -27.9 (Concentration = 0.5, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60	3.78	13.99
Found	59.86	3.8	13.85

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

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Description:

Inactive control for BAY 678 (Cat.No.5706).

Physical and Chemical Properties:

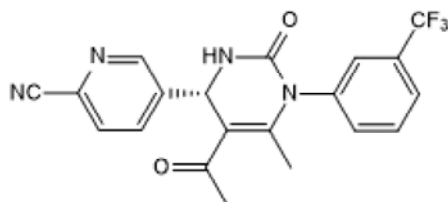
Batch Molecular Formula: C₂₀H₁₅F₃N₄O₂

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 probe 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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