

Product Name:

Certificate of Analysis

Print Date: Mar 21st 2022

Batch No.: 1

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Catalog No.: 6874

CAS Number: 1416799-28-4

IUPAC Name: 6-[[(S)-(3-Fluoro-2-pyridinyl)]3-fluoro-4-(trifluoromethoxy)phenyl]methyl]amino]carbonyl]-3-pyridinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

AMG 333

Batch Molecular Formula: $C_{20}H_{12}F_5N_3O_4$

Batch Molecular Weight: 453.33 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.23 (Ethyl acetate:Methanol [9:1])

HPLC: Shows 99.6% purity
Chiral HPLC: Shows 99.52% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.99 2.67 9.27 Found 53.03 2.56 9.25

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Product Information

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IUPAC Name: 6-[[[(S)-(3-Fluoro-2-pyridinyl)[3-fluoro-4-(trifluoromethoxy)phenyl]methyl]amino]carbonyl]-3-pyridinecarboxylic acid

Description:

AMG 333 is a potent and selective TRPM8 antagonist (IC $_{50}$ values are 13 and 20 nM for hTRPM8 and rTRPM8, respectively). Displays high selectivity over other TRP channels (IC $_{50}$ >20 μ M, TRPV1/V3/V4/A1). Inhibits icilin-induced wet-dog shake in rats and suppresses cold-induced increases in blood pressure in the rat cold-pressor test.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₁₂F₅N₃O₄

Batch Molecular Weight: 453.33 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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.

References:

Horne *et al* (2018) Discovery of TRPM8 antagonist (*S*)-6-(((3-Fluoro-4-(trifluoromethoxy)phenyl)(3-fluoropyridin-2-yl)methyl)carbamoyl) nicotinic acid (AMG 333), a clinical candidate for the treatment of migraine. J.Med.Chem. *61* 8186. PMID: 30148953.

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