

Certificate of Analysis

Print Date: Oct 10th 2019

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Product Name: VX 702 Catalog No.: 3916 Batch No.: 1

CAS Number: 745833-23-2

IUPAC Name: 6-[(Aminocarbonyl)(2,6-difluorophenyl)amino]-2-(2,4-difluorophenyl)-3-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{12}F_4N_4O_2.H_2O$

Batch Molecular Weight: 422.34

Physical Appearance: White solid

Solubility: DMSO to 100 mM

ethanol to 5 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.04 3.34 13.27 Found 54.32 3.05 13.4

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Product Information

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IUPAC Name: 6-[(Aminocarbonyl)(2,6-difluorophenyl)amino]-2-(2,4-difluorophenyl)-3-pyridinecarboxamide

Description:

Orally active, ATP-competitive inhibitor of p38 α MAPK; also inhibits p38 β (K_D values are 3.7 and 17 nM respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₂F₄N₄O₂.H₂O

Batch Molecular Weight: 422.34 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 5 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:

Goldstein *et al* (2010) Selective p38α inhibitors clinically evaluated for the treatment of chronic inflammatory disorders. J.Med.Chem. **53** 2345. PMID: 19950901.

Damjanov et al (2009) Efficacy, pharmacodynamics, and safety of VX-702, a novel p38 MAPK inhibitor, in rheumatoid arthritis. Arthrit.Rheumat. **60** 1232.

Din (2006) Drug evaluation: VX-702, a MAP kinase inhibitor for rheumatoid arthritis and acute coronary syndrome. Curr.Opin.Investig.Drugs **7** 1020. PMID: 17117592.