Certificate of Analysis

www.tocris.com

Product Name: GNF 5

CAS Number: 778277-15-9

IUPAC Name: N-(2-Hydroxyethyl)-3-[6-[[4-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: **Batch Molecular Structure:** $C_{20}H_{17}F_3N_4O_3.^{3}_4H_2O$ 431.88 Off-white solid DMSO to 100 mM Store at +4°C

HC OCF₃ ΗN

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: **Microanalysis:**

R_f = 0.28 (Chloroform:Methanol [9:1]) Shows 99.9% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 55.62 4.32 12.97 Found 55.34 4.05 12.96

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

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Print Date: Dec 13th 2021

Catalog No.: 4908

Batch No.: 1

TOCRIS a biotechne brand

Product Information

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Print Date: Dec 13th 2021

Product Name: GNF 5

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N-(2-Hydroxyethyl)-3-[6-[[4-(trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]benzamide

Description:

IUPAC Name:

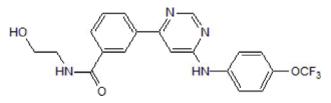
GNF 5 is a selective, non-ATP competitive allosteric inhibitor of Bcr-Abl (IC_{50} = 220 nM for wild-type Abl). Binds the myristatebinding site of Abl. Acts in combination with nilotinib to inhibit T315I Bcr-Abl in vitro and in vivo. Analog of GNF 2 (Cat. No. 4399). GNF 5 decreases mitochondrial function in lung cancer cells.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{20}H_{17}F_3N_4O_3.^3H_2O$ Batch Molecular Weight: 431.88 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°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).

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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:

Luttman et al (2021) ABL allosteric inhibitors synergize with statins to enhance apoptosis of metastatic lung cancer cells. Cell Rep. 37 109880. PMID: 34706244.

lacob *et al* (2011) Allosteric interactions between the myristate- and ATP-site of the Abl kinase. PLoS One **6** e15929. PMID: 21264348. **Deng** *et al* (2010) Expanding the diversity of allosteric Bcr-Abl inhibitors. J.Med.Chem. **53** 6934. PMID: 20828158.

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