

Product Name: GNF 5

Catalog No.: 4908

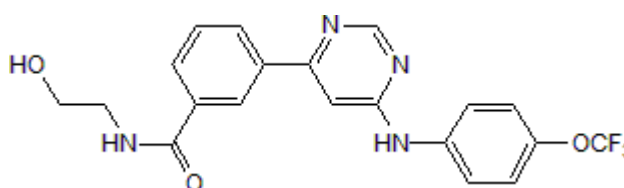
Batch No.: 1

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: $C_{20}H_{17}F_3N_4O_3 \cdot \frac{3}{4}H_2O$
Batch Molecular Weight: 431.88
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.28$ (Chloroform:Methanol [9:1])
HPLC: Shows >99.9% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	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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 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

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Description:

Selective, non-ATP competitive allosteric inhibitor of Bcr-Abl (IC₅₀ = 220 nM for wild-type Abl). Binds the myristate-binding 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).

Physical and Chemical Properties:

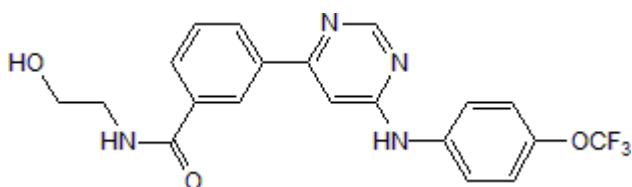
Batch Molecular Formula: C₂₀H₁₇F₃N₄O₃·¾H₂O

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).

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:

Zhang et al (2010) Targeting Bcr-Abl by combining allosteric with ATP-binding-site inhibitors. *Nature* **463** 501. PMID: 20072125.

Deng et al (2010) Expanding the diversity of allosteric Bcr-Abl inhibitors. *J.Med.Chem.* **53** 6934. PMID: 20828158.

Iacob et al (2011) Allosteric interactions between the myristate- and ATP-site of the Abl kinase. *PLoS One* **6** e15929. PMID: 21264348.

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