

**Product Name:** GNF 2

**Catalog No.:** 4399

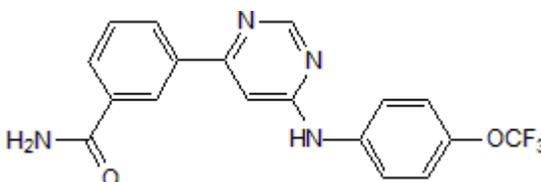
**Batch No.:** 1

CAS Number: 778270-11-4

IUPAC Name: 3-[6-[[4-(Trifluoromethoxy)phenyl]amino]-4-pyrimidinyl]benzamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>13</sub>F<sub>3</sub>N<sub>4</sub>O<sub>2</sub>  
**Batch Molecular Weight:** 374.32  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 50 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.31 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 99% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	57.76	3.5	14.97
Found	57.78	3.5	14.85

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**Description:**

Allosteric inhibitor of Bcr-Abl tyrosine kinase activity ( $IC_{50} = 267$  nM); inhibits proliferation and induces apoptosis in Bcr-Abl-expressing cells. Selective for Bcr-Abl over a panel of serine, threonine and tyrosine kinases. Non-ATP-competitive.

**Physical and Chemical Properties:**

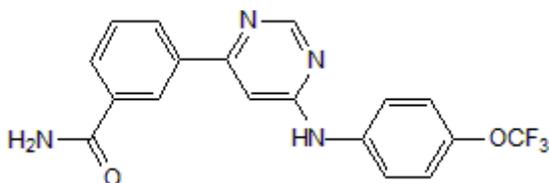
Batch Molecular Formula:  $C_{18}H_{13}F_3N_4O_2$

Batch Molecular Weight: 374.32

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Adrián et al** (2006) Allosteric inhibitors of Bcr-abl-dependent cell proliferation. *Nat.Chem.Biol.* **2** 95. PMID: 16415863.

**Ohren & Sebolt-Leopold et al** (2006) Inhibitors of Bcr-abl... breaking new ground again. *Nat.Chem.Biol.* **2** 63. PMID: 16421581.

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

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 50 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.

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