



# **Certificate of Analysis**

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Product Name: LFM-A13 Catalog No.: 1300 Batch No.: 2

CAS Number: 62004-35-7

IUPAC Name: 2-Cyano-N-(2,5-dibromophenyl)-3-hydroxy-2-butenamide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{11}H_8Br_2N_2O_2$ 

Batch Molecular Weight: 360

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM

Storage: Store at RT

**Batch Molecular Structure:** 

2. ANALYTICAL DATA

**TLC:**  $R_f = 0.2$  (Ethyl acetate:Petroleum ether [4:1])

**HPLC:** Shows 98.3% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 36.7 2.24 7.78 Found 36.59 2.26 7.59



# **Product Information**

Print Date: Feb 26<sup>th</sup> 2016 **WWW.tocris.com** 

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CAS Number: 62004-35-7

IUPAC Name: 2-Cyano-*N*-(2,5-dibromophenyl)-3-hydroxy-2-butenamide

#### **Description:**

Potent and selective inhibitor of Bruton's tyrosine kinase (BTK). Inhibits recombinant BTK with an IC $_{50}$  value of 2.5  $\mu$ M and has no activity on other protein kinases ( including JAK1, JAK3, HCK, EGFR kinase and insulin receptor kinase) at concentrations of up to 278  $\mu$ M.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>11</sub>H<sub>8</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>2</sub>

Batch Molecular Weight: 360

Physical Appearance: Off White solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

Storage: Store at RT

### 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:

**Mahajan** *et al* (1999) Rational design and synthesis of a novel anti-leukemic agent targeting Bruton's tyrosine kinase (BTK), LFM-A13 [α-cyano-β-hydroxy-β-methyl-N-(2,5-dibromophenyl)propenamide]. J.Biol.Chem. **274** 9587. PMID: 10092645.

Vassilev et al (1999) Bruton's tyrosine kinase as an inhibitor of the Fas/CD95 death-inducing signaling complex. J.Biol.Chem. 274 1646. PMID: 9880544.

Crosby and Pool (2002) Interaction of Bruton's tyrosine kinase and protein kinase Cθ in platelets. J.Biol.Chem. 277 9958. PMID: 11788586