



Certificate of Analysis

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Product Name: BM -IN-1 Catalog No.: 123 Batch No.: 1

1431525-23-3 CAS Number:

IUPAC Name: N-2-Methyl-5-9-4- (methylsulfonyl)amino phenyl -2-oxobenzo h -1,6-naphthyridin-1(2H)-yl phenyl -2-propenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

C₂₉H₂₄N₄O₄S.H₂O **Batch Molecular Formula:**

542.61 **Batch Molecular Weight: Physical Appearance:** White solid

DMSO to 1 mM with gentle warming Solubility:

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 64.19 4.83 10.33 Found 64.33 4.71 10.18

Tel: +44 (0)1235 529449 www.tocris.com/distributors Tel:+1 612 379 2956



Product Information

Print Date: Jan 12th 2018

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Product Name: BMX-IN-1 Catalog No.: 5123 Batch No.: 1

CAS Number: 1431525-23-3

 $IUPAC\ Name: \ N-[2-Methyl-5-[9-[4-[(methylsulfonyl)amino]phenyl]-2-oxobenzo[h]-1,6-naphthyridin-1(2\textit{H})-yl]phenyl]-2-propenamide$

Description:

Potent and irreversible BMX inhibitor ($IC_{50} = 25$ nM). Covalently modifies Cysteine 496. Demonstrates selectivity over other Tec family members with identically positioned reactive cysteine residue in vitro. Reduces cell number and induces apoptosis in prostate cancer cell lines. Also inhibits proliferation and reduces viability in HeLa and SiHa cell lines.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₂₄N₄O₄S.H₂O

Batch Molecular Weight: 542.61 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 1 mM with gentle warming

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.

Licensing Information:

Sold under license from Dana-Farber Cancer Institute.

References:

Li et al (2017) BMX/Etk promotes cell proliferation and tumorigenicity of cervical cancer cells through PI3K/AKT/mTOR and STAT3 pathways. Oncotarget. 8 49238. PMID: 28514765.

Liu et al (2013) Discovery of a selective irreversible BMX inhibitor for prostate cancer. ACS Chem.Biol. 8 1423. PMID: 23594111.