Print Date: Feb 1st 2023

Certificate of Analysis

www.tocris.com

Product Name: **BAY 707** **Catalog No.: 6562** **Batch No.: 1**

CAS Number: 2109805-96-9

IUPAC Name: *N*-Ethyl-4-[(3*S*)-3-methyl-4-morpholinyl]-1*H*-pyrrolo[2,3-*b*]pyridine-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{20}N_4O_2$

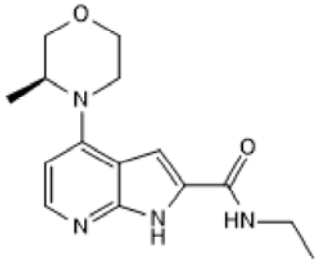
Batch Molecular Weight: 288.34

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

Chiral HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.48	6.99	19.43
Found	62.07	7.03	19.24

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Description:

BAY 707 is a potent and selective MTH1 inhibitor (IC_{50} = 2.3 nM); exhibits no significant activity at 1 µM concentration against a panel of 97 kinases. BAY 707 is cell-permeable and active in vivo, and displays no antitumor activity in vitro or in vivo.

Physical and Chemical Properties:

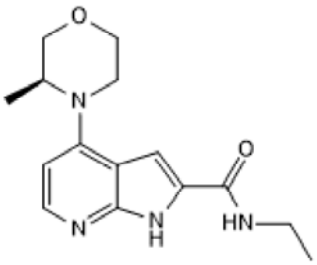
Batch Molecular Formula: $C_{15}H_{20}N_4O_2$

Batch Molecular Weight: 288.34

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 10 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY-707 probe summary on the SGC website.

References:

Rahm *et al* (2018) Creation of a novel class of potent and selective MutT Homologue 1 (MTH1) inhibitors using fragment-based screening and structure-based drug design. J.Med.Chem. ***61*** 2533. PMID: 29485874.

Ellermann *et al* (2017) Novel class of potent and cellularly active inhibitors devalidates MTH1 as broad-spectrum cancer target. ACS Chem.Biol. ***12*** 1986. PMID: 28679043.