



Certificate of Analysis

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Product Name: BMS 345541 Catalog No.: 4806 Batch No.: 1

CAS Number: 547757-23-3

IUPAC Name: N^{1} -(1,8-Dimethylimidazo[1,2-a]quinoxalin-4-yl)-1,2-ethanediamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₇N₅.HCI.H₂O

309.8 **Batch Molecular Weight:**

Physical Appearance: Pale yellow solid Solubility: water to 100 mM DMSO to 100 mM

Store at -20°C

Batch Molecular Structure:

.HCI NH_2

2. ANALYTICAL DATA

Storage:

TLC: $R_f = 0.29$ (Methanol 100%)

HPLC: Shows 99.4% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 54.28 6.51 22.61 Found 54.09 6.28 22.68

Tel: +44 (0)1235 529449



Product Information

Print Date: Apr 24th 2020

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Description:

Selective allosteric inhibitor of IKK (IC $_{50}$ values are 0.3 and 4.0 μ M for IKK β and IKK α respectively). Exhibits no effect against a panel of 15 other kinases. Attenuates LPS-induced cytokine production in vitro and blocks NF κ B dependent transcription in mice. Also suppresses joint destruction in a mouse model of arthritis.

Physical and Chemical Properties:

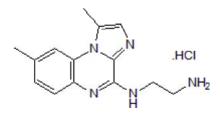
Batch Molecular Formula: C₁₄H₁₇N₅.HCl.H₂O

Batch Molecular Weight: 309.8

Physical Appearance: Pale yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM 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:

De Silva *et al* (2010) Inhibition of choriodecidual cytokine production and inflammatory gene expression by selective IκB kinase (IKK) inhibitors. Br.J.Pharmacol. *160* 1808. PMID: 20649582.

Pattoli *et al* (2005) Collagen and aggrecan degradation is blocked in interleukin-1-treated cartilage explants by an inhibitor of IκB kinase through suppression of metalloproteinase expression. J.Pharmacol.Exp.Ther. *315* 382. PMID: 16009742.

Burke *et al* (2003) BMS-345541 is a highly selective inhibitor of $l\kappa B$ kinase that binds at an allosteric site of the enzyme and blocks NF- κB -dependent transcription in mice. J.Biol.Chem. **278** 1450. PMID: 12403772.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use