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Print Date: Jan 16th 2016

# Certificate of Analysis

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**Product Name:** **BMS 566419** **Catalog No.: 5492** **Batch No.: 1**

CAS Number: 566161-24-8

IUPAC Name: *N*-[1-[6-(4-Ethyl-1-piperazinyl)-3-pyridinyl]-1-methylethyl]-2-fluoro-9,10-dihydro-9-oxo-3-acridinecarboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{28}H_{30}FN_5O_2 \cdot ¼H_2O$

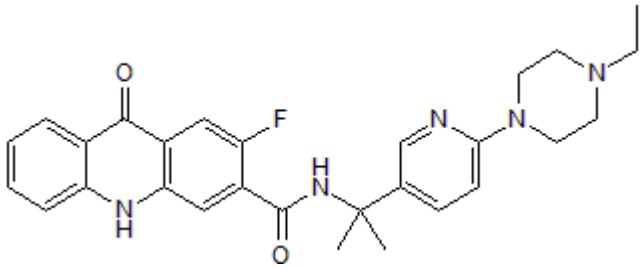
**Batch Molecular Weight:** 492.07

**Physical Appearance:** Yellow solid

**Solubility:** 1eq. HCl to 50 mM
DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.11 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99.2% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 68.34 | 6.25 | 14.23 |
| Found | 68.4 | 6.24 | 14.16 |



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**Description:**

Potent inosine monophosphate dehydrogenase (IMPDH) inhibitor ($IC_{50}$ = 17 nM). Inhibits proliferation of human T-lymphoblasts and PBMCs in vitro. Reduces paw swelling in a rat adjuvant arthritis model. Orally available.

**Physical and Chemical Properties:**

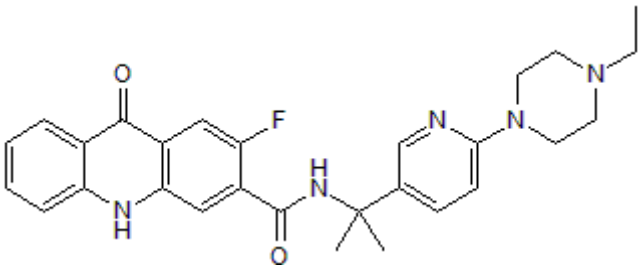
Batch Molecular Formula: $C_{28}H_{30}FN_5O_2.¼H_2O$

Batch Molecular Weight: 492.07

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Usage Info:**

1eq. HCl to 50 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:**

**Watterson** *et al* (2007) Acridone-based inhibitors of inosine 5'-monophosphate dehydrogenase: discovery and SAR leading to the identification of *N*-(2-(6-(4-ethylpiperazin-1-yl)pyridin-3-yl)propan-2-yl)-2- fluoro-9-oxo-9,10-dihydroacridine-3-carboxamide (BMS-566419). J.Med.Chem. ***50*** 3730. PMID: 17585753.