Print Date: Jan 15th 2018

# Certificate of Analysis

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**Product Name:** **Halofuginone hydrobromide** **Catalog No.: 1993** **Batch No.: 1**

CAS Number: 64924-67-0

IUPAC Name: (2*R**,3*S**)-7-Bromo-6-chloro-3-[3-(3-hydroxy-2-piperidinyl)-2-oxopropyl]-4-3*H*-quinazolinone hydrobromide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{16}H_{17}BrClN_3O_3.HBr$

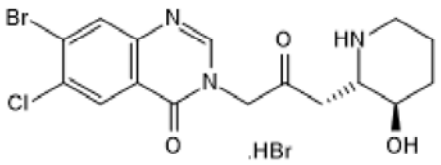
**Batch Molecular Weight:** 495.59

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**




(and enantiomer)

## 2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 38.78 | 3.66 | 8.48 |
| Found | 38.98 | 3.63 | 8.33 |



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# Product Information



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**Description:**

High affinity competitive prolyl-tRNA synthetase inhibitor ($K_i$ = 18.3 nM). Blocks expression of MMP2. Inhibits ECM invasion in vitro and lung metastasis by bladder cancer cells in mice. Inhibits the development of Th17-driven autoimmunity in a mouse model of multiple sclerosis by activating the amino acid response (AAR) pathway. Also antiparasitic.

**Physical and Chemical Properties:**

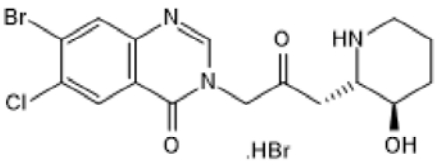
Batch Molecular Formula: $C_{16}H_{17}BrClN_3O_3.HBr$

Batch Molecular Weight: 495.59

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




(and enantiomer)

**Storage:** Store at -20°C

**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:**

**Keller** *et al* (2012) Halofuginone and other febrifugine derivatives inhibit prolyl-tRNA synthetase. Nat Chem Biol. ***8*** 311. PMID: 22327401.

**Elkin** *et al* (1999) Inhibition of matrix metalloproteinase-2 expression and bladder carcinoma metastasis by halofuginone. Clin.Cancer.Res. ***5*** 1982. PMID: 10473075 .

**Anderson** *et al* (1979) Analysis of the anti-coccidial drug, halofunginone, in chicken feed using gas-liquid chromatography and high-performance liquid chromatography. J.Chromatogr. ***168*** 471. PMID: 570196.



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