TOCRIS
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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **Phortress** **Catalog No.: 4995** **Batch No.: 1**

CAS Number: 328087-38-3

IUPAC Name: (2*S*)-2,6-Diamino-*N*-[4-(5-fluoro-2-benzothiazolyl)-2-methylphenyl]hexanamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{23}FN_4OS.2HCl.H_2O$

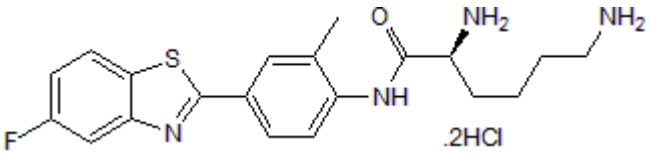
Batch Molecular Weight: 477.43

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.32	5.7	11.74
Found	50.43	5.57	11.6

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Description:

Prodrug of the antitumor agent 5F 203, which acts via binding to aryl hydrocarbon receptors. Induces expression of CYP1A1 and generates adducts in the DNA of sensitive MCF7 and IGROV-1 cells.

Physical and Chemical Properties:

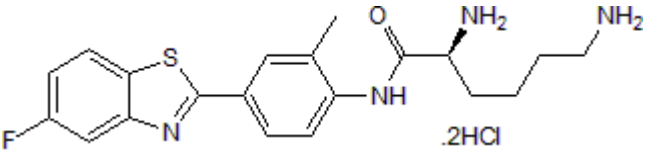
Batch Molecular Formula: $C_{20}H_{23}FN_4OS.2HCl.H_2O$

Batch Molecular Weight: 477.43

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



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:

Leong *et al* (2003) Antitumour 2-(4-aminophenyl)benzothiazoles generate DNA adducts in sensitive tumour cells *in vitro* and *in vivo*. Br.J.Cancer ***88*** 470. PMID: 12569393.

Trapani *et al* (2003) DNA damage and cell cycle arrest induced by 2-(4-amino-3-methylphenyl)-5-fluorobenzothiazole (5F 203, NSC 703786) is attenuated by aryl hydrocarbon receptor deficient MCF-7 cells. Br.J.Cancer ***88*** 599. PMID: 12592376.

Bradshaw and Westwell (2004) The development of the antitumour benzothiazole prodrug, phortress, as a clinical candidate. Curr.Med.Chem. ***11*** 1241. PMID: 15078163.

Leong *et al* (2004) In vitro, in vivo and in silico analyses of the antitumor activity of 2(-4-amino-3-methylphenyl)-5-fluorobenzothiazoles. Mol.Cancer Ther. ***3*** 1565. PMID: 15634650.

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