



Certificate of Analysis

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Product Name: MC 1568 Catalog No.: 4077 Batch No.: 1

CAS Number: 852475-26-4

IUPAC Name: 3-[5-(3-(3-Fluorophenyl)-3-oxopropen-1-yl)-1-methyl-1*H*-pyrrol-2-yl]-*N*-hydroxy-2-propenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{15}FN_2O_3$. ¹/₄ H_2O

Batch Molecular Weight: 318.81

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.34$ (Dichloromethane:Methanol [9:1])

HPLC: Shows 96.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 64.04 4.9 8.79 Found 64.37 4.72 8.69



Product Information

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Print Date: Jan 14th 2016

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Description:

Selective inhibitor of class IIa histone deacetylases (HDACs). Exhibits tissue-selective inhibition between members of class II deacetylases in vivo; inhibits HDAC4 and HDAC5 in skeletal muscle and the heart without affecting HDAC3 activity. Arrests myogenesis through the stabilization of myocyte enhancer factor 2D (MEF2D)-HDAC3/4 complex. Displays no inhibition of class I HDAC activity or expression.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₅FN₂O₃.1/4H₂O

Batch Molecular Weight: 318.81 Physical Appearance: Orange solid

Minimum Purity: >96%

Batch Molecular Structure:

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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:

Mai et al (2005) Class II (IIa)-selective histone deacetylase inhibitors. 1. Synthesis and biological evaluation of novel (aryloxopropenyl) pyrrolyl hydroxyamines. J.Med.Chem. 48 3344. PMID: 15857140.

Mai et al (2007) Identification of two new synthetic histone deacetylase inhibitors that modulate globin gene expression in erythroid cells from healthy donors and patients with thalassemia. Mol.Pharmacol. **72** 1111. PMID: 17666592.

Nebbioso *et al* (2009) Selective class II HDAC inhibitors may impaor myogenesis by modulating the stability and activity of HDAC-MEF2 complexes. EMBO J. *10* 776.