

**Product Name:** MC 1742

**Catalog No.:** 5727

**Batch No.:** 1

CAS Number: 1776116-74-5

IUPAC Name: 5-[(4-[1,1'-Biphenyl]-4-yl)-1,6-dihydro-6-oxo-2-pyrimidinyl]thio]-*N*-hydroxypentanamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>21</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>S·¼H<sub>2</sub>O

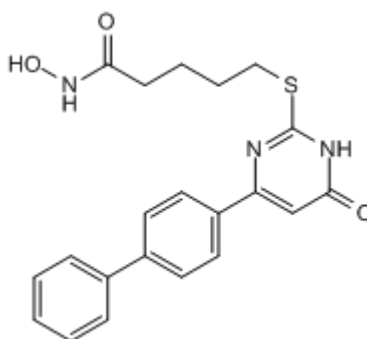
**Batch Molecular Weight:** 399.97

**Physical Appearance:** Off White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.4 (Dichloromethane:Methanol [85:15])

**HPLC:** Shows >99.1% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	63.06	5.42	10.51
Found	62.89	5.22	10.55

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**Description:**

Potent class I and IIb HDAC inhibitor (IC<sub>50</sub> values are 7, 20, 40, 100, 110 and 610 nM for HDAC6, HDAC3, HDAC10, HDAC1, HDAC2 and HDAC8, respectively). Suppresses proliferation and induces apoptosis of sarcoma cancer stem cells (CSCs) at concentrations >500 nM. Also induces osteogenesis in sarcoma CSCs at concentrations of 25 - 500 nM .

**Physical and Chemical Properties:**

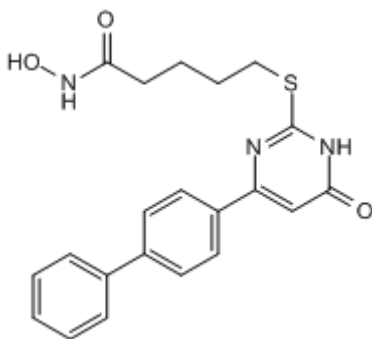
Batch Molecular Formula: C<sub>21</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>S. ¼H<sub>2</sub>O

Batch Molecular Weight: 399.97

Physical Appearance: Off White 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:**

**Di Pompo et al** (2015) Novel histone deacetylase inhibitors induce growth arrest, apoptosis, and differentiation in sarcoma cancer stem cells. *J.Med.Chem.* **58** 4073. PMID: 25905694.

**Mai et al** (2008) Novel uracil-based 2-aminoanilide and 2-aminoanilide-like derivatives: histone deacetylase inhibition and in-cell activities. *Bioorg.Med.Chem.Lett.* **18** 2530. PMID: 18381238.

**Mai et al** (2006) Synthesis and biological properties of novel, uracil-containing histone deacetylase inhibitors. *J.Med.Chem.* **49** 6046. PMID: 17004718.

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956