

Certificate of Analysis

Print Date: Jul 19th 2018

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Product Name: CI 994 Catalog No.: 2952 Batch No.: 1

CAS Number: 112522-64-2

IUPAC Name: 4-(Acetylamino)-N-(2-aminophenyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{15}N_3O_2$ **Batch Molecular Weight:** 269.3

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.33$ (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 66.9 5.61 15.6 Found 66.46 5.69 15.56



Product Information

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IUPAC Name: 4-(Acetylamino)-*N*-(2-aminophenyl)benzamide

Description:

Orally active class I histone deacetylase (HDAC) inhibitor (K_i values are 0.41, 0.75, >100 and >100 μ M for HDAC1, HDAC3, HDAC6 and HDAC8 respectively). Mediates G_1 cell cycle arrest, inhibits proliferation and induces apoptosis in vitro and in vivo. Increases neuroplasticity during memory extinction. Also increases efficiency of hepatic differentiation of hPSCs

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₅N₃O₂ Batch Molecular Weight: 269.3 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°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:

Gräff et al (2014) Epigenetic priming of memory updating during reconsolidation to attenuate remote fear memories. Cell **156** 261. PMID: 24439381.

Beckers *et al* (2007) Distinct pharamacological properties of second generation HDAC inhibitors with the benzamide or hydroxamate head group. Int.J.Cancer **121** 1138. PMID: 17455259.

Kraker *et al* (2003) Modulation of histone acetylation by [4-(acetylamino)-*N*-(2-amino-phenyl) benamide] in HCT-8 colon carcinoma. Mol.Cancer Ther. **2** 401. PMID: 12700284.