

Certificate of Analysis

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Product Name: PCI 34051 Catalog No.: 4643 Batch No.: 1

CAS Number: 950762-95-5

IUPAC Name: N-Hydroxy-1-[(4-methoxyphenyl)methyl]-1H-indole-6-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{16}N_2O_3$ Batch Molecular Weight: 296.32

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

1eq. NaOH to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.18$ (Dichloromethane:Methanol [96:4])

HPLC: Shows >99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 68.91 5.44 9.45 Found 68.91 5.39 9.48







Product Information

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IUPAC Name: N-Hydroxy-1-[(4-methoxyphenyl)methyl]-1H-indole-6-carboxamide

Description:

Potent and selective histone deacetylase 8 (HDAC8) inhibitor (IC $_{50}$ = 10 nM). Displays >200 fold selectivity over HDAC isoforms 1, 2, 3, 6 and 10. Induces apoptosis in cell lines derived from T cell lymphomas or leukemias.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₆N₂O₃ Batch Molecular Weight: 296.32 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM 1eq. NaOH to 20 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:

Balasubramanian et al (2008) A novel histone deacetylase 8 (HDAC8)-specific inhibitor PCI-34051 induces apoptosis in T-cell lymphomas. Leukemia 22 (5) 1026. PMID: 18256683.

Pipalia et al (2011) Histone deacetylase inhibitor treatment dramatically reduces cholesterol accumulation in Niemann-Pick type C1 mutant human fibroblasts. Proc.Natl.Acad.Sci.U.S.A. **108** (14) 5620. PMID: 21436030.

