

Certificate of Analysis

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Product Name: Sodium 4-Phenylbutyrate

Catalog No.: 2682

Batch No.: 5

CAS Number: 1716-12-7

IUPAC Name: 4-Phenylbutyric acid, sodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₀H₁₁NaO₂·¼H₂O

Batch Molecular Weight: 190.68

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 25 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.99	6.08	
Found	63.16	5.81	

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: 4-Phenylbutyric acid, sodium salt

Description:

Sodium 4-Phenylbutyrate is a histone deacetylase inhibitor that displays anticancer activity. Inhibits cell proliferation, invasion and migration and induces apoptosis in glioma cells. Sodium 4-Phenylbutyrate also inhibits protein isoprenylation, depletes plasma glutamine, increases production of fetal hemoglobin through transcriptional activation of the γ -globin gene and affects hPPAR γ activation.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₀H₁₁NaO₂· $\frac{1}{4}$ H₂O

Batch Molecular Weight: 190.68

Physical Appearance: White solid

Minimum Purity: \geq 99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 25 mM

This compound is hygroscopic and may absorb atmospheric moisture during prolonged storage, causing the solid to become sticky and/or collapse into a gel or glass-like form. Although purity is unaffected, it may be difficult to extract the full quantity from the vial. In such a situation, we recommend that solutions are made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Khan *et al* (2011) HDAC inhibitor 4-phenylbutyrate preserves immature phenotype of human embryonic midbrain stem cells: implications for the involvement of DNA methyltransferase. *Int.J.Mol.Med.* **28** 977. PMID: 21894430.

Ammerpohl *et al* (2007) Complementary effects of HDAC inhibitor 4-PB on gap junction communication and cellular export mechanisms support restoration of chemosensitivity of PDAC cells. *Br.J.Cancer* **96** 73. PMID: 17164759.

Appelskog *et al* (2004) Histone deacetylase inhibitor 4-phenylbutyrate suppresses GADPH mRNA expression in glioma cells. *Int.J.Oncol.* **24** 1419. PMID: 15138583.

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