PRODUCT INFORMATION



Sodium 4-Phenylbutyrate-d₁₁

Item No. 22085

CAS Registry No.:	1392208-11-5	
Formal Name:	benzene-d ₅ -butanoic-d ₆ acid, monosodium salt	
Synonyms:	Benzenebutanoic acid-d ₁₁ , TriButyrate-d ₁₁	5
MF:	$C_{10}D_{11}O_2 \bullet Na$	
FW:	197.3	
Chemical Purity:	≥98% (Sodium 4-Phenylbutyrate)	
Deuterium		- Na ⁺
Incorporation:	≥99% deuterated forms (d ₁ -d ₁₁); ≤1% d ₀	D' D'
Supplied as:	A solid	D
Storage:	-20°C	
Stability:	≥4 years	
Special Conditions	: Hygroscopic	
Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.		

Laboratory Procedures

Sodium 4-phenylbutyrate-d₁₁ is intended for use as an internal standard for the quantification of sodium 4-phenylbutyrate (Item No. 11323) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Sodium 4-phenylbutyrate-d₁₁ is supplied as a solid. Sodium 4-phenylbutyrate-d₁₁ is soluble in the organic solvent DMSO, which should be purged with an inert gas. It is also soluble in water. The solubility of sodium 4-phenylbutyrate-d₁₁ in DMSO and water is approximately 25 and 100 mM, respectively. We do not recommend storing the aqueous solution for more than one day.

Description

Sodium 4-phenylbutyrate is a chemical chaperone that has been shown to rescue the trafficking of misfolded proteins.^{1,2} It also weakly blocks histone deacetylase activity (IC₅₀ = 0.4 mM), which results in cell cycle arrest, differentiation, and/or apoptosis of various tumors.^{3,4} Formulations containing sodium 4-phenylbutyrate have been used for the treatment of urea cycle disorders.

References

- 1. Majed, B.H. and Khalil, R.A. Molecular mechanisms regulating the vascular prostacyclin pathways and their adaptation during pregnancy and in the newborn. Pharmacol. Rev. 64(3), 540-582 (2012).
- 2. Bradbury, N.A. Focus on "sodium 4-phenylbutyrate downregulates Hsc70: Implications for intracellular trafficking of △F508-CFTR". Am. J. Physiol. Cell Physiol. 278(2), C257-C258 (2000).
- 3. Lu, Q., Wang, D.S., Chen, C.S., et al. Structure-based optimization of phenylbutyrate-derived histone deacetylase inhibitors. J. Med. Chem. 48(17), 5530-5535 (2005).
- 4. Ammerpohl, O., Trauzold, A., Schniewind, B., et al. 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(1), 73-81 (2007).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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1180 EAST ELLSWORTH RD ANN ARBOR, MI 48108 · USA PHONE: [800] 364-9897 [734] 971-3335 FAX: [734] 971-3640 CUSTSERV@CAYMANCHEM.COM WWW.CAYMANCHEM.COM