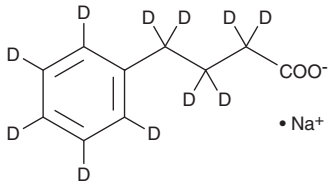
PRODUCT INFORMATION

Sodium 4-Phenylbutyrate-d_{11}

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}
MF: $C_{10}D_{11}O_2 \bullet Na$
FW: 197.3
Chemical Purity: ≥98% (Sodium 4-Phenylbutyrate)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_{11}); ≤1% d_0
Supplied as: A solid
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-d_{11} 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-d_{11} is supplied as a solid. Sodium 4-phenylbutyrate-d_{11} 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-d_{11} 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 (IC_{50} = 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 ΔF508-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).

CAYMAN CHEMICAL
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