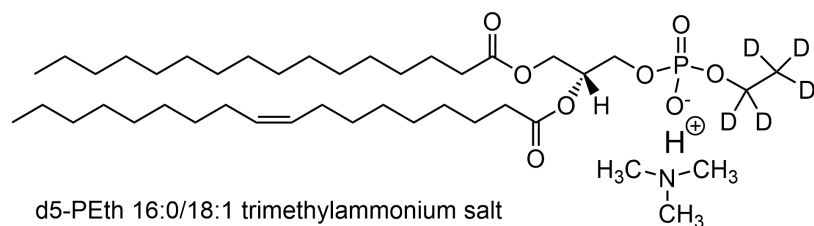

Deuterated Phosphatidylethanol (D5-PEth) 16:0/18:1 Internal Standard

Cat. No. 50-1021, 50-1023

Background: Phosphatidylethanol (PEth) is a group of homologous unnatural phospholipids formed by phospholipase D catalyzed ethanolysis in-vivo of mainly endogenous phosphatidylcholine. The half-life of PEth is about three to eight days, which makes PEth suitable as a biomarker for a person's ethanol consumption over longer period. PEth-16:0/18:1 is the most abundant individual form of the PEth-homologues. It is used in quantitative LC-MS/MS analysis of blood from patients to estimate the level of alcohol consumption.

Description: 1-Palmitoyl-2-oleoyl-3-d5-ethoxyhydroxyphosphinyl-sn-glyceroltrimethyl ammonium salt (PEth-d5 16:0/18:1); solution in methanol.

Structure:



Quantity: 50-1021: 10nmol D5-PEth 16:0/18:1
50-1023: 100nmol D5-PEth 16:0/18:1

Concentration: Within range of 1.0 to 2.0 $\mu\text{mol/g}$ as precisely determined by $^1\text{H-qNMR}$.

Molecular Weight: Most Abundant Isotope of Parent: $^{12}\text{C}_{39}\text{H}_{70}\text{H}_5\text{O}_8\text{P}$ =707.55 g/mol.

Solution: Methanol.

Storage: Dark at +2°C + 8°C, expiration date on the vial. Protect from air - subject to oxidation. Diluted solution should be stored at -20° C.

Application note:

For use as internal standard in LC-MS(/MS) applications for the qualitative and quantitative analysis of, for example, PEth-16:0/18:1. This product may be diluted directly with isopropanol or any other appropriate solutions to obtain a secondary solution having any concentration of PEth-d516:0/18:1 of choice.

Important! Centrifuge the ampule briefly before opening it to collect the content (centrifuge, 2000 RCF, 2 min).

Important Safety Notes:

The pharmacological and toxicological properties of this product have not been fully investigated. Use general laboratory practice and caution in the use and handling of this product. This product must not be used in humans.

References:

1. Gustavsson L, Alling C. Formation of phosphatidylethanol in rat brain by phospholipase D. *Biochem Biophys Res Com* 1987, 142(3):958-63.
2. Helander A. and Zheng Y. Molecular Species of the Alcohol Biomarker Phosphatidylethanol in Human Blood Measured by LC-MS. *Clinical Chemistry* 2009, 55(7):1395-1405.
3. Gnann H, Engelmann C, Skopp G, Winkler M, Auwärter V, Dresen S, Ferreirós N, Wurst FM, Weinmann W. Identification of 48 homologues of phosphatidylethanol in blood by LC-ESI-MS/MS. *Anal Bioanal Chem* 2010, 396(7):2415-23.
4. Furey A, Moriarty M, Bane V, Kinsella B, Lehane M. Ion suppression; a critical review on causes, evaluation, prevention and applications. *Talanta* 2013, 15(115):104-22.
5. Wensbo, D. et al Differentiation and quantification of synthetic phosphatidylethanol (PEth) homologues by ¹H- and ¹³C-NMR in polar organic solvents. *Anal. Bio. Chem.* In press, DOI 10.1007/s00216-014-7826-4.