

INSTRUCTIONS FOR USE

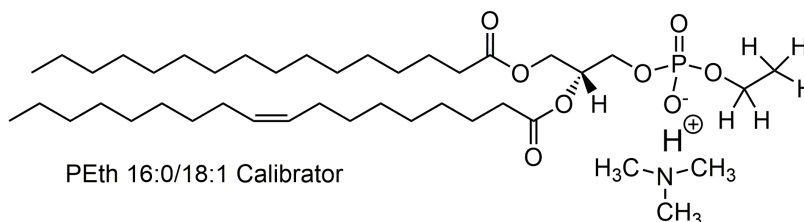
PEth 16:0/18:1 Calibrator

Cat. No. 50-1014, 50-1015

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 five 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 has been used in quantitative LC-MS/MS analysis of blood from patients to estimate the level of alcohol consumption.

Description: 1-Palmitoyl-2-oleoyl-3-ethoxyhydroxyphosphinyl-sn-glyceroltrimethyl ammonium salt (PEth-16:0/18:1); solution in hexadeuterodimethyl sulfoxide (DMSO-d₆) [patent pending].

Structure:



Quantity: Precise quantity (P=0.95, ±<3%).

Concentration: Within range of 1.0 to 2.0 µmol/g as precisely determined by ¹H-qNMR.

Molecular Weight: Most Abundant Isotope of Parent: ¹²C₃₉¹H₇₅¹⁶O₈³¹P=702.52 g/mol.

Solution: MeOH.

Solubility: Soluble in isopropanol

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

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

Important! Centrifuge the ampule briefly before opening it to collect the content (e.g Eppendorf centrifuge, 4000 RCF, 3 min).

Application example:

Make an initial dilution by addition of 1.0 ml (corresponding to 10 μ M) of e.g. blood or plasma directly to the original 10 nmol vial, followed by consecutive serial dilutions to the desired range of concentrations to be used for the generation of a calibration curve in LC-MS/MS applications. As an example for an 5 points calibrator curve; add 1.0 ml of e.g. PEth-free blood to the original calibrator vial, vortex thoroughly, and transfer 500 μ l to a second vial containing 500 μ l of PEth-free blood, to make a 2-fold dilution, repeat the procedure 6 times. This will generate a calibrator curve with concentration of: 10.0, 4.0, 1.0, 0.4, 0.1, and 0.05 μ M.

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 ^{13}C -NMR in polar organic solvents. *Anal. Bio. Chem.* In press, DOI 10.1007/s00216-014-7826-4.