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## PEth-d5 16:0/18:1 Internal Standard

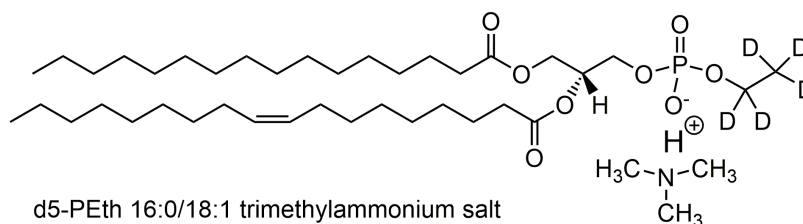
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**Background:** Phosphatidylethanol (PEth) is a group of homologous unnatural phospholipids formed by phospholipase D catalyzed ethanolysis in-vivo of mainly endogenous phosphatidylcholine. The half-life of PEth is about five days, which makes PEth 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-d5-ethoxyhydroxyphosphinyl-sn-glyceroltrimethyl ammonium salt (PEth-d5 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 <sup>1</sup>H-qNMR.

**Molecular Weight:** Most Abundant Isotope of Parent: <sup>12</sup>C<sub>39</sub><sup>1</sup>H<sub>70</sub><sup>2</sup>H<sub>5</sub><sup>16</sup>O<sub>8</sub><sup>31</sup>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 (e.g Eppendorf centrifuge, 4000 RCF, 3 min).

**Application example:** Transfer quantitatively entire content of the vial to a secondary container, to ensure complete transfer of the content, wash the container and transfer to the secondary container, at least three times with transfer-solution (isopropanol or acetonitrile). Example of manual extraction procedure for whole blood: add 400  $\mu$ l of isopropanol, containing 0.4  $\mu$ M of d5-PEth internal standard, to a 2 mL micro tube containing 100  $\mu$ l of patient blood. Put the tubes directly on a 64 position mixer and shake for 10 minutes. After centrifugation at 10.000 g for 5 minutes transfer the supernatants to a 1 mL 96 well plate and seal with a pre-slit silicon mat, put the 96 well plate in the autosampler and analyze by LC-MS(MS).

**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:**

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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  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR in polar organic solvents. *Anal. Bio. Chem.* In press, DOI 10.1007/s00216-014-7826-4.