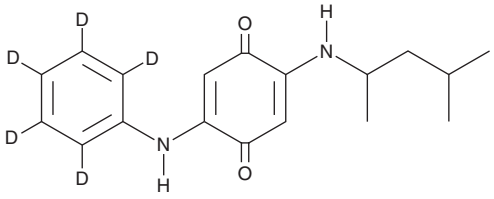
PRODUCT INFORMATION

6-PPD-Q-d_5

Item No. 40784

CAS Registry No.: 2750119-14-1
Formal Name: 2-[(1,3-dimethylbutyl)amino]-5-(phenyl-2,3,4,5,6-d_5-amino)-2,5-cyclohexadiene-1,4-dione
Synonym: 6-PPD-quinone-d_5
MF: $C_{18}H_{17}D_5N_2O_2$
FW: 303.4
Chemical Purity: ≥95% (6-PPD-Q)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_5); ≤1% d_0
Supplied as: A solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

6-PPD-Q-d_5 is intended for use as an internal standard for the quantification of 6-PPD-Q (Item No. 38247) 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).

6-PPD-Q-d_5 is supplied as a solid. A stock solution may be made by dissolving the 6-PPD-Q-d_5 in the solvent of choice, which should be purged with an inert gas. 6-PPD-Q-d_5 is slightly soluble in chloroform and methanol (warmed).

Description

6-PPD-Q is an oxidized derivative of the tire antiozonant and substituted *p*-phenylenediamine 6-PPD (Item No. 38246).[1] It is toxic to rainbow trout (*O. mykiss*) and brook trout (*S. fontinalis*; LC_{50}s = 0.59 and 1.96 µg/L, respectively) but not to artic char (*S. alpinus*) and white sturgeon (*A. transmontanus*; LC_{50}s = >12.7 µg/L for both). 6-PPD-Q (10 µg/L) induces cell death and germline DNA damage, as well as decreases the number of mitotic cells, in *C. elegans* gonads.[2] Urine levels of 6-PPD-Q are increased in pregnant women compared to non-pregnant adults and children.[3]

References

1. Brinkmann, M., Montgomery, D., Selinger, S., *et al.* Acute toxicity of the tire rubber-derived chemical 6PPD-quinone to four fishes of commercial, cultural, and ecological importance. *Environ. Sci. Tech. Lett.* **9(4)**, 333-338 (2022).
2. Hua, X., Feng, X., Liang, G., *et al.* Long-term exposure to 6-PPD quinone reduces reproductive capacity by enhancing germline apoptosis associated with activation of both DNA damage and cell corpse engulfment in *Caenorhabditis elegans*. *J. Hazard. Mater.* **454**, 131495 (2023).
3. Du, B., Liang, B., Li, Y., *et al.* First report on the occurrence of *N*-(1,3-dimethylbutyl)-*N′*-phenyl-*p*-phenylenediamine (6PPD) and 6PPD-quinone as pervasive pollutants in human urine from south China. *Environ. Sci. Tech. Lett.* **9(12)**, 1056-1062 (2022).

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