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SZABO-SCANDIC HandelsgmbH

Quellenstraße 110, A-1100 Wien

T. +43(0)1 489 3961-0

F. +43(0)1 489 3961-7

mail@szabo-scandic.com

www.szabo-scandic.com

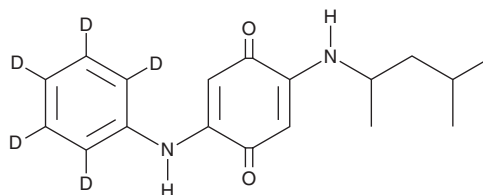
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PRODUCT INFORMATION



6-PPD-Q-d₅ Item No. 40784

CAS Registry No.: 2750119-14-1
Formal Name: 2-[(1,3-dimethylbutyl)amino]-5-(phenyl-2,3,4,5,6-d₅-amino)-2,5-cyclohexadiene-1,4-dione
Synonym: 6-PPD-quinone-d₅
MF: C₁₈H₁₇D₅N₂O₂
FW: 303.4
Chemical Purity: ≥90% (6-PPD-Q)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₅); ≤1% d₀
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-d₅ 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-d₅ is supplied as a solid. A stock solution may be made by dissolving the 6-PPD-Q-d₅ in the solvent of choice, which should be purged with an inert gas. 6-PPD-Q-d₅ 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*; LC₅₀s = 0.59 and 1.96 µg/L, respectively) but not to arctic char (*S. alpinus*) and white sturgeon (*A. transmontanus*; LC₅₀s = >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).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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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