PRODUCT INFORMATION



(±)-Ibuprofen-d₃

Item No. 18255

CAS Registry No.: 121662-14-4

Formal Name: α -(methyl-d₃)-4-(2-methylpropyl)-

benzeneacetic acid

Synonym: DL-Ibuprofen-d₂ MF: $C_{13}H_{15}D_3O_2$ 209.3 FW:

≥98% Ibuprofen **Chemical Purity:**

Deuterium

Incorporation: ≥99% deuterated forms (d₁-d₃); ≤1% d₀

 λ_{max} : 212, 219, 263 nm UV/Vis.: A crystalline solid Supplied as:

-20°C Storage: Stability: ≥4 years

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

Laboratory Procedures

 (\pm) -Ibuprofen- d_3 contains three deuterium atoms located on the methyl group. It is intended for use as an internal standard for the quantification of ibuprofen (Item No. 70280) by GC- or LC-mass spectrometry (MS). For long term storage, we suggest that (\pm)-ibuprofen-d₃ be stored as supplied at -20°C. It should be stable for at least two years.

(±)-Ibuprofen-d3 is supplied as a crystalline solid. A stock solution may be made by dissolving the (\pm) -ibuprofen- d_3 in the solvent of choice, which should be purged with an inert gas. (\pm) -Ibuprofen- d_3 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of (±)-ibuprofen-d3 in these solvents is approximately 60, 50, and 45 mg/ml, respectively.

(±)-Ibuprofen-d₂ is used as an internal standard for the quantification of ibuprofen by stable isotope dilution 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).

Description

(±)-Ibuprofen is a non-steroidal anti-inflammatory drug (NSAID) and non-selective COX inhibitor (IC₅₀s = 2.6 and 1.3 μM for human recombinant COX-1 and COX-2, respectively). In vivo, (±)-ibuprofen inhibits late-phase formalin-induced paw licking in mice (ED₅₀ = 6.1 mg/kg).² It also inhibits acetic acid-induced writhing in mice (ED₅₀ = 0.47 mg/kg). Formulations containing (±)-ibuprofen have been used in the treatment of fever and mild to severe pain.

References

- 1. Johnson, J.L., Wimsatt, J., Buckel, S.D., et al. Purification and characterization of prostaglandin H synthase-2 from sheep placental cotyledons. Arch. Biochem. Biophys. 324, 26-34 (1995).
- 2. Seguin, L., Le Marouille-Girardon, S., and Millan, M.J. Antinociceptive profiles of non-peptidergic neurokinin, and neurokinin, receptor antagonists: A comparison to other classes of antinociceptive agent. Pain 61(2), 325-343 (1995).

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

SAFEI Y DAIA
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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