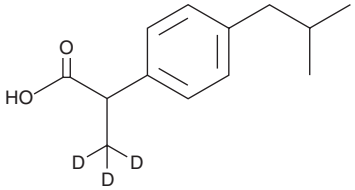
PRODUCT INFORMATION

(±)-Ibuprofen-d_3

Item No. 18255

CAS Registry No.:	121662-14-4
Formal Name:	α-(methyl-d_3)-4-(2-methylpropyl)-benzeneacetic acid
Synonym:	DL-Ibuprofen-d_3
MF:	$C_{13}H_{15}D_3O_2$
FW:	209.3
Chemical Purity:	≥98% Ibuprofen
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_3); ≤1% d_0
UV/Vis.:	λ_{max}: 212, 219, 263 nm
Supplied as:	A crystalline 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

(±)-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 (±)-ibuprofen-d_3 be stored as supplied at -20°C. It should be stable for at least two years.

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

(±)-Ibuprofen-d_3 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 (IC_{50}s = 2.6 and 1.3 µM for human recombinant COX-1 and COX-2, respectively).[1] *In vivo*, (±)-ibuprofen inhibits late-phase formalin-induced paw licking in mice (ED_{50} = 6.1 mg/kg).[2] It also inhibits acetic acid-induced writhing in mice (ED_{50} = 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$_1$ and neurokinin$_2$ receptor antagonists: A comparison to other classes of antinociceptive agent. *Pain* **61(2)**, 325-343 (1995).

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