(S)-(+)-Ibuprofen

Cat. No.: HY-78131A

CAS No.: 51146-56-6

Molecular Formula: $C_{13}H_{18}O_2$

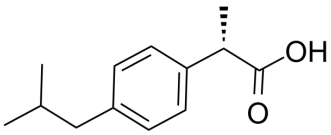
Molecular Weight: 206.28

Target: COX

Pathway: Immunology/Inflammation

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (484.78 mM; Need ultrasonic)

Ethanol : 100 mg/mL (484.78 mM; Need ultrasonic)

H_2O : 1 mg/mL (4.85 mM; Need ultrasonic and warming)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	4.8478 mL	24.2389 mL	48.4778 mL
5 mM	0.9696 mL	4.8478 mL	9.6956 mL
10 mM	0.4848 mL	2.4239 mL	4.8478 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 6.67 mg/mL (32.33 mM); Clear solution; Need ultrasonic and warming and heat to 60°C
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (12.12 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (12.12 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (12.12 mM); Clear solution
5. Add each solvent one by one: 10% EtOH >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (12.12 mM); Clear solution
6. Add each solvent one by one: 10% EtOH >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (12.12 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	(S)-(+)-Ibuprofen ((S)-Ibuprofen), a S(+)-enantiomer of Ibuprofen, is a potent COX-1 and COX-2 inhibitor with IC_{50}s of 2.1 μM and 1.6 μM, respectively. (S)-(+)-Ibuprofen has analgesic, anti-inflammatory, anticancer and antipyretic effects[1][2].

IC_{50} & Target	COX-1	COX-2
	2.1 μM (IC_{50})	1.6 μM (IC_{50})

In Vitro

(S)-(+)-Ibuprofen (HCT-15 and HCA-7 cells; 0-1000 μM; 8 days) treatment reduces concentration dependently cell survival in both cell lines to a similar extent[2].
(S)-(+)-Ibuprofen (HCT-15 and HCA-7 cells; 0-1000 μM; 20-72 hours) treatment causes a G0/G1 phase block as well as apoptosis[2].
(S)-(+)-Ibuprofen (HCT-15 and HCA-7 cells; 900 μM; 4-72 hours) treatment shows a down regulation of cyclin A and B and an increase of the cell cycle inhibitory protein p27Kip-1[2].
(S)-(+)-Ibuprofen inhibits COX activity, thromboxane formation, and platelet aggregation[1].
(S)-(+)-Ibuprofen inhibits the activation of NF-κB in response to T-cell stimulation with an IC_{50} of 61.7 μM[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[2]

Cell Line:	HCT-15 and HCA-7 cells
Concentration:	0 μM, 200 μM, 400 μM, 600 μM, 700 μM, 800 μM, 900 μM, and 1000 μM
Incubation Time:	8 days
Result:	Reduced concentration dependently cell survival in both cell lines to a similar extent.

Cell Cycle Analysis[2]

Cell Line:	HCT-15 and HCA-7 cells
Concentration:	0 μM, 200 μM, 400 μM, 600 μM, 800 μM, 900 μM, and 1000 μM
Incubation Time:	24 hours (HCT-15) or 20 hours (HCA-7)
Result:	Caused a G0/G1 phase block.

Apoptosis Analysis[2]

Cell Line:	HCT-15 and HCA-7 cells
Concentration:	0 μM, 200 μM, 400 μM, 600 μM, 800 μM, 900 μM, and 1000 μM
Incubation Time:	72 hours
Result:	Induced cell apoptosis.

Western Blot Analysis[2]

Cell Line:	HCT-15 and HCA-7 cells
Concentration:	900 μM
Incubation Time:	4 hours, 8 hours, 16 hours, 24 hours, 32 hours, 48 hours and 72 hours
Result:	Decreased levels of Cyclin D1 protein.

In Vivo

(S)-(+)-Ibuprofen (15 mg/kg/day; intraperitoneal injection; five days a week; for 4 weeks) treatment inhibits tumor growth of HCA-7 and HCT-15 xenografts in the nude mice model[2].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	NMRI (nu/nu) male mice (6-8 week old) injected with HCA-7 and HCT-15 cells[2]
Dosage:	15 mg/kg/day
Administration:	Intraperitoneal injection; five days a week; for 4 weeks
Result:	Inhibited tumor growth of HCA-7 and HCT-15 xenografts in mice.

REFERENCES

[1]. Evans AM, et al. Comparative pharmacology of S(+)-ibuprofen and (RS)-ibuprofen. Clin Rheumatol. 2001 Nov;20 Suppl 1:S9-14.

[2]. N Scheuren, et al. Modulation of transcription factor NF-kappaB by enantiomers of the nonsteroidal drug ibuprofen. Br J Pharmacol. 1998 Feb;123(4):645-52.

[3]. Astrid Janssen, et al. Evidence of COX-2 independent induction of apoptosis and cell cycle block in human colon carcinoma cells after S- or R-ibuprofen treatment. Eur J Pharmacol. 2006 Jul 1;540(1-3):24-33.

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