ADL-5859 hydrochloride

Cat. No.: HY-13044

CAS No.: 850173-95-4

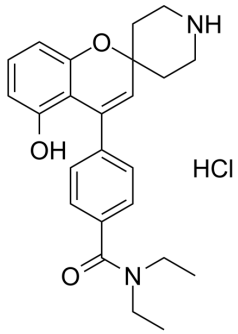
Molecular Formula: $C_{24}H_{29}ClN_2O_3$

Molecular Weight: 428.95

Target: Opioid Receptor; Potassium Channel; Cytochrome P450

Pathway: GPCR/G Protein; Neuronal Signaling; Membrane Transporter/Ion Channel; Metabolic Enzyme/Protease

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (233.13 mM)

H_2O : 5 mg/mL (11.66 mM; ultrasonic and warming and heat to 60°C)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.3313 mL	11.6564 mL	23.3127 mL
5 mM	0.4663 mL	2.3313 mL	4.6625 mL
10 mM	0.2331 mL	1.1656 mL	2.3313 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.75 mg/mL (6.41 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.75 mg/mL (6.41 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

ADL-5859 hydrochloride (compound 20) is a selective and orally active δ opioid receptor (DOR) agonist with an K_i and an EC_{50} value of 0.84 and 20 nM, respectively. ADL-5859 hydrochloride also shows inhibitory activity to hERG channel with an IC_{50} value of 78 μM. ADL-5859 hydrochloride can be used for the research of pain[1][2].

IC_{50} & Target

δ Opioid Receptor/DOR

In Vitro

ADL-5859 (0-10 μM) hydrochloride shows activities to δ opioid receptor with an K_i and an EC_{50} value of 0.84 and 20 nM, and inhibits 32% and 37% activities to μ and κ opioid receptor, respectively[1].

ADL-5859 (0-100 μM) hydrochloride exhibits inhibitory activity to hERG channel with an IC_{50} value of 78 μM[1].

ADL-5859 (0-100 μM) hydrochloride inhibits activity of the drug metabolizing enzyme cytochrome P450 2D6 (CYP2D6) in vitro with an IC_{50} value of 43 μM[2].

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

In Vivo

ADL-5859 (0.3-10 mg/kg; p.o. once) hydrochloride reverses hyperalgesia in inflamed paw of rats and shows robust antidepressant-like activity[1].

Pharmacokinetic Properties of ADL-5859 in Rats and Dogs[1].

	Rats IV 0.25 mg/kg and PO 3 mg/kg	Dogs IV 1 mg/kg and PO 3 mg/kg
CLs (L/h/kg)	1.8±0.5	0.4±0.1
Vdss (L/kg)	10.7±1.9	2.5±0.5
$t_{1/2}$ (oral, h)	5.3±0.7	4.7±0.2
F (%)	33.4±3.2	66.5±6.8

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

Animal Model:	Rats with Freund's Complete Adjuvant (FCA) injection induced mechanical hyperalgesia[1]
Dosage:	0.3-10 mg/kg
Administration:	Oral gavage; 0.3-10 mg/kg once
Result:	Produced 100% reversal of hyperalgesia in the inflamed paw with a dose of 3 mg/kg and showed an oral ED_{50} value of 1.4 mg/kg.

Animal Model:	Male Sprague-Dawley rats[1]
Dosage:	0.3 and 3 mg/kg
Administration:	Oral gavage; 0.3 and 3 mg/kg once
Result:	Produced robust antidepressant-like activity in the rat forced swim assay with a dose of 3 mg/kg.

CUSTOMER VALIDATION

- Eur J Pharmacol. 2016 Jun 15;781:53-9.

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REFERENCES

[1]. Le Bourdonnec B, et al. Potent, orally bioavailable delta opioid receptor agonists for the treatment of pain: discovery of N,N-diethyl-4-(5-hydroxyspiro[chromene-2,4'-piperidine]-4-yl)benzamide (ADL5859). J Med Chem. 2008 Oct 9;51(19):5893-6.

[2]. Le Bourdonnec B, et al. Spirocyclic delta opioid receptor agonists for the treatment of pain: discovery of N,N-diethyl-3-hydroxy-4-(spiro[chromene-2,4'-piperidine]-4-yl) benzamide (ADL5747).J Med Chem. 2009 Sep 24;52(18):5685-702.

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