ADL-5859 hydrochloride

Cat. No.:	HY-13044	
CAS No.:	850173-95-4	
Molecular Formula:	C ₂₄ H ₂₉ CIN ₂ O 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	o [⊥] Ņ∕
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	H ₂ O : 5 mg/mL (11.66	DMSO : ≥ 100 mg/mL (233.13 mM) H ₂ O : 5 mg/mL (11.66 mM; ultrasonic and warming and heat to 60°C) * "≥" means soluble, but saturation unknown.					
		Solvent Mass Concentration	1 mg	5 mg	10 mg		
	Preparing Stock Solutions	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	 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 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				
BIOLOGICALIACIA				
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 μ M. 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 μ M) 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 μ M) hydrochloride exhibits inhibitory activity to hERG channel with an IC ₅₀ value of 78 μ M ^[1] .			



ADL-5859 (0-100 µM) hydrochloride inhibits activity of the drug metabolizing enzyme cytochrome P450 2DG (CYP2DG) in vitro with an IC ₂₀ 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. onco) hydrochloride reverses hyperalgesia in inflamed paw of rats and shows robust antidepressant-like activity ¹¹ . Pharmacokinetic Properties of ADL-5859 in Rats and Dogr ^[11] . In Vivo Rats Dogs In Vivo Rats Dogs In Vizo S mg/kg and PO 3 mg/kg 0.440.1 In Vizo S (L/k/kg) 10.7±1.9 2.540.5 In Vizo (L/k/kg) 0.3.34±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 ¹¹¹ Dosage: 0.3.10 mg/kg 0.3.10 mg/kg once Initial Model: Mate spraye; 0.3.10 mg/kg once Animal Model: Male Sprayue-Dawley rats ^[11] Dosage: Initial Model: Male Sprayue-Dawley rats ^[11] Dosage: 0.3 and 3 mg/kg Initial Model: Male Sprayue-Dawley rats ^[11] Initial Model: Animal Model: Male Sprayue-Dawley rats ^[11] Initial Model: Initial Model: Initititial model: <						
antidepressant-like activity ^[1] . Pharmacokinetic Properties of ADL-S859 in Rats and Dogs ^[1] . Image: The second secon		with an IC ₅₀ value of 43 μ M ^[2] .				
IV 0.25 mg/kg and PO 3 mg/kgIV 1 mg/kg and PO 3 mg/kgCLs (L/h/kg)1.8±0.50.4±0.1Vdss (L/kg)10.7±1.92.5±0.5t_1/2 (oral, h)5.3±0.74.7±0.2F (%)33.4±3.266.5±6.8MCE has not independently comfirmed the accuracy of these methods. They are for reference only.Nimal Model:Animal Model:Rats with Freund's Complete Adjuvant (FCA) injection induced mechanical hyperalgesia ¹¹ Dosage:0.3-10 mg/kgAdministration:Oral gavage; 0.3-10 mg/kg onceResult:Produced 100% reversal of hyperalgesia in the inflamed paw with a dose of 3 mg/kg and showed an oral ED50 value of 1.4 mg/kg.Animal Model:Male Sprague-Dawley rats ^[1] Dosage:0.3 and 3 mg/kgAdministration:Oral gavage; 0.3 and 3 mg/kg onceResult:Oral gavage; 0.3 and 3 mg/kg onceRuinistration:Oral gavage; 0.3 and 3 mg/kg onceRuinistration: <th rowspan="7">In Vivo</th> <th colspan="5">antidepressant-like activity^[1].</th>	In Vivo	antidepressant-like activity ^[1] .				
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		Administration:	Oral gavage;	Oral gavage; 0.3 and 3 mg/kg once		
		Result:				

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• 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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