Bufuralol

Cat. No.: HY-105124

CAS No.: 54340-62-4

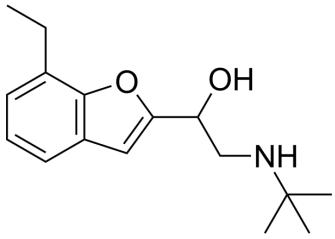
Molecular Formula: $C_{16}H_{23}NO_2$

Molecular Weight: 261.36

Target: Adrenergic Receptor

Pathway: GPCR/G Protein; Neuronal Signaling

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (382.61 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.8261 mL	19.1307 mL	38.2614 mL
	5 mM	0.7652 mL	3.8261 mL	7.6523 mL
	10 mM	0.3826 mL	1.9131 mL	3.8261 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: ≥ 3.5 mg/mL (13.39 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 3.5 mg/mL (13.39 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3.5 mg/mL (13.39 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Bufuralol (Ro 3-4787) is a potent non-selective, orally active β-adrenoreceptor antagonist with partial agonist activity. Bufuralol hydrochloride is a CYP2D6 probe substrate[1][2][3][4].

IC_{50} & Target

β-adrenoceptor

In Vitro

Bufuralol (Ro 3-4787) is widely used in the characterization of CYP2D6 activity, and possesses aromatic rings and a basic nitrogen that are characteristic of CYP2D6 substrates[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo	Bufuralol (Ro 3-4787) metabolism mediated by NADPH exhibits biphasic kinetics and is less efficient than that observed in the presence of cumene hydroperoxide (CuOOH) in and monkey intestines, in agreement with the observations in the livers [4]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- J Pharmaceut Biomed. 2020, 113870.

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REFERENCES

[1]. T H Pringle, et al. Pharmacodynamic and pharmacokinetic studies on bufuralol in man. Br J Clin Pharmacol. 1986 Nov;22(5):527-34.

[2]. Jie Cai, et al. Effects of 22 Novel CYP2D6 Variants Found in the Chinese Population on the Bufuralol and Dextromethorphan Metabolisms In Vitro. Basic Clin Pharmacol Toxicol. 2016 Mar;118(3):190-9.

[3]. Sarah M Glass, et al. CYP2D6 Allelic Variants *34, *17-2, *17-3, and *53 and a Thr309Ala Mutant Display Altered Kinetics and NADPH Coupling in Metabolism of Bufuralol and Dextromethorphan and Altered Susceptibility to Inactivation by SCH 66712. Drug Metab Dispos. 2018 Aug;46(8):1106-1117.

[4]. T Prueksaritanont, et al. (+)-bufuralol 1'-hydroxylation activity in human and rhesus monkey intestine and liver. Biochem Pharmacol. 1995 Oct 26;50(9):1521-5.

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