3-Hydroxy agomelatine

Cat. No.: HY-133111

CAS No.: 166526-99-4

Molecular Formula: $C_{15}H_{17}NO_3$

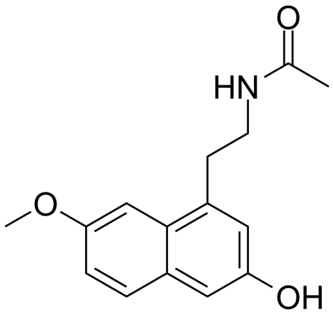
Molecular Weight: 259.3

Target: 5-HT Receptor

Pathway: GPCR/G Protein; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (964.13 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.8565 mL	19.2827 mL	38.5654 mL
5 mM	0.7713 mL	3.8565 mL	7.7131 mL
10 mM	0.3857 mL	1.9283 mL	3.8565 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: ≥ 2.08 mg/mL (8.02 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (8.02 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

3-Hydroxy agomelatine is a metabolite of Agomelatine. 3-Hydroxy agomelatine is a 5-HT_{2C} receptor antagonist with an IC_{50} of 3.2 μM and a K_i of 1.8 μM[1].

IC_{50} & Target

5-HT_{2C} Receptor 3.2 μM (IC_{50})	5-HT_{2C} Receptor 1.8 μM (Ki)

In Vitro

Agomelatine and S 21517 have moderately high affinities for 5-HT_{2C} receptors (K_i = 0.21 μM and 0.13 μM, respectively). The metabolite 3-Hydroxy agomelatine (S 21540) has a 10-fold lower affinity (K_i = 1.8 μM). Agomelatine, S 21517 and 3-Hydroxy agomelatine (10^{-7}-10^{-4} M) are antagonists at 5-HT_{2C} receptors, with a rank order of efficacy as follows: S 21517>Agomelatine>3-Hydroxy agomelatine[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Increasing doses (from 1.25 to 40 mg/kg, intraperitoneal injection) of 3-Hydroxy agomelatine (S 21540) does not affect the penile erections induced by mCPP and Ro 60-0175 in Wistar rat[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Chagraoui A, et al. Agomelatine(S 20098) antagonizes the penile erections induced by the stimulation of 5-HT2C receptors in Wistar rats. Psychopharmacology (Berl). 2003 Oct;170(1):17-22.

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