Agomelatine hydrochloride

Cat. No.: HY-17038A

CAS No.: 1176316-99-6

Molecular Formula: $C_{15}H_{18}ClNO_2$

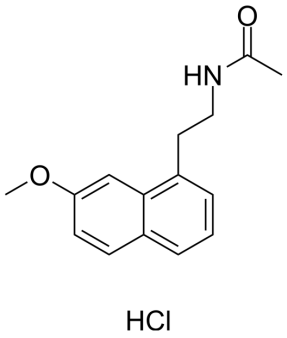
Molecular Weight: 279.76

Target: 5-HT Receptor; Melatonin Receptor; Endogenous Metabolite

Pathway: GPCR/G Protein; Neuronal Signaling; 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 (357.45 mM)

H_2O : < 0.1 mg/mL (insoluble)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.5745 mL	17.8725 mL	35.7449 mL
5 mM	0.7149 mL	3.5745 mL	7.1490 mL
10 mM	0.3574 mL	1.7872 mL	3.5745 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: ≥ 2.5 mg/mL (8.94 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (8.94 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (8.94 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Agomelatine hydrochloride (S-20098 hydrochloride) is a specific agonist of MT1 and MT2 receptors with K_is of 0.1, 0.06, 0.12, and 0.27 nM for CHO-hMT1, HEK-hMT1, CHO-hMT2, and HEK-hMT2, respectively[1]. Agomelatine hydrochloride is a selective 5-HT2C receptor antagonist with pK_is of 6.4 and 6.2 at native (porcine) and cloned, human 5-HT2C receptors, respectively[2].

IC_{50} & Target				
	5-HT_{2C} Receptor 6.4 (pKi, native porcine)	5-HT_{2C} Receptor 6.2 (pKi, human)	hMT1 0.1 (Ki, CHO Cells)	hMT1 0.06 (Ki, HEK Cells)

	hMT2 0.12 (Ki, CHO Cells)	hMT2 0.27 (Ki, HEK Cells)

In Vitro

Agomelatine (S 20098) acts as a full agonist of MT1 and MT2 receptors with EC_{50}s of 1.6±0.4, 0.10±0.04 nM for CHO hMT1 CHO-hMT2 (hMT1 and hMT2 receptors expressed in CHO or HEK cell membranes)[1].
Agomelatine (S20098) also interacts with h5-HT2B receptors (6.6), whereas it shows low affinity at native (rat)/cloned, human 5-HT2A (<5.0/5.3) and 5-HT1A (<5.0/5.2) receptors, and negligible (<5.0) affinity for other 5-HT receptors[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

Agomelatine (25, 50, or 75 mg/kg; i.p.) has antioxidant activity in Strychnine (75 mg/kg, i.p.) or Pilocarpine (400 mg/kg, i.p.) induced seizure models in mice. Agomelatine dose not have any antioxidant effects on parameters of oxidative stress produced by Pentylenetetrazole (PTZ) or Picrotoxin (PTX) induced seizure models when compared to controls[3].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female Swiss mice (20-30 g) were administered PTZ (85 mg/kg, i.p.), PTX (7 mg/kg, i.p.), strychnine (75 mg/kg, i.p.), Pilocarpine (400 mg/kg, i.p.), respectively[3]
Dosage:	25, 50, or 75 mg/kg
Administration:	Administered intraperitoneally (i.p.)
Result:	All dosages showed a significant decrease in thiobarbituric acid reactive substances (TBARS) levels and nitrite content in all brain areas when compared to controls in the Pilocarpine induced seizure model. All dosages decreased TBARS levels in all brain areas, and at low doses (25 or 50 mg/kg) decreased nitrite contents, but only at 25 or 50 mg/kg showed a significant increase in catalase activity in three brain areas when compared to controls in the Strychnine-induced seizure model. Did not have any antioxidant effects on parameters of oxidative stress produced by PTX- or PTZ-induced seizure models when compared to controls.

CUSTOMER VALIDATION

- Protein Cell. 2019 Mar;10(3):178-195.
- Cell Commun Signal. 2023 May 25;21(1):123.
- Pest Manag Sci. 2021 Jul;77(7):3561-3570.

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REFERENCES

[1]. Audinot V, et al. New selective ligands of human cloned melatonin MT1 and MT2 receptors. Naunyn Schmiedebergs Arch Pharmacol. 2003 Jun;367(6):553-61.

[2]. Millan MJ, et al. The novel melatonin agonist agomelatine (S20098) is an antagonist at 5-hydroxytryptamine2C receptors, blockade of which enhances the activity of frontocortical dopaminergic and adrenergic pathways. J Pharmacol Exp Ther. 2003 Sep;306(3):954-64.

[3]. Aguiar CC, et al. Effects of agomelatine on oxidative stress in the brain of mice after chemically induced seizures. Cell Mol Neurobiol. 2013 Aug;33(6):825-35.

Caution: Product has not been fully validated for medical applications. For research use only.

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