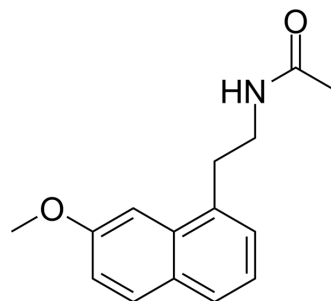


## Agomelatine

<b>Cat. No.:</b>	HY-17038		
<b>CAS No.:</b>	138112-76-2		
<b>Molecular Formula:</b>	C <sub>15</sub> H <sub>17</sub> NO <sub>2</sub>		
<b>Molecular Weight:</b>	243.3		
<b>Target:</b>	5-HT Receptor; Melatonin Receptor; Endogenous Metabolite		
<b>Pathway:</b>	GPCR/G Protein; Neuronal Signaling; Metabolic Enzyme/Protease		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : ≥ 100 mg/mL (411.02 mM)  
 \* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	4.1102 mL	20.5508 mL	41.1015 mL
	5 mM	0.8220 mL	4.1102 mL	8.2203 mL
	10 mM	0.4110 mL	2.0551 mL	4.1102 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: ≥ 2.5 mg/mL (10.28 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
 Solubility: ≥ 2.5 mg/mL (10.28 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
 Solubility: ≥ 2.5 mg/mL (10.28 mM); Clear solution

### BIOLOGICAL ACTIVITY

#### Description

Agomelatine (S-20098) is a specific agonist of MT1 and MT2 receptors with K<sub>i</sub>s of 0.1, 0.06, 0.12, and 0.27 nM for CHO-hMT1, HEK-hMT1, CHO-hMT2, and HEK-hMT2, respectively<sup>[1]</sup>. Agomelatine is a selective 5-HT<sub>2C</sub> receptor antagonist with pK<sub>i</sub>s of 6.4 and 6.2 at native (porcine) and cloned, human 5-HT<sub>2C</sub> receptors, respectively<sup>[2]</sup>.

#### IC<sub>50</sub> & Target

5-HT <sub>2C</sub> Receptor 6.4 (pKi, native porcine)	5-HT <sub>2C</sub> Receptor 6.2 (pKi, human)	hMT1 0.1 nM (K <sub>i</sub> , CHO Cells)	hMT1 0.06 nM (K <sub>i</sub> , HEK Cells)
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	hMT2 0.12 nM (Ki, CHO Cells)	hMT2 0.27 nM (Ki, HEK Cells)								
<b>In Vitro</b>	<p>Agomelatine (S 20098) acts as a full agonist of MT1 and MT2 receptors with EC<sub>50</sub>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)<sup>[1]</sup>.</p> <p>Agomelatine (S20098) also interacts with h5-HT2B receptors (6.6), whereas Agomelatine shows low affinity at native (rat)/cloned, human 5-HT2A (&lt;5.0/5.3) and 5-HT1A (&lt;5.0/5.2) receptors, and negligible (&lt;5.0) affinity for other 5-HT receptors [2].</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>									
<b>In Vivo</b>	<p>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 Pentylentetrazole (PTZ) or Picrotoxin (PTX) induced seizure models when compared to controls<sup>[3]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> <table border="1"> <tr> <td>Animal Model:</td> <td>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<sup>[3]</sup>.</td> </tr> <tr> <td>Dosage:</td> <td>25, 50, or 75 mg/kg</td> </tr> <tr> <td>Administration:</td> <td>Administered intraperitoneally (i.p.)</td> </tr> <tr> <td>Result:</td> <td> <p>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.</p> <p>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.</p> <p>Did not have any antioxidant effects on parameters of oxidative stress produced by PTX- or PTZ-induced seizure models when compared to controls.</p> </td> </tr> </table>		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 <sup>[3]</sup> .	Dosage:	25, 50, or 75 mg/kg	Administration:	Administered intraperitoneally (i.p.)	Result:	<p>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.</p> <p>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.</p> <p>Did not have any antioxidant effects on parameters of oxidative stress produced by PTX- or PTZ-induced seizure models when compared to controls.</p>
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## 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-hydroxytryptamine<sub>2C</sub> 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.

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

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