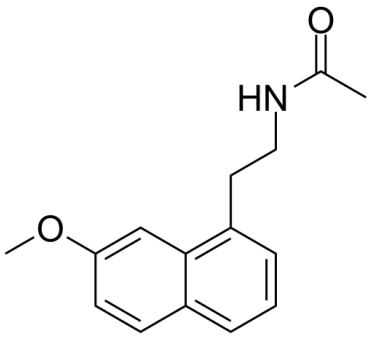
Data Sheet

Product Name:	Agomelatine
Cat. No.:	CS-0740
CAS No.:	138112-76-2
Molecular Formula:	$C_{15}H_{17}NO_2$
Molecular Weight:	243.30
Target:	5-HT Receptor; Melatonin Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : ≥ 100 mg/mL (411.02 mM)



BIOLOGICAL ACTIVITY:

Agomelatine (S-20098) is a specific agonist of **MT1** and **MT2** receptors with **K_i**s of 0.1, 0.06, 0.12, and 0.27 nM for CHO-hMT1, HEK-hMT1, CHO-hMT2, and HEK-hMT2, respectively[1]. Agomelatine is a selective **5-HT2C receptor** antagonist with **pK_i**s of 6.4 and 6.2 at native (porcine) and cloned, human 5-HT2C receptors, respectively[2]. IC50 & Target: Ki: 0.1 nM (CHO-hMT1), 0.06 nM (HEK-hMT1), 0.12 nM (CHO-hMT2), and 0.27 nM (HEK-hMT2)[1]

pKi: 6.4 (native porcine 5-HT2C receptor), 6.2 (human 5-HT2C receptor)[2] **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 Agomelatine 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]. **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].

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.

CAIndexNames:

Acetamide, N-[2-(7-methoxy-1-naphthalenyl)ethyl]-

SMILES:

CC(NCCC1=C2C=C(OC)C=CC2=CC=C1)=O

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

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