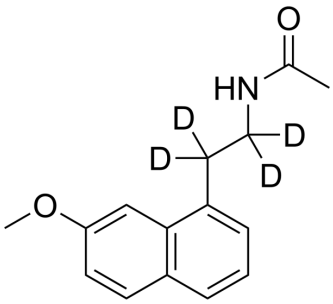
Agomelatine-d_4

Cat. No.:	HY-17038S1
CAS No.:	1079389-44-8
Molecular Formula:	$C_{15}H_{13}D_4NO_2$
Molecular Weight:	247.33
Target:	Melatonin Receptor; 5-HT Receptor; Endogenous Metabolite; Isotope-Labeled Compounds
Pathway:	GPCR/G Protein; Neuronal Signaling; Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Agomelatine-d_4 is the deuterium labeled Agomelatine. Agomelatine (S-20098) is a specific agonist of MT1 and MT2 receptors with Kis 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 pKis of 6.4 and 6.2 at native (porcine) and cloned, human 5-HT2C receptors, respectively[2].	
IC_{50} & Target	MT2	MT1
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[2]. 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.

[3]. 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.

[4]. 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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