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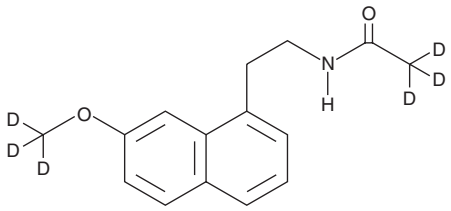
PRODUCT INFORMATION

Agomelatine-d_6

Item No. 26447

CAS Registry No.: 1079389-42-6
Formal Name: N-[2-[7-(methoxy-d_3)-1-naphthalenyl] ethyl]-acetamide-2,2,2-d_3
MF: $C_{15}H_{11}D_6NO_2$
FW: 249.3
Chemical Purity: 98% (Agomelatine)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_6); ≤1% d_0
Supplied as: A solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Agomelatine-d_6 is intended for use as an internal standard for the quantification of agomelatine (Item No. 13203) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated *versus* unlabeled).

Agomelatine-d_6 is supplied as a solid. A stock solution may be made by dissolving the agomelatine-d_6 in the solvent of choice, which should be purged with an inert gas. Agomelatine-d_6 is soluble in the organic solvent methanol.

Description

Agomelatine is an agonist of melatonin (MT) receptors and a derivative of melatonin (Item No. 14427).[1] It binds to MT_1 and MT_2 receptors (K_is = 0.14 and 0.41 nM, respectively) and has an EC_{50} value of 0.1 nM in a [^{35}S]GTPγS binding assay using CHO cells expressing MT_2 receptors. Agomelatine is also an antagonist of the serotonin (5-HT) receptor subtypes 5-HT_{2B} and 5-HT_{2C} (K_is = 0.26 and 0.71 nM, respectively, for the human receptors).[2] Agomelatine (40 mg/kg) inhibits the penile erection response induced by the 5-HT_2 agonist Ro 60-0175 (Item No. 29520) in rats. It also increases extracellular levels of noradrenaline and dopamine in the frontal cortex of freely moving rats when administered at doses ranging from 20 to 80 mg/kg. Agomelatine (10 mg/kg) reduces immobility time in the forced swim test and increases the amount of time spent in the open arms of the elevated plus maze, indicating antidepressant-like and anxiolytic-like activity, in a transgenic neuroendocrine model of depression.[3] It also increases the rate of readjustment to circadian activity cycles following an induced phase shift.

References

1. Poissonnier-Durieux, S., Ettaoussi, M., Pérès, B., *et al.* Synthesis of 3-phenylnaphthalenic derivatives as new selective MT_2 melatoninergic ligands. *Bioorg. Med. Chem.* **16(18)**, 8339-8348 (2008).
2. Millan, M.J., Gobert, A., Lejeune, F., *et al.* The novel melatonin agonist agomelatine (S20098) is an antagonist at 5-hydroxytryptamine$_{2C}$ receptors, blockade of which enhances the activity of frontocortical dopaminergic and adrenergic pathways. *J. Pharmacol. Exp. Ther.* **306(3)**, 954-964 (2003).
3. Barden, N., Shink, E., Labbé, M., *et al.* Antidepressant action of agomelatine (S 20098) in a transgenic mouse model. *Prog. Neuropsychopharmacol. Biol. Psychiatry* **29(6)**, 908-916 (2005).

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