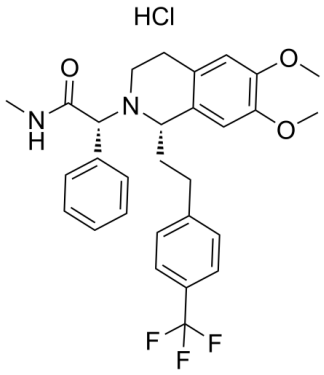
Data Sheet

Product Name:	Almorexant (hydrochloride)
Cat. No.:	CS-2485
CAS No.:	913358-93-7
Molecular Formula:	$C_{29}H_{32}ClF_3N_2O_3$
Molecular Weight:	549.02
Target:	Apoptosis; Calcium Channel; Caspase; Orexin Receptor (OX Receptor)
Pathway:	Apoptosis; GPCR/G Protein; Membrane Transporter/Ion Channel; Neuronal Signaling
Solubility:	DMSO : ≥ 46 mg/mL;H_2O : < 0.1 mg/mL (ultrasonic;warming;heat to 60°C)



BIOLOGICAL ACTIVITY:

Almorexant (ACT 078573) hydrochloride is an orally active, potent and competitive dual **orexin receptor** antagonist, with **K_d** values of 1.3 nM (**OX1**) and 0.17 nM (**OX2**), respectively. Almorexant hydrochloride reversibly blocks signaling of orexin-A and orexin-B peptides. Almorexant hydrochloride totally blocked the intracellular **Ca^{2+}** signal pathway. Almorexant hydrochloride stimulates **caspase-3** activity in AsPC-1 cells and induces **apoptosis**[1][2][3][4]. IC50 & Target: Kd: 0.17 nM (hOX2), 1.3 nM (hOX1)[2] ***In Vitro:*** Almorexant hydrochloride (1 μM) promote tyrosine phosphorylation of SHP2/OX1R complex[1].

Almorexant hydrochloride (1 μM) inhibits the cellular growth of AsPC-1 cells[1]. ***In Vivo:*** Almorexant hydrochloride (1.8 μmol/kg, 100 μL; IP, daily) reduces the volume of tumors[2].

Almorexant hydrochloride (300 mg/kg, PO, once) can help rats to be fully capable of spatial and avoidance learning[4].

Almorexant hydrochloride (30-300 mg/kg) dose-dependently increases rapid eye movement (REM) and non-REM (NREM) sleep and decreases wakefulness apparently without inducing either cataplexy18 or deficits in next-day performance[3].

PROTOCOL (Extracted from published papers and Only for reference)

Please refer to Almorexant (HY-10805).

References:

[1]. Dayot S, et al. In vitro, in vivo and ex vivo demonstration of the antitumoral role of hypocretin-1/orexin-A and almorexant in pancreatic ductal adenocarcinoma. Oncotarget. 2018 Jan 9;9(6):6952-6967.

[2]. Malherbe P, et al. Biochemical and electrophysiological characterization of almorexant, a dual orexin 1 receptor (OX1)/orexin 2 receptor (OX2) antagonist: comparison with selective OX1 and OX2 antagonists. Mol Pharmacol. 2009 Sep;76(3):618-31.

[3]. Black SW, et al. Almorexant promotes sleep and exacerbates cataplexy in a murine model of narcolepsy. Sleep. 2013 Mar 1;36(3):325-36.

[4]. Dietrich H, et al. Intact learning and memory in rats following treatment with the dual orexin receptor antagonist almorexant. Psychopharmacology (Berl). 2010 Oct;212(2):145-54.

CAIndexNames:

2(1H)-Isoquinolineacetamide, 3,4-dihydro-6,7-dimethoxy-N-methyl-α-phenyl-1-[2-[4-(trifluoromethyl)phenyl]ethyl]-, hydrochloride (1:1), (αR,1S)-

SMILES:

CNC([C@@H](C1=CC=CC=C1)N2CCC3=CC(OC)=C(OC)C=C3[C@@H]2CCC4=CC=C(C(F)(F)F)C=C4)=O.Cl

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

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