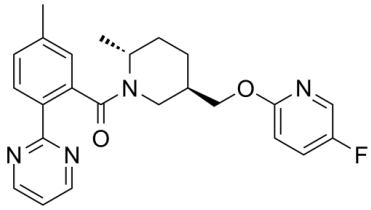
Data Sheet

Product Name:	Filorexant
Cat. No.:	CS-4437
CAS No.:	1088991-73-4
Molecular Formula:	C24H25FN4O2
Molecular Weight:	420.48
Target:	Orexin Receptor (OX Receptor)
Pathway:	GPCR/G Protein; Neuronal Signaling
Solubility:	DMSO : 12.61 mg/mL (29.99 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

Filorexant (MK-6096) is an orally bioavailable potent and selective reversible antagonist of OX1 and OX2 receptor(<3 nM in binding). IC50 & Target: Ki: < 3 nM(Orexin receptor)[1]. **In Vitro:** In radioligand binding and functional cell based assays Filorexant (MK-6096) demonstrated potent binding and antagonism of both human OX(1)R and OX(2)R (<3 nM in binding, 11 nM in FLIPR), with no significant off-target activities against a panel of >170 receptors and enzymes. Filorexant (MK-6096) occupies 90% of human OX(2)Rs expressed in transgenic rats at a plasma concentration of 142 nM. **In Vivo:** Filorexant (MK-6096) dose-dependently reduced locomotor activity and significantly increased sleep in rats (3-30 mg/kg) and dogs (0.25 and 0.5 mg/kg).

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: [1]Animal administration[1]

The male Sprague Dawley rats (n = 8/study; age: 3-6 months; weight: 450-600 g) were singly housed with water and food ad libitum and a 12 h light: 12 h dark cycle with lights on at 04:00 and off at 16:00. Sleep studies were conducted to evaluate Filorexant (3 and 10 mg/kg, p.o.), DORA-22 (10 mg/kg, p.o.) and almorexant (3 and 30 mg/kg, p.o.), employing a counterbalanced crossover design in which all animals were alternatively treated with drug and vehicle daily for either 3 or 7 consecutive days (for DORA-22 and Filorexant, respectively): 2 baseline days (no dosing), a 2 day vehicle-only run-in, a 3 or 7-day arm of drug or vehicle followed by 3 or 7 days of conditional crossover. Effects of compound treatments relative to vehicle (20% Vitamin E TPGS, p.o.) were evaluated following administration in the active phase).

References:

[1]. Winrow CJ, et al. Pharmacological characterization of MK-6096 - a dual orexin receptor antagonist for insomnia. Neuropharmacology. 2012 Feb;62(2):978-87.

[2]. Coleman PJ, et al. Discovery of [(2R,5R)-5-<[(5-fluoropyridin-2-yl)oxy]methyl>-2-methylpiperidin-1-yl][5-methyl-2-(pyrimidin-2-yl)phenyl]methanone (MK-6096): a dual orexin receptor antagonist with potent sleep-promoting properties. ChemMedChem. 2012 Mar 5;7(3):415-24, 337.

CAIndexNames:

Methanone, [(2R,5R)-5-[[(5-fluoro-2-pyridinyl)oxy]methyl]-2-methyl-1-piperidinyl][5-methyl-2-(2-pyrimidinyl)phenyl]-

SMILES:

CC1=CC(C(N2C[C@H](COC3=CC=C(F)C=N3)CC[C@H]2C)=O)=C(C4=NC=CC=N4)C=C1

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

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