Pavinetant

Cat. No.: HY-14432

CAS No.: 941690-55-7

Molecular Formula: $C_{26}H_{25}N_3O_3S$

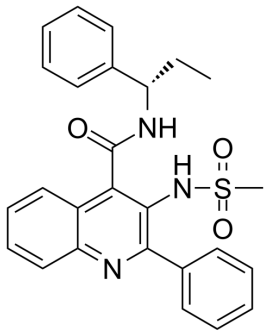
Molecular Weight: 459.56

Target: Neurokinin Receptor

Pathway: GPCR/G Protein; Neuronal Signaling

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (108.80 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.1760 mL	10.8800 mL	21.7599 mL
5 mM	0.4352 mL	2.1760 mL	4.3520 mL
10 mM	0.2176 mL	1.0880 mL	2.1760 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 3 mg/mL (6.53 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3 mg/mL (6.53 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Pavinetant (MLE-4901) is a neurokinin-3 receptor (NK3R) antagonist.

IC_{50} & Target

NK3R[1]

In Vitro

Pavinetant (AZD2624) is a potent and selective NK3 receptor antagonist which is developed for the treatment of schizophrenia. Pavinetant exhibits an inhibitory effect on microsomal CYP3A4/5 activities with apparent IC_{50} values of 7.1 and 19.8 μM for midazolam and testosterone assays, respectively. No time-dependent inactivation of CYP3A4/5 activity by Pavinetant is observed. Pavinetant demonstrates weak to no inhibition of CYP1A2, CYP2B6, CYP2C8, CYP2C9, CYP2C19, and CYP2D6[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Kinase Assay [1]

The potential of Pavinetant (AZD2624) to cause time-dependent inhibition of CYP3A activities is evaluated by pre-incubating 10 μM of Pavinetant at 37°C for 0, 3, 10, 20, and 30 min in 0.1 M pH 7.4 phosphate buffer incubation mixture (0.2 mL) containing 2 mg/mL HLM and 1 mM NADPH. Verapamil, tested at 10 μM, is also incubated separately as a positivecontrol. An aliquot of 20 μL is removed from pre-incubation tube at each time point and added to a secondary 5-min incubation(180 μL) containing 15 μM of midazolam and 1 mM of NADPH. The formation of 1′-hydroxymidazolam is used as the marker activity for CYP3A enzymes and analyzed using LC-MS. CYP3A enzyme activities after pre-incubation with Pavinetant arecompared to activities following incubation with vehicle solvent (1% methanol) and without pre-incubation[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Li Y, et al. In vitro assessment of metabolic drug–drug interaction potential of AZD2624, neurokinin-3 receptor antagonist, through cytochrome P(450) enzyme identification, inhibition, and induction studies. Xenobiotica. 2010 Nov;40(11):721-9.

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

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