VU0463271 quarterhydrate

Cat. No.: HY-110110A

Molecular Formula: $C_{19}H_{18}N_4OS_2 \cdot 1/4H_2O$

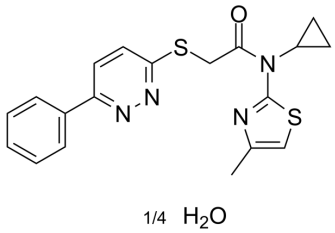
Molecular Weight: 387

Target: Potassium Channel

Pathway: Membrane Transporter/Ion Channel

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 19 mg/mL (49.10 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5840 mL	12.9199 mL	25.8398 mL
	5 mM	0.5168 mL	2.5840 mL	5.1680 mL
	10 mM	0.2584 mL	1.2920 mL	2.5840 mL

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

BIOLOGICAL ACTIVITY

Description

VU0463271 quarterhydrate is a potent KCC2 antagonist, with an IC_{50} of 61 nM[1].

IC_{50} & Target

IC50: 61 nM (KCC2)[1].

In Vitro

VU0463271 is a potent antagonist of the neuronal-specific potassium-chloride cotransporter 2 (KCC2), with an IC_{50} of 61 nM and >100-fold selectivity versus the closely related Na-K-2Cl cotransporter 1 (NKCC1) and no activity in a larger panel of GPCRs, ion channels and transporters. It is also found rapidly cleared in vitro[1].

VU0463271 is applied to the transected CNS preparation and resulted in a significant increase in firing rates of the Drosophila CNS with 1 μM VU0463271 resulting in a peak firing rate that was a 2.7- and 2.5-fold increase over baseline firing rate for OR and rdl strains, respectively[2].

VU0463271 (10-100 nM) results in approximately 20% reduction of CNS firing frequency within asmall percentage of preparations[2].

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

In Vivo

VU0463271 is found to be a moderate-to-high clearance compound in rat (CL=57 mL/min/kg) following intravenous administration (1 mg/kg); the low volume of distribution at steady state (Vss 0.4 L/kg), coupled with moderate-to-high

	clearance produce a relatively short t1/2 (9 min) in vivo[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Delpire E, et al. Further optimization of the K-Cl cotransporter KCC2 antagonist ML077: development of a highly selective and more potent in vitro probe. Bioorg Med Chem Lett. 2012 Jul 15;22(14):4532-5.

[2]. Rui Chen, et al. Functional Coupling of K +-Cl - Cotransporter (KCC) to GABA-Gated Cl - Channels in the Central Nervous System of Drosophila melanogaster Leads to Altered Drug Sensitivities. ACS Chem Neurosci. 2019 Jun 19;10(6):2765-2776.

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