

Product Data Sheet

Product Name: VU0463271 quarterhydrate

Cat. No.: GC61379

Chemical Properties

Cas. No.

SMILES O=C(N(C1CC1)C2=NC(C)=CS2)CSC3=NN=C(C4=CC=CC=C4)C=C3.[1/4].O

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

M.Wt 387

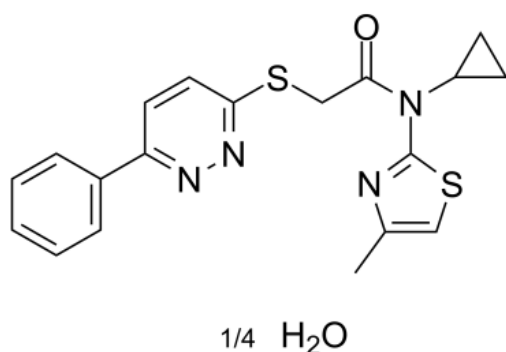
Solubility

Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure



Background

VU0463271 quarterhydrate is a potent KCC2 antagonist, with an IC₅₀ of 61 nM[1].

VU0463271 is a potent antagonist of the neuronal-specific potassium-chloride cotransporter 2 (KCC2), with an IC₅₀ of 61 nM and >100-fold selectivity versus the closely related Na-K-2Cl

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

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com

Address: 10292 Central Ave. #205, Montclair, CA, USA

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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 μ M 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 a small percentage of preparations[2].

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 t_{1/2} (9 min) in vivo[1].

[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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