Quetiapine hemifumarate

Cat. No.: HY-B0031

CAS No.: 111974-72-2

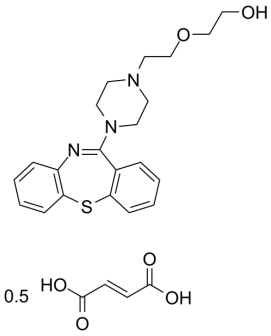
Molecular Formula: $C_{23}H_{27}N_3O_4S$

Molecular Weight: 441.54

Target: 5-HT Receptor; Dopamine Receptor

Pathway: GPCR/G Protein; Neuronal Signaling

Storage: 4°C, sealed storage, away from moisture
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 50 mg/mL (113.24 mM; Need ultrasonic)
H_2O : 1.25 mg/mL (2.83 mM; Need ultrasonic)

Preparing Stock Solutions

Concentration \ Solvent \ Mass	1 mg	5 mg	10 mg
1 mM	2.2648 mL	11.3240 mL	22.6480 mL
5 mM	0.4530 mL	2.2648 mL	4.5296 mL
10 mM	0.2265 mL	1.1324 mL	2.2648 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: ≥ 2.5 mg/mL (5.66 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.66 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Quetiapine hemifumarate is a 5-HT receptors agonist with a pEC_{50} of 4.77 for human 5-HT1A receptor. Quetiapine hemifumarate is a dopamine receptor antagonist with a pIC_{50} of 6.33 for human D2 receptor. Quetiapine hemifumarate has moderate to high affinity for the human D2, HT1A, 5-HT2A, 5-HT2C receptor with pK_is of 7.25, 5.74, 7.54, 5.55. Antidepressant and anxiolytic effects[1].

IC_{50} & Target				
	5-HT_{1A} Receptor 5.74 (pKi)	5-HT_{2A} Receptor 7.54 (pKi)	5-HT_{2C} Receptor 5.55 (pKi)	D2 Receptor 7.25 (pKi)

	5-HT_{1A} Receptor 4.77 (pEC50)	D2 Receptor 6.33 (pIC_{50})

In Vitro

Quetiapine (<100 μM; 24 hours) has no significant effect on cell viabilities[2].
Quetiapine (10 μM) inhibits NO release, which increased by LPS (0.1-100 ng/mL) in concentration-dependent manner[2].
Quetiapine (10 μM) also inhibits TNF-α synthesis[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay[2]

Cell Line:	N9 microglial cells
Concentration:	0, 0.1, 1, 10, 50, and 100 μM
Incubation Time:	24 hours
Result:	Had no significant effect on cell viabilities at various concentrations under 100 μM, in which significant toxicity could be observed.

RT-PCR[2]

Cell Line:	N9 microglial cells
Concentration:	10 μM
Incubation Time:	24 hours
Result:	Dramatically inhibited TNF-α synthesis.

In Vivo

Quetiapine (10 mg/kg/day; ingested) can alleviate the recruitment and activation of microglia and promote myelin repair in Cuprizone (CPZ)-induced chronic mouse model of demyelination[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	C57BL/6 mice[2]
Dosage:	10 mg/kg/day
Administration:	Ingested
Result:	Significantly increased in optical density of myelin basic protein (MBP) staining compared to Veh group.

CUSTOMER VALIDATION

- Chemosphere. 2019 Jun;225:378-387.

See more customer validations on www.MedChemExpress.com

REFERENCES

[1]. Cross AJ, et al. Quetiapine and its metabolite norquetiapine: translation from in vitro pharmacology to in vivo efficacy in rodent models. Br J Pharmacol. 2016 Jan;173(1):155-66.

[2]. Hanzhi Wang, et al. Quetiapine Inhibits Microglial Activation by Neutralizing Abnormal STIM1-Mediated Intercellular Calcium Homeostasis and Promotes Myelin Repair in a Cuprizone-Induced Mouse Model of Demyelination. Front Cell Neurosci. 2015 Dec 21;9:492.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA