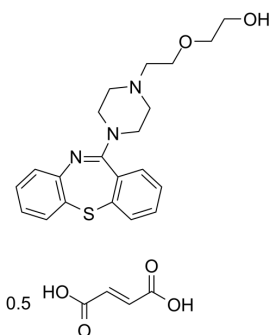


## Quetiapine hemifumarate

<b>Cat. No.:</b>	HY-B0031
<b>CAS No.:</b>	111974-72-2
<b>Molecular Formula:</b>	C <sub>23</sub> H <sub>27</sub> N <sub>3</sub> O <sub>4</sub> S
<b>Molecular Weight:</b>	441.54
<b>Target:</b>	5-HT Receptor; Dopamine Receptor
<b>Pathway:</b>	GPCR/G Protein; Neuronal Signaling
<b>Storage:</b>	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



### SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 50 mg/mL (113.24 mM; Need ultrasonic)					
	H <sub>2</sub> O : 1.25 mg/mL (2.83 mM; Need ultrasonic)					
	<b>Preparing Stock Solutions</b>	<b>Solvent</b>	<b>Mass</b>	<b>1 mg</b>	<b>5 mg</b>	<b>10 mg</b>
		<b>Concentration</b>				
		<b>1 mM</b>		2.2648 mL	11.3240 mL	22.6480 mL
<b>5 mM</b>			0.4530 mL	2.2648 mL	4.5296 mL	
	<b>10 mM</b>		0.2265 mL	1.1324 mL	2.2648 mL	
Please refer to the solubility information to select the appropriate solvent.						
<b>In Vivo</b>	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

<b>Description</b>	Quetiapine hemifumarate is a 5-HT receptors agonist with a pEC <sub>50</sub> of 4.77 for human 5-HT <sub>1A</sub> receptor. Quetiapine hemifumarate is a dopamine receptor antagonist with a pIC <sub>50</sub> of 6.33 for human D <sub>2</sub> receptor. Quetiapine hemifumarate has moderate to high affinity for the human D <sub>2</sub> , HT <sub>1A</sub> , 5-HT <sub>2A</sub> , 5-HT <sub>2C</sub> receptor with pK <sub>i</sub> s of 7.25, 5.74, 7.54, 5.55. Antidepressant and anxiolytic effects <sup>[1]</sup> .			
<b>IC<sub>50</sub> &amp; Target</b>	5-HT <sub>1A</sub> Receptor 5.74 (pKi)	5-HT <sub>2A</sub> Receptor 7.54 (pKi)	5-HT <sub>2C</sub> Receptor 5.55 (pKi)	D <sub>2</sub> Receptor 7.25 (pKi)

	5-HT <sub>1A</sub> Receptor 4.77 (pEC <sub>50</sub> )	D2 Receptor 6.33 (pIC <sub>50</sub> )
<b>In Vitro</b>	<p>Quetiapine (&lt;100 μM; 24 hours) has no significant effect on cell viabilities<sup>[2]</sup>.            Quetiapine (10 μM) inhibits NO release, which increased by LPS (0.1-100 ng/mL) in concentration-dependent manner<sup>[2]</sup>.            Quetiapine (10 μM) also inhibits TNF-α synthesis<sup>[2]</sup>.            MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>	
	Cell Viability Assay <sup>[2]</sup>	
	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 <sup>[2]</sup>	
	Cell Line:	N9 microglial cells
	Concentration:	10 μM
	Incubation Time:	24 hours
Result:	Dramatically inhibited TNF-α synthesis.	
<b>In Vivo</b>	<p>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<sup>[1]</sup>.            MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>	
	Animal Model:	C57BL/6 mice <sup>[2]</sup>
	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.

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## 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.

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[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.

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

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