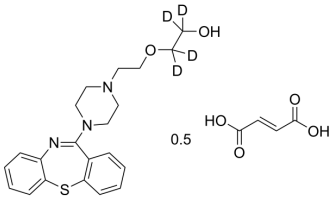
Quetiapine-d_4-1 fumarate

Cat. No.:	HY-B0031S5
CAS No.:	2820085-77-4
Molecular Formula:	$C_{21}H_{21}D_4N_3O_2S.1/2C_4H_4O_4$
Molecular Weight:	445.57
Target:	Dopamine Receptor; 5-HT Receptor; Isotope-Labeled Compounds
Pathway:	GPCR/G Protein; Neuronal Signaling; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Quetiapine-d_4-1 fumarate is deuterated labeled Quetiapine (hemifumarate) (HY-B0031). 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].
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1]. Quetiapine (<100?μM; 24?hours) has no significant effect on cell viabilities[3]. Quetiapine (10?μM) inhibits NO release, which increased by LPS (0.1-100 ng/mL) in concentration-dependent manner[3]. Quetiapine (10?μM) also inhibits TNF-α synthesis[3]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
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[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

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.

[3]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.

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

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