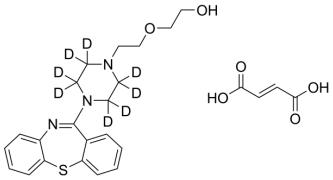
Quetiapine hemifumarate-d8

Cat. No.:	HY-B0031S4
CAS No.:	1435938-24-1
Molecular Formula:	$C_{25}H_{21}D_8N_3O_6S$
Molecular Weight:	507.63
Target:	Dopamine Receptor; 5-HT Receptor
Pathway:	GPCR/G Protein; Neuronal Signaling
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Quetiapine (hemifumarate)-d_8 is the deuterium labeled Quetiapine hemifumarate[1]. Quetiapine hemifumarate is a 5-HT receptors agonist with a pEC50 of 4.77 for human 5-HT1A receptor. Quetiapine hemifumarate is a dopamine receptor antagonist with a pIC50 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 pKis of 7.25, 5.74, 7.54, 5.55. Antidepressant and anxiolytic effects[2].
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]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

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

[2]. 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.

[3]. 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 219:492.

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