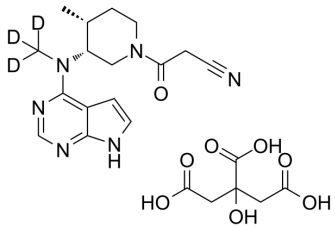
Tofacitinib-d3 citrate

Cat. No.:	HY-40354AS
CAS No.:	2701680-77-3
Molecular Formula:	$C_{22}H_{25}D_3N_6O_8$
Molecular Weight:	507.51
Target:	Fungal; Apoptosis; JAK; Bacterial; Influenza Virus
Pathway:	Anti-infection; Apoptosis; Epigenetics; JAK/STAT Signaling; Protein Tyrosine Kinase/RTK; Stem Cell/Wnt
Storage:	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



BIOLOGICAL ACTIVITY

Description	Tofacitinib-d_3 (citrate) is deuterium labeled Tofacitinib (citrate). Tofacitinib citrate is an orally available JAK1/2/3 inhibitor with IC50s of 1, 20, and 112 nM, respectively. Tofacitinib citrate has antibacterial, antifungal and antiviral activities.
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;53(2):211-216.

[2]. Jiang JK, et al. Examining the chirality, conformation and selective kinase inhibition of 3-((3R,4R)-4-methyl-3-(methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile (CP-690,550). J Med Chem. 2008 Dec 25;51(24):8012-8.

[3]. LaBranche TP, et al. JAK inhibition with tofacitinib suppresses arthritic joint structural damage through decreased RANKL production. Arthritis Rheum. 2012 Nov;64(11):3531-42.

[4]. Onda M, et al. Tofacitinib suppresses antibody responses to protein therapeutics in murine hosts. J Immunol. 2014 Jul 1;193(1):48-55.

[5]. Yagi K, et al. Pharmacological inhibition of JAK3 enhances the antitumor activity of STI571 in human chronic myeloid leukemia. Eur J Pharmacol. 2018 Apr 15;825:28-33.

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