Vimirogant hydrochloride

Cat. No.: HY-103637A

CAS No.: 1802678-42-7

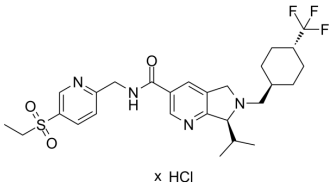
Molecular Formula: $C_{27}H_{35}F_3N_4O_3S.xHCl$

Target: ROR

Pathway: Metabolic Enzyme/Protease; Vitamin D Related/Nuclear Receptor

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 : 125 mg/mL (Need ultrasonic) Ethanol : 50 mg/mL (Need ultrasonic)
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 6.25 mg/mL (Infinity mM); Clear solution 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 6.25 mg/mL (Infinity mM); Clear solution 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 6.25 mg/mL (Infinity mM); Clear solution 4. Add each solvent one by one: 10% EtOH >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (Infinity mM); Clear solution 5. Add each solvent one by one: 10% EtOH >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (Infinity mM); Clear solution 6. Add each solvent one by one: 10% EtOH >> 90% corn oil Solubility: ≥ 2.5 mg/mL (Infinity mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Vimirogant (VTP-43742) hydrochloride is a potent, selective, and orally active RORγt inhibitor (K_i=3.5 nM; IC_{50}=17 nM). Vimirogant hydrochloride exhibits >1000-fold selectivity versus the RORα and RORβ isotypes. Vimirogant hydrochloride inhibits Th17 differentiation and IL-17A secretion from mouse splenocytes (IC_{50}=57 nM) without affecting Th1, Th2, or Treg cell differentiation. Vimirogant hydrochloride has the potential for autoimmune disorders research[1][2].	
IC_{50} & Target	RORγt 3.5 nM (Ki)	RORγt 17 nM (IC_{50})
In Vitro	Vimirogant hydrochloride inhibits the secretion of IL-17A from activated hPBMCs (IC_{50}=18 nM) and human whole blood (IC_{50} =192 nM)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.	

In Vivo	In the MOG35-55/CFA immunized mouse EAE model, Vimirogant hydrochloride (p.o.) significantly suppresses clinical symptoms, demyelination and mRNA expression of multiple inflammatory markers in the spinal cord[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Gege C. RORγt inhibitors as potential back-ups for the phase II candidate VTP-43742 from Vitae Pharmaceuticals: patent evaluation of WO2016061160 and US20160122345. Expert Opin Ther Pat. 2017;27(1):1-8.

[2]. Gerard McGeehan, et al. VTP-43742 is a potent and selective RORγt blocker that demonstrates oral efficacy in a mouse model of autoimmunity through suppression of IL-17A production (THER7P.945). J Immunol May 1, 2015, 194 (1 Supplement) 208.5-208.5.

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