Dagrocorat hydrochloride

Cat. No.: HY-16718A

CAS No.: 1044535-61-6

Molecular Formula: $C_{29}H_{30}ClF_3N_2O_2$

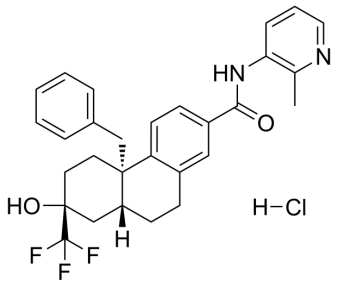
Molecular Weight: 531.01

Target: Glucocorticoid Receptor; Cytochrome P450

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

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (188.32 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.8832 mL	9.4160 mL	18.8320 mL
5 mM	0.3766 mL	1.8832 mL	3.7664 mL
10 mM	0.1883 mL	0.9416 mL	1.8832 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 7.5 mg/mL (14.12 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 7.5 mg/mL (14.12 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 7.5 mg/mL (14.12 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Dagrocorat (PF-00251802) hydrochloride is an orally active and selective high-affinity partial agonist of the glucocorticoid receptor. Dagrocorat hydrochloride is also a time-dependent reversible inhibitor of CYP3A (IC_{50}=1.3 μM in human liver microsomes) and CYP2D6 (K_i=0.57 μM in human liver microsomes). Dagrocorat hydrochloride can be used for the research of rheumatoid arthritis[1].

IC_{50} & Target	CYP3A	CYP2D6

In Vitro	Dagrocorat hydrochloride is metabolized by cytochrome P450 (CYP)3A to an N-oxide metabolite. Dagrocorat hydrochloride is a reversible inhibitor of several CYPs, such as CYP3A and CYP2D6[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Ripp SL, et al. In Vitro and In Vivo Investigation of Potential for Complex CYP3A Interaction for PF-00251802 (Dagrocorat), a Novel Dissociated Agonist of the Glucocorticoid Receptor. Clin Pharmacol Drug Dev. 2018;7(3):244-255.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA