Dagrocorat

Cat. No.: HY-16718

CAS No.: 1044535-52-5

Molecular Formula: $C_{29}H_{29}F_3N_2O_2$

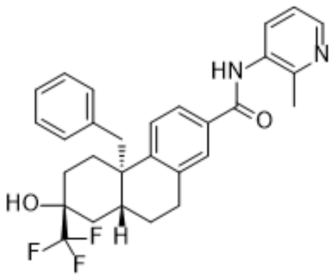
Molecular Weight: 494.55

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 : 250 mg/mL (505.51 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.0220 mL	10.1102 mL	20.2204 mL
	5 mM	0.4044 mL	2.0220 mL	4.0441 mL
	10 mM	0.2022 mL	1.0110 mL	2.0220 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: ≥ 6.25 mg/mL (12.64 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 6.25 mg/mL (12.64 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Dagrocorat (PF-00251802) is an orally active and selective high-affinity partial agonist of the glucocorticoid receptor. Dagrocorat 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 can be used for the research of rheumatoid arthritis[1].

IC_{50} & Target	CYP3A	CYP2D6

In Vitro

Dagrocorat is metabolized by cytochrome P450 (CYP)3A to an N-oxide metabolite. Dagrocorat 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 Mar;7(3):244-255.

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