Abemaciclib metabolite M18-d8

Cat. No.: HY-126534S

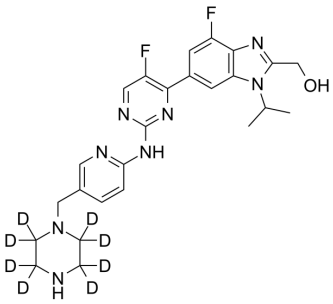
Molecular Formula: $C_{25}H_{20}D_8F_2N_8O$

Molecular Weight: 502.59

Target: Ligands for Target Protein for PROTAC; CDK

Pathway: PROTAC; Cell Cycle/DNA Damage

Storage: -20°C, sealed storage, away from moisture and light
* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 32 mg/mL (63.67 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9897 mL	9.9485 mL	19.8969 mL
	5 mM	0.3979 mL	1.9897 mL	3.9794 mL
	10 mM	0.1990 mL	0.9948 mL	1.9897 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: ≥ 1.78 mg/mL (3.54 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 1.78 mg/mL (3.54 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Abemaciclib metabolite M18-d_8 is the deuterium labeled Abemaciclib metabolite M18. Abemaciclib metabolite M18 (LSN3106729), the metabolite of Abemaciclib (HY-16297A), is a CDK inhibitor with antitumor activity. Abemaciclib metabolite M18 and a CRBN ligand have been used to design PROTAC CDK4/6 degrader[1][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;53(2):211-216.

[2]. Nathanael Gray, et al. Degradation of cyclin-dependent kinase 4/6 (cdk4/6) by conjugation of cdk4/6 inhibitors with e3 ligase ligand and methods of use. WO2017185031A1.

[3]. Edward S. Kim, et al. Abemaciclib in Combination with Single-Agent Options in Patients with Stage IV Non–Small Cell Lung Cancer: A Phase Ib Study.

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