Dihydrodiol-Ibrutinib

Cat. No.: HY-100659 CAS No.: 1654820-87-7 Molecular Formula: $C_{25}H_{26}N_{6}O_{4}$ Molecular Weight: 474.51

Btk Target:

Pathway: Protein Tyrosine Kinase/RTK

Storage: Powder -20°C 3 years 2 years

> -80°C In solvent 6 months

> > -20°C 1 month

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 100 mg/mL (210.74 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.1074 mL	10.5372 mL	21.0744 mL
	5 mM	0.4215 mL	2.1074 mL	4.2149 mL
	10 mM	0.2107 mL	1.0537 mL	2.1074 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: ≥ 2.5 mg/mL (5.27 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (5.27 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (5.27 mM); Clear solution

BIOLOGICAL ACTIVITY

Description Dihydrodiol-Ibrutinib (PCI-45227) is a dihydrodiol active metabolite of Ibrutinib (HY-10997), has inhibitory activity towards BTK approximately 15 times lower than that of ibrutinib^[1].

IC50: BTK[1] IC₅₀ & Target

REFERENCES

1]. Sridhar Veeraraghavan, et al. Simultaneous quantification of lenalidomide, ibrutinib and its active metabolite PCI-45227 in rat plasma by LC-MS/MS: application to a sharmacokinetic study. J Pharm Biomed Anal						
Caution: Product has not been fully validated for medical applications. For research use only.						
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