Ibrutinib-MPEA

Cat. No.: HY-43521

CAS No.: 1710768-30-1

Molecular Formula: $C_{32}H_{39}N_9O_2$

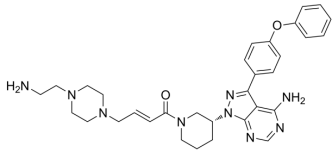
Molecular Weight: 581.71

Target: Btk

Pathway: Protein Tyrosine Kinase/RTK

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 : 33.33 mg/mL (57.30 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7191 mL	8.5953 mL	17.1907 mL
	5 mM	0.3438 mL	1.7191 mL	3.4381 mL
	10 mM	0.1719 mL	0.8595 mL	1.7191 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 5 mg/mL (8.60 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 3.33 mg/mL (5.72 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3.33 mg/mL (5.72 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Ibrutinib-MPEA (Compound 20) is ibrutinib derivative. Ibrutinib is a covalent and irreversible inhibitor of Bruton's tyrosine kinase (BTK) that has been used to treat haematological malignancies[1].

REFERENCES

[1]. Liu N, et al. Direct and two-step bioorthogonal probes for Bruton's tyrosine kinase based on ibrutinib: a comparative study. Org Biomol Chem. 2015 May 14;13(18):5147-57.

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