Enitociclib

Cat. No.: HY-103019

CAS No.: 1610358-56-9

Molecular Formula: $C_{19}H_{18}F_2N_4O_2S$

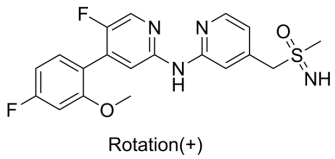
Molecular Weight: 404.43

Target: CDK

Pathway: Cell Cycle/DNA Damage

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



Rotation(+)

SOLVENT & SOLUBILITY

In Vitro

DMSO : 113.3 mg/mL (280.15 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4726 mL	12.3631 mL	24.7262 mL
	5 mM	0.4945 mL	2.4726 mL	4.9452 mL
	10 mM	0.2473 mL	1.2363 mL	2.4726 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 (6.18 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.18 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (6.18 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Enitociclib ((+)-Enitociclib) is an enanthiomer of BAY-1251152 with rotation (+). Enitociclib is a potent and selective CDK9 inhibitor with an IC_{50} of 3 nM. Enitociclib has anti-tumour activity[1][2].

IC_{50} & Target

CDK9/CycT1
3 nM (IC_{50})

In Vitro

Enitociclib (Example 2) inhibits HeLa, HeLa-MaTu-ADR, NCI-H460, DU145, Caco-2, B16F10, A2780 and MOLM-13 cells

	proliferation with IC_{50} values of 110 nM, 33 nM, 75 nM, 33 nM, 62 nM, 240 nM, 110 nM and 29 nM, respectively[1]. An efficient inhibition of the proliferation of both ABC (Activated B-cell type) and GCB (Germinal-centre B-cell type) subtypes of diffuse large B-cell lymphoma (DLBCL) by Enitociclib (Compound A')[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	Enitociclib (Compound A'; 10 mg/kg; intravenous injection; once every seven days; for 14 days; female SCID mice) reaches a Treatment to Control ratios (T/C) by area of 0.29 and a T/C by weight of 0.24. Enitociclib inhibits tumour growth and had good tolerability[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female SCID mice with OCI-LY-3 cells[2]
Dosage:	10 mg/kg
Administration:	Intravenous injection; once every seven days; for 14 days
Result:	Inhibited tumour growth and had good tolerability.

CUSTOMER VALIDATION

- Acta Pharm Sin B. 2023 May 26.

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REFERENCES

[1]. Ulrich LÜCKING, et al. 5-fluoro-n-(pyridin-2-yl)pyridin-2-amine derivatives containing a sulfoximine group. WO2014076091A1.

[2]. Use of Arne Scholz, et al. 5-fluoro-4-(4-fluoro-2-methoxyphenyl)-n-{4-[(s-methylsulfonimidoyl)methyl]pyridin-2-yl}pyridin-2-amine for treating diffuse large b-cell lymphoma. WO2019158517A1.

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