CDK2/4/6-IN-1

Cat. No.: HY-148213

CAS No.: 2803837-13-8

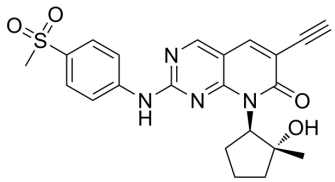
Molecular Formula: $C_{22}H_{22}N_4O_4S$

Molecular Weight: 438.5

Target: CDK

Pathway: Cell Cycle/DNA Damage

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

CDK2/4/6-IN-1(example 29) is a CDK2/4/6 inhibitor with IC_{50} values of 2.5, 23.7 and 44.3 nM for CDK2, CDK4 and CDK6, respectively. CDK2/4/6-IN-1 can be used in cancer research[1]. CDK2/4/6-IN-1 is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

CDK2	CDK4	CDK6
2.5 nM (IC_{50})	23.7 nM (IC_{50})	44.3 nM (IC_{50})

In Vitro

CDK2/4/6-IN-1(example 29) (0-600 nM, 24 h) inhibits the proliferation of OVCAR3 and MCF7 cells with the IC_{50} values of 14.6 and 117.8 nM, respectively[1].

CDK2/4/6-IN-1(example 29) (0-600 nM, 24 h) inhibits phosphorylation of Rb protein in OVCAR3 and MCF7 cells with the IC_{50} values of 18 and 581 nM, respectively[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

CDK2/4/6-IN-1(example 29) (25 mg/kg or 50 mg/kg, once a day, orally) has a significant inhibitory effect on tumor growth[1].

The pharmacokinetic parameters of example 29 in BALB/c mice (10 mg/kg, p.o.)

Parameters	C_{max}(ng/mL)	T_{max}(hr)	AUC_{last}(hr*ng/mL)	$T_{1/2}$(hr)
PO	4050	0.5	10050	4.8

The pharmacokinetic parameters of example 29 in BALB/c mice (3 mg/kg, i.v.)

Parameters	C_0(ng/mL)	$T_{1/2}$(hr)	AUC_{last}(hr*ng/mL)	V_{ss}(L/Kg)
IV	4407	0.7	3245	0.9

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. ZHANG YAN, et al. Cdk2/4/6 inhibitor, preparation method therefor, and application thereof. WO2022152259 A1.

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