Product Datasheet

Palbociclib Isethionate

Catalog No. **BP-02086** · CAS **827022-33-3** · Form **free base** · Physical state **other** · Color **Light yellow to yellow** · Version **1.0** · Revision **2026-09-14**

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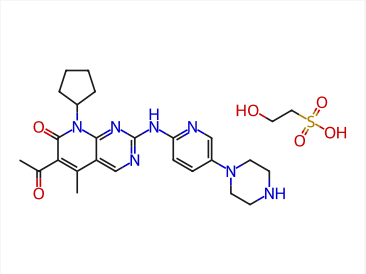
Target	Research area
CDK	**Infection; Neurological Disease; Cancer**

Molecular formula	$C_{26}H_{35}N_7O_6S$
Molecular weight	**573.6640**

STRUCTURE



DESCRIPTION

Palbociclib (PD 0332991) isethionate is an orally active selective CDK4 and CDK6 inhibitor with IC50 values of 11 and 16 nM, respectively. Palbociclib isethionate has potent anti-proliferative activity and induces cell cycle arrest in cancer cells, which can be used in the research of HR-positive and HER2-negative breast cancer and hepatocellular carcinoma.

BIOLOGICAL ACTIVITY

In Vitro

Palbociclib dihydrochloride (0-1 μM, 24 h) inhibits Rb Phosphorylation at Ser795 in MDA-MB-435 cells with an IC50 value of 0.063 μM, and obtains similar effects on both Ser780 and Ser795 phosphorylation in the Colo-205 colon carcinoma.

Palbociclib dihydrochloride (0-10 μM, 24 h) arrests MDA-MB-453 cells exclusively in G1 phase.

Palbociclib dihydrochloride (500 nM, 7 days) increases expression of homologous genes (H2d1, H2k1, and B2m) in MDA-MB-453 and MDA-MB-361 cells.

Palbociclib dihydrochloride (0-1 μM, 6 days) inhibits growth of several luminal ER-positive as well as HER2-amplified breast cancer cell lines, with IC50 values ranging from 4 nM to 1 μM.

Palbociclib dihydrochloride (0-1 μM, 3 days) inhibits the proliferation of human liver cancer cell lines with IC50 values ranging from 0.01 μM to 3.49 μM, and induces a reversible cell cycle arrest.

In Vivo

Palbociclib isethionate (oral adminstration, 75 or 150 mg/kg, daily for 14 days) produces rapid tumor regressions and delays tumor growth.

Palbociclib isethionate (oral adminstration, 90 mg/kg, daily for 12 days) reduces Treg numbers and the Treg:CD8 ratio in the spleen and lymph nodes in tumor-free mice, demonstrating the tumor-independent effects.

Palbociclib isethionate (oral administration, 100 mg/kg, daily for 1 week) has potent antitumour effects in genetically engineered mosaic mouse model of liver cancer.

SOLUBILITY

Soluble in H2O 50 mg/mL DMSO 10 mg/mL

REFERENCES

[1]. Fry DW, et al. Specific inhibition of cyclin-dependent kinase 4/6 by PD 0332991 and associated antitumor activity in human tumor xenografts. Mol Cancer Ther. 2004 Nov;3(11):1427-38.

[2]. Goel S, et al. CDK4/6 inhibition triggers anti-tumour immunity. Nature. 2017 Aug 24;548(7668):471-475.

[3]. Richard S Finn, et al. PD 0332991, a selective cyclin D kinase 4/6 inhibitor, preferentially inhibits proliferation of luminal estrogen receptor-positive human breast cancer cell lines in vitro. Breast Cancer Res. 2009;11(5):R77.

[4]. Bollard J, et al. Palbociclib (PD-0332991), a selective CDK4/6 inhibitor, restricts tumour growth in preclinical models of hepatocellular carcinoma. Gut. 2017 Jul;66(7):1286-1296.