Web: www.taiclone.com
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Erismodegib diphosphate

Catalog No: tcsc1175

Available Sizes

Size: 5mg

Size: 10mg

Size: 50mg

Size: 100mg

Size: 200mg

Size: 500mg

Specifications

CAS No:
1218778-77-8

Formula:
$C_{26}H_{32}F_3N_3O_{11}P_2$

Pathway:
Stem Cell/Wnt

Target:
Smo

Purity / Grade:
>98%

Solubility:
DMSO : ≥ 31 mg/mL (45.49 mM)

Alternative Names:
LDE225 diphosphate; NVP-LDE 225 diphosphate

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Observed Molecular Weight:
681.49

Product Description

Erismodegib diphosphate (LDE225 diphosphate) is a potent and selective **Smo** antagonist with **IC_{50}** of 1.3 nM and 2.5 nM for mouse and human Smo in binding assay, respectively.

IC50 & Target: IC50: 1.3 nM (mSmo), 2.5 nM (hSmo)[1]

In Vitro: The IC_{50} values for Erismodegib (NVP-LDE225) for the major human CYP450 drug metabolizing enzymes is greater than 10 μM[1]. Erismodegib (LDE225), a small molecule, clinically investigated SMO inhibitor, used alone and in combination with Nilotinib, inhibits the Hh pathway in $CD34^+$ chronic phase (CP)-chronic myeloid leukaemia (CML) cells, reducing the number and self-renewal capacity of CML leukaemia stem cell (LSC). Erismodegib interacts directly with SMO, in a similar fashion to cyclopamine, to reduce expression of downstream Hh signaling targets. Primary $CD34^+$ CP-CML cells are cultured in serum free media (SFM)±Erismodegib for 6, 24 and 72 hours (h). At 72 h, while there is variability between the biological samples, *GLI1* is significantly downregulated following exposure to Erismodegib (10 nM; 0.78-fold and 100 nM; 0.73-fold, respectively (p[2].

In Vivo: Erismodegib (NVP-LDE225) is a weak base with a measured pK_a of 4.2 and exhibits relatively poor aqueous solubility. In the subcutaneous $Ptch^{+/-}p53^{-/-}$ medulloblastoma allograft mouse model, Erismodegib demonstrates dose-related antitumor activity after 10 days of oral administration of a suspension of the diphosphate salt. At a dose of 5 mg/kg/day qd, Erismodegib significantly inhibits tumor growth, corresponding to a T/C value of 33% (p[1]. Bone marrow cells and spleen cells from a subset of treated mice are transplanted into secondary recipient mice. Transplantation of either bone marrow (BM) or spleen cells from mice treated with Erismodegib (LDE225)+ Nilotinib results in reduced white cell count (WCC) and reduces leukaemia development in secondary recipients compared to Erismodegib or Nilotinib alone[2].