

## Product Datasheet

# NVP-LDE225

Catalog No. **BP-02471** · CAS **956697-53-3** · Form **free base** · Physical state **solid** · Color **White to light yellow** · Version **1.0** · Revision **2026-09-10**

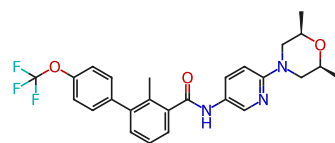
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|                      |                                |
|----------------------|--------------------------------|
| Target<br><b>Smo</b> | Research area<br><b>Cancer</b> |
|----------------------|--------------------------------|

Molecular formula **C<sub>26</sub>H<sub>26</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>**

Molecular weight **485.4981**

### STRUCTURE



## DESCRIPTION

Sonidegib (Erismodegib) is a potent and selective Smo antagonist with IC<sub>50</sub> of 1.3 nM and 2.5 nM for mouse and human Smo in binding assay, respectively .

## BIOLOGICAL ACTIVITY

### In Vitro

The IC<sub>50</sub> values for Sonidegib (NVP-LDE225) for the major human CYP450 drug metabolizing enzymes is greater than 10 μM[1]. Sonidegib (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). Sonidegib 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)±Sonidegib 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 Sonidegib (10 nM; 0.78-fold and 100 nM; 0.73-fold, respectively (p<0.01).

### In Vivo

Sonidegib (NVP-LDE225) is a weak base with a measured pKa of 4.2 and exhibits relatively poor aqueous solubility. In the subcutaneous Ptch+/-p53-/- medulloblastoma allograft mouse model, Sonidegib 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, Sonidegib significantly inhibits tumor growth, corresponding to a T/C value of 33% (p<0.05 as compared to vehicle controls). When dosed at 10 and 20 mg/kg/day qd, Sonidegib affords 51 and 83% regression, respectively[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 Sonidegib (LDE225)+Nilotinib results in reduced white cell count (WCC) and reduces leukaemia development in secondary recipients compared to Sonidegib or Nilotinib alone.

## SOLUBILITY

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Soluble in DMSO

## REFERENCES

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[1].Pan S, et al. Discovery of NVP-LDE225, a Potent and Selective Smoothened Antagonist. ACS Med Chem Lett. 2010 Mar 16;1(3):130-4.

[2]. Irvine DA, et al. Deregulated hedgehog pathway signaling is inhibited by the smoothened antagonist LDE225 (Sonidegib) in chronic phase chronic myeloid leukaemia. Sci Rep. 2016 May 9;6:25476.

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Tel: +86 20 31130026 · Fax: +86 20 36822386 · tech@biochemprobe.com · www.biochemprobe.com

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