

# Product data sheet



MedKoo Cat#: 205510 Name: Sonidegib (LDE-225) CAS#: 956697-53-3 (free base) Chemical Formula: C <sub>26</sub> H <sub>26</sub> F <sub>3</sub> N <sub>3</sub> O <sub>3</sub> Exact Mass: 485.1926 Molecular Weight: 485.50		
Product supplied as:		Powder
Purity (by HPLC):		≥ 98%
Shipping conditions		Ambient temperature
Storage conditions:		Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.

## 1. Product description:

Sonidegib (also known as erismodegib, LDE225, and NVP-LDE225) is an orally bioavailable small-molecule Smoothened (Smo) antagonist with potential antineoplastic activity. Erismodegib selectively binds to the Hedgehog (Hh)-ligand cell surface receptor Smo, which may result in the suppression of the Hh signaling pathway and, so, the inhibition of tumor cells in which this pathway is abnormally activated. It was approved by the FDA for treating basal cell carcinoma in July 2015.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	73.50	151.39
Ethanol	48.0	98.87

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.06 mL	10.30 mL	20.60 mL
5 mM	0.41 mL	2.06 mL	4.12 mL
10 mM	0.21 mL	1.03 mL	2.06 mL
50 mM	0.04 mL	0.21 mL	0.41 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

- Jalili A, Mertz KD, Romanov J, Wagner C, Kalthoff F, Stuetz A, Pathria G, Gschaider M, Stingl G, Wagner SN. NVP-LDE225, a potent and selective SMOOTHENED antagonist reduces melanoma growth in vitro and in vivo. PLoS One. 2013 Jul 30;8(7):e69064. doi: 10.1371/journal.pone.0069064. Erratum in: PLoS One. 2013;8(9). doi:10.1371/annotation/ddd22094-5d8d-43ef-ad81-b95afe392ec7. PMID: 23935925; PMCID: PMC3728309.
- Irvine DA, Zhang B, Kinstrie R, Tarafdar A, Morrison H, Campbell VL, Moka HA, Ho Y, Nixon C, Manley PW, Wheadon H, Goodlad JR, Holyoake TL, Bhatia R, Copland M. 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. doi: 10.1038/srep25476. PMID: 27157927; PMCID: PMC4860619.

### In vivo study

- Cantisani C, Musolff N, Longo C, Di Guardo A, Rovaldi E, Rossi G, Sasso F, Farnetani F, Rega F, Bánvölgyi A, Azzella G, Paolino G, Pellacani G. Dynamic optical coherence tomography evaluation in locally advanced basal cell carcinoma during sonidegib treatment. J Eur Acad Dermatol Venereol. 2024 Jan 25. doi: 10.1111/jdv.19806. Epub ahead of print. PMID: 38270330.

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- Nazzaro G, Benzecry V, Mattioli MA, Denaro N, Beltramini GA, Marzano AV, Passoni E. Sonidegib in Locally Advanced Basal Cell Carcinoma: A Monocentric Retrospective Experience and a Review of Published Real-Life Data. *Cancers (Basel)*. 2023 Jul 14;15(14):3621. doi: 10.3390/cancers15143621. PMID: 37509282; PMCID: PMC10377077.

## 7. Bioactivity

### Biological target:

Sonidegib is a Smo antagonist with IC50 of 1.3 nM (mouse) and 2.5 nM (human) in cell-free assays.

### In vitro activity

Sonidegib may have potential therapeutic use in melanoma, even without BRAF(V600E). Inhibition of SONIC HEDGEHOG (SHH)-GLI pathway by the novel small molecule inhibitor of smoothened sonidegib was followed by inhibition of cell growth and induction of apoptosis in human melanoma cell lines, interestingly with both BRAF(V600E) and BRAF(Wild Type) status. Sonidegib was potent in reducing cell proliferation in vitro, and these effects were superior to cyclopamine.

Reference: PLoS One. 2013 Jul 30;8(7):e69064. <https://pubmed.ncbi.nlm.nih.gov/23935925/>

### In vivo activity

Sonidegib has therapeutic potential in the treatment of locally advanced basal cell carcinoma. Eleven patients, including four with Basal Cell Naevus syndrome, received sonidegib. Results showed 50% achieved complete remission, 37.5% had partial response, and 12.5% had stable disease. No signs of progression were observed. All four patients suffering from Basal Cell Naevus syndrome achieved disease control by being treated with sonidegib.

Reference: *Cancers (Basel)*. 2023 Jul 14;15(14):3621. <https://pubmed.ncbi.nlm.nih.gov/37509282/>

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*