

Product Name: Sonidegib

Catalog No.: 7826

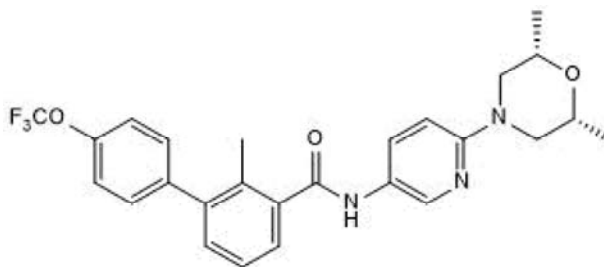
Batch No.: 1

CAS Number: 956697-53-3

IUPAC Name: *rel-N*-[6-[(2*R*,6*S*)-2,6-Dimethyl-4-morpholinyl]-3-pyridinyl]-2-methyl-4'-(trifluoromethoxy)[1,1'-biphenyl]-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₆ H ₂₆ F ₃ N ₃ O ₃
Batch Molecular Weight:	485.51
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 99.8% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

Microanalysis:	Carbon Hydrogen Nitrogen		
Theoretical	64.32	5.4	8.66
Found	64.07	5.39	8.59

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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IUPAC Name: *rel-N-[6-[(2R,6S)-2,6-Dimethyl-4-morpholinyl]-3-pyridinyl]-2-methyl-4'-(trifluoromethoxy)[1,1'-biphenyl]-3-carboxamide*

Description:

Sonidegib is a potent Smoothed (Smo) receptor antagonist (IC₅₀ values are 1.3 nM and 2.5 nM at mouse and human receptors, respectively). Inhibits growth of a variety of tumor types including basal cell carcinoma, small cell lung cancer and medulloblastoma. Sonidegib inhibits Hh pathway in CD34+ chronic myeloid leukemia cells; it reduces both the number of cells and self-renewal ability. Brain penetrant and orally bioavailable.

Physical and Chemical Properties:

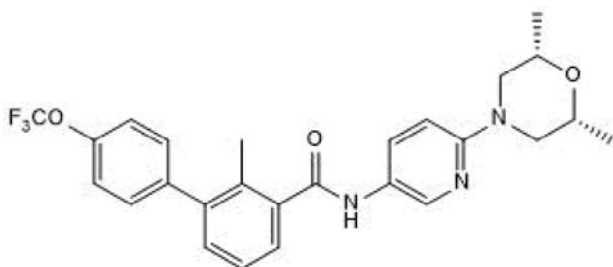
Batch Molecular Formula: C₂₆H₂₆F₃N₃O₃

Batch Molecular Weight: 485.51

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Irvine et al (2016) Deregulated hedgehog pathway signaling is inhibited by the smoothed antagonist LDE225 (Sonidegib) in chronic phase chronic myeloid leukaemia. *Sci.Rep.* **6** 25476. PMID: 27157927.

Pan et al (2010) Discovery of NVP-LDE225, a potent and selective smoothed antagonist. *ACS Med.Chem.Lett.* **1** 130. PMID: 24900187.

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