

Product data sheet



MedKoo Cat#: 203500 Name: Vismodegib CAS#: 879085-55-9 Chemical Formula: C ₁₉ H ₁₄ Cl ₂ N ₂ O ₃ S Exact Mass: 420.0102 Molecular Weight: 421.30	
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:

Vismodegib, also known as GDC-0449 or RG3616, is a hedgehog antagonist, is also a n orally bioavailable small molecule with potential antineoplastic activity. Hedgehog antagonist GDC-0449 targets the Hedgehog signaling pathway, blocking the activities of the Hedgehog-ligand cell surface receptors PTCH and/or SMO and suppressing Hedgehog signaling.

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	50.0	118.68

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.37 mL	11.87 mL	23.74 mL
5 mM	0.47 mL	2.37 mL	4.75 mL
10 mM	0.24 mL	1.19 mL	2.37 mL
50 mM	0.05 mL	0.24 mL	0.47 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

1. Ishii A, Shigemura K, Kitagawa K, Sung SY, Chen KC, Yi-Te C, Liu MC, Fujisawa M. Anti-tumor Effect of Hedgehog Signaling Inhibitor, Vismodegib, on Castration-resistant Prostate Cancer. *Anticancer Res.* 2020 Sep;40(9):5107-5114. doi: 10.21873/anticancerres.14514. PMID: 32878799.

In vivo study

1. Meerang M, Bérard K, Felley-Bosco E, Lauk O, Vrugt B, Boss A, Kenkel D, Broggin-Tenzer A, Stahel RA, Arni S, Weder W, Opitz I. Antagonizing the Hedgehog Pathway with Vismodegib Impairs Malignant Pleural Mesothelioma Growth In Vivo by Affecting Stroma. *Mol Cancer Ther.* 2016 May;15(5):1095-105. doi: 10.1158/1535-7163.MCT-15-0583. Epub 2016 Feb 2. PMID: 26839306.

2. Ishii A, Shigemura K, Kitagawa K, Sung SY, Chen KC, Yi-Te C, Liu MC, Fujisawa M. Anti-tumor Effect of Hedgehog Signaling Inhibitor, Vismodegib, on Castration-resistant Prostate Cancer. *Anticancer Res.* 2020 Sep;40(9):5107-5114. doi: 10.21873/anticancerres.14514. PMID: 32878799.

7. Bioactivity

Biological target: Vismodegib (GDC-0449) is a hedgehog pathway inhibitor with an IC₅₀ of 3 nM.

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In vitro activity

Cell proliferation, apoptosis and the expression of EMT (epithelial mesenchymal transition) related genes for three prostate cancer cell lines were evaluated; androgen-dependent LNCaP and independent C4-2B and PC-3 in the presence of vismodegib in vitro. Vismodegib significantly inhibited cell proliferation and induced cell apoptosis in all cell lines in vitro ($p < 0.05$). The results indicate that vismodegib inhibited cell proliferation via apoptosis and also suppressed EMT.

Reference: Anticancer Res. 2020 Sep;40(9):5107-5114. <https://ar.iiarjournals.org/content/40/9/5107.long>

In vivo activity

The effects of the SMO (Smoothened) antagonist, vismodegib, were investigated in the rat MPM (malignant pleural mesothelioma) model to elaborate the role of Hh (Hedgehog) signaling. Vismodegib was administered and six days later, it was observed that tumor volume measured by MRI was significantly reduced in the treated group compared with control (3-fold difference, $P = 0.03$; Fig. 3B). Consistently, significant reduction in macroscopic tumor volume ($P = 0.03$) of the treated group was detected (Fig. 3D). Tumor growth monitored by BLI (bioluminescence) seems to be reduced in the treated group compared with control (see images in Fig. 3E).

Reference: Mol Cancer Ther. 2016 May;15(5):1095-105. <https://mct.aacrjournals.org/content/15/5/1095.long>

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.