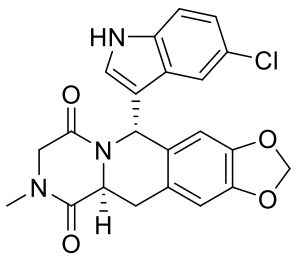
Product data sheet

MedKoo Cat#: 406643 Name: ISA-2011B CAS: 1395347-24-6 Chemical Formula: $C_{22}H_{18}ClN_3O_4$ Exact Mass: 423.0986 Molecular Weight: 423.853	
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:

ISA-2011B is a PIP5Kα (Phosphatidylinositol-4-phosphate 5-kinase-α) inhibitor. The overexpression of PIP5K1α is associated with poor prognosis in prostate cancer and correlates with an elevated level of the androgen receptor. ISA-2011B significantly inhibits growth of tumor cells in xenograft mice, which is mediated by targeting PIP5K1α-associated PI3K/AKT and the downstream survival, proliferation, and invasion pathways. PIP5K1α has high potential as a drug target, and compound ISA-2011B is interesting for further development of targeted cancer therapy.

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	100.0	235.93

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	2.36 mL	11.80 mL	23.59 mL
5 mM	0.47 mL	2.36 mL	4.72 mL
10 mM	0.24 mL	1.18 mL	2.36 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. Wang T, Sarwar M, Whitchurch JB, Collins HM, Green T, Semenas J, Ali A, Roberts CJ, Morris RD, Hubert M, Chen S, El-Schich Z, Wingren AG, Grundström T, Lundmark R, Mongan NP, Gunhaga L, Heery DM, Persson JL. PIP5K1α is Required for Promoting Tumor Progression in Castration-Resistant Prostate Cancer. Front Cell Dev Biol. 2022 Mar 21;10:798590. doi: 10.3389/fcell.2022.798590. PMID: 35386201; PMCID: PMC8979106.
2. Kunkl M, Porciello N, Mastrogiovanni M, Capuano C, Lucantoni F, Moretti C, Persson JL, Galandrini R, Buzzetti R, Tuosto L. ISA-2011B, a Phosphatidylinositol 4-Phosphate 5-Kinase α Inhibitor, Impairs CD28-Dependent Costimulatory and Pro-inflammatory Signals in Human T Lymphocytes. Front Immunol. 2017 Apr 26;8:502. doi: 10.3389/fimmu.2017.00502. PMID: 28491063; PMCID: PMC5405084.

In vivo study

1. Sarwar M, Semenas J, Miftakhova R, Simoulis A, Robinson B, Gjörloff Wingren A, Mongan NP, Heery DM, Johnsson H, Abrahamsson PA, Dizeyi N, Luo J, Persson JL. Targeted suppression of AR-V7 using PIP5K1α inhibitor overcomes enzalutamide resistance in prostate cancer cells. Oncotarget. 2016 Sep 27;7(39):63065-63081. doi: 10.18632/oncotarget.11757. PMID: 27588408; PMCID: PMC5325347.

2. Semenas J, Hedblom A, Miftakhova RR, Sarwar M, Larsson R, Shcherbina L, Johansson ME, Härkönen P, Sterner O, Persson JL. The role of PI3K/AKT-related PIP5K1α and the discovery of its selective inhibitor for treatment of advanced prostate cancer. Proc Natl Acad Sci U S A. 2014 Sep 2;111(35):E3689-98. doi: 10.1073/pnas.1405801111. Epub 2014 Jul 28. PMID: 25071204; PMCID: PMC4156761.

7. Bioactivity

Biological target:

ISA-2011B is a PIP5K1α inhibitor with promising anticancer effects .

In vitro activity

ISA-2011B exhibited a significant inhibitory effect on AR target genes including CDK1 and MMP9 in CRPC cells with wild-type PIP5K1α and in CRPC cells lacking the N-terminal domain of PIP5K1α.

Reference: Front Cell Dev Biol. 2022 Mar 21;10:798590. https://pubmed.ncbi.nlm.nih.gov/35386201/

In vivo activity

This study established 22Rv1 tumors overexpressing AR-V7 in mice, and then treated these mice bearing AR-V7-overexpressing tumors (100-150 mm^3 in mean volumes) with ISA-2011B or vehicle control. ISA-2011B-treatment also led to an inhibition in the expression of vimentin, a bio-marker for metastatic tumors, in the infiltrating tumor cells at the invasive front (Figure 3f).

Reference: Oncotarget. 2016 Sep 27;7(39):63065-63081. https://pubmed.ncbi.nlm.nih.gov/27588408/

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.