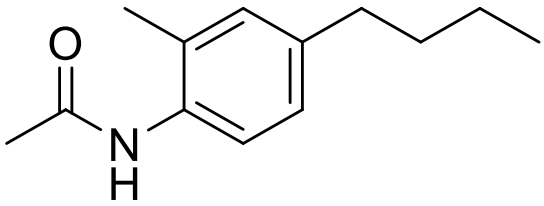
Product data sheet

MedKoo Cat#: 406809 Name: SMIP004 CAS#: 143360-00-3 Chemical Formula: $C_{13}H_{19}NO$ Exact Mass: 205.1467 Molecular Weight: 205.301	
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:

SMIP004 is a novel inducer of cancer-cell selective apoptosis of human prostate cancer cells. SMIP004 decreased the levels of positive cell cycle regulators, upregulated cyclin-dependent kinase inhibitors, and resulted in G1 arrest, inhibition of colony formation in soft agar, and cell death. SMIP004 potently inhibits the growth of prostate and breast cancer xenografts in mice. SMIP004, by inducing mitochondrial ROS formation, targets specific sensitivities of prostate cancer cells to redox and bioenergetic imbalances that can be exploited in 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	20.53	100

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	4.87 mL	24.35 mL	48.71 mL
5 mM	0.97 mL	4.87 mL	9.74 mL
10 mM	0.49 mL	2.44 mL	4.87 mL
50 mM	0.10 mL	0.49 mL	0.97 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. Rico-Bautista E, Zhu W, Kitada S, Ganapathy S, Lau E, Krajewski S, Ramirez J, Bush JA, Yuan Z, Wolf DA. Small molecule-induced mitochondrial disruption directs prostate cancer inhibition via UPR signaling. Oncotarget. 2013 Aug;4(8):1212-29. doi: 10.18632/oncotarget.1130. PMID: 23902736; PMCID: PMC3787152.
2. Rico-Bautista E, Yang CC, Lu L, Roth GP, Wolf DA. Chemical genetics approach to restoring p27Kip1 reveals novel compounds with antiproliferative activity in prostate cancer cells. BMC Biol. 2010 Dec 23;8:153. doi: 10.1186/1741-7007-8-153. PMID: 21182779; PMCID: PMC3025922.

In vivo study

1. Li C, Du L, Ren Y, Liu X, Jiao Q, Cui D, Wen M, Wang C, Wei G, Wang Y, Ji A, Wang Q. SKP2 promotes breast cancer tumorigenesis and radiation tolerance through PDCD4 ubiquitination. J Exp Clin Cancer Res. 2019 Feb 13;38(1):76. doi: 10.1186/s13046-019-1069-3. PMID: 30760284; PMCID: PMC6375223.
2. Wang D, Xu X, Wu Y, Lin Y, Gao M, Hu P, Chen D, Lu X, Chen Z, Wang H, Huang C. SMIP004: A compound with antidepressant-like activities in mouse models. Eur J Pharmacol. 2019 Jan 15;843:260-267. doi: 10.1016/j.ejphar.2018.11.039. Epub 2018 Nov 29. PMID: 30502341.

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7. Bioactivity

Biological target:

SMIP004 upregulates p27 and activates the unfolded protein response (UPR) in LNCaP prostate cancer cells overexpressing SKP2. SMIP004 also induces oxidative stress. SMIP004 induces proteasomal degradation of cyclin D1 and acts as CDK2 inhibitor.

In vitro activity

Results from this study suggest that SMIP004 could have potential in prostate cancer treatment. SMIP004 upregulated p21(Cip)[1], inhibited cellular CDK2 activity, induced G1 delay, inhibited colony formation in soft agar, and exhibited preferential cytotoxicity in LNCaP cells relative to normal human fibroblasts. SMIP004 was found to downregulate SKP2 and to stabilize p27, although it is not a proteasome inhibitor.

Reference: BMC Biol. 2010 Dec 23;8:153. https://pubmed.ncbi.nlm.nih.gov/21182779/

In vivo activity

SMIP004 has potential to be a novel antidepressant. In C57BL6/J mice, SMIP004 displayed obvious antidepressant-like activities in all conducted tests. The antidepressant-like activity of SMIP004 in naïve mice occurred at day 11; SMIP004 also produced antidepressant-like activities in naïve mice after three times in a 24-h administration scheme, but not before the test. Combined SMIP004-fluoxetine administration induced coordinated antidepressant-like effects in the tail suspension test and forced swim test.

Reference: Eur J Pharmacol. 2019 Jan 15;843:260-267. https://pubmed.ncbi.nlm.nih.gov/30502341/

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.