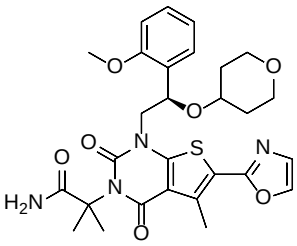
Product data sheet

MedKoo Cat#: 406951 Name: ND-646 CAS: 1434639-57-2 Chemical Formula: $C_{28}H_{32}N_4O_7S$ Exact Mass: 568.1992 Molecular Weight: 568.645	
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:

ND-646 is-an allosteric inhibitor of the ACC enzymes ACC1 and ACC2 that prevents ACC subunit dimerization-to suppress fatty acid synthesis in vitro and in vivo. Chronic ND-646 treatment of xenograft and genetically engineered mouse models of NSCLC inhibited tumor growth. When administered as a single agent or in combination with the standard-of-care drug carboplatin, ND-646 markedly suppressed lung tumor growth in the Kras;Trp53-/- (also known as KRAS p53) and Kras;Stk11-/- (also known as KRAS Lkb1) mouse models of NSCLC. ND-646 had enhanced efficacy when combined with carboplatin, a common component of chemotherapeutic regimens used to treat human NSCLC.

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
DMF	30.0	52.76
DMSO	76.67	134.82
DMSO:PBS (pH 7.2) (1:4)	0.20	0.35
Ethanol	60.0	105.51

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	**1 mg**	**5 mg**	**10 mg**
1 mM	1.76 mL	8.79 mL	17.59 mL
5 mM	0.35 mL	1.76 mL	3.52 mL
10 mM	0.18 mL	0.88 mL	1.76 mL
50 mM	0.04 mL	0.18 mL	0.35 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

Duan X, Tang X, Nair MS, Zhang T, Qiu Y, Zhang W, Wang P, Huang Y, Xiang J, Wang H, Schwartz RE, Ho DD, Evans T, Chen S. An airway organoid-based screen identifies a role for the HIF1α-glycolysis axis in SARS-CoV-2 infection. Cell Rep. 2021 Nov 9;37(6):109920. doi: 10.1016/j.celrep.2021.109920. Epub 2021 Oct 15. PMID: 34731648; PMCID: PMC8516798.

In vivo study

Svensson RU, Parker SJ, Eichner LJ, Kolar MJ, Wallace M, Brun SN, Lombardo PS, Van Nostrand JL, Hutchins A, Vera L, Gerken L, Greenwood J, Bhat S, Harriman G, Westlin WF, Harwood HJ Jr, Saghatelian A, Kapeller R, Metallo CM, Shaw RJ. Inhibition of acetyl-CoA carboxylase suppresses fatty acid synthesis and tumor growth of non-small-cell lung cancer in preclinical models. Nat Med. 2016 Oct;22(10):1108-1119. doi: 10.1038/nm.4181. Epub 2016 Sep 19. PMID: 27643638; PMCID: PMC5053891.

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7. Bioactivity

Biological target:

ND-646 is an orally bioavailable and steric inhibitor of acetyl-CoA carboxylase (ACC) with IC_{50}s of 3.5 nM and 4.1 nM for recombinant hACC1 and hACC2, respectively.

In vitro activity

Finally, 5-(tetradecyloxy)-2-furoic acid (TOFA) (Parker et al., 1977) and ND-646 (Svensson et al., 2016), two inhibitors of acetyl-coenzyme A (CoA) carboxylase 1, the key enzyme involved in fatty acid de novo synthesis, were tested to further validate the role of fatty acid metabolism in SARS-CoV-2 infection. Both qRT-PCR (Figure 6M) and immunostaining (Figures 6N and 6O) confirmed that TOFA or ND-646 blocks SARS-CoV-2 infection in hPSC-AOs.

Reference: Cell Rep. 2021 Nov 9;37(6):109920. https://pubmed.ncbi.nlm.nih.gov/34731648/

In vivo activity

Chronic ND-646 treatment of xenograft and genetically engineered mouse models of NSCLC inhibited tumor growth. When administered as a single agent or in combination with the standard-of-care drug carboplatin, ND-646 markedly suppressed lung tumor growth in the Kras;$Trp53^{-/-}$ (also known as KRAS p53) and Kras;$Stk11^{-/-}$ (also known as KRAS Lkb1) mouse models of NSCLC.

Reference: Nat Med. 2016 Oct;22(10):1108-1119. https://pubmed.ncbi.nlm.nih.gov/27643638/

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.