# Product Data Sheet

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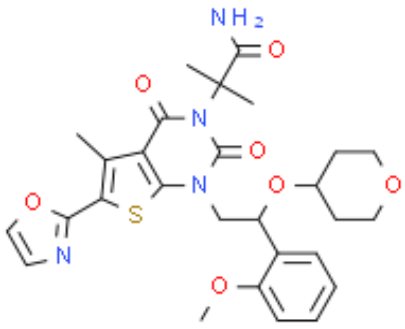
| Cas No.: | 1434639-57-2 | Cat. No: | PL01297 |
| Product Name: | ND-646 | | |
| Product synonym: | ND-646 | | |
| Chemical name: | ND-646 | | |
| MF: | C28H32N4O7S | FW: | 568.641285896301 |
| Purity: | ≥99% | Batch No.: | - |
| Storage: | | | |
| Structural formula: |  | | |
| λmax： | - | Formulation： | - |
| Solubility : | | | |
| SMILES : | O=C(N)C(C)(C)N(C(N(C[C@@H](C1=CC=CC=C1OC)OC2CCOCC2)C3=C4C(C)=C(C5=NC=CO5)S3)=O)C4=O | | |
| InChI Code: | - | | |
| InChI Key: | | | |

**WARNING This product is not for human or veterinary use.**

## Product Description

ND-646 是一种有效的乙酰辅酶 A 羧化酶 (ACC) 抑制剂，抑制重组 hACC1 和 hACC2，$IC_{50}$ 分别为 3.5 nM 和 4.1 nM。

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| 生物活性 | 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. |
| IC50 & Target[1][2] | IC50: 3.5 nM (hACC1), 4.1 nM (hACC2) |
| 体外研究(In Vitro) | ND-646 inhibits both ACC1 and ACC2 and therefore precludes the ability of ACC2 to compensate for ACC1 inhibition. ND-646 inhibits dimerization of recombinant human ACC2 BC domain (hACC2-BC) under native conditions; hACC2-BC migrates as a dimer in its absence and a monomer in its presence. In cell free systems, ND-646 inhibits enzymatic activity of recombinant human ACC1 (hACC1) with an IC50 of 3.5 nM and recombinant human ACC2 (hACC2) with an IC50 of 4.1 nM. has not independently confirmed the accuracy of these methods. They are for reference only. |

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| 体内研究(In Vivo) | To explore the impact of chronic ND-646 treatment on NSCLC tumor growth and to determine the efficacy of twice-daily dosing, athymic nude mice bearing established A549 subcutaneous tumors are treated orally with either vehicle twice daily (BID), 25 mg/kg ND-646 once daily (QD), 25 mg/kg ND-646 BID or 50 mg/kg ND-646 QD for 31 days. ND-646 at 25 mg/kg QD is ineffective at inhibiting tumor growth. However, ND-646 administered at 25 mg/kg BID or 50 mg/kg QD significantly inhibits subcutaneous A549 tumor growth. ND-646 is well tolerated throughout the treatment period, with no significant weight loss occurring after chronic ND-646 dosing, suggesting that the maximum tolerated dose (MTD) has not been reached. Mice are sacrificed at 1 hr post final dose and tissues are either prepared for immunohistochemistry (IHC) or immunoblot analysis. Tumors treated with all doses of ND-646 have |
| 包装储存 | Powder -20°C 3 years；4°C 2 years |
| 溶解度数据 | In Vitro: DMSO : ≥ 100 mg/mL (175.86 mM)配制储备液 |