

Product data sheet



MedKoo Cat#: 463165 Name: PANKi CAS: 902614-04-4 Chemical Formula: C ₂₁ H ₂₁ N ₅ O Exact Mass: 391.1467 Molecular Weight: 391.493	
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:

Pantothenate Kinase Inhibitor (PANKi) is a reversible inhibitor of pantothenate kinase, the rate-limiting enzyme in the synthesis of coenzyme A. It binds to the ATP-PanK3 complex with an apparent binding constant of 300 nM and exhibits mixed-type inhibition with respect to ATP and pantothenate. PANKi inhibits CoA biosynthesis in C3A cells with no effect on cell viability when used at concentrations up to 8 μM. PANKi synergizes with BSO to induce ferroptosis in PANC-1 cells and sensitizes the cells to imidazole ketone erastin-induced ferroptosis.

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	1.0	2.55
DMSO	1.0	2.55
DMSO:PBS (pH 7.2) (1:4)	0.25	0.64

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.55 mL	12.77 mL	25.54 mL
5 mM	0.51 mL	2.55 mL	5.11 mL
10 mM	0.26 mL	1.28 mL	2.55 mL
50 mM	0.05 mL	0.26 mL	0.51 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

Sharma LK, Leonardi R, Lin W, Boyd VA, Goktug A, Shelat AA, Chen T, Jackowski S, Rock CO. A high-throughput screen reveals new small-molecule activators and inhibitors of pantothenate kinases. *J Med Chem.* 2015 Feb 12;58(3):1563-8. doi: 10.1021/jm501585q. Epub 2015 Jan 21. PMID: 25569308; PMCID: PMC4357395.

In vivo study

TBD

7. Bioactivity

Biological target:

Pantothenate Kinase Inhibitor (PANKi) is a reversible inhibitor of pantothenate kinase.

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In vitro activity

Pantothenate kinase (PanK) is a regulatory enzyme that controls coenzyme A (CoA) biosynthesis. The association of PanK with neurodegeneration and diabetes suggests that chemical modifiers of PanK activity may be useful therapeutics. This study performed a high throughput screen of >520000 compounds from the St. Jude compound library and identified new potent PanK inhibitors and activators with chemically tractable scaffolds. The HTS identified PanK inhibitors exemplified by the detailed characterization of a tricyclic compound (7) and a preliminary SAR. Biophysical studies reveal that the PanK inhibitor acts by binding to the ATP-enzyme complex.

Reference: J Med Chem. 2015 Feb 12;58(3):1563-8. <https://pubmed.ncbi.nlm.nih.gov/25569308/>

In vivo activity

TBD

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.