

# Product data sheet



MedKoo Cat#: 585022 Name: DPTIP CAS: 351353-48-5 Chemical Formula: C <sub>21</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> S Exact Mass: 378.1038 Molecular Weight: 378.446	
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:

DPTIP is a potent and selective N-SMase2 inhibitor and brain penetrant.

## 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	143.92	380.29

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.64 mL	13.21 mL	26.42 mL
5 mM	0.53 mL	2.64 mL	5.28 mL
10 mM	0.26 mL	1.32 mL	2.64 mL
50 mM	0.05 mL	0.26 mL	0.53 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. Álvarez-Fernández H, Mingo-Casas P, Blázquez AB, Caridi F, Saiz JC, Pérez-Pérez MJ, Martín-Acebes MA, Priego EM. Allosteric Inhibition of Neutral Sphingomyelinase 2 (nSMase2) by DPTIP: From Antiflaviviral Activity to Deciphering Its Binding Site through In Silico Studies and Experimental Validation. *Int J Mol Sci.* 2022 Nov 11;23(22):13935. doi: 10.3390/ijms232213935. PMID: 36430407; PMCID: PMC9697135.

2. Rojas C, Barneva E, Thomas AG, Hu X, Southall N, Marugan J, Chaudhuri AD, Yoo SW, Hin N, Stepanek O, Wu Y, Zimmermann SC, Gadiano AG, Tsukamoto T, Rais R, Haughey N, Ferrer M, Slusher BS. DPTIP, a newly identified potent brain penetrant neutral sphingomyelinase 2 inhibitor, regulates astrocyte-peripheral immune communication following brain inflammation. *Sci Rep.* 2018 Dec 7;8(1):17715. doi: 10.1038/s41598-018-36144-2. PMID: 30531925; PMCID: PMC6286365.

### In vivo study

1. Tallon C, Bell BJ, Sharma A, Pal A, Malvankar MM, Thomas AG, Yoo SW, Hollinger KR, Coleman K, Wilkinson EL, Kannan S, Haughey NJ, Kannan RM, Rais R, Slusher BS. Dendrimer-Conjugated nSMase2 Inhibitor Reduces Tau Propagation in Mice. *Pharmaceutics.* 2022 Sep 28;14(10):2066. doi: 10.3390/pharmaceutics14102066. PMID: 36297501; PMCID: PMC9609094.

2. Pal A, Gori S, Yoo SW, Thomas AG, Wu Y, Friedman J, Tenora L, Bhasin H, Alt J, Haughey N, Slusher BS, Rais R. Discovery of Orally Bioavailable and Brain-Penetrable Prodrugs of the Potent nSMase2 Inhibitor DPTIP. *J Med Chem.* 2022 Aug 25;65(16):11111-11125. doi: 10.1021/acs.jmedchem.2c00562. Epub 2022 Aug 5. PMID: 35930706.

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## 7. Bioactivity

### Biological target:

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DPTIP is a potent brain penetrant neutral sphingomyelinase 2 (N-SMase 2) inhibitor (exosome inhibitor), with an IC<sub>50</sub> of 30 nM.

### In vitro activity

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Even more, DPTIP showed potent antiviral activity against both viruses with half-maximal effective concentrations (EC<sub>50</sub>) of 0.26 μM in Vero cells and 2.81 μM in HeLa cells for WNV.

Reference: Int J Mol Sci. 2022 Nov 11;23(22):13935. <https://pubmed.ncbi.nlm.nih.gov/36430407/>

### In vivo activity

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Male mice treated with D-DPTIP had significant and robust reduction of hippocampal nSMase2 activity (dark red vs. dark blue;  $p = 4.5 \times 10^{-7}$ ) (Figure 7B). Similarly, female mice treated with D-DPTIP had significantly reduced nSMase2 activity (light red vs. light blue;  $p = 0.0013$ ).

Reference: Pharmaceutics. 2022 Sep 28;14(10):2066. <https://pubmed.ncbi.nlm.nih.gov/36297501/>

*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.*