# **Product data sheet**



MedKoo Cat#: 407376				
Name: SHD000 free base				
Name: SHP099 free base				
CAS#: 1801747-42-1 (free base)				
Chemical Formula: C <sub>16</sub> H <sub>19</sub> Cl <sub>2</sub> N <sub>5</sub>				
Exact Mass: 351.1018				
Molecular Weight: 352.263				
Product supplied as:	Powder			
Purity (by HPLC):	$\geq 98\%$			
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:

SHP099 is a potent, selective, orally bioavailable, and efficacious SHP2 inhibitor with IC50 =0.07  $\mu$ M and p-ERK modulation in cells IC50 = 0.250  $\mu$ M. SHP099 exhibits dose-dependent pathway inhibition and antitumor activity in xenograft models. SHP2 is a nonreceptor protein tyrosine phosphatase (PTP) encoded by the PTPN11 gene involved in cell growth and differentiation via the MAPK signaling pathway. SHP2 also purportedly plays an important role in the programmed cell death pathway (PD-1/PD-L1).

#### 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	12.0	34.07
Water	1.0	2.84

#### 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.84 mL	14.19 mL	28.39 mL
5 mM	0.57 mL	2.84 mL	5.68 mL
10 mM	0.28 mL	1.42 mL	2.84 mL
50 mM	0.06 mL	0.28 mL	0.57 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
- Tani H, Kurita S, Miyamoto R, Ochiai K, Tamura K, Bonkobara M. Canine histiocytic sarcoma cell lines with SHP2 p.Glu76Gln or p.Glu76Ala mutations are sensitive to allosteric SHP2 inhibitor SHP099. Vet Comp Oncol. 2020 Jun;18(2):161-168. doi: 10.1111/vco.12524. Epub 2019 Aug 19. PMID: 31339650.
- Hao HX, Wang H, Liu C, Kovats S, Velazquez R, Lu H, Pant B, Shirley M, Meyer MJ, Pu M, Lim J, Fleming M, Alexander L, Farsidjani A, LaMarche MJ, Moody S, Silver SJ, Caponigro G, Stuart DD, Abrams TJ, Hammerman PS, Williams J, Engelman JA, Goldoni S, Mohseni M. Tumor Intrinsic Efficacy by SHP2 and RTK Inhibitors in KRAS-Mutant Cancers. Mol Cancer Ther. 2019 Dec;18(12):2368-2380. doi: 10.1158/1535-7163.MCT-19-0170. Epub 2019 Aug 22. PMID: 31439712.

In vivo study

 Ye S, Zuo B, Xu L, Wu Y, Luo R, Ma L, Yao W, Chen L, Liang G, Zhang Y. Inhibition of SHP2 by the Small Molecule Drug SHP099 Prevents Lipopolysaccharide-Induced Acute Lung Injury in Mice. Inflammation. 2023 Jun;46(3):975-986. doi: 10.1007/s10753-023-01784-8. Epub 2023 Feb 3. PMID: 36732395.

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 Sun Z, Xu X, Lv Z, Li J, Shi T, Sun H, Sun K, Tan G, Yan W, Yang YX, Wu R, Xu J, Guo H, Jiang Q, Shi D. Intraarticular injection of SHP2 inhibitor SHP099 promotes the repair of rabbit full-thickness cartilage defect. J Orthop Translat. 2022 Feb 17;32:112-120. doi: 10.1016/j.jot.2022.01.001. PMID: 35228993; PMCID: PMC8857578.

#### 7. Bioactivity

**Biological target:** 

SHP099 is an SHP2 inhibitor with an IC50 of 70 nM.

In vitro activity

Targeting cells harboring SHP2 p.Glu76Gln and p.Glu76Ala with SHP099 may be useful in the treatment of canine histiocytic sarcoma (HS). Of five of canine HS cell lines expressing SHP2, SHP099 potently suppressed the growth of two of the mutant cell lines (SHP2 p.Glu76Gln or p.Glu76Ala) but not that of the other three cell lines. SHP099 suppressed ERK activation in the cell line harbouring the SHP2 p.Glu76Ala mutation.

Reference: Vet Comp Oncol. 2020 Jun;18(2):161-168. https://pubmed.ncbi.nlm.nih.gov/31339650/

#### In vivo activity

SHP099 has potential for acute lung injury (ALI) treatment. Giving SHP099 to mice with ALI and sepsis relieved ALI and significantly increased animal survival.

Reference: Inflammation. 2023 Jun;46(3):975-986. https://pubmed.ncbi.nlm.nih.gov/36732395/

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.