

Product data sheet



MedKoo Cat#: 555361 Name: S18-000003 CAS#: 2068119-11-7 Chemical Formula: C ₂₆ H ₂₅ F ₃ N ₂ O ₄ S Exact Mass: 518.1487 Molecular Weight: 518.5512	
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:

S18-000003 is a potent orally bioavailable retinoic acid receptor-related orphan receptor-gamma-t (RORγt) inhibitor with IC₅₀ = 30 nM. S18-000003 inhibited IL-17 production in the skin of IL-23-treated mice by oral administration.

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	100	192.85

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.93 mL	9.64 mL	19.28 mL
5 mM	0.39 mL	1.93 mL	3.86 mL
10 mM	0.19 mL	0.96 mL	1.93 mL
50 mM	0.04 mL	0.19 mL	0.39 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

To be determined

In vivo study

- Imura C, Ueyama A, Sasaki Y, Shimizu M, Furue Y, Tai N, Tsujii K, Katayama K, Okuno T, Shichijo M, Yasui K, Yamamoto M. A novel RORγt inhibitor is a potential therapeutic agent for the topical treatment of psoriasis with low risk of thymic aberrations. *J Dermatol Sci.* 2019 Mar;93(3):176-185. doi: 10.1016/j.jdermsci.2019.03.002. Epub 2019 Mar 8. PMID: 30905492.
- Sasaki Y, Odan M, Yamamoto S, Kida S, Ueyama A, Shimizu M, Haruna T, Watanabe A, Okuno T. Discovery of a potent orally bioavailable retinoic acid receptor-related orphan receptor-gamma-t (RORγt) inhibitor, S18-000003. *Bioorg Med Chem Lett.* 2018 Dec 1;28(22):3549-3553. doi: 10.1016/j.bmcl.2018.09.032. Epub 2018 Sep 27. PMID: 30301676.

7. Bioactivity

Biological target:

S18-000003 is a potent, selective and orally active inhibitor of retinoic acid receptor-related orphan receptor-gamma-t (RORγt), with an IC₅₀ of <30 nM towards human RORγt in competitive binding assays.

In vitro activity

To be determined

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In vivo activity

S18-000003, a potential psoriasis treatment with a low risk of thymic lymphoma, was tested topically in a mouse psoriasis model. It effectively reduced psoriatic skin inflammation by targeting the IL-17 pathway. The treatment inhibited various types of IL-17-producing cells in the skin without causing harm to thymocytes or cell cycle disruptions, even at high doses.

Reference: J Dermatol Sci. 2019 Mar;93(3):176-185. <https://pubmed.ncbi.nlm.nih.gov/30905492/>

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.