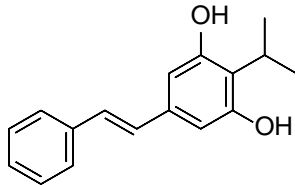


Product data sheet



MedKoo Cat#: 326981 Name: Benvitimod CAS#: 79338-84-4 Chemical Formula: C ₁₇ H ₁₈ O ₂ Exact Mass: 254.1307 Molecular Weight: 254.33	
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:

Benvitimod, also known as tapinarof, WB-1001; GSK-2894512 and WBI-1001, is a non-steroidal anti-inflammatory drug (NSAID) potentially for the treatment of atopic dermatitis. WBI-1001 is an efficacious novel topical anti-inflammatory molecule for the treatment of AD.

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	88.0	346.01
Ethanol	51.0	200.53

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.93 mL	19.66 mL	39.32 mL
5 mM	0.79 mL	3.93 mL	7.86 mL
10 mM	0.39 mL	1.97 mL	3.93 mL
50 mM	0.08 mL	0.39 mL	0.79 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. Smith SH, Jayawickreme C, Rickard DJ, Nicodeme E, Bui T, Simmons C, Coquery CM, Neil J, Pryor WM, Mayhew D, Rajpal DK, Creech K, Furst S, Lee J, Wu D, Rastinejad F, Willson TM, Viviani F, Morris DC, Moore JT, Cote-Sierra J. Tapinarof Is a Natural AhR Agonist that Resolves Skin Inflammation in Mice and Humans. *J Invest Dermatol.* 2017 Oct;137(10):2110-2119. doi: 10.1016/j.jid.2017.05.004. Epub 2017 Jun 6. PMID: 28595996.

In vivo study

1. Smith SH, Jayawickreme C, Rickard DJ, Nicodeme E, Bui T, Simmons C, Coquery CM, Neil J, Pryor WM, Mayhew D, Rajpal DK, Creech K, Furst S, Lee J, Wu D, Rastinejad F, Willson TM, Viviani F, Morris DC, Moore JT, Cote-Sierra J. Tapinarof Is a Natural AhR Agonist that Resolves Skin Inflammation in Mice and Humans. *J Invest Dermatol.* 2017 Oct;137(10):2110-2119. doi: 10.1016/j.jid.2017.05.004. Epub 2017 Jun 6. PMID: 28595996.

7. Bioactivity

Biological target:

Tapinarof (WBI-1001) is a natural aryl hydrocarbon receptor (AhR) agonist with an EC₅₀ of 13 nM.

Product data sheet



In vitro activity

At $<1 \mu\text{M}$, tapinarof was antiproliferative to B cells, coronary smooth muscle cells, and endothelial cells (Figure 2a; gray arrows). Furthermore, tapinarof induced tissue factor (CD142), E-selectin, IL-8, IL-1 α , and sIgG and decreased eotaxin 3, sTNF α , sIL-10, sIL-6 (Figure 2a). Tapinarof also induced cellular apoptosis in CD4⁺ T cells in a dose-dependent manner (IC50 = 5.2 μM).

Reference: J Invest Dermatol. 2017 Oct;137(10):2110-2119. [https://www.jidonline.org/article/S0022-202X\(17\)31543-9/fulltext](https://www.jidonline.org/article/S0022-202X(17)31543-9/fulltext)

In vivo activity

Mice treated topically with tapinarof showed significantly less inflammation, epidermal thickening, and proinflammatory cytokine expression than mice treated for 10 days with vehicle alone (Figure 4a–c). Decreased tissue cytokine expression was observed in tapinarof-treated mice, including IL17a, IL17f, IL19, IL22, IL23a, and IL1 β , which were dose-dependently inhibited by tapinarof (Figure 4d, Supplementary Table S4 online). Interestingly, this activity was restricted to select biomarkers, as IMQ-induced expression of other cytokines was either not affected (IL6) or increased (IL10 and IP10) by tapinarof (Supplementary Table S4).

Reference: J Invest Dermatol. 2017 Oct;137(10):2110-2119. [https://www.jidonline.org/article/S0022-202X\(17\)31543-9/fulltext](https://www.jidonline.org/article/S0022-202X(17)31543-9/fulltext)

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.