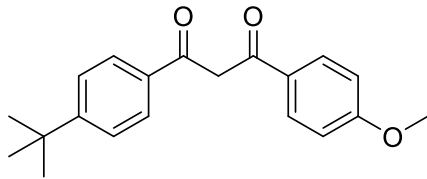


Product data sheet



MedKoo Cat#: 531005 Name: Avobenzone CAS#: 70356-09-1 Chemical Formula: C ₂₀ H ₂₂ O ₃ Exact Mass: 310.1569 Molecular Weight: 310.393	
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:

Avobenzone is a dibenzoylmethane compound commonly found in sunscreens and can photoisomerize after exposure to near-ultraviolet light. At equilibrium, Avobenzone exists as a chelated enol characterized by a strong intramolecular hydrogen bond. The photochemistry of Avobenzone includes keto-enol tautomerization, cis-trans isomerization, rotation about the single bond and α bond cleavages of carbonyl groups. Findings suggest that torsion around the double C2-C3 bond of photoexcited chelated enol leads to internal conversion to the ground state and formation of rotamer E. In addition, opening of the chelated hydrogen ring by torsion of the hydroxyl group creates non-chelated enol. The possible mechanisms of rotamer Z formation are discussed.

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	47.33	152.48
DMSO:PBS (pH 7.2) (1:2)	0.33	1.06
DMF	30.0	96.65
Ethanol	5.0	16.11

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.22 mL	16.11 mL	32.22 mL
5 mM	0.64 mL	3.22 mL	6.44 mL
10 mM	0.32 mL	1.61 mL	3.22 mL
50 mM	0.06 mL	0.32 mL	0.64 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

- Ahn S, An S, Lee M, Lee E, Pyo JJ, Kim JH, Ki MW, Jin SH, Ha J, Noh M. A long-wave UVA filter avobenzone induces obesogenic phenotypes in normal human epidermal keratinocytes and mesenchymal stem cells. Arch Toxicol. 2019 Jul;93(7):1903-1915. doi: 10.1007/s00204-019-02462-1. Epub 2019 Apr 23. PMID: 31016361.
- Yang C, Lim W, Bazer FW, Song G. Avobenzone suppresses proliferative activity of human trophoblast cells and induces apoptosis mediated by mitochondrial disruption. Reprod Toxicol. 2018 Oct;81:50-57. doi: 10.1016/j.reprotox.2018.07.003. Epub 2018 Jul 4. PMID: 29981360.

In vivo study

TBD

Product data sheet



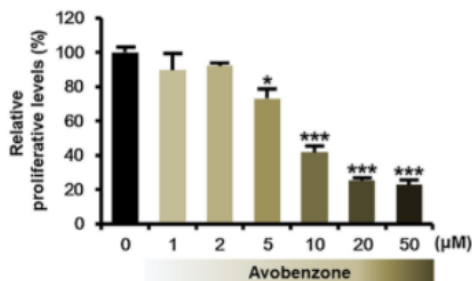
7. Bioactivity

Biological target:

Avobenzone is an endocrine disruptor that directly binds to estrogen receptor β and acts as an estrogen agonist

In vitro activity

HTR8/SVneo cells were treated with various concentrations (0, 1, 2, 5, 10, 20, and 50 μM) of avobenzone with 50 μM being the maximum concentration. A significant decrease in cell proliferation was observed at 5 μM (Fig. 1A). Avobenzone at 10 μM produced more than 50% inhibition of cell proliferation and 74.6% ($P < 0.001$) and 77.2% ($P < 0.001$) cell proliferation were observed at 20 and 50 μM , respectively.



Reference: Reprod Toxicol. 2018 Oct;81:50-57. <https://pubmed.ncbi.nlm.nih.gov/29981360/>

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.