Product data sheet



| MedKoo Cat#: 561250 | | |
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| Name: Shikonin | | |
| CAS#: 517-89-5 | | |
| Chemical Formula: C ₁₆ H ₁₆ O ₅ | | |
| Exact Mass: 288.0998 | | |
| Molecular Weight: 288.30 | | |
| Product supplied as: | Powder | |
| Purity (by HPLC): | ≥ 98% | |
| Shipping conditions | Ambient temperature | |
| Storage conditions: | Powder: -20°C 3 years; 4°C 2 years. | OH O OH |
| | In solvent: -80°C 3 months; -20°C 2 weeks. | 911 9 911 |

1. Product description:

Shikonin is a natural product from the root of Lithospermum erythrorhizon and a specific inhibitor of pyruvate kinase M2 (PKM2). Shikonin also suppresses the ATF2 pathway in skin carcinogenesis.

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 | 125 | 433.58 |

4. Stock solution preparation table:

| Concentration / Solvent Volume / Mass | 1 mg | 5 mg | 10 mg |
|---------------------------------------|---------|----------|----------|
| 1 mM | 3.47 mL | 17.34 mL | 34.69 mL |
| 5 mM | 0.69 mL | 3.47 mL | 6.94 mL |
| 10 mM | 0.35 mL | 1.73 mL | 3.47 mL |
| 50 mM | 0.07 mL | 0.35 mL | 0.69 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. Ahmad H, Crotts MS, Jacobs JC, Baer RW, Cox JL. Shikonin Causes Non-apoptotic Cell Death in B16F10 Melanoma. Anticancer Agents Med Chem. 2023;23(16):1880-1887. doi: 10.2174/1871520623666230701000338. PMID: 37393553.
- 2. Chen Q, Han H, Lin F, Yang L, Feng L, Lai X, Wen Z, Yang M, Wang C, Ma Y, Yin T, Lu G, Lin H, Qi J, Yang Y. Novel shikonin derivatives suppress cell proliferation, migration and induce apoptosis in human triple-negative breast cancer cells via regulating PDK1/PDHC axis. Life Sci. 2022 Dec 1;310:121077. doi: 10.1016/j.lfs.2022.121077. Epub 2022 Oct 13. PMID: 36244412.

In vivo study

- 1. Luo Q, Ji XY, Zhang L, Huang X, Wang XQ, Zhang B. Shikonin prevents mice from heat stroke-induced death via suppressing a trigger IL-17A on the inflammatory and oxidative pathways. Biomed Pharmacother. 2023 Oct;166:115346. doi: 10.1016/j.biopha.2023.115346. Epub 2023 Aug 27. PMID: 37643485.
- 2. He Y, Luo K, Hu X, Liu J, Hao M, Li Y, Xia X, Lü X, Shi C. Antibacterial Mechanism of Shikonin Against Vibrio vulnificus and Its Healing Potential on Infected Mice with Full-Thickness Excised Skin. Foodborne Pathog Dis. 2023 Feb;20(2):67-79. doi: 10.1089/fpd.2022.0065. PMID: 36779943.

7. Bioactivity

Biological target:

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Shikonin is a potent TMEM16A chloride channel inhibitor with an IC50 of $6.5 \mu M$. Shikonin is a specific PKM2 inhibitor and can inhibit TNF- α and NF- κ B pathway. Shikonin decreases exosome secretion through the inhibition of glycolysis. Shikonin inhibits AIM2 inflammasome activation.

In vitro activity

Shikonin has potential for melanoma treatment, as it causes non-apoptotic cell death in B16F10 melanoma cells. There was a large decrease in cellular growth and proliferation with increasing shikonin concentrations. MTT assays suggested that necroptosis, autophagy, and reactive oxygen species are a part of shikonin's mechanism of action. Western blotting confirmed that shikonin-treated melanoma cells had increased levels of stress-related proteins, such as CHOP, RIP, pRIP.

Reference: Anticancer Agents Med Chem. 2023;23(16):1880-1887. https://pubmed.ncbi.nlm.nih.gov/37393553/

In vivo activity

In a murine model of heat stroke, shikonin demonstrated anti-inflammatory and antioxidative characteristics by reducing the production of IL-17A and inhibiting its expression. SK delayed the rising rate of core temperature, prolonged the survival time of mice, and improved organ injury and coagulation function markedly. Serum HS biomarkers were decreased significantly by SK, which contribute to liver and lung protection in the models.

Reference: Biomed Pharmacother. 2023 Oct;166:115346. https://pubmed.ncbi.nlm.nih.gov/37643485/

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.