

**Product Name:** (R)-Shikonin

**Catalog No.:** 6829

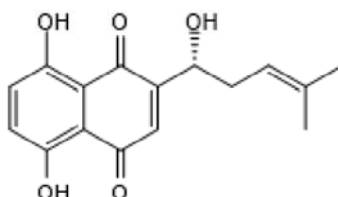
**Batch No.:** 1

CAS Number: 517-89-5

IUPAC Name: 5,8-Dihydroxy-2-[(1R)-1-hydroxy-4-methyl-3-penten-1-yl]-1,4-naphthalenedione

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>16</sub>H<sub>16</sub>O<sub>5</sub>  
**Batch Molecular Weight:** 288.3  
**Physical Appearance:** Red/brown solid  
**Solubility:** DMSO to 100 mM  
ethanol to 20 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.8% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	66.66	5.59	
Found	66.63	5.61	

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

PTEN and inflammasome inhibitor. Inhibits PTEN's phosphatase activity ( $IC_{50} = 2.7 \mu M$ ) and NLRP3 activation. Also blocks TNF- $\alpha$  and NF- $\kappa B$  signaling. Attenuates HIV-1 replication at nanomolar concentrations. Suppresses glycolysis in cancer cells by inhibiting tumor-specific pyruvate kinase M2 (PKM2) ( $IC_{50} = 0.3 \mu M$ ). Induces necroptosis in MCF-7 and HEK293 cancer cell lines. Displays anti-inflammatory activity in a mouse model of collagen-induced arthritis.

**Physical and Chemical Properties:**

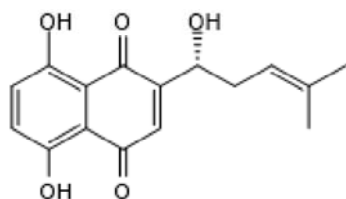
Batch Molecular Formula:  $C_{16}H_{16}O_5$

Batch Molecular Weight: 288.3

Physical Appearance: Red/brown solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

**Hafner-Bratkovic et al** (2018) NLRP3 lacking the leucine-rich repeat domain can be fully activated via the canonical inflammasome pathway. *Nat. Commun.* **9** 5182. PMID: 30518920.

**McLoughlin et al** (2018) The therapeutic potential of PTEN modulation: targeting strategies from gene to protein. *Cell Chem. Biol.* **25** 19. PMID: 29153852.

**Chen et al** (2011) Shikonin and its analogs inhibit cancer cell glycolysis by targeting tumor pyruvate kinase-M2. *Oncogene* **30** 4297. PMID: 21516121.

**Storage:** Store at  $-20^{\circ}C$

**CAUTION** - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a  $45-60^{\circ}C$  water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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