Print Date: May 2nd 2019

Certificate of Analysis

www.tocris.com

Product Name: **(R)-Shikonin** **Catalog No.: 6829** **Batch No.: 1**

CAS Number: 517-89-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

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

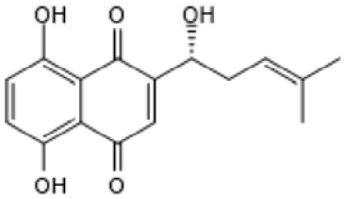
Batch Molecular Weight: 288.3

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

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.66	5.59	
Found	66.63	5.61	

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Description:

PTEN and inflammasome inhibitor. Inhibits PTEN's phosphatase activity (IC_{50} = 2.7 µM) and NLRP3 activation. Also blocks TNF-α and NF-κB 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 µM). 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:

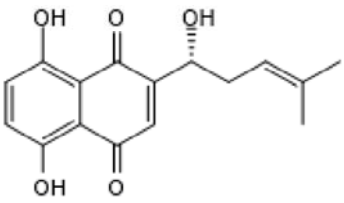
Batch Molecular Formula: $C_{16}H_{16}O_5$

Batch Molecular Weight: 288.3

Physical Appearance: Red/brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°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°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°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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.

Kim *et al* (2010) The efficacy of shikonin on cartilage protection in a mouse model of rheumatoid arthritis. Korean J.Physiol.Pharmacol. ***14*** 199. PMID: 20827333.

Han *et al* (2007) Shikonin circumvents cancer drug resistance by induction of a necroptotic death. Mol. Cancer Ther. ***6*** 1641. PMID: 17513612.

Nigorikawa *et al* (2006) A naphthoquinone derivative, shikonin, has insulin-like actions by inhibiting both phosphatase and tensin homolog deleted on chromosome 10 and tyrosine phosphatases. Mol.Pharmacol. ***70*** 1143. PMID: 16804092.

Chen *et al* (2003) Shikonin, a Component of Chinese Herbal Medicine, Inhibits Chemokine Receptor Function and Suppresses Human Immunodeficiency Virus Type 1 Antimicrob. Agents Chemother. ***47*** 2810. PMID: 12936978.