# TOCRIS a biotechne brand

#### Print Date: Jan 19th 2023

# **Certificate of Analysis**

### www.tocris.com

Batch No.: 2

Catalog No.: 4962

### Product Name: SB 204990

CAS Number: 154566-12-8

IUPAC Name: (3R,5S)-rel-5-[6-(2,4-Dichlorophenyl)hexyl]tetrahydro-3-hydroxy-2-oxo-3-furanacetic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>18</sub>H<sub>22</sub>Cl<sub>2</sub>O<sub>5</sub> 389.27 White solid DMSO to 100 mM ethanol to 100 mM Store at -20°C

**Batch Molecular Structure:** C

CI CO<sub>2</sub>H 0 (and enantiomer) 0

2. ANALYTICAL DATA

Storage:

TLC:Rf = 0.4 (Dichloromethane:Methanol [9:1])HPLC:Shows 98.1% purity<sup>1</sup>H NMR:Consistent with structureMass Spectrum:Consistent with structureMicroanalysis:Carbon Hydrogen NitrogenTheoretical 55.545.7

Found

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

55.74

5.82

0.1

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# **Product Information**

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#### Product Name: SB 204990

CAS Number: 154566-12-8

IUPAC Name:

(3R,5S)-rel-5-[6-(2,4-Dichlorophenyl)hexyl]tetrahydro-3-hydroxy-2-oxo-3-furanacetic acid

#### Description:

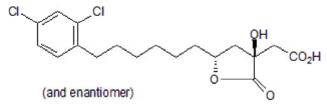
SB 204990 is an ATP citrate lyase (ACLY) inhibitor; it is a prodrug of SB 201076. SB 204990 inhibits cholesterol and fatty acid synthesis in a dose-dependent manner in HepG2 cells. Suppresses growth of cancer cells showing aerobic glycolysis in vitro and in vivo. Orally active.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>18</sub>H<sub>22</sub>Cl<sub>2</sub>O<sub>5</sub> Batch Molecular Weight: 389.27 Physical Appearance: White solid

#### Minimum Purity: ≥98%

#### **Batch Molecular Structure:**



#### **Storage:** Store at -20°C

#### Solubility & Usage Info: DMSO to 100 mM

ethanol to 100 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°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

#### Licensing Information:

Sold for research purposes under agreement from GlaxoSmithKline

#### **References:**

Hatzivassiliou et al (2005) ATP citrate lyase inhibition can suppress tumor cell growth. Cancer Cell 8 311. PMID: 16226706.

**Gribble** *et al* (1998) ATP-Citrate lyase as a target for hypolipidemic intervention. 2. Synthesis and evaluation of (3R\*,5S\*)-ω-substituted-3-carboxy-3, 5-dihydroxyalkanoic acids and their gamma-lactone prodrugs as inhibitors of the enzy J.Med.Chem. **41** 3582. PMID: 9733484.

**Pearce** *et al* (1998) The role of ATP citrate-lyase in the metabolic regulation of plasma lipids. Hypolipidaemic effects of SB-204990, a lactone prodrug of the potent ATP citrate-lyase inhibitor SB-201076. Biochem.J. **334** 113. PMID: 9693110.

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