



# **Certificate of Analysis**

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Product Name: SB 204990 Catalog No.: 4962 Batch No.: 1

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:  $C_{18}H_{22}CI_2O_5$ . <sup>1</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 393.77

Physical Appearance: White solid

**Solubility:** DMSO to 100 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.42$  (Chloroform:Methanol [9:1])

HPLC: Shows >98.3% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.9 5.76

Found 55.04 5.7 0.05



## **Product Information**

Print Date: Oct 11th 2013

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#### **Description:**

ATP-citrate lyase (ACL) inhibitor. Prodrug of SB 201076. Inhibits cholesterol and fatty acid synthesis in a dose-dependent manner in HepG2 cells. Orally active in vivo.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>18</sub>H<sub>22</sub>Cl<sub>2</sub>O<sub>5</sub>. ¼H<sub>2</sub>O

Batch Molecular Weight: 393.77 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°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:

**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.

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

