



# **Certificate of Analysis**

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Product Name: NSC 668036 Catalog No.: 5813 Batch No.: 1

CAS Number: 144678-63-7

IUPAC Name: N-[(1,1-dimethylethoxy)carbonyl]-L-alanyl-(2S)-2-hydroxy-3-methylbutanoyl-L-alanine-(1S)-1-carboxy-2-methylpropyl

ester

**Batch Molecular Structure:** 

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{36}N_2O_9$ Batch Molecular Weight:460.52Physical Appearance:White solid

Solubility: DMSO to 100 mM ethanol to 100 mM

Ctare of 20°C

Storage: Store at -20°C

# 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.7$  (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.9% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.77 7.88 6.08 Found 54.65 7.82 6.14





# **Product Information**

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#### **Description:**

Wnt signaling inhibitor. Binds the PDZ domain of the Dishevelled (DvI) protein. Inhibits proliferation, migration and TGF-β-induced differentiation of fibroblasts in vitro. Reduces severity of pulmonary fibrosis in a mouse model.

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

Batch Molecular Formula: C<sub>21</sub>H<sub>36</sub>N<sub>2</sub>O<sub>9</sub> Batch Molecular Weight: 460.52 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:

Wang et al (2015) Targeted inhibition of disheveled PDZ domain via NSC668036 depresses fibrotic process. Exp.Cell Res. 331 115. PMID: 25445788.

Shan et al (2005) Identification of a specific inhibitor of the dishevelled PDZ domain. Biochemistry 44 15495. PMID: 16300398.