

# **Certificate of Analysis**

# www.tocris.com

Product Name: Betulinic acid Catalog No.: 3906 Batch No.: 1

CAS Number: 472-15-1 EC Number: 207-448-8

IUPAC Name: (+)- $(3\beta)$ -3-Hydroxylup-20(29)-en-28-oic acid

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{30}H_{48}O_3$ . 1/4  $H_2O$ 

Batch Molecular Weight: 461.2

Physical Appearance: White solid

Solubility: DMSO to 50 mM Storage: Store at +4°C

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

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

**Optical Rotation:**  $[\alpha]_D = +9.8$  (Concentration = 1, Solvent = pyridine)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 78.13 10.6 Found 78.24 10.7





## Print Date: May 18th 2012

**Product Information** 

www.tocris.com

Product Name: Betulinic acid Catalog No.: 3906 Batch No.: 1

CAS Number: 472-15-1 EC Number: 207-448-8

IUPAC Name: (+)- $(3\beta)$ -3-Hydroxylup-20(29)-en-28-oic acid

#### **Description:**

Natural triterpenoid that displays anti-HIV and antitumor activity. Induces the production of reactive oxygen species (ROS) and activates NF- $\kappa$ B. Exhibits TGR5 agonist activity (EC50 = 1.04  $\mu$ M).

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

Batch Molecular Formula: C<sub>30</sub>H<sub>48</sub>O<sub>3</sub>. ¼H<sub>2</sub>O

Batch Molecular Weight: 461.2 Physical Appearance: White solid

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

Storage: Store at +4°C

## Solubility & Usage Info:

DMSO to 50 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:

Kashiwada et al (1996) Betulinic acid and dihydrobetulinic acid derivatives as potent anti-HIV agents. J.Med.Chem. 39 1016. PMID: 8676334.

Fulda (2008) Betulinic acid for cancer treatment and prevention. Int.J.Mol.Sci. 9 1096. PMID: 19325847.

**Genet** *et al* (2010) Structure-activity relationship study of betulinic acid, a novel and selective TGR5 agonist, and its synthetic derivatives: potential impact in diabetes. J.Med.Chem. *53* 178. PMID: 19911773.

