



# **Certificate of Analysis**

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Product Name: CU CPT 22 Catalog No.: 4884 Batch No.: 1

CAS Number: 1416324-85-0

**Batch Molecular Structure:** 

IUPAC Name: 3,4,6-Trihydroxy-2-methoxy-5-oxo-5*H*-benzocycloheptene-8-carboxylic acid hexyl ester

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{19}H_{22}O_7.H_2O$ 

Batch Molecular Weight: 380.39

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM ethanol to 50 mM

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Storage: Store at -20°C

OMe OH OH

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.6$  (Dichloromethane:Methanol [97:3])

HPLC: Shows >99.6% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.99 6.36

Found 59.79 6.43 0.05



# **Product Information**

Print Date: Oct 10th 2013

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#### **Description:**

Selective toll-like receptor 1/2 (TLR1/2) inhibitor (IC $_{50}$  = 0.58  $\mu$ M). Exhibits no activity at TRL2/TLR6, TLR3, TLR4 and TLR7 or a panel of 10 representative kinases. Inhibits the release of proinflammatory cytokines TNF- $\alpha$  and IL-1 $\beta$ .

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

Batch Molecular Formula: C<sub>19</sub>H<sub>22</sub>O<sub>7</sub>.H<sub>2</sub>O Batch Molecular Weight: 380.39 Physical Appearance: Orange 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 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:

Cheng et al (2012) Discovery of small-molecule inhibitors of the TLR1/TLR2 complex. Angew Chem.Int.Ed.Engl. 51 12246. PMID: 22969053.

