



# **Certificate of Analysis**

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Product Name: TCS 3035 Catalog No.: 4244 Batch No.: 1

CAS Number: 871085-49-3

IUPAC Name: 2-[4-[(Z)-(2,4-Dioxo-5-thiazolidinylidene)methyl]phenoxyacetic acid

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{12}H_9NO_5S.4H_2O$ 

Batch Molecular Weight: 283.77

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM

ethanol to 10 mM with sonication

Storage: Store at +4°C

**Batch Molecular Structure:** 

HO<sub>2</sub>C O

#### 2. ANALYTICAL DATA

**HPLC:** Shows 99.7% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen

Carbon Hydrogen Nitrogen

Theoretical 50.79 3.37 4.94 Found 50.66 3.29 4.9



## **Product Information**

Print Date: Sep 12<sup>th</sup> 2014

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IUPAC Name: 2-[4-[(Z)-(2,4-Dioxo-5-thiazolidinylidene)methyl]phenoxyacetic acid

### **Description:**

GPR35 agonist (pEC $_{50}$  values are 5.13 and 5.86 for rat and human GPR35 orthologs, respectively).

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

Batch Molecular Formula: C<sub>12</sub>H<sub>9</sub>NO<sub>5</sub>S.<sup>1</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 283.77 Physical Appearance: Off White solid

**Minimum Purity:** >98%

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

Storage: Store at +4°C

#### Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with sonication

#### 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:

**Jenkins** *et al* (2011) Agonist activation of the G protein-coupled receptor GPR35 involves transmembrane domain III and is transduced via  $G_{\alpha13}$  and  $\beta$ -arrestin-2. Br.J.Pharmacol. *162* 733. PMID: 20958291.

