# TOCRIS a biotechne brand

Batch No.: 2

## **Certificate of Analysis**

## www.tocris.com

Catalog No.: 4959

#### Product Name: CID 16020046

CAS Number: IUPAC Name:

834903-43-4

4-[4,6-Dihydro-4-(3-hydroxyphenyl)-3-(4-methylphenyl)-6-oxopyrrolo[3,4-c]pyrazol-5(1H)-yl]benzoic acid

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure:  $C_{25}H_{19}N_3O_4$ .<sup>1/4</sup> $H_2O$ 429.94 Off White solid DMSO to 100 mM Store at +4°C

CO<sub>2</sub>H

### 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis:

Shows 99.7% purity Consistent with structure Consistent with structure

	Carbon H	Hydrogen	Nitrogen
Theoretical	69.84	4.57	9.77
Found	69.73	4.69	9.75

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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4-[4,6-Dihydro-4-(3-hydroxyphenyl)-3-(4-methylphenyl)-6-oxopyrrolo[3,4-c]pyrazol-5(1H)-yl]benzoic acid

#### **Description:**

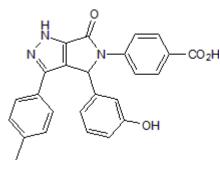
Selective GPR55 antagonist. Inhibits LPI-induced Ca<sup>2+</sup> signaling (IC<sub>50</sub> = 0.21  $\mu$ M in HEK-GPR55 cells), ERK1/2 phosphorylation and GPR55-mediated transcription factor activation. Displays weak inhibition of acetylcholinesterase,  $\mu$ -opioid receptor, KCNH2 and hERG. Decreases LPI-induced GPR55 internalization. Reduces experimental intestinal inflammation in mice.

#### Physical and Chemical Properties:

Batch Molecular Formula:  $C_{25}H_{19}N_3O_4$ . <sup>1</sup>/<sub>4</sub> $H_2O$ Batch Molecular Weight: 429.94 Physical Appearance: Off White solid

#### Minimum Purity: >99%

**Batch Molecular Structure:** 



#### **Storage:** Store at +4°C

Solubility & Usage Info: DMSO 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  $45-60^{\circ}C$  water bath).

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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:**

Kargl *et al* (2013) A selective antagonist reveals a potential role of G protein-coupled receptor 55 in platelet and endothelial cell function. J.Pharmacol.Exp.Ther. **346** 54. PMID: 23639801.

Stančić et al (2015) The GPR55 antagonist CID16020046 protects against intestinal inflammation. Neurogastroenterol.Motil. PMID: 26227635.

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