



Certificate of Analysis

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Product Name: CID 16020046 Catalog No.: 4959 Batch No.: 1

CAS Number: 834903-43-4

IUPAC Name: 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: $C_{25}H_{19}N_3O_4.H_2O$

Batch Molecular Weight: 443.46

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.71 4.77 9.48 Found 67.8 4.71 9.57



Product Information

Print Date: Sep 6th 2013

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Description:

Selective GPR55 antagonist. Inhibits LPI-induced Ca²⁺ signaling (IC $_{50}$ = 0.21 μ M in HEK-GPR55 cells), ERK1/2 phosphorylation and GPR55-mediated transcription factor activation. Displays weak inhibition of acetylcholinesterase, μ -opioid receptor, KCNH2 and hERG. Decreases LPI-induced GPR55 internalization.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{25}H_{19}N_3O_4.H_2O$

Batch Molecular Weight: 443.46 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°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:

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.

