

Product Name: CID 16020046

Catalog No.: 4959

Batch No.: 3

CAS Number: 834903-43-4

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₁₉N₃O₄·½H₂O

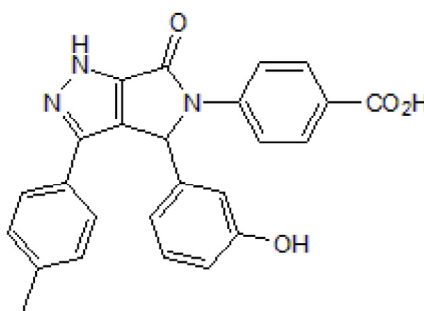
Batch Molecular Weight: 434.45

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69.12	4.64	9.67
Found	68.17	4.52	9.46

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Description:

CID 16020046 is a selective GPR55 antagonist. Inhibits LPI-induced Ca²⁺ signaling (IC₅₀ = 0.21 μM 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. Reduces experimental intestinal inflammation in mice.

Physical and Chemical Properties:

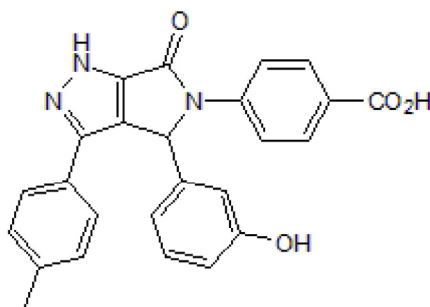
Batch Molecular Formula: C₂₅H₁₉N₃O₄·½H₂O

Batch Molecular Weight: 434.45

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Stančić *et al* (2015) The GPR55 antagonist CID16020046 protects against intestinal inflammation. *Neurogastroenterol.Motil* **27** 1432. PMID: 26227635.

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.

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

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