1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $\text{C}_{25}\text{H}_{19}\text{N}_{3}\text{O}_{4} \cdot \frac{1}{4}\text{H}_{2}\text{O}$
- **Batch Molecular Weight:** 429.94
- **Physical Appearance:** Off White solid
- **Solubility:** DMSO to 100 mM
- **Storage:** Store at +4°C

2. ANALYTICAL DATA

- **HPLC:** Shows 99.7% purity
- **$^1\text{H NMR}:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  - Carbon Hydrogen Nitrogen
  - Theoretical: 69.84 4.57 9.77
  - Found: 69.73 4.69 9.75
Product Name: CID 16020046
Catalog No.: 4959  Batch No.: 2

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

Description:
Selective GPR55 antagonist. Inhibits LPI-induced Ca\(^{2+}\) signaling (IC\(_{50}\) = 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, KCNQ2 and hERG. Decreases LPI-induced GPR55 internalization. Reduces experimental intestinal inflammation in mice.

Physical and Chemical Properties:
Batch Molecular Formula: C\(_{29}\)H\(_{23}\)N\(_3\)O\(_4\).\(\frac{1}{4}\)H\(_2\)O
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°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: