



Certificate of Analysis

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Product Name: GPBAR-A Catalog No.: 4478 Batch No.: 1

CAS Number: 877052-79-4

IUPAC Name: 4-[[3,5-Bis(trifluoromethyl)phenyl]methyl]-6-(2-fluorophenyl)-4,5-dihydro-pyrido[3,2-f]-1,4-oxazepin-3(2H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{15}F_7N_2O_2$

Batch Molecular Weight: 484.37

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.73$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.03 3.12 5.78 Found 57.37 2.96 5.72



Product Information

Print Date: May 25th 2016

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Description:

GPBA receptor agonist. Upregulates GLP-1 secretion from intestinal cultures. Increases MQAE-fluorescence suggesting a decrease in intracellular chloride concentration in gallbladder epithelial cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₁₅F₇N₂O₂ Batch Molecular Weight: 484.37 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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:

Parker et al (2012) Molecular mechanisms underlying bile acid-stimulated glucagon-like peptide-1 secretion. Br.J.Pharmacol. 165 414. PMID: 21718300.

Keitel *et al* (2009) The membrane-bound bile acid receptor TGR5 is localized in the epithelium of human gallbladders. Hepatology *50* 861. PMID: 19582812.

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