

Certificate of Analysis

Print Date: Nov 9th 2016

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Product Name: ZQ 16 Catalog No.: 6001 Batch No.: 1

CAS Number: 376616-73-8

IUPAC Name: 2-(Hexylthio)-6-hydroxy-4(3*H*)-pyrimidinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{10}H_{16}N_2O_2S$

Batch Molecular Weight: 228.31 **Physical Appearance:** White solid

Solubility: DMSO to 50 mM

ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

S N OH

2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 52.61 7.06 12.26 Found 52.62 7.36 12.1



Product Information

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IUPAC Name: 2-(Hexylthio)-6-hydroxy-4(3*H*)-pyrimidinone

Description:

Selective medium-chain free fatty acid receptor GPR84 agonist (EC $_{50}$ = 139 nM). Exhibits no response at GPR40, GPR41, GPR119 or GPR120 at 100 uM. Activates calcium mobilization, inhibits cAMP accumulation, and induces ERK1/2 phosphorylation, receptor desensitization and internalization in vitro.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₀H₁₆N₂O₂S Batch Molecular Weight: 228.31 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM ethanol 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:

Liu et al (2016) Design and synthesis of 2-alkylpyrimidine-4,6-diol and 6-alkylpyridine-2,4-diol as potent GPR84 agonists. ACS Med.Chem.Lett. **7**579. PMID: 27326330.

Zhang *et al* (2016) Discovery and characterization of a novel small-molecule agonist for medium-chain free fatty acid receptor G protein-coupled receptor 84. J.Pharmacol.Exp.Ther. **357** 337. PMID: 26962172.