

Certificate of Analysis

Print Date: Jan 13th 2016

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Product Name: YM 976 Catalog No.: 1821 Batch No.: 3

CAS Number: 191219-80-4

IUPAC Name: 4-(3-Chlorophenyl)-1,7-diethylpyrido[2,3-d]pyrimidin-2(1H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{16}CIN_3O$

Batch Molecular Weight: 313.79

Physical Appearance: Pale yellow solid

Solubility: ethanol to 100 mM

DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.35$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows >98.3% purity

1H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.07 5.14 13.39 Found 64.94 5.17 13.37



Product Information

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IUPAC Name: 4-(3-Chlorophenyl)-1,7-diethylpyrido[2,3-d]pyrimidin-2(1H)-one

Description:

Orally active PDE4 inhibitor ($IC_{50} = 2.2$ nM). Low emetogenic activity, suggested to be due to poor brain penetration.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₁₆ClN₃O Batch Molecular Weight: 313.79

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

ethanol to 100 mM 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:

Aoki *et al* (2000) A novel phosphodiesterase type 4 inhibitor, YM976 (4-(3-chlorophenyl)-1,7-diethylpyrido[2,3-d]pyrimidin-2(1H)-one), with little emetogenic activity. J.Pharmacol.Exp.Ther. **295** 255. PMID: 10991987.

Aoki et al (2001) Studies on mechanisms of low emetogenicity of YM976, a novel phosphodiesterase type 4 inhibitor. J.Pharmacol.Exp.Ther. **298** 1142. PMID: 11504812.

Moriuchi *et al* (2003) Relaxant effect of YM976, a novel phosphodiesterase 4 inhibitor, on bovine tracheal smooth muscle. Eur.J.Pharmacol. **470** 57. PMID: 12787831.