

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: TC-G 1006 Catalog No.: 4747 Batch No.: 1

CAS Number: 1324003-64-6

IUPAC Name: 4-Methoxy-N-[[[2-trifluoromethyl)[1,1'-biphenyl]-4-yl]amino]carbonyl]-3-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{16}F_3N_3O_3$

Batch Molecular Weight: 415.37 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.6$ (Dichloromethane:Methanol [9:1])

HPLC: Shows >98.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.72 3.88 10.12 Found 60.6 3.97 10.04



Product Information

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Description:

Potent and selective sphingosine-1-phosphate receptor 1 (S1P $_1$) agonist (EC $_{50}$ = 35 nM), displays >100-fold selectivity against receptor subtypes S1P $_{2\cdot5}$. Induces a dose-dependent reduction in circulating blood lymphocyte counts in rodent models. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₁₆F₃N₃O₃ Batch Molecular Weight: 415.37 Physical Appearance: White solid

Minimum Purity: >98%

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:

Pennington *et al* (2011) 4-Methoxy-*N*-[2-(trifluoromethyl)biphenyl-4-ylcarbamoyl]nicotinamide: A Potent and Selective Agonist of S1P₁. ACS Med.Chem.Lett. **2** 752. PMID: 24900263.