

Product Name: TC-G 1006

Catalog No.: 4747

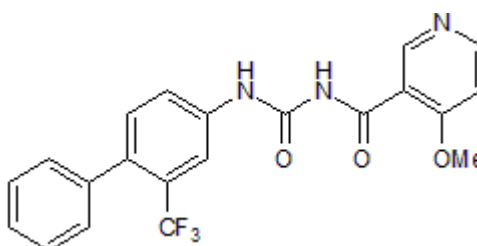
Batch No.: 1

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: C₂₁H₁₆F₃N₃O₃
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

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent and selective sphingosine-1-phosphate receptor 1 (S1P₁) agonist (EC₅₀ = 35 nM), displays >100-fold selectivity against receptor subtypes S1P₂₋₅. Induces a dose-dependent reduction in circulating blood lymphocyte counts in rodent models. Orally bioavailable.

Physical and Chemical Properties:

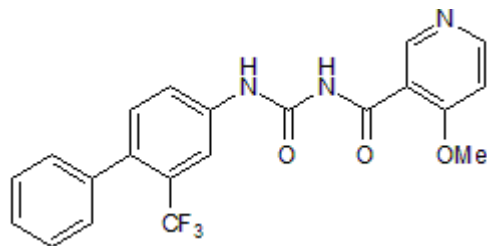
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Batch Molecular Weight: 415.37

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-ylcarbonyl]nicotinamide: A Potent and Selective Agonist of S1P₁. ACS Med.Chem.Lett. **2** (10) 752.

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