

Certificate of Analysis

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Print Date: Jan 14th 2016

Product Name: SEW 2871 Catalog No.: 2284 Batch No.: 2

CAS Number: 256414-75-2

IUPAC Name: 5-[4-Phenyl-5-(trifluoromethyl)thiophen-2-yl]-3-[3-(trifluoromethyl)phenyl]1,2,4-oxadiazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{10}F_6N_2OS$

Batch Molecular Weight: 440.36
Physical Appearance: White solid

Solubility: DMSO to 20 mM

ethanol to 20 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: Between 93 - 94°C HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.55 2.29 6.36 Found 54.56 2.16 6.39



Product Information

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IUPAC Name: 5-[4-Phenyl-5-(trifluoromethyl)thiophen-2-yl]-3-[3-(trifluoromethyl)phenyl]1,2,4-oxadiazole

Description:

Novel, potent and selective sphingosine-1-phosphate 1 (S1P₁) receptor agonist. Activates S1P₁ receptor with an EC₅₀ of 13 nM, but does not activate S1P₂, S1P₃, S1P₄ or S1P₅ receptors at concentrations up to 10 μ M. Cell-permeable and active in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₀H₁₀F₆N₂OS Batch Molecular Weight: 440.36 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 20 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:

Hale *et al* (2004) A rational utilization of high-throughput screening affords selective, orally bioavailable 1-benzyl-3-carboxyazetidine sphingosine-1-phosphate-1 receptor agonists. J.Med.Chem. *47* 6662. PMID: 15615513.

Sanna *et al* (2004) Sphingosine 1-phosphate (S1P) receptor subtypes S1P₁ and S1P₃, respectively, regulate lymphocyte recirculation and heart rate. J.Biol.Chem. **279** 13839. PMID: 14732717.

Bolick *et al* (2005) Sphingosine-1-phosphate prevents tumor necrosis factor-α-mediated monocyte adhesion to aortic endothelium in mice. Arterioscler.Thromb.Vasc.Biol. *25* 976. PMID: 15761190.