

Certificate of Analysis

Print Date: May 1st 2019

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Product Name: PF 514273 Catalog No.: 3676 Batch No.: 2

CAS Number: 851728-60-4

IUPAC Name: 2-(2-Chlorophenyl)-3-(4-chlorophenyl)-7-(2,2-difluoropropyl)-6,7-dihydro-2*H*-pyrazolo[3,4-*f*][1,4]oxazepin-8(5*H*)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{17}CI_2F_2N_3O_2$

Batch Molecular Weight: 452.28 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.77 3.79 9.29 Found 55.84 3.76 9.34

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Product Information

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Description:

High affinity and selective CB_1 receptor antagonist (K_i values are 1 and > 10000 nM at CB_1 and CB_2 receptors respectively). Inhibits food intake in vivo following oral administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₁H₁₇Cl₂F₂N₃O₂

Batch Molecular Weight: 452.28 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 50 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:

Dow *et al* (2009) Discovery of 2-(2-chlorophenyl)-3-(4-chlorophenyl)-7-(2,2-difluoropropyl)-6,7-dihydro-2*H*-pyrazole[3,4-f][1,4]oxazepin-8-(5*H*)-one (PF-514273), a novel, bicyclic lactam-based cannabinoid-1 receptor antagonist for the treatment of J.Med.Chem. *52* 2652. PMID: 19351113.

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