

Certificate of Analysis

Print Date: Aug 8th 2019

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Product Name: C 021 dihydrochloride Catalog No.: 3581 Batch No.: 3

CAS Number: 1784252-84-1

IUPAC Name: 2-[1,4'-Bipiperidin]-1'-yl-N-cycloheptyl-6,7-dimethoxy-4-quinazolinamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{41}N_5O_2.2HCl.2H_2O$

Batch Molecular Weight: 576.6

Physical Appearance: White solid

Solubility: water to 50 mM

DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Dichloromethane:Methanol [4:1])

HPLC: Shows 99.7% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.24 8.22 12.15 Found 56.18 8.18 12.03

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



Product Information

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Description:

Potent CCR4 chemokine receptor antagonist (IC_{50} values are 0.14 and 0.039 μM for inhibition of chemotaxis in human and mouse respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₇H₄₁N₅O₂.2HCl.2H₂O

Batch Molecular Weight: 576.6 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at RT

Solubility & Usage Info:

water to 50 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:

Yokoyama et al (2009) Potent and orally bioavailable CCR4 antagonists: synthesis and structure-activity relationship study of 2-aminoquinazolines. Bioorg.Med.Chem. 17 64. PMID: 19081254.

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