

Certificate of Analysis

Print Date: Nov 4th 2021

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Product Name: CGI 1746 Catalog No.: 6965 Batch No.: 1

CAS Number: 910232-84-7

IUPAC Name: N-[3-[4,5-Dihydro-4-methyl-6-[[4-(4-morpholinylcarbonyl)phenyl]amino]-5-oxo-2-pyrazinyl]-2-methylphenyl]

-4-(1,1-dimethylethyl)benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{34}H_{37}N_5O_4$.

Batch Molecular Weight: 579.7

Physical Appearance: Cream solid

Solubility: ethanol to 20 mM

DMSO to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.45 6.43 12.08 Found 70.16 6.42 12.03



Product Information

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Description:

CGI 1746 is a potent, reversible inhibitor of Bruton's tyrosine kinase (Btk) (IC₅₀ = 1.9 nM). CGI 1746 decreases cell survival in prostate cancer cell lines. In a cell model, CGI 1746 blocks the production of Fc γ R-induced cytokines IL-1 β , TNF α and IL-6 (IC₅₀ values are 36 nM, 47 nM and 353 nM, respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₃₄H₃₇N₅O₄. Batch Molecular Weight: 579.7 Physical Appearance: Cream solid

Minimum Purity: ≥97%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

ethanol to 20 mM DMSO to 5 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:

Kokabee *et al* (2015) Bruton's tyrosine kinase is a potential therapeutic target in prostate cancer. Cancer Biol. Ther. *16* 1604. PMID: 26383180.

Di Paolo et al (2011) Specific Btk inhibition suppresses B cell- and myeloid cell-mediated arthritis. Nat.Chem.Biol. 7 41. PMID: 21113169.

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