

Certificate of Analysis

Print Date: Sep 22nd 2022

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Product Name: BIRB 796 Catalog No.: 5989 Batch No.: 2

CAS Number: 285983-48-4

IUPAC Name: N-[3-(1,1-Dimethylethyl)-1-(4-methylphenyl)-1H-pyrazol-5-yl]-N'-[4-[2-(4-morpholinyl)ethoxy]-1-naphthalenyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{31}H_{37}N_5O_3$ Batch Molecular Weight: 527.66

Physical Appearance: Off-white solid
Solubility: DMSO to 10 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.56 7.07 13.27 Found 70.21 6.69 13.35

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

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Product Information

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Description:

BIRB 796 is a high affinity and selective p38 kinase inhibitor (K_d = 50-100 pM). Exhibits no significant inhibition on a panel of related kinases. Inhibits LPS-induced TNF α production in human PBMCs and whole blood (IC $_{50}$ values are 21 and 960 nM, respectively). Also inhibits JNK2 α 2 and c-Raf-1 (IC $_{50}$ values are 98 nM and 1.4 μ M, respectively). BIRB 796 can be used in protocols for the chemical reprogramming of somatic cells to iPSCs. Cell permeable.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{31}H_{37}N_5O_3$ Batch Molecular Weight: 527.66 Physical Appearance: Off-white solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 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:

Guan et al (2022) Chemical reprogramming of human somatic cells to pluripotent stem cells. Nature 605 325. PMID: 35418683.

Goldstein *et al* (2010) Selective p38 α inhibitors clinically evaluated for the treatment of chronic inflammatory disorders. J.Med.Chem. **53** 2345. PMID: 19950901.

Laufer *et al* (2008) Design, synthesis, and biological evaluation of novel Tri- and tetrasubstituted imidazoles as highly potent and specific ATP-mimetic inhibitors of p38 MAP kinase: focus on optimized interactions with the enzyme's surface-exposed front region. J.Med.Chem. *51* 4122. PMID: 18578517.

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