Certificate of Analysis

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PF CBP1 Product Name:

Catalog No.: 5801 Batch No.: 2

CAS Number: **IUPAC Name:** 1962928-21-7

5-(Dimethyl-1,2-oxazol-4-yl)-1-[2-(morpholin-4-yl)ethyl]-2-[2-(4-propoxyphenyl)ethyl]-1H-1,3-benzodiazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

 $C_{29}H_{36}N_4O_3$ 488.62 White solid DMSO to 100 mM ethanol to 100 mM Store at +4°C

Storage: **Batch Molecular Structure:**

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: Microanalysis:

R_f = 0.44 (Ethyl acetate:Methanol [9:1]) Shows 99.4% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 71.28 7.43 11.47 Found 71.21 7.73 11.45

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

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Print Date: Nov 12th 2019

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5-(Dimethyl-1,2-oxazol-4-yl)-1-[2-(morpholin-4-yl)ethyl]-2-[2-(4-propoxyphenyl)ethyl]-1H-1,3-benzodiazole

Description:

IUPAC Name:

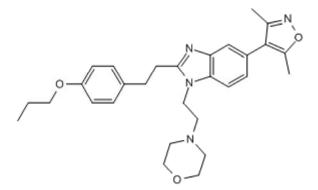
Selective CBP/p300 bromodomain inhibitor (IC₅₀ values are 125 and 363 nM, respectively). Exhibits >100-fold selectivity for CBP over BRD4. Also exhibits selectivity over a panel of other bromodomains. Reduces LPS-induced IL-1 β , IL-6 and IFN- β expression in macrophages in vitro. Also downregulates RGS4 expression in primary cortical neurons in vitro. Negative Control also available.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{29}H_{36}N_4O_3$ Batch Molecular Weight: 488.62 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info: DMSO to 100 mM

ethanol 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 $45-60^{\circ}C$ water bath).

Catalog No.: 5801

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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevent licence or be exempt from restrictions in order to purchase and posess this material.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

References:

Chekler *et al* (2015) Transcriptional profiling of a selective CREB binding protein bromodomain inhibitor highlights therapeutic opportunities. Chem.Biol. **22** 1588. PMID: 26670081.

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