

Certificate of Analysis

Print Date: Apr 6th 2020

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Product Name: NBC 19 Catalog No.: 6722 Batch No.: 1

CAS Number: 2068818-75-5

IUPAC Name: (T4)-[2-Acetyl-4,4,4-trichloro-*N*-cyclohexyl-3-(imino- κN)butanamidato- κO]diphenylboron

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{24}H_{26}BCI_3N_2O_2$ **Batch Molecular Formula:**

Batch Molecular Weight: 491.64

Physical Appearance: Light yellow solid DMSO to 100 mM Solubility:

ethanol to 100 mM

Storage: Store at -20°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 58.63 5.33 5.7 Found 58.47 5.3 5.4

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

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Product Information

Print Date: Apr 6th 2020

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Product Name: NBC 19 Catalog No.: 6722 Batch No.: 1

CAS Number: 2068818-75-5

IUPAC Name: (74)-[2-Acetyl-4,4,4-trichloro-N-cyclohexyl-3-(imino-κN)butanamidato-κO]diphenylboron

Description:

Potent NLRP3 inflammasome inhibitor ($IC_{50} = 60-80$ nM). Inhibits nigericin- and ATP-induced IL-1 β release.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₂₆BCl₃N₂O₂

Batch Molecular Weight: 491.64

Physical Appearance: Light yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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°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.

Licensing Information:

Sold under license from the University of Manchester.

References:

Redondo-Castro *et al* (2018) Development of a characterised tool kit for the interrogation of NLRP3 inflammasome-dependent responses. Sci.Rep. *8* 5667. PMID: 29618797.

Baldwin et al (2017) Boron-Based Inhibitors of the NLRP3 Inflammasome. Cell Chem.Biol. 24 1321. PMID: 28943355.