

# **Certificate of Analysis**

Print Date: Sep 13th 2021

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Product Name: ML 299 Catalog No.: 4894 Batch No.: 1

CAS Number: 1426916-00-8

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>26</sub>BrFN<sub>4</sub>O<sub>2</sub>.

Batch Molecular Weight: 489.39

Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

Chiral HPLC: Shows 100.0% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 56.45 5.36 11.45

Found 56.36 5.37 11.41

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# **Product Information**

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CAS Number: 1426916-00-8

#### **Description:**

ML 299 is a selective allosteric modulator and potent inhibitor of phospholipases D1 and D2 (IC $_{50}$  values are 6 and 12 nM, respectively). ML 299 decreases invasive migration in glioblastoma cells and increases caspase 3/7 activity in serum-free conditions. ML 299 is non-cytotoxic, active in vivo and CNS penetrant.

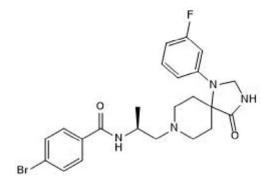
# **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{23}H_{26}BrFN_4O_2$ .

Batch Molecular Weight: 489.39 Physical Appearance: White solid

Minimum Purity: ≥98%

#### **Batch Molecular Structure:**



Storage: Store at -20°C

# Solubility & Usage Info:

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:

**O'Reilly** *et al* (2013) Development of dual PLD1/2 and PLD2 selective inhibitors from a common 1,3,8-triazaspiro[4.5]decane core: discovery of ML298 and ML299 that decrease invasive migration in U87-MG glioblastoma cells. J.Med.Chem. *56* 2695. PMID: 23445448.