



Certificate of Analysis

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Product Name: ML 240 Catalog No.: 5153 Batch No.: 1

CAS Number: 1346527-98-7

IUPAC Name: 2-(2-Amino-1*H*-benzimidazole-1-yl)-8-methoxy-*N*-(phenylmethyl)-4-quinazolinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\begin{array}{lll} \textbf{Batch Molecular Formula:} & \textbf{C_{23}H}_{20}$N}_{6}$O \\ \textbf{Batch Molecular Weight:} & 396.44 \\ \textbf{Physical Appearance:} & \textbf{White solid} \\ \textbf{Solubility:} & \textbf{DMSO to 20 mM} \\ \end{array}$

Batch Molecular Structure:

Storage:

Store at +4°C

2. ANALYTICAL DATA

TLC: $R_f = 0.31$ (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 69.68 5.08 21.2 Found 69.33 5.06 21.07



Product Information

Print Date: Jun 10th 2017

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Description:

ATP-competitive inhibitor of p97 ATPase (VCP, IC $_{50}$ = 110 nM). Exhibits antiproliferative activity in NCI-60 cancer cell lines and rapidly induces executioner caspases 3 and 7 in multiple colon cancer cells. Promotes accumulation of LC3-II and impairs autophagosome maturation. Also impairs the endoplasmic-reticulum-associated degradation (ERAD) pathway.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₂₀N₆O Batch Molecular Weight: 396.44 Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 20 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:

Chou et al (2013) Structure-activity relationship study reveals ML240 and ML241 as potent and selective inhibitors of p97 ATPase. ChemMedChem 8 297. PMID: 23316025.