Print Date: Nov 13th 2017

Certificate of Analysis

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Product Name: **ML 311** **Catalog No.: 5733** **Batch No.: 1**

CAS Number: 315698-17-0

IUPAC Name: 7-[(4-Ethyl-1-piperazinyl)[4-(trifluoromethyl)phenyl]methyl]-8-quinolinol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{24}F_3N_3O$

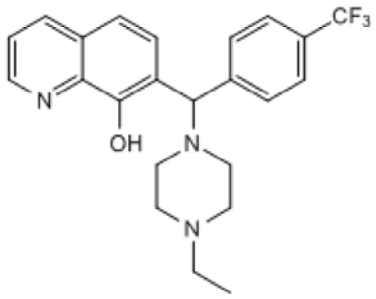
Batch Molecular Weight: 415.45

Physical Appearance: White solid

Solubility: DMSO to 50 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (20% MeOH/DCM/4 drops NH4OH)

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.49	5.82	10.11
Found	66.52	5.74	10.14

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Product Information

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CAS Number: 315698-17-0

IUPAC Name: 7-[(4-Ethyl-1-piperazinyl)[4-(trifluoromethyl)phenyl]methyl]-8-quinolinol

Description:

Inhibits Mcl1-BIM interaction. Inhibits viability of Mcl1-dependent tumor cell lines. Induces cell death and decreased spheroid formation in Her2 positive breast cancer cells.

Physical and Chemical Properties:

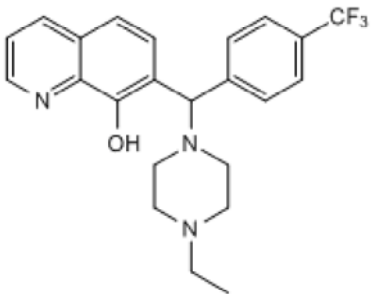
Batch Molecular Formula: $C_{23}H_{24}F_3N_3O$

Batch Molecular Weight: 415.45

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 mM
ethanol to 50 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:

Bashari *et al* (2016) Mcl-1 confers protection of Her2-positive breast cancer cells to hypoxia: therapeutic implications. Breast Cancer Res. ***18*** 26. PMID: 26921175.

Bannister *et al* (2012) ML311: A small molecule that potently and selectively disrupts the protein-protein interaction of Mcl-1 and Bim: a probe for studying lymphoid tumorigenesis. Probe Reports from the NIH Molecular Libraries Program. PMID: 23762927.