

Print Date: Jan 16th 2016

Certificate of Analysis

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Product Name: ML 349 Catalog No.: 5344 Batch No.: 1

CAS Number: 890819-86-0

IUPAC Name: (5,5-Dioxido-4*H*-thieno[3,2-c][1]benzothiopyran-2-yl)[4-(4-methoxyphenyl)-1-piperazinyl]methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}N_2O_4S_2.^{1/4}H_2O$

Batch Molecular Weight: 459.06

Physical Appearance: Off-white solid
Solubility: DMSO to 20 mM
Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity **1H NMR:** Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 60.18 4.94 6.1 Found 60.18 4.8 6.11



Product Information

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Description:

Selective and reversible lysophospholipase 2 (LYPLA2) inhibitor ($IC_{50} = 144$ nM). Displays selectively over LYPLA1 and 20 other serine hydrolases (IC_{50} values are >3000 and >10,000 nM respectively).

Physical and Chemical Properties:

Batch Molecular Formula: $C_{23}H_{22}N_2O_4S_2$. $\frac{1}{4}H_2O$

Batch Molecular Weight: 459.06 Physical Appearance: Off-white solid

Minimum Purity: >98%

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:

Adibekian et al (2010) Characterization of a selective, reversible inhibitor of lysophospholipase 2 (LYPLA2). Probe Reports from the NIH Molecular Libraries Program. PMID: 24624468.

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