

# **Certificate of Analysis**

Print Date: Jul 28th 2020

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Product Name: MS049 oxalate salt Catalog No.: 5685 Batch No.: 1

IUPAC Name: N-Methyl-4-(phenylmethoxy)-1-piperidineethanamine oxalate salt

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{15}H_{24}N_2O.C_2H_2O_4.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 347.41

Physical Appearance: White solid

Solubility: water to 100 mM

DMSO to 20 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.06 (Dichloromethane:Methanol:Ammonia soln. [95:5:1])

**HPLC:** Shows 100% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.77 7.83 8.06 Found 58.73 7.57 7.99

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# **Product Information**

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IUPAC Name: N-Methyl-4-(phenylmethoxy)-1-piperidineethanamine oxalate salt

#### **Description:**

Potent and selective PRMT4 and PRMT6 inhibitor (IC $_{50}$  values are 44 and 63 nM, respectively). Reduces Med12me2a and H3R2me2a levels in HEK293 cells in vitro. To request the negative control for MS049, please fill out the MS049N request form on the SGC website.

# **Physical and Chemical Properties:**

Batch Molecular Formula:  $C_{15}H_{24}N_2O.C_2H_2O_4.\frac{1}{2}H_2O$ 

Batch Molecular Weight: 347.41 Physical Appearance: White solid

Minimum Purity: ≥98%

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

Storage: Desiccate at RT

# Solubility & Usage Info:

water to 100 mM 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.

### **Licensing Information:**

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the MS049 probe summary on the SGC website.

#### References:

**Scheer** *et al* (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. Nat.Commun. *10* 19. PMID: 30604761.

**Shen** et al (2016) Discovery of a potent, selective, and cell-active dual inhibitor of protein arginine methyltransferase 4 and protein arginine methyltransferase 6. J.Med.Chem. **59** 9124. PMID: 27584694.