Certificate of Analysis

Product Name: **MS 023 dihydrochloride** **Catalog No.: 5713** **Batch No.: 2**

CAS Number: 1992047-64-9

IUPAC Name: N^1-Methyl-N^1-[[4-[4-(1-methylethoxy)phenyl]-1*H*-pyrrol-3-yl]methyl]-1,2-ethanediamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{25}N_3O.2HCl.1½H_2O$

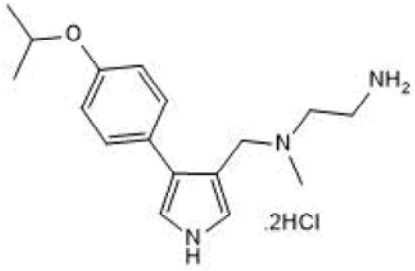
Batch Molecular Weight: 387.34

Physical Appearance: Pink solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.71	7.81	10.85
Found	53.1	7.79	10.75

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Description:

MS 023 dihydrochloride is a potent and selective type I PRMT inhibitor (IC_{50} values are 8, 8, 30, 83 and 119 nM for PRMT6, PRMT8, PRMT1, PRMT4 and PRMT3, respectively). Exhibits no significant activity against type II and III PRMTs, PKMTs, DNMTs, KDMs and reader proteins. Reduces global arginine asymmetric dimethylation levels in vitro. Also inhibits and reduces TGF-β-activated kinase 1 expression and protein levels.

Physical and Chemical Properties:

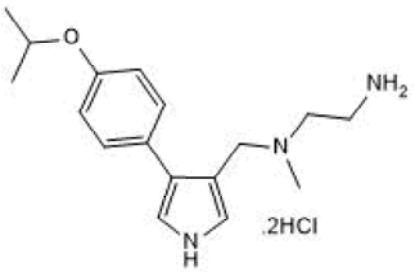
Batch Molecular Formula: $C_{17}H_{25}N_3O.2HCl.1½H_2O$

Batch Molecular Weight: 387.34

Physical Appearance: Pink solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM
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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the MS023 probe summary on the SGC website.

References:

Scheer *et al* (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. Nat.Commun. ***11*** 19. PMID: 30604761.

Eram *et al* (2016) A potent, selective, and cell-active inhibitor of human type I protein arginine methyltransferases. ACS Chem.Biol. ***11*** 772. PMID: 26598975.