



Certificate of Analysis

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Product Name: A 366 Catalog No.: 5163 Batch No.: 1

CAS Number: 1527503-11-2

IUPAC Name: 5'-Methoxy-6'-[3-(1-pyrrolidinyl)propoxy]spiro[cyclobutane-1,3'-[3*H*]indol]-2'-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{27}N_3O_2$. $^{1/2}H_2O$

Batch Molecular Weight: 338.45 **Physical Appearance:** Cream solid

Solubility: 1eq. HCl to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

N O NH2

2. ANALYTICAL DATA

TLC: $R_f = 0.26 (10\% 2M NH3/MeOH in DCM)$

HPLC: Shows 99.2% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 67.43 8.34 12.42 Found 67.04 8.18 12.25



Product Information

Print Date: Oct 9th 2014

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Description:

Potent and selective G9a/GLP histone lysine methyltransferase inhibitor (IC $_{50}$ = 3.3 nM). Exhibits >1000-fold selectivity for G9a/GLP over 21 other methyltransferases. Decreases levels of lysine 9 dimethylation on histone H3 (H3K9Me2) in PC3 cells.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{19}H_{27}N_3O_2$. $1/2H_2O$

Batch Molecular Weight: 338.45 Physical Appearance: Cream solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl 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.

References:

Sweis et al (2014) Discovery and development of potent and selective inhibitors of histone methyltransferase G9a. ACS Med.Chem.Lett. 5 205. PMID: 24900801.

