

Certificate of Analysis

Print Date: Jan 17th 2017

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Product Name: RN 1 dihydrochloride Catalog No.: 4977 Batch No.: 2

CAS Number: 1781835-13-9

IUPAC Name: $1-(4-\text{methyl}-1-\text{piperazinyl})-2-[[(1R^*,2S^*)-2-[4-\text{phenylmethoxy})\text{phenyl}]\text{cyclopropyl}]$ amino]ethanone dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{29}N_3O_2.2HCI.H_2O$

Batch Molecular Weight: 470.44

Physical Appearance: White solid

Solubility: water to 20 mM

DMSO to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

.2HCl (and enantiomer)

2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.72 7.07 8.93 Found 58.74 7.16 8.83



Product Information

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IUPAC Name: 1-(4-methyl-1-piperazinyl)-2-[[(1R*,2S*)-2-[4-phenylmethoxy)phenyl]cyclopropyl]amino]ethanone dihydrochloride

Description:

Potent lysine specific demethylase 1 (LSD1) inhibitor (IC $_{50}$ = 70 nM). Exhibits selectivity for LSD1 over MAO-A and MAO-B (IC $_{50}$ values are 0.51 and 2.79 μ M for MAO-A and MAO-B, respectively). Impairs long-term, but not short-term memory in mice. Brain penetrant following systemic administration.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{23}H_{29}N_3O_2.2HCI.H_2O$

Batch Molecular Weight: 470.44 Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

water to 20 mM

DMSO to 20 mM with gentle warming

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).

Catalog No.: 4977

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:

Neelamegam et al (2012) Brain-penetrant LSD1 inhibitors can block memory consolidation. ACS Chem.Neurosci. 3 120. PMID: 22754608.