

Certificate of Analysis

Print Date: Sep 22nd 2020

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Product Name: ABT 089 dihydrochloride Catalog No.: 5079 Batch No.: 1

CAS Number: 161416-61-1

IUPAC Name: 2-Methyl-3-[(2S)-pyrrolidinylmethoxy]pyridine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{11}H_{16}N_2O.2HCI.H_2O$

Batch Molecular Weight: 283.2

Physical Appearance: White solid

Solubility: water to 100 mM

DMSO to 20 mM

Storage: Desiccate at RT

Batch Molecular Structure:

N 2HCI

2. ANALYTICAL DATA

TLC: R_f = 0.31 (Dichloromethane / 2M Ammonia in Methanol 19:1)

HPLC: Shows 99.6% purity
Chiral HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +20.4$ (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 46.65 7.12 9.89 Found 46.69 6.85 9.76

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Product Information

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Batch No.: 1

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CAS Number: 161416-61-1

IUPAC Name: 2-Methyl-3-[(2S)-pyrrolidinylmethoxy]pyridine dihydrochloride

Description:

High affinity and selective $\alpha 4\beta 2$ partial agonist ($K_i = 16$ nM). Exhibits >1000-fold and >10,000-fold selectivity for $\alpha 4\beta 2$ over $\alpha 1\beta 1\gamma 1$ and $\alpha 7$ receptors respectively. Neuroprotective against glutamate-induced toxicity in rat cortical neurons in vitro. Enhances cognitive performance in vivo. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₁H₁₆N₂O.2HCl.H₂O

Batch Molecular Weight: 283.2 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).

Catalog No.: 5079

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:

Rueter *et al* (2004) ABT-089: pharmacological properties of a neuronal nicotinic acetylcholine receptor agonist for the potential treatment of cognitive disorders. CNS Drug Rev. *10* 167. PMID: 15179445.

Decker *et al* (1997) ABT-089 [2-methyl-3-(2-(S)-pyrrolidinylmethoxy)pyridine dihydrochloride]: II. A novel cholinergic channel modulator with effects on cognitive performance in rats and monkeys. J.Pharmacol.Exp.Ther. **283** 247. PMID: 9336330.

Sullivan *et al* (1997) ABT-089 [2-methyl-3-(2-(S)-pyrrolidinylmethoxy)pyridine]: I. A potent and selective cholinergic channel modulator with neuroprotective properties. J.Pharmacol.Exp.Ther. **283** 235. PMID: 9336329.

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