

Certificate of Analysis

Print Date: Jan 14th 2016

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Product Name: AR-R 17779 hydrochloride Catalog No.: 3964 Batch No.: 2

CAS Number: 178419-42-6

IUPAC Name: (3S)-Spiro[1-azabicyclo[2.2.2]octane-3,5'-oxazolidine]-2'-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_0H_{14}N_2O_2.HCI.\frac{1}{2}H_2O$

Batch Molecular Weight: 227.69

Physical Appearance: Off-white solid

Solubility: DMSO to 50 mM water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

NH O HCI

2. ANALYTICAL DATA

TLC: $R_f = 0.1$ (Chloroform:Methanol [2:1])

Chiral HPLC: Shows 99.3% purity

Consistent with struct

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

Optical Rotation: $[\alpha]_D = +62$ (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.48 7.08 12.3 Found 47.14 7 12.37



Product Information

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Description:

Selective agonist of $\alpha 7$ nAChRs (K $_i$ values are 190 and 16000 nM for rat $\alpha 7$ and $\alpha 4\beta 2$ receptors respectively). CNS penetrant after systemic administration.

Physical and Chemical Properties:

Batch Molecular Formula: C₉H₁₄N₂O₂.HCl.½H₂O

Batch Molecular Weight: 227.69 Physical Appearance: Off-white solid

Batch Molecular Structure:

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 50 mM water to 100 mM

CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival.

Catalog No.: 3964

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:

Grottick *et al* (2000) Evidence that nicotinic α_7 receptors are not involved in the hyperlocomotor and rewarding effects of nicotine. J.Pharmacol.Exp.Ther. **294** 1112. PMID: 10945867.

Mullen *et al* (2000) (-)-spiro[1-azabicyclo[2.2.2]octane-3,5'-oxazolidin-2'-one], a conformationally restricted analogue of acetylcholine, is a highly selective full agonist at the α7 nicotinic acetylcholine receptor. J.Med.Chem. *43* 4045. PMID: 11063601.

Huang *et al* (2010) Activation of presynaptic α7 nicotinic receptors evokes an excitatory response in hippocampal CA3 neurones in anaesthetized rats: an *in vivo* iontophoretic study. Br.J.Pharmacol. *159* 554. PMID: 20105181.

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