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Certificate of Analysis

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Print Date: Oct 30th 2019

Product Name: (S)-(-)-5-lodowillardiine CAS Number: 140187-25-3 Catalog No.: 0307 Batc

Batch No.: 6

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure:

C₇H₈IN₃O₄ 325.06 White solid 1.1eq. NaOH to 25 mM Store at RT

2. ANALYTICAL DATA

TLC: Chiral HPLC: ¹H NMR: Mass Spectrum: Optical Rotation: Microanalysis: $\label{eq:response} \begin{array}{l} \mathsf{R}_{\mathsf{f}} = 0.29 \ (\mathsf{Pyridine:Acetic acid:Water:Butanol [3:8:11:33]}) \\ \mathsf{Shows } 98.1\% \ \mathsf{purity} \\ \mathsf{Consistent with structure} \\ \mathsf{Consistent with structure} \\ [\alpha]_{\mathsf{D}} = +14.8 \ (\mathsf{Concentration} = 0.5, \ \mathsf{Solvent} = 6\mathsf{N} \ \mathsf{HCI}) \\ & \mathsf{Carbon} \ \mathsf{Hydrogen} \ \mathsf{Nitrogen} \\ \mathsf{Theoretical} \ 25.86 \ 2.48 \ 12.92 \\ \mathsf{Found} \ 25.85 \ 2.56 \ 12.71 \end{array}$

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Product Name: (*S*)-(-)-5-lodowillardiine

CAS Number: 140187-25-3

Catalog No.: 0307 Ba

Batch No.: 6

Description:

Demonstrates high affinity for the kainate receptor subtype hGluK1 (formerly hGluR5) ($K_i = 0.24$ nM) and 600-4000-fold selectivity over both the AMPA receptor subtypes and the homomeric kainate receptor hGluK2 (formerly hGluR6). Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions.

Physical and Chemical Properties:

Batch Molecular Formula: C₇H₈IN₃O₄ Batch Molecular Weight: 325.06 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

1.1eq. NaOH to 25 mM

Solutions of this product of up to 50mM (14mg/ml) are best prepared using 1eq. of NaOH solution with gentle warming if necessary (avoid excessive heating). Occasionally a slight excess - up to 15% - of NaOH may be advantageous. Aqueous solutions of pH7-9 are stable for several days; they should be kept frozen (-20°C) when not in use

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:

Swanson et al (1998) Kainate receptors exhibit differential sensitivities to (S)-5-iodowillardiine. Mol. Pharmacol. 53 942. PMID: 9584222.

Jane et al (1997) Synthesis of willardiine and 6-azawillardiine analogs: pharmacological characterization on cloned homomeric human AMPA and kainate receptor subtypes. J.Med.Chem. **40** 3645. PMID: 9357531.

Thompson *et al* (1996) Depolarising effects of certain derivatives of (S) willardiine upon *in vitro* neonatal rat dorsal roots. Br.J.Pharmacol. **117** 331P.

Wong *et al* (1994) Willardiines differentiate agonist binding sites for kainate-versus AMPA-preferring glutamate receptors in DRG and hippocampal neurones. J.Neurosci. **14** 3881. PMID: 7515954.

Patneau *et al* (1992) Activation and desensitization of AMPA/kainate receptors by novel derivatives of willardiine. J.Neurosci. **12** 595. PMID: 1371315.

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