Certificate of Analysis

Print Date: Oct 16th 2024

Product Name: CGP 78608 hydrochloride

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Catalog No.: 1493 Batch No.: 2

CAS Number: IUPAC Name:

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1135278-54-4

[(1S)-1-[[(7-Bromo-1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxalinyl)methyl]amino]ethyl]phosphonic acid hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C₁₁H₁₃BrN₃O₅P.HCl.½H₂O 423.59 White solid 2.2eq. NaOH to 100 mM Store at RT



31.21

3.44

9.73

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Butanol:Acetic acid:Water [40:10:25])Melting Point:At 260°C(dec)HPLC:Shows 98.4% purity¹H NMR:Consistent with structureMicroanalysis:Carbon Hydrogen NitrogenTheoretical 31.193.579.92

Found

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

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2

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Description:

CGP 78608 hydrochloride is a potent and selective NMDA antagonist that acts through the glycine site ($IC_{50} = 5 \text{ nM}$). Displays > 500-fold selectivity over kainate and AMPA receptors (IC_{50} values are 2.7 and 3 μ M respectively). Also potentiates GluN1/GluN3A-mediated glycine currents ($EC_{50} = 26.3 \text{ nM}$). Anticonvulsant in vivo following systemic administration.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{11}H_{13}BrN_3O_5P.HCl.\frac{1}{2}H_2O$ Batch Molecular Weight: 423.59 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info: 2.2eq. NaOH 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).

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Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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.

Licensing Information:

Sold with the permission of Novartis Pharma AG

References:

Grand et al (2018) Unmasking GluN1/GluN3A excitatory glycine NMDA receptors. Nat.Commun. 9 4769. PMID: 30425244.

Ametamey *et al* (2000) Synthesis, radiolabelling and biological characterization of (D)-7-iodo-*N*-(1-phosphonoethyl)l-5aminomethylquinoxaline-2,3-dione, a glycine-binding site antagonist of NMDA receptors. Bioorg.Med.Chem.Lett. **10** 75. PMID: 10636248.

Auberson *et al* (1999) N-phosphonoalkyl-5-aminomethylquinoxaline-2,3-diones: *in vivo* active AMPA and NMDA(glycine) antagonists. Bioorg.Med.Chem.Lett. **9** 249. PMID: 10021939.

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