

Certificate of Analysis

Print Date: Nov 10th 2021

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Product Name: CGP 54626 hydrochloride Catalog No.: 1088 Batch No.: 2

CAS Number: 149184-21-4

 $IUPAC \ Name: \ [S-(R^*,R^*)]-[3-[[1-(3,4-Dichlorophenyl)ethyl]amino]-2-hydroxypropyl] (cyclohexylmethyl) \ phosphinic \ acid$

DMSO to 50 mM

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₈Cl₂NO₃P.HCl

Batch Molecular Weight: 444.76 **Physical Appearance:** White solid

ethanol to 10 mM with gentle warming

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Solubility:

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -32.7$ (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 48.61 6.57 3.15 Found 48.51 6.6 2.96

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Product Information

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CAS Number: 149184-21-4

IUPAC Name: [S-(R*,R*)]-[3-[[1-(3,4-Dichlorophenyl)ethyl]amino]-2-hydroxypropyl](cyclohexylmethyl) phosphinic acid

Description:

CGP 54626 hydrochloride is a potent, selective GABA $_{\rm B}$ receptor antagonist (IC $_{50}$ = 4 nM).

Physical and Chemical Properties:

Batch Molecular Formula: C₁₈H₂₈Cl₂NO₃P.HCl

Batch Molecular Weight: 444.76 Physical Appearance: White solid

Minimum Purity: ≥96%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:

DMSO to 50 mM

ethanol to 10 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.: 1088

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.

Licensing Information:

Sold with the permission of Novartis Pharma AG

References:

Kaupmann *et al* (1998) GABA_B-receptor subtypes assemble into functional heteromeric complexes. Nature **396** 683. PMID: 9872317. **Froestl** *et al* (1996) Potent, orally active GABA_B receptor antagonists. Pharmacol.Rev.Comm. **8** 127.

Brugger *et al* (1993) The action of new potent GABA_B receptor antagonists in the hemisected spinal cord preparation of the rat. Eur.J.Pharmacol. *235* 153. PMID: 8390938.

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