

Certificate of Analysis

Print Date: May 17th 2022

Batch No.: 1

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Catalog No.: 4236

Product Name: CP 945598 hydrochloride

CAS Number: 686347-12-6

IUPAC Name: 1-[8-(2-Chlorophenyl)-9-(4-chlorophenyl)-9*H*-purin-6-yl]-4-(ethylamino)piperidine-4-carboxamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₅Cl₂N₇O.HCl

Batch Molecular Weight: 546.88

Physical Appearance: White solid

Solubility: DMSO to 20 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 54.91 4.79 17.93 Found 54.89 4.72 17.68

Tel: +44 (0)1235 529449 www.tocris.com/distri Tel:+1 612 379 2956



Product Information

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IUPAC Name: 1-[8-(2-Chlorophenyl)-9-(4-chlorophenyl)-9H-purin-6-yl]-4-(ethylamino)piperidine-4-carboxamide hydrochloride

Description:

CP 945598 hydrochloride is a selective, high affinity CB_1 antagonist (K_i values are 0.7 and 0.12 nM in binding and functional assays respectively). Displays low affinity for CB_2 receptors (K_i = 7600 nM).

Physical and Chemical Properties:

Batch Molecular Formula: C25H25Cl2N7O.HCl

Batch Molecular Weight: 546.88 Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

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).

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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. 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 for research purposes under agreement from Pfizer Inc.

References:

Hadcock *et al* (2010) *In vitro* and *in vivo* pharmacology of CP-945,598, a potent and selective cannabinoid CB₁ receptor antagonist for the management of obesity. Biochem.Biophys.Res.Commun. **394** 366. PMID: 20211605.

Griffith *et al* (2009) Discovery of 1-[9-(4-Chlorophenyl)-8-(2-chlorophenyl)-9H-purin-6-yl]-4-ethylaminopiperidine-4-carboxylic acid amide hydrochloride (CP-945,598), a novel, potent, and selective cannabinoid type 1 receptor antagonist. J.Med.Chem. *52* 234. PMID: 19102698.

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