

Certificate of Analysis

Product Name: CP 945598 hydrochloride

Catalog No.: 4236

Batch No.: 1

CAS Number: 686347-12-6

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₅Cl₂N₇O.HCl

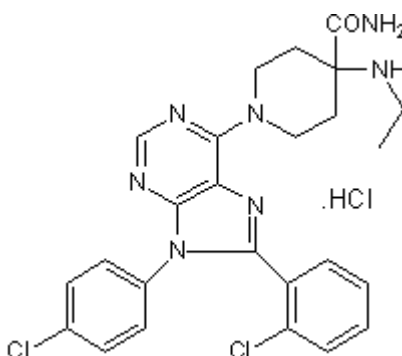
Batch Molecular Weight: 546.88

Physical Appearance: White solid

Solubility: DMSO to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% 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

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

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Description:

Selective, high affinity CB₁ antagonist (K_i values are 0.7 and 0.12 nM in binding and functional assays respectively). Displays low affinity for CB₂ receptors (K_i = 7600 nM).

Physical and Chemical Properties:

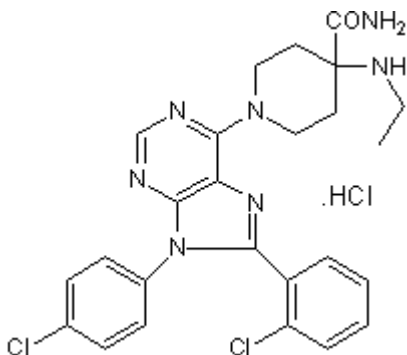
Batch Molecular Formula: C₂₅H₂₅Cl₂N₇O.HCl

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).

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:

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.

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.

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