



# **Certificate of Analysis**

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Batch No.: 7

**Product Name:** SCH 79797 dihydrochloride Catalog No.: 1592

CAS Number: 1216720-69-2

**IUPAC Name:** N<sup>3</sup>-Cyclopropyl-7-[[4-(1-methylethyl)phenyl]methyl]-7*H*-pyrrolo[3,2-f]quinazoline-1,3-diamine dihydrochloride

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C23H25N5.2HCI

444.41 **Batch Molecular Weight:** 

**Physical Appearance:** Yellow solid Solubility: ethanol to 5 mM

DMSO to 50 mM

Desiccate at RT Storage:

**Batch Molecular Structure:** 

# 2. ANALYTICAL DATA

**HPLC**: Shows 99.0% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

> Theoretical 62.16 6.12 15.76 15.96 Found 61.99 6.02 16.34 15.84

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# **Product Information**

Print Date: Nov 18th 2020

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## **Description:**

Potent, selective non-peptide PAR<sub>1</sub> receptor antagonist (IC<sub>50</sub> = 70 nM). Inhibits haTRAP-induced- but not  $\gamma$ -thrombin-, ADP- or collagen-induced human platelet aggregation. Selectively blocks PAR<sub>1</sub> agonist- or thrombin-induced increases in cytosolic Ca<sup>2+</sup> in vascular smooth muscle cells. Also broad spectrum antibiotic. Kills bacteria by a dual action of inhibiting dihydrofolate reductase and interfering with bacterial cell membrane integrity.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C23H25N5.2HCI

Batch Molecular Weight: 444.41 Physical Appearance: Yellow solid

**Minimum Purity**: ≥99%

#### **Batch Molecular Structure:**

Storage: Desiccate at RT

### Solubility & Usage Info:

ethanol to 5 mM DMSO to 50 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).

Catalog No.: 1592

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:

Martin et al (2020) A dual-mechanism antibiotic kills Gram-negative bacteria and avoids drug resistance. Cell **\$0092-8674** 30567. PMID: 32497502.

**Lidington** *et al* (2005) A role for proteinase-activated receptor 2 and PKC-ε in thrombin-mediated induction of decay-accelerating factor on human endothelial cells. Am.J.Physiol.Cell Physiol. **289** C1437. PMID: 16079188.

**Ahn** et al (2000) Inhibition of cellular action of thrombin by N3-cyclopropyl-7-{[4-(1-methylethyl)phenyl]methyl}-7H-pyrrolo[3,2-f] quinazoline-1,3-diamine (SCH 79797), a nonpeptide thrombin receptor antagonist. Biochem.Pharmacol. **60** 1425. PMID: 11020444.

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