Print Date: Feb 16th 2014

Certificate of Analysis

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Product Name: **SCH 79797 dihydrochloride** **Catalog No.: 1592** **Batch No.: 4**

CAS Number: 1216720-69-2

IUPAC Name: N^3-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: $C_{23}H_{25}N_5.2HCl$

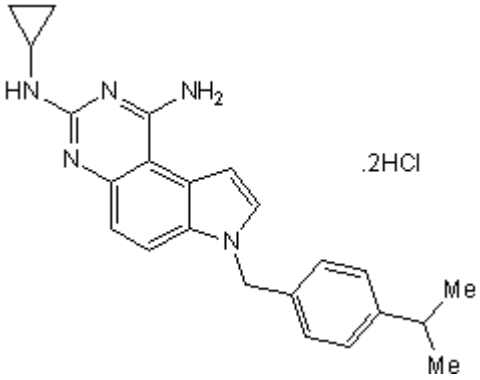
Batch Molecular Weight: 444.41

Physical Appearance: Yellow solid

Solubility: ethanol to 25 mM
DMSO to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.16	6.12	15.76
Found	62.01	6.08	15.55

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Description:

Potent, selective non-peptide PAR_1 receptor antagonist (IC_{50} = 70 nM). Inhibits haTRAP-induced- but not γ-thrombin-, ADP- or collagen-induced human platelet aggregation. Also selectively blocks PAR_1 agonist- or thrombin-induced increases in cytosolic Ca^{2+} in vascular smooth muscle cells.

Physical and Chemical Properties:

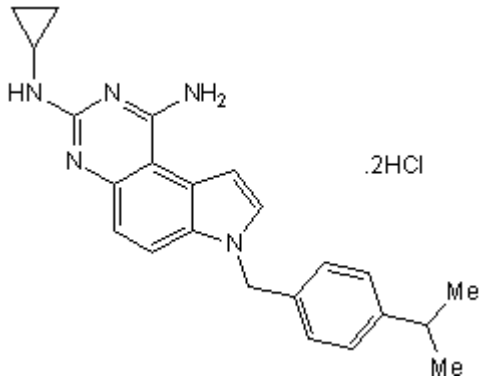
Batch Molecular Formula: $C_{23}H_{25}N_5.2HCl$

Batch Molecular Weight: 444.41

Physical Appearance: Yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

ethanol to 25 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).

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:

Ahn *et al* (1999) Structure-activity relationships of pyrroloquinazolines as thrombin receptor antagonists. Bioorg.Med.Chem.Lett. ***9*** 2073. PMID: 10450984.

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

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.