

Certificate of Analysis

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Product Name: Q94 hydrochloride

Catalog No.: 4755

Batch No.: 1

CAS Number: 1052076-77-3

IUPAC Name: 1-[(4-Chlorophenyl)methyl]-2-(phenylmethyl)-1*H*-benzimidazole hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₁₇ClN₂.HCl

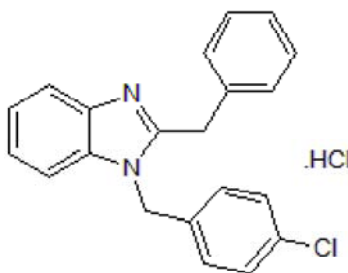
Batch Molecular Weight: 369.29

Physical Appearance: Grey solid

Solubility: DMSO to 50 mM
ethanol to 50 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	68.3	4.91	7.59
Found	68.3	4.97	7.64

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

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Description:

PAR₁ negative allosteric modulator (IC₅₀ = 916 nM); inhibits PAR₁-Gα_q interaction. Selective for PAR₁ over PAR₂. Blocks thrombin-induced intracellular calcium mobilization (IC₅₀ = 10.3 nM), CCL2 expression, ERK1/2 and MLC phosphorylation, and IP₃ production in cells.

Physical and Chemical Properties:

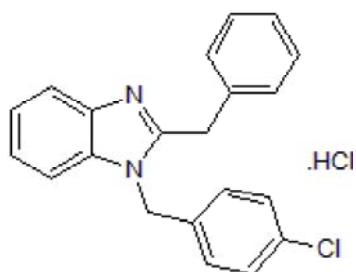
Batch Molecular Formula: C₂₁H₁₇ClN₂.HCl

Batch Molecular Weight: 369.29

Physical Appearance: Grey solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol 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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

References:

Asteriti *et al* (2012) Modulation of PAR₁ signalling by benzimidazole compounds. *Br.J.Pharmacol.* **167** 80. PMID: 22519452.

Scotton *et al* (2009) Increased local expression of coagulation factor X contributes to the fibrotic response in human and murine lung injury. *J.Clin.Invest.* **119** 2550. PMID: 19652365.

Deng *et al* (2008) Thrombin induces fibroblast CCL2/JE production and release via coupling of PAR₁ to Gα_q and cooperation between ERK1/2 and Rho kinase signaling pathways. *Mol.Biol.Cell* **19** 2520. PMID: 18353977.

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