



Certificate of Analysis

www.tocris.com

Product Name: Ro 1138452 hydrochloride Catalog No.: 4268 Batch No.: 1

IUPAC Name: 4,5-Dihydro-*N*-[4-[[4-(1-methylethoxy)phenyl]methyl]phenyl]-1*H*-imidazol-2-amine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{23}N_3O.HCI$

Batch Molecular Weight: 345.87 **Physical Appearance:** White solid

Solubility: water to 100 mM DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.3 (40\% Dichloromethane: Methanol + 2\% NH4OH)$

HPLC: Shows 99% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.98 6.99 12.15 Found 65.87 6.93 12.16



Product Information

Print Date: Jan 16th 2016

www.tocris.com

Product Name: Ro 1138452 hydrochloride Catalog No.: 4268 Batch No.: 1

IUPAC Name: 4,5-Dihydro-*N*-[4-[[4-(1-methylethoxy)phenyl]methyl]phenyl]-1*H*-imidazol-2-amine hydrochloride

Description:

Selective prostacyclin IP receptor antagonist (pK_i = 8.3). Exhibits no affinity at other prostanoid receptors (EP₁₋₄, FP and TP) in a radioligand binding assay. Demonstrates analgesic activity in rats. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₂₃N₃O.HCl

Batch Molecular Weight: 345.87 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate at RT

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM

CAUTION - This product is hygroscopic and we recommend that it is desiccated upon arrival.

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:

Clark et al (2004) Discovery and SAR development of 2-(phenylamino) imidazolines as prostacyclin receptor antagonists. Bioorg.Med.Chem.Lett. 14 1053. PMID: 15013022.

Jones *et al* (2006) Investigation of the prostacyclin (IP) receptor antagonist RO1138452 on isolated blood vessel and platelet preparations. Br.J.Pharmacol. *149* 110. PMID: 16880763.

Bley et al (2006) RO1138452 and RO3244794: characterization of structurally distinct, potent and selective IP (prostacyclin) receptor antagonists. Br.J.Pharmacol. **147** 335. PMID: 16331286.