Certificate of Analysis

Product Name: ICI 118,551 hydrochloride

Catalog No.: 0821

CAS Number: **IUPAC Name:** 72795-01-8

(±)-erythro-(S*,S*)-1-[2,3-(Dihydro-7-methyl-1H-inden-4-yl)oxy]-3-[(1-methylethyl)amino]-2-butanol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility:

C17H27NO2.HCI 313.87 White solid DMSO to 10 mM water to 10 mM Store at RT

Storage: **Batch Molecular Structure:**

.HCI ōн

2. ANALYTICAL DATA

TLC: HPLC: ¹H NMR: Mass Spectrum: **Microanalysis:**

R_f = 0.68 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33]) Shows 100% purity Consistent with structure Consistent with structure Carbon Hydrogen Nitrogen Theoretical 65.05 8.99 4.46 Found 65.04 9.03 4.56

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

bio-techne.com	North America	China	Europe Middle East Africa	Rest of World
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Batch No.: 5

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CAS Number: 72795-01-8

IUPAC Name: (±)-erythro-(S*,S*)-1-[2,3-(Dihydro-7-methyl-1H-inden-4-yl)oxy]-3-[(1-methylethyl)amino]-2-butanol hydrochloride

Description:

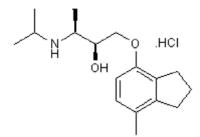
Very selective β_2 adrenergic inverse agonist (K_i values are 1.2, 120 and 257 nM for β_2 , β_1 and β_3 receptors respectively). Active in vivo. Also available as part of the β -Adrenoceptor Antagonist TocrisetTM.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₇NO₂.HCl Batch Molecular Weight: 313.87 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info: DMSO to 10 mM water to 10 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.

Licensing Information:

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References:

Strosberg and Pietri-Rouxel (1996) Function and regulation of the β_3 -adrenoceptor. TiPS **17** 373. PMID: 8979772.

Bond *et al* (1995) Physiological effects of inverse agonists in transgenic mice with myocardial overexpression of the β_2 -adrenoceptor. Nature **374** 272. PMID: 7885448.

Ten Berge *et al* (1995) β_2 -but not β_3 -adrenoceptors mediate prejunctional inhibition of non-adrenergic non cholinergic contraction of guinea pig main bronchi. Eur.J.Pharmacol. **275** 199. PMID: 7796855.

Cook *et al* (1993) β-Adrenoceptor subtypes and the opening of plasmalemmal K⁺-channels in trachealis muscle: electrophysiological and mechanical studies in guinea-pig tissue. Br.J.Pharmacol. **109** 1140. PMID: 8104643.

Bilski *et al* (1983) The pharmacology of a β2-selective adrenoceptor antagonist (ICI-118,551). J.Cardiovasc.Pharmacol. **5** 430. PMID: 6191142.

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Catalog No.: 0821 Ba

Batch No.: 5