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TOCRIS

Print Date: May 9th 2023

Certificate of Analysis

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Product Name: **CL 316243 disodium salt** **Catalog No.: 1499** **Batch No.: 9**

CAS Number: 138908-40-4

IUPAC Name: 5-[(2*R*)-2-[[(2*R*)-2-(3-Chlorophenyl)-2-hydroxyethyl]amino]propyl]-1,3-benzodioxole-2,2-dicarboxylic acid disodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{18}ClNNa_2O_7.½H_2O$

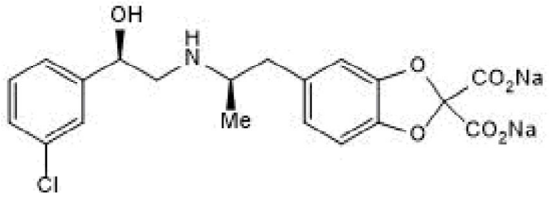
Batch Molecular Weight: 474.81

Physical Appearance: Pale yellow solid

Solubility: water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.59	4.03	2.95
Found	49.96	4.04	2.89

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Description:

CL 316243 disodium salt is a potent and highly selective β_3-adrenoceptor agonist (EC_{50} = 3 nM); > 10000-fold selective over β_1 and β_2 receptors. Increases brown adipose tissue thermogenesis and metabolic rate, and decreases blood insulin and glucose levels following oral administration in vivo.

Physical and Chemical Properties:

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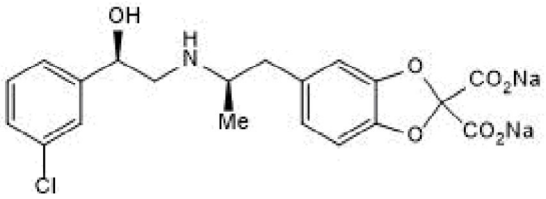
Batch Molecular Weight: 474.81

Physical Appearance: Pale yellow solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 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:

Woods *et al* (2001) Efficacy of the β3-adrenergic receptor agonist CL-316243 on experimental bladder hyperflexia and detrusor instability in the rat. J.Urol. ***166*** 1142. PMID: 11490313.

Yoshida *et al* (1994) Anti-obesity and anti-diabetic effects of CL 316,243, a highly specific β_3-adrenoceptor agonist, in yellow KK mice. Life Sci. ***54*** 491. PMID: 8309351.

Bloom *et al* (1992) Disodium(R,R)-5-[2-[[2-(3-chlorophenyl)-2-hydroxyethyl]-amino]propyl]-1,3-benzodioxole-2,2-dicarboxylate (CL 316,243). A potent β-adrenergic agonist virtually specific for β3 receptors. A promising antidiabetic and a J.Med.Chem. ***35*** 3081. PMID: 1354264.

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