

**Product Name:** CL 316243 disodium salt

**Catalog No.:** 1499

**Batch No.:** 8

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<sub>20</sub>H<sub>18</sub>ClNa<sub>2</sub>O<sub>7</sub> · 1¼H<sub>2</sub>O

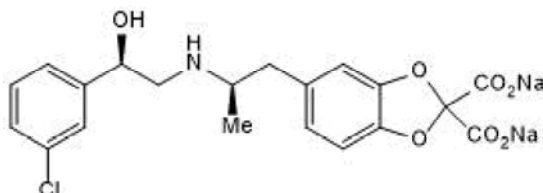
**Batch Molecular Weight:** 488.32

**Physical Appearance:** Pale yellow solid

**Solubility:** water to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.33 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

**HPLC:** Shows 98.0% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	49.19	4.23	2.87
Found	49.15	4.32	2.92

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**Description:**

CL 316243 disodium salt is a potent and highly selective  $\beta_3$ -adrenoceptor agonist ( $EC_{50} = 3 \text{ nM}$ ); > 10000-fold selective over  $\beta_1$  and  $\beta_2$  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:**

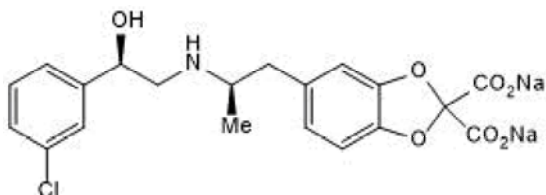
Batch Molecular Formula:  $C_{20}H_{18}ClNa_2O_7 \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 488.32

Physical Appearance: Pale yellow solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^\circ\text{C}$

**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  $45\text{-}60^\circ\text{C}$  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  $-20^\circ\text{C}$  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  $\beta_3$ -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  $\beta_3$ -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  $\beta$ -adrenergic agonist virtually specific for  $\beta_3$  receptors. A promising antidiabetic and a *J.Med.Chem.* **35** 3081. PMID: 1354264.

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