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Print Date: Jan 13th 2016

# Certificate of Analysis

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**Product Name:** **(±)-AC 7954 hydrochloride** **Catalog No.: 2484** **Batch No.: 2**

CAS Number: 477313-09-0

IUPAC Name: (±)-3-(4-Chlorophenyl)-3-[2-(dimethylamino)ethyl]-3,4-dihydro-1*H*-2-benzopyran-1-one hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{19}H_{20}ClNO_2.HCl.½H_2O$

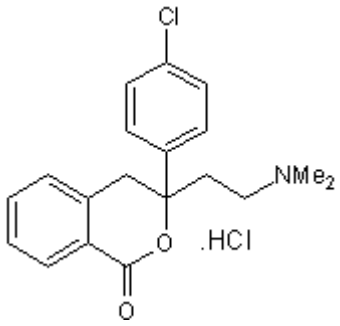
**Batch Molecular Weight:** 375.29

**Physical Appearance:** Beige solid

**Solubility:** water to 75 mM
DMSO to 75 mM
ethanol to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.44 (Dichloromethane:Methanol:Ammonia soln. [90:10:2])

**HPLC:** Shows >98.4% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 62.3 | 5.78 | 3.82 |
| Found | 60.87 | 5.63 | 3.75 |



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IUPAC Name: (±)-3-(4-Chlorophenyl)-3-[2-(dimethylamino)ethyl]-3,4-dihydro-1*H*-2-benzopyran-1-one hydrochloride

**Description:**

Highly selective, non-peptide urotensin-II (UT) receptor agonist that displays potent activity at human and rat UT receptors ($pEC_{50}$ values are 6.5 and 6.7 respectively).

**Physical and Chemical Properties:**

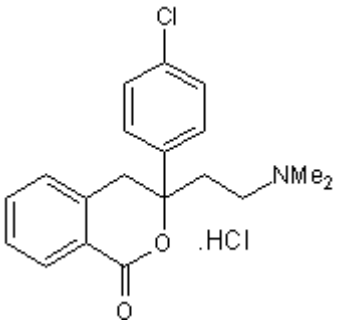
Batch Molecular Formula: $C_{19}H_{20}ClNO_2.HCl.½H_2O$

Batch Molecular Weight: 375.29

Physical Appearance: Beige solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Usage Info:**

water to 75 mM
DMSO to 75 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.

**References:**

**Croston** *et al* (2002) Discovery of the first nonpeptide agonist of the GPR14/urotensin-II receptor: 3-(4-chlorophenyl)-3-(2-(dimethylamino)ethyl)isochroman-1-one (AC-7954). J.Med.Chem. ***45*** 4950. PMID: 12408704.

**Lavecchia** *et al* (2005) Architecture of the human urotensin II receptor: comparison of the binding domains of peptide and non-peptide urotensin II agonists. J.Med.Chem. ***48*** 2480. PMID: 15801838.

**Lehmann** *et al* (2006) Novel potent and efficacious nonpeptidic urotensin II receptor agonists. J.Med.Chem. ***49*** 2232. PMID: 16570919.



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