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-1H-2-benzopyran-1-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES
Batch Molecular Formula: $C_{19}H_{20}ClNO_2\cdot HCl\cdot \frac{1}{2}H_2O$
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:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>62.3</td>
<td>60.87</td>
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<tr>
<td>Hydrogen</td>
<td>5.78</td>
<td>5.63</td>
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<tr>
<td>Nitrogen</td>
<td>3.82</td>
<td>3.75</td>
</tr>
</tbody>
</table>
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Description:
Highly selective, non-peptide urotensin-II (UT) receptor agonist that displays potent activity at human and rat UT receptors (pEC50 values are 6.5 and 6.7 respectively).

Physical and Chemical Properties:
Batch Molecular Formula: C19H19ClNO2.HCl.½H2O
Batch Molecular Weight: 375.29
Physical Appearance: Beige solid
Minimum Purity: >98%

Batch Molecular Structure:

![Molecular Structure Image]

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: