Product Name: Tiotropium bromide
Catalog No.: 5902
Batch No.: 2
CAS Number: 136310-93-5
IUPAC Name: \((1\alpha, 2\beta, 4\beta, 5\alpha, 7\beta)-7-[(2\text{-Hydroxy-2,2-di-2-thienylacetyl})\text{oxy}]-9,9\text{-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0^{2,4}]}\text{nonane} \) bromide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \(C_{19}H_{22}BrNO_4S_2\cdot\frac{1}{2}H_2O\)
Batch Molecular Weight: 481.43
Physical Appearance: White solid
Solubility: water to 20 mM
DMSO to 100 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
\(^1\text{H NMR:}\) Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<tbody>
<tr>
<td>Theoretical</td>
<td>47.4</td>
<td>4.82</td>
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<tr>
<td>Found</td>
<td>47.21</td>
<td>4.75</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** Tiotropium bromide  
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\[\text{bromide}\]

**Description:**
Potent muscarinic receptor antagonist. Inhibits electrical field stimulation-induced contraction of guinea pig trachea in vitro (IC\text{50} = 0.17 nM). Induces smooth muscle relaxation and bronchodilation.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** \(C_{19}H_{22}BrNO_3S_2\cdot\frac{1}{2}H_2O\)
- **Batch Molecular Weight:** 481.43
- **Physical Appearance:** White solid
- **Minimum Purity:** >98%
- **Batch Molecular Structure:**

![Molecular Structure](image)

**Storage:** Store at +4°C

**Solubility & Usage Info:**
- **Water to 20 mM**
- **DMSO 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:**