1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $\text{C}_{17}\text{H}_{21}\text{NO}_4\cdot\text{HBr}\cdot\text{H}_2\text{O}$
- **Batch Molecular Weight:** 429.31
- **Physical Appearance:** White solid
- **Solubility:**
  - Water to 100 mM
  - DMSO to 50 mM
- **Storage:** Store at RT
- **Batch Molecular Structure:**

2. ANALYTICAL DATA

- **Melting Point:** At 196°C
- **HPLC:** Shows 100% purity
- **$^1$H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Optical Rotation:** $[\alpha]_D = -21.8$ (Concentration = 1, Solvent = Water)
- **Microanalysis:**
  - Carbon 47.56
  - Hydrogen 6.34
  - Nitrogen 3.26
  - Theoretical:
  - Found:
  - Carbon 47.61
  - Hydrogen 6.22
  - Nitrogen 3.18

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Scopolamine hydrobromide
Catalog No.: 1414
Batch No.: 6
CAS Number: 114-49-8
EC Number: 204-050-6
IUPAC Name: \((\alpha, S)-\alpha-((\text{Hydroxymethyl})\text{benzeneacetic\ acid\ }1\alpha, 2\beta, 4\beta, 5\alpha, 7\beta)-9\text{-methyl-3-oxa-9-aza}\text{tricyclo[3.3.1.0}2, 4\text{]}\text{non-7-yl ester}\) hydrobromide

Description:
Non-selective muscarinic antagonist. Widely used clinically to treat motion sickness.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{17}$H$_{21}$NO$_4$.HBr.2½H$_2$O
Batch Molecular Weight: 429.31
Physical Appearance: White solid
Minimum Purity: >99%
Batch Molecular Structure:

![Batch Molecular Structure](image)

Storage: Store at RT

Solubility & Usage Info:
- Water to 100 mM
- DMSO 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: