Product Name: Cocaine hydrochloride
Catalog No.: 2833
Batch No.: 3
CAS Number: 53-21-4
EC Number: 200-167-1
IUPAC Name: 3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid methyl ester benzoate hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: C_{17}H_{21}NO_4.HCl
   Batch Molecular Weight: 339.81
   Physical Appearance: White crystalline solid
   Solubility: water to 100 mM
   Storage: Store at RT
   Batch Molecular Structure:

   ![Molecular Structure]

2. ANALYTICAL DATA

   HPLC: Shows >99% purity
   Optical Rotation: \([\alpha]_D = -72.2\) (Concentration = 2.5, Solvent = Water)
Description:
Competitive inhibitor of monoamine neurotransmitter transporters. Inhibits dopamine (DAT), serotonin (SERT) and noradrenalin (NET) transporters with \( K_i \) values are 267, 392 and 872 nM respectively. Psychostimulant.

Physical and Chemical Properties:
- **Batch Molecular Formula:** \( \text{C}_{17}\text{H}_{21}\text{NO}_4\cdot\text{HCl} \)
- **Batch Molecular Weight:** 339.81
- **Physical Appearance:** White crystalline solid
- **Minimum Purity:** >99%

Storage:
- Store at RT
- CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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 45-60°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.

Other Information:
**INFORMATION FOR CUSTOMERS IN THE UK ONLY**
This product is a Schedule 2 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

**INFORMATION FOR CUSTOMERS IN THE USA ONLY**
This product is a Schedule II DEA controlled substance and customers in the USA are required to hold a controlled substance registration in order to purchase and possess this material (in accordance with Title 21 code of federal regulations part 1300 to end).

**INFORMATION FOR CUSTOMERS IN CANADA ONLY**
This product is a Schedule I CDSA controlled substance and customers in Canada require an import permit to purchase this material.

References: