Print Date: Jul 25th 2017

# Certificate of Analysis

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**Product Name:** **ML 133 hydrochloride** **Catalog No.: 4549** **Batch No.: 1**

CAS Number: 1222781-70-5

IUPAC Name: *N*-[(4-Methoxyphenyl)methyl]-1-naphthalenemethanamine hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{19}H_{19}NO.HCl$

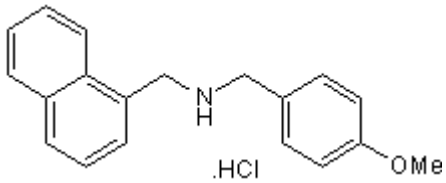
**Batch Molecular Weight:** 313.82

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 100 mM
ethanol to 20 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**HPLC:** Shows 99.0% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 72.71 | 6.42 | 4.46 |
| Found | 72.42 | 6.4 | 4.52 |



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# Product Information



**Product Name:** **ML 133 hydrochloride** **Catalog No.: 4549** **Batch No.: 1**

CAS Number: 1222781-70-5

IUPAC Name: *N*-[(4-Methoxyphenyl)methyl]-1-naphthalenemethanamine hydrochloride

**Description:**

Selective blocker of inwardly rectifying $K_{ir}2$ potassium channels ($IC_{50}$ values are 1.8, 2.8, 2.9 and 4.0 μM at pH 7.4 for $mK_{ir}2.1$, $hK_{ir}2.6$, $hK_{ir}2.2$ and $hK_{ir}2.3$ respectively). Exhibits no effect on $rK_{ir}1.1$ ($IC_{50}$ > 300 μM); displays weak activity at $hK_{ir}7.1$ and $rK_{ir}4.1$ ($IC_{50}$ values are 33 and 76 μM).

**Physical and Chemical Properties:**

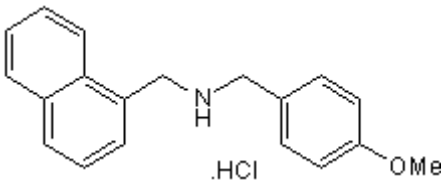
Batch Molecular Formula: $C_{19}H_{19}NO.HCl$

Batch Molecular Weight: 313.82

Physical Appearance: Off-white solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**




**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM
ethanol to 20 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:**

**Wang** *et al* (2011) Selective inhibition of the $K_{ir}2$ family of inward rectifier potassium channels by a small molecule probe: the discovery, SAR, and pharmacological characterization of ML133. ACS Chem.Biol. ***6*** 845. PMID: 21615117.

**Wu** *et al* (2010) A potent and selective small molecule $K_{ir}2.1$ inhibitor. Probe Reports from the NIH Molecular Libraries Pro. PMID: 21433384.