

# **Certificate of Analysis**

Print Date: Feb 9th 2024

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Product Name: E-4031 dihydrochloride Catalog No.: 1808 Batch No.: 5

CAS Number: 113559-13-0

IUPAC Name: N-[4-[[1-[2-(6-Methyl-2-pyridinyl)ethyl]-4-piperidinyl]carbonyl]phenyl]methanesulfonamide dihydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{21}H_{27}N_3O_3S.2HCI.$ 

**Batch Molecular Weight:** 474.44 **Physical Appearance:** White solid

**Solubility:** water to 100 mM

DMSO to 20 mM with gentle warming

Storage: Desiccate at RT

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.1% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

Theoretical 53.16 6.16 8.86 14.94 Found 52.64 6.06 8.61 13.93

## **Product Information**

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### **Description:**

E-4031 dihydrochloride is a selective blocker of  $K_V11.1$  (hERG) channels; inhibits the rapid delayed-rectifier  $K^+$  current ( $I_{Kr}$ ). Reversibly prolongs action potential duration in guinea pig papillary muscle and isolated ventricular myocytes, without affecting Na+ or Ca²+ inward currents. Class III antiarrhythmic agent

### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>21</sub>H<sub>27</sub>N<sub>3</sub>O<sub>3</sub>S.2HCl.

Batch Molecular Weight: 474.44 Physical Appearance: White solid

### Minimum Purity: ≥98%

### **Batch Molecular Structure:**

Storage: Desiccate at RT

### Solubility & Usage Info:

water to 100 mM

DMSO to 20 mM with gentle warming

### 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).

Catalog No.: 1808

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

**Ficker** *et al* (2002) The binding site for channel blockers that rescue misprocessed human long QT syndrome type 2 *ether-a-gogo*-related gene (HERG) mutations. J.Biol.Chem. **277** 4989. PMID: 11741928.

**Verheijck** *et al* (1995) Effects of the delayed rectifier current blockade by E-4031 on impulse generation in single sinoatrial nodal myocytes of the rabbit. Circ.Res. **76** 607. PMID: 7895335.

**Wettwer** *et al* (1991) Effects of the new class III antiarrhythmic drug E-4031 on myocardial contractility and electrophysiological parameters. J.Cardiovasc.Pharmacol. *17* 480. PMID: 1711611.