TOCRIS
a bio-techne brand

Print Date: Feb 4th 2019

Certificate of Analysis

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Product Name: **E-4031 dihydrochloride** **Catalog No.: 1808** **Batch No.: 4**

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: $C_{21}H_{27}N_3O_3S.2HCl.¼H_2O$

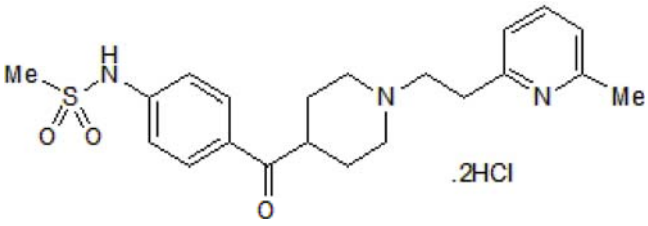
Batch Molecular Weight: 478.94

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 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.66	6.21	8.77
Found	52.72	6.14	8.79

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Description:

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 Ca^{2+} inward currents. Class III antiarrhythmic agent.

Physical and Chemical Properties:

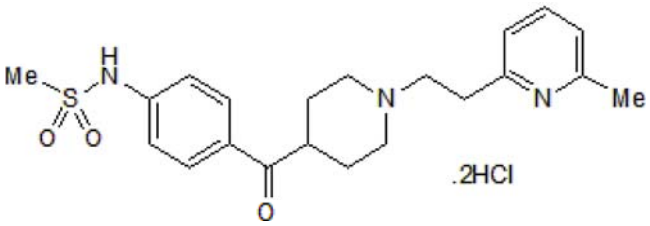
Batch Molecular Formula: $C_{21}H_{27}N_3O_3S.2HCl.¼H_2O$

Batch Molecular Weight: 478.94

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).

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:

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.