

Certificate of Analysis

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Product Name: Ibutilide hemifumarate

Catalog No.: 3908

Batch No.: 1

CAS Number: 122647-32-9

IUPAC Name: (±)-N-[4-[4-(Ethylheptylamino)-1-hydroxybutyl]phenyl]methanesulfonamide hemifumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{36}N_2O_3S \cdot 0.5C_4H_4O_4$

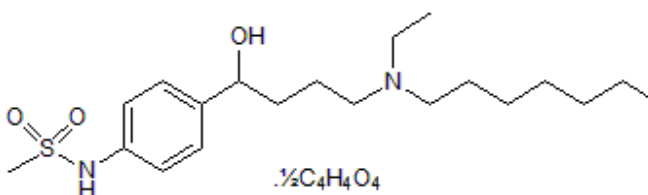
Batch Molecular Weight: 442.61

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM
water to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.7	8.65	6.33
Found	59.65	8.74	6.43

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Class III antiarrhythmic. Blocks the rapid component of delayed rectifier K⁺ current (I_{Kr}); also blocks hERG channels and L-type Ca²⁺ channels. Shown to activate a slow inward Na⁺ current in guinea pig ventricular cells. Used to terminate atrial fibrillation and atrial flutter; can prolong QT.

Physical and Chemical Properties:

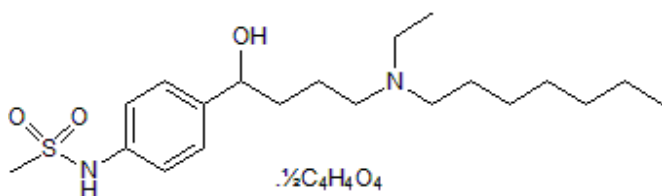
Batch Molecular Formula: C₂₀H₃₆N₂O₃S. 0.5C₄H₄O₄

Batch Molecular Weight: 442.61

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Merck Index **12** 4927.

Murray (1998) Ibutilide. *Circulation* **97** 493. PMID: 9490245.

Lee and Lee (1998) Ionic mechanism of ibutilide in human atrium: evidence for a drug-induced Na⁺ current through nifedipine inhibited inward channel. *J.Pharmacol.Exp.Ther.* **286** 9. PMID: 9655836.

Perry et al (2004) Structural determinants of HERG channel block by clofilium and ibutilide. *Mol.Pharmacol.* **66** 240. PMID: 15266014.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM
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.

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