

Product Name: HMR 1556

Catalog No.: 5011

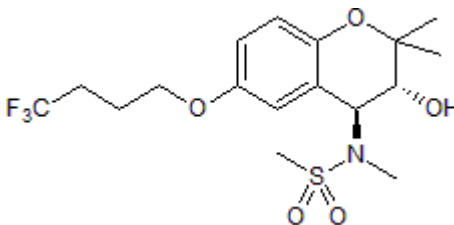
Batch No.: 1

CAS Number: 223749-46-0

IUPAC Name: *N*-[(3*R*,4*S*)-3,4-Dihydro-3-hydroxy-2,2-dimethyl-6-(4,4,4-trifluorobutoxy)-2*H*-1-benzopyran-4-yl]-*N*-methylmetanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₂₄F₃NO₅S
Batch Molecular Weight: 411.44
Physical Appearance: Off White solid
Solubility: DMSO to 100 mM
 ethanol to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.06 (Ethyl acetate:Petroleum ether [3:7])
HPLC: Shows 98.9% purity
Chiral HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +3.8 (Concentration = 1, Solvent = Methanol)
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.63	5.88	3.4
Found	49.66	5.83	3.38

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

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Description:

Potent and selective I_{ks} channel blocker (IC₅₀ values are 10.5 and 34 nM in canine and guinea pig ventricular myocytes respectively). Selectively inhibits I_{ks} currents over I_{Kr}, I_{K1}, I_{to} and L-type Ca²⁺ channel currents. Also has little or no effect on K_v11.1, K_v1.5, K_v1.3, K_{ir}2.1 and HCN2 channel currents. Potentiates E-4031-induced arrhythmias in vivo.

Physical and Chemical Properties:

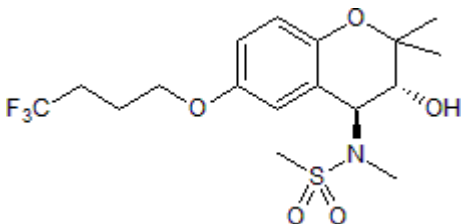
Batch Molecular Formula: C₁₇H₂₄F₃NO₅S

Batch Molecular Weight: 411.44

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Gerlach et al (2001) Synthesis and activity of novel and selective I(Ks)-channel blockers. *J.Med.Chem.* **44** 3831. PMID: 11689069.

Thomas et al (2003) HMR 1556, a potent and selective blocker of slowly activating delayed rectifier potassium current. *J.Cardiovasc.Pharmacol.* **41** 140. PMID: 12500032.

Michael et al (2007) Potentiation of E-4031-induced torsade de pointes by HMR1556 or ATX-II is not predicted by action potential short-term variability or triangulation. *Br.J.Pharmacol.* **152** 1215. PMID: 17965747.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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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