Product Name: HMR 1556
Catalog No.: 5011      Batch No.: 3
CAS Number: 223749-46-0
IUPAC Name: N-[(3R,4S)-3,4-Dihydro-3-hydroxy-2,2-dimethyl-6-(4,4,4-trifluorobutoxy)-2H-1-benzopyran-4-yl]-N-methylmetanesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{17}H_{24}F_{3}NO_{5}S \)
Batch Molecular Weight: 411.44
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 20 mM
Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.06 \) (Ethyl acetate:Petroleum ether [3:7])
HPLC: Shows >99.8% purity
Chiral HPLC: Shows >99.7% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon (C)</td>
<td>49.63</td>
<td>49.94</td>
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<tr>
<td>Hydrogen (H)</td>
<td>5.88</td>
<td>5.88</td>
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<tr>
<td>Nitrogen (N)</td>
<td>3.40</td>
<td>3.30</td>
</tr>
</tbody>
</table>
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Description:
Potent and selective I\textsubscript{ks} channel blocker (IC_{50} values are 10.5 and 34 nM in canine and guinea pig ventricular myocytes respectively). Selectively inhibits I\textsubscript{ks} currents over I\textsubscript{Ks}, I\textsubscript{K1.5}, I\textsubscript{K1.3}, I\textsubscript{K1.1}, and I\textsubscript{L}-type Ca\textsuperscript{2+} channel currents. Also has little or no effect on K\textsubscript{v1.1}, K\textsubscript{v1.5}, K\textsubscript{v1.3}, K\textsubscript{v2.1}, and HCN2 channel currents. Potentiates E-4031-induced arrhythmias in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{21}H\textsubscript{22}F\textsubscript{3}NO\textsubscript{5}S
Batch Molecular Weight: 411.44
Physical Appearance: White solid
Minimum Purity: >98%

References: