Product Name: SK1-I

CAS Number: 1072443-89-0
IUPAC Name: 1,2,4-Trideoxy-4-(methylamino)-1-(4-pentylphenyl)-D-erythro-pent-1-enitol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_{17}\text{H}_{27}\text{NO}_2\cdot\text{HCl}$
Batch Molecular Weight: 313.86
Physical Appearance: White solid
Solubility: water to 100 mM
DMSO to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: $R_f = 0.15$ (Dichloromethane7N NH3 in Methanol [9:1])
HPLC: Shows >99.7% purity
Chiral HPLC: Shows >99.1% purity
$^1\text{H NMR}$: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>65.05</td>
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<tr>
<td>Hydrogen</td>
<td>8.99</td>
<td>8.93</td>
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<tr>
<td>Nitrogen</td>
<td>4.46</td>
<td>4.49</td>
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</tbody>
</table>

Certificate of Analysis

Print Date: Feb 11th 2014

www.tocris.com

Tocris Bioscience is an R&D Systems company

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Description:
Sphingosine kinase (SphK) inhibitor. Isoenzyme-selective for SphK1; displays no activity at SphK2. Also displays no inhibitory activity against a range of protein kinases including PKC, PKA, ERK1, EGFR and CDK2. Exhibits potent antileukemic activity in vivo; inhibits the growth of both U937 and Jurkat T cells. Also suppresses proliferation and induces apoptosis in several human glioblastoma cell lines.

Physical and Chemical Properties:
Batch Molecular Formula: C_{17}H_{27}NO_{4}.HCl
Batch Molecular Weight: 313.86
Physical Appearance: White solid

Minimum Purity: >98%

Storage: Store at -20°C

Solubility & Usage Info:
water to 100 mM
DMSO 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.

References: