1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_{25}\text{H}_{26}\text{N}_{4}\text{O}_{3}\cdot\frac{1}{4}\text{H}_{2}\text{O}$

Batch Molecular Weight: 435

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

TLC: $R_f = 0.15$ (Dichloromethane:Methanol [5:1])

HPLC: Shows 98.5% 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>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>69.03</td>
<td>68.91</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.14</td>
<td>6.14</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.88</td>
<td>12.8</td>
</tr>
</tbody>
</table>
Product Name: SM 16  
Catalog No.: 6245  
Batch No.: 1

CAS Number: 614749-78-9  
IUPAC Name: 4-[4-(1,3-Benzodioxol-5-yl)-5-(6-methyl-2-pyridinyl)-1H-imidazol-2-yl]bicyclo[2.2.2]octane-1-carboxamide

Description: Potent TGF-β receptor type 1 (TGF-βRI) inhibitor (IC$_{50}$ = 64 nM in luciferase assay). Selective for TGF-βRI over other ALK family members. Decreases Smad phosphorylation and inhibits tumor growth in a mouse xenograft model. Attenuates increased TGF-β signaling in retinal vessels of diabetic rats. Also prevents intimal thickening and vascular remodeling in rat carotid balloon injury model. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{25}$H$_{26}$N$_{3}$O$_{3}$·½H$_{2}$O  
Batch Molecular Weight: 435  
Physical Appearance: White solid  
Minimum Purity: >98%

 physically and chemical properties:
Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:  
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:


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