1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** C\textsubscript{22}H\textsubscript{16}N\textsubscript{4}O\textsubscript{3}.2\textsubscript{1/4}H\textsubscript{2}O
- **Batch Molecular Weight:** 424.92
- **Physical Appearance:** Pale yellow solid
- **Solubility:**
  - ethanol to 10 mM
  - DMSO to 100 mM with gentle warming
- **Storage:** Store at RT
- **Batch Molecular Structure:**

![Molecular Structure](image)

2. ANALYTICAL DATA

- **TLC:**
  - R\textsubscript{f} = 0.2 (Dichloromethane:Methanol:Ammonia soln. [95:5:0.1])
- **HPLC:** Shows >99.5% purity
- **\textsuperscript{1}H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  
<table>
<thead>
<tr>
<th>Component</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>62.19</td>
<td>62.24</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.86</td>
<td>4.6</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>13.19</td>
<td>13.42</td>
</tr>
</tbody>
</table>

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

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Product Name: SB 431542
Catalog No.: 1614
Batch No.: 12

CAS Number: 301836-41-9
IUPAC Name: 4-[4-(1,3-benzodioxol-5-yl)-5-(2-pyridinyl)-1H-imidazol-2-yl]benzamide

Description:
Potent and selective inhibitor of the transforming growth factor-β (TGF-β) type I receptor activin receptor-like kinase ALK5 (IC₅₀ = 94 nM), and its relatives ALK4 and ALK7. Suppresses TGF-β-induced proliferation of human osteosarcoma cells. Replaces SOX2 in reprogramming of fibroblasts into iPSCs. Stimulates proliferation, differentiation and sheet formation of ESC-derived endothelial cells. Inhibits TGF-β-induced EMT, migration, invasion and VEGF secretion in several human cancer cell lines.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₂H₁₆N₄O₂.2½H₂O
Batch Molecular Weight: 424.92
Physical Appearance: Pale yellow solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
ethanol to 10 mM
DMSO to 100 mM with gentle warming

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.

Licensing Information:
Sold for research purposes under agreement from GlaxoSmithKline

References: