# Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Name:</strong></td>
<td>IPI-504 (Retaspimycin hydrochloride)</td>
</tr>
<tr>
<td><strong>Cas No.:</strong></td>
<td>857402-63-2</td>
</tr>
<tr>
<td><strong>M.Wt:</strong></td>
<td>624.2</td>
</tr>
<tr>
<td><strong>Formula:</strong></td>
<td>C31H46ClN3O8</td>
</tr>
<tr>
<td><strong>Synonyms:</strong></td>
<td>IPI 504, IPI504</td>
</tr>
<tr>
<td><strong>Chemical Name:</strong></td>
<td>[(3R,5S,6R,7S,8E,10S,11S,12Z,14E)-6,20,22-trihydroxy-5,11-dimethoxy-5,11-dimethoxy-3,7,9,15-tetramethyl-16-oxo-21-{prop-2-enylamino}-17-azabicyclo[16.3.1]docosa-1(22),8,12,14,18,20-hexaen-10-yl]carbamate;hydrochloride</td>
</tr>
<tr>
<td><strong>Canonical SMILES:</strong></td>
<td>CC1CC(C(C=C(C(C=C(C(C=CC=C(C(=O)NC2=CC(=C(C(=C2O)C1)NCC=C)O)C)OC)OC(=O)N)C)C)O)OC.Cl</td>
</tr>
<tr>
<td><strong>Solubility:</strong></td>
<td>$\geq26.1$mg/mL in DMSO with gentle warming</td>
</tr>
<tr>
<td><strong>Storage:</strong></td>
<td>Store at -20°C</td>
</tr>
<tr>
<td><strong>General tips:</strong></td>
<td>For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.</td>
</tr>
<tr>
<td><strong>Shopping Condition:</strong></td>
<td>Evaluation sample solution: ship with blue ice</td>
</tr>
<tr>
<td></td>
<td>All other available size: ship with RT, or blue ice upon request</td>
</tr>
</tbody>
</table>

# Biological Activity

**Targets:** Proteases  
**Pathways:** HSP  
**Description:** Retaspimycin hydrochloride (also known as IPI-504), a hydroquinone hydrochloride salt derivative of 17-AAG, is a novel, potent and selective inhibitor of heat shock protein 90 (Hsp90) that binds to
the amino-terminal ATP/ADP-binding site of Hsp90. As a highly water-soluble version of 17-AAG, IPI-504 (solubility > 200 mg/mL) does not need prior dissolution in organic solvents and hence can be delivered in high concentrations. Once in the systemic circulation, IPI-504 is deprotonated and converted into the free base IPI-504 which is subsequently oxidized to 17-AAG. IPI-504 potently inhibits proliferation in several tumor cell lines with 50% inhibition concentration IC50 values ranging from 10-40 nmol/L and has been used for the treatment of gastrointestinal stromal tumors, soft-tissue sarcomas and non-small cell lung cancer.

Reference:

Protocol

Cell experiment:

Cell lines
Glioma cell lines (D-54 MG and U-251 MG cells)

Preparation method
This compound was soluble in DMSO. General tips for obtaining a higher concentration: Please warm the tube at 37°C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Reacting conditions
1 or 2.5 μM; 24 or 48 hrs

Applications
In glioma cells, IPI-504 inhibited cell proliferation through increasing sub-G1 population of cells and dose-dependently inducing fragmented DNA of the apoptotic cells.

Animal experiment [3]:

Animal models
Mice bearing human brain tumor D-54MG xenografts

Dosage form
100 mg/kg; i.p.; b.i.d., twice weekly or 5/2/5 schedule (5 days on, 2 days off, and then 5 days on), for 6 weeks
Applications

In immunocompromised mice, IPI-504 mildly attenuated tumor growth.

Other notes

Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Reference:

Product Citations


Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.