Product Name: Sitagliptin phosphate monohydrate

Revision Date: 6/30/2016

Product Data Sheet

Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Name:</strong></td>
<td>Sitagliptin phosphate monohydrate</td>
</tr>
<tr>
<td><strong>Cas No.:</strong></td>
<td>654671-77-9</td>
</tr>
<tr>
<td><strong>M.Wt:</strong></td>
<td>523.3</td>
</tr>
<tr>
<td><strong>Formula:</strong></td>
<td>C16H15F6N5O.H3PO4.H2O</td>
</tr>
<tr>
<td><strong>Synonyms:</strong></td>
<td>Tesavel, MK-0431, MK0431</td>
</tr>
<tr>
<td><strong>Chemical Name:</strong></td>
<td>(3R)-3-amino-1-[3-(trifluoromethyl)-6,8-dihydro-5H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]-4-(2,4,5-trifluorophenyl)butan-1-one; phosphoric acid; hydrate</td>
</tr>
<tr>
<td><strong>Canonical SMILES:</strong></td>
<td>[HH].C1CN2C(=NN=C2(C(F)(F)F)CN1C(=O)CC(CC3=CC(=C(C=C3F)F)F)F)N.O.OOP(=O)=O</td>
</tr>
<tr>
<td><strong>Solubility:</strong></td>
<td>&gt;26.2mg/mL in DMSO</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:** DPP-4

**Pathways:** Proteases >> DPP-4

**Description:**
Sitagliptin phosphate monohydrate is the phosphate salt of its active component, sitagliptin, with one molecule of water. Sitagliptin is a potent inhibitor of dipeptidyl peptidase 4 (DPP-4), an enzyme catalyzing the cleavage of peptides with an N-terminal alanine or proline amino acid.
residue, that selectively inhibits DPP-4 with 50% inhibition concentration IC50 value of 18 nM and shows no affinity towards other DDP enzymes (such as DDP-8 and DDP-9). The inhibition of DPP4 by sitagliptin has been found to be mediated by increasing levels of two DPP-4 substrates, including glucagon-like peptide-1 (GLP-1) and gastric inhibitory polypeptide (GIP). Sitagliptin is currently being investigated in the treatment of type II diabetes.

**Reference:**

**Protocol**

**Cell experiment:**

**Cell lines**
Endothelial progenitor cells (EPCs) and bone marrow mesenchymal stem cells (MSC)

**Preparation method**
The solubility of this compound in DMSO is >10 mM. 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**
14 d; 25 μmol/L

**Applications**
To determine whether sitagliptin treatment participated in enhancing the differentiation of EPCs and MSCs and cells expressing its ligand, SDF-1α, adipose tissues were co-cultured with sitagliptin (25 μmol/L) in M199 culture medium for 14 d and examined by flow cytometric analysis. The results show that compared with the 7 d cell culture, the numbers of EPCs [CD31/Sca-1+(double-stained) and CXCR4+ (single-stained)] were remarkably higher at day 14 in both the non-sitagliptin-treated (Si-T) group and the Si-T group.

**Animal experiment [3]:**

**Animal models**
ApoE−/−mice with the C57BL/6 genetic background

**Dosage form**
200 mg/kg/day; oral taken

**Applications**
In ApoE−/−mice, the sitagliptin group showed fewer atherosclerotic plaques than in controls (7.64±1.98% [range 4.62–10.13%] vs 12.91±1.15% [range 11.55–14.37%], p<0.001). Compared with control mice, atherosclerotic plaque areas decreased respectively 1.92- and 2.74-fold in the aortic root and abdominal aorta of mice fed sitagliptin (p=0.011 and p=0.006). Our data show that sitagliptin...
can inhibit the formation of atherosclerotic areas in entire aorta, aortic root and abdominal aorta of ApoE−/− mice.

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


Product Validation

Sitagliptin increased (p < 0.05) the inhibitory effect of PYY(1-36) on alanine-induced insulin release without affecting the inhibitory actions of PYY(3-36). Effects of sitagliptin (500 nM) on the insulin secretory actions of GLP-1 (10-6 M) and ability of PYY peptides (10-6 M) to inhibit alanine-induced insulin secretion in isolated mouse islets. Mol Cell Endocrinol. 2016 Jul 25;436:102-113.

MK0431 inhibits plasma DPP-IV activity and increases plasma active GLP-1 levels in STZ-induced diabetic mice.
Treatment of sitagliptin decreased insulin resistance (33% reduction; P<0.01) and enhanced β-cell function (3.9-fold; P<0.05) by the calculations of HOMA-IR and HOMA-β.

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.