Product Data Sheet

Chemical Properties

Product Name: Olcegepant
Cas No.: 204697-65-4
M.Wt: 869.66
Formula: C38H47Br2N9O5

Synonyms: BIBN-4096; BIBN-4096BS; BIBN4096BS; BIBN 4096BS

Chemical Name: N-[(2R)-1-[[[2S]-6-amino-1-oxo-1-(4-pyridin-4-yl)piperazin-1-yl]hexan-2-yl]amino]-3-(3,5-dibromo-4-hydroxyphenyl)-1-oxopropan-2-yl]-4-(2-oxo-1,4-dihydroquinazolin-3-yl)piperidine-1-carboxamide

Canonical SMILES: C1CN(CCC1N2CC3=CC=CC3NC2=O)C(=O)NC(CC4=CC(=C(C(=C4)Br)O)Br)C(=O)NC(CCCCN)C(=O)N5CCN(CC5)C6=CC=NC=C6

Solubility: ≥87mg/mL in DMSO with gentle warming

Storage: Store at -20°C

General tips: 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.

Shopping Condition: Evaluation sample solution: ship with blue ice
All other available size: ship with RT, or blue ice upon request

Biological Activity

Targets: Neuroscience
Pathways: CGRP

Description:
Olcegepant Description: IC50: 0.1nM on human brain vessels [1]
Olcegepant is the first potent and selective non-peptide antagonist of the calcitonin gene-related
peptide 1 (CGRP1) receptor, a key modulator in neurogenic inflammatory pain. Under development by Boehringer Ingelheim GmbH, olcegepant is an intravenously formulated treatment for acute attacks of migraine.

**In vitro:** Functional studies with SK-N-MC cells demonstrated that CGRP-induced cAMP production was antagonised by both CGRP-(8-37) and olcegepant with pA2 values of 7.8 and 11.2, respectively. [1].

**In vivo:** Pre-treatment with olcegepant (900 mg/kg) inhibited the capsaicin-induced expression of Fos throughout the spinal trigeminal nucleus by 57%. In contrast, the expression of phosphorylated extracellular signal-regulated kinase in the trigeminal ganglion was not changed by olcegepant pre-treatment. CGRP receptor inhibition, which has been shown to decrease spinal trigeminal activity, is likely to occur in the central nervous system rather than in the periphery including the trigeminal ganglion. This may be important for future therapeutic interventions with CGRP receptor antagonists in migraine. [2].

**Clinical trial:** In a phase II clinical trial, olcegepant reduced the severity of headache in 60% of migraine sufferers and met secondary endpoints including headache-free rate and rate of sustained response. Only mild-to-moderate transient adverse events were observed, with no adverse cardiovascular symptoms reported. The compound appears to be an effective anti-migraine medication that is well tolerated and does not display the vasoconstrictive effect that precludes the use of triptans and dihydroergotamine in certain patients [3].

**Reference:**

**Protocol**

**Cell experiment:**

<table>
<thead>
<tr>
<th>Cell lines</th>
<th>SK-N-MC cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Preparation method</td>
<td>The solubility of this compound in DMSO is &gt;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.</td>
</tr>
<tr>
<td>Reacting conditions</td>
<td>In SK-N-MC cells, CGRP-induced cAMP production was antagonised by both CGRP-(8-37) and Olcegepant with pA2 values of 7.8 and 11.2, respectively.</td>
</tr>
</tbody>
</table>

**Applications**

In SK-N-MC cells, CGRP-induced cAMP production was antagonised by both CGRP-(8-37) and Olcegepant with pA2 values of 7.8 and 11.2, respectively.
**Animal experiment [3]:**

<table>
<thead>
<tr>
<th>Animal models</th>
<th>Rats</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dosage form</td>
<td>900 μg/kg; i.v.; 10 mins</td>
</tr>
</tbody>
</table>

**Applications**

Pre-treatment with Olcegepant (900 μg/kg) inhibited the capsaicin-induced expression of Fos (57%) throughout the spinal trigeminal nucleus, but did not change the expression of phosphorylated extracellular signal-regulated kinase in the trigeminal ganglion.

**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.

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**Reference:**


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**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 datasheet.

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