Product Name: Tofacitinib (CP-690550) Citrate

Revision Date: 6/30/2018

Product Data Sheet

Chemical Properties

Product Name: Tofacitinib (CP-690550) Citrate

Cas No.: 540737-29-9

M.Wt: 504.49

Formula: C16H20N6O.C6H8O7

Synonyms: Tasocitinib citrate, CP 690550 citrate

Chemical Name: 2-hydroxypropane-1,2,3-tricarboxylic acid; 3-[(3R,4R)-4-methyl-3-[methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino]piperidin-1-yl]-3-oxopropanenitrile

Canonical SMILES: CC1CCN(CC1N(C)C2=NC=NC3=C2C=CN3)(=O)CC#N.C(C(=O)O)C(CC(=O)O)(C(=O)O)O

Solubility: \( \geq 25.22 \text{ mg/mL in DMSO, } <2.53 \text{ mg/mL in EtOH, } \geq 3.4 \text{ mg/mL in H}_2\text{O with ultrasonic and warming} \)

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: Chromatin/Epigenetics

Pathways: JAK

Description: Tofacitinib citrate, also known as CP-690550 citrate, is a potent inhibitor of janus kinase 3 (JAK3), a hematopoetic cell-restricted tyrosine kinase involved in signal transduction regulating
lymphocyte survival, proliferation, differentiation, and apoptosis. The inhibition is JAK3 specific with a selectivity 1000-fold more than other non-JAK family kinases. Besides inhibiting JAKS (IC50 = 1 nM), tofacitinib citrate also inhibits janus kinase 2 (JAK2) and janus kinase 1 (JAK1) with 20- and 100-fold less in potency respectively. However, in a recent study, the binding affinities (Ki) of tofacitinib citrate towards JAK1, JAK2, and JAK3 were reported to be 1.6 nM, 21.7 nM, and 6.5 nM respectively.

Reference:
Lalitha Vijayakrishnan, R. Venkataramanan and Palak Gulati. Treating inflammation with the janus kinase inhibitor CP-690,550. Trends in Pharmacological Sciences 2011: 32 (1); 25-34

### Protocol

**Cell experiment:**

<table>
<thead>
<tr>
<th>Cell lines</th>
<th>Naïve T cell</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>16h; 50 nM</td>
</tr>
<tr>
<td>Applications</td>
<td>A concentration of 100 nM. 50 nM, but not 10 nM, CP-690,550 suppressed IFN-γ production 4 days after Th1 differentiation conditions were established, while both 10 nM and 50 nM CP-690,550 strongly suppressed IL-4 production under Th2 differentiation conditions. This suggests that CP-690,550 inhibits both Th1 and Th2 differentiation, and that Th2 is more sensitive than Th1 to this drug. We then examined the effect of CP-690,550 on Th17 and induced T regulatory (iTreg) cells. CP-690,550 enhanced IL-17 production while suppressing Foxp3 and IL-10 induction in a dose-dependent manner under Th17 differentiation conditions. These data indicate that &lt;100 nM CP-690,550 efficiently inhibits Th1, Th2 and iTreg while promoting Th17, in vitro.</td>
</tr>
</tbody>
</table>

**Animal experiment [3]:**

| Animal models | C57BL6/J mice and DBA/1J mice |
| Dosage form | 30 nM; intraperitoneal injection |
| Applications | Naïve CD4+T cells isolated from mice were stimulated with various cytokines in the presence of various concentrations of CP-690,550. |
CP-690,550 selectively inhibited IFN-γ-induced STAT1, IL-4-induced STAT6, and IL-2-induced STAT5 at 3–30 nM, while 30 nM CP-690,550 did not suppress IL-6-induced STAT3 phosphorylation. A concentration greater than 100 nM was required for the partial suppression of STAT3.

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.