TLR7 agonist 2

Cat. No.: HY-103039
CAS No.: 1642857-69-9
Molecular Formula: C₁₇H₁₆N₆O₂
Molecular Weight: 336.35
Target: Toll-like Receptor (TLR)
Pathway: Immunology/Inflammation
Storage:
- Powder: -20°C 3 years, 4°C 2 years
- In solvent: -80°C 6 months, -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro DMSO: 160 mg/mL (475.69 mM; Need ultrasonic and warming)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>Mass 1 mg</th>
<th>Mass 5 mg</th>
<th>Mass 10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td></td>
<td>2.9731 mL</td>
<td>14.8655 mL</td>
<td>29.7309 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td>0.5946 mL</td>
<td>2.9731 mL</td>
<td>5.9462 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td>0.2973 mL</td>
<td>1.4865 mL</td>
<td>2.9731 mL</td>
</tr>
</tbody>
</table>

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description TLR7 agonist 2 is a potent and selective Toll-like Receptor 7 (TLR7) agonist with a LEC of 0.4 μM.

IC₅₀ & Target LEC: 0.4 μM (TLR7) [1]

In Vitro TLR7 agonist 2 is a potent and selective Toll-like Receptor 7 (TLR7) agonist with a lowest effective concentration (LEC) of 0.4 μM in HEK293 cell. TLR7 agonist 2 is found to be selective for TLR7 over TLR8 with LEC of >100 μM for human TLR8. TLR7 agonist 2 demonstrates low inhibition across five CYP450 isozymes (IC₅₀ > 10 μM) and is also not a time dependent inhibitor of CYP450 3A4. TLR7 agonist 2 has limited inhibition of the hERG potassium ion channel ³H-dofetilide binding in vitro (IC₅₀ > 50 μM) [1].

In Vivo TLR7 agonist 2 is found to be rapidly cleared in conjunction with our target profile. Both Cmax and AUC increase less than dose proportionally between 0.3 and 3 mg/kg and more than dose-proportionally between 3 and 10 mg/kg. TLR7 agonist 2 can induce an antiviral interferon stimulated gene (ISG) response without inducing an IFNα response at a low dose. TLR7 agonist 2 also induces a 2.7 log decrease in serum HBV viral load from 0.3 mg/kg, and a
The ability of TLR7 agonist 2 to activate human TLR7 and/or TLR8 is assessed by using HEK293 cells. Briefly, HEK293 cells are grown in culture medium (DMEM supplemented with 10% FCS and 2 mM Glutamine). Transfected cells are then detached with Trypsin-EDTA, washed in PBS and resuspended in medium to a density of $1.67 \times 10^5$ cells/mL. Thirty microliters of cells are then dispensed into each well in 384-well plates, where 10 μL of TLR7-agonist-1 in 4% DMSO is already present. Following 6 hours incubation at 37°C, 5% CO$_2$, the luciferase activity is determined by adding 15 μL of Steady Lite Plus substrate to each well and readout performed on a microplate imager. Lowest effective concentrations (LEC) values are determined for TLR7-agonist-1.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

**REFERENCES**