**TES-991**

**Cat. No.:** HY-112619  
**CAS No.:** 1883602-20-7  
**Molecular Formula:** C₁₇H₁₁N₇OS₂  
**Molecular Weight:** 393.45  
**Target:** Others  
**Pathway:** Others  
**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 : 62.5 mg/mL (158.85 mM; Need ultrasonic)  
H₂O : < 0.1 mg/mL (insoluble)

<table>
<thead>
<tr>
<th>Preparing Stock Solutions</th>
<th>Solvent Concentration</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mM</td>
<td></td>
<td>2.5416 mL</td>
<td>12.7081 mL</td>
<td>25.4162 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td>0.5083 mL</td>
<td>2.5416 mL</td>
<td>5.0832 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td>0.2542 mL</td>
<td>1.2708 mL</td>
<td>2.5416 mL</td>
</tr>
</tbody>
</table>

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

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
   Solubility: ≥ 2.08 mg/mL (5.29 mM); Clear solution  
2. Add each solvent one by one: 10% DMSO >> 90% corn oil  
   Solubility: ≥ 2.08 mg/mL (5.29 mM); Clear solution

**BIOLOGICAL ACTIVITY**

**Description**

TES-991 is a potent and selective human α-Amino-β-carboxymuconate-ε-semialdehyde Decarboxylase (ACMSD) inhibitor, with an IC₅₀ of 3 nM.

**IC₅₀ & Target**

IC₅₀: 3 nM (hACMSD)[¹].

**In Vitro**

TES-991 (compounds 21) is able to significantly increase intracellular NAD⁺ levels, providing further proof of their mechanism of action. TES-991 shows an inhibition of cytochrome P450 2C19, suggesting a possible involvement of the 2H-tetrazole motif in this interaction[¹].
<table>
<thead>
<tr>
<th>In Vivo</th>
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<tbody>
<tr>
<td>After the intravenous administration of 0.5 mg/kg, TES-991 (compound 21) shows low blood clearance, with low volumes of distribution and halflives ($t_{1/2}$) of about 4.0 and 5.0 h, respectively, although after oral administration at 5 mg/kg, the blood concentrations of TES-991 is quantifiable for up to 8 h. A moderate systemic exposure is observed for the 2H-tetrazole analogue, TES-991, a good systemic exposure is recorded for the free acid[1].</td>
</tr>
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REFERENCES