Atuveciclib Racemate

**Cat. No.:** HY-12871  
**CAS No.:** 1414943-88-6  
**Molecular Formula:** C₁₈H₁₈FN₅O₂S  
**Molecular Weight:** 387.43  
**Target:** CDK  
**Pathway:** Cell Cycle/DNA Damage  
**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: 100 mg/mL (258.11 mM; Need ultrasonic)

<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></td>
<td>1 mM</td>
<td>2.5811 mL</td>
<td>12.9056 mL</td>
<td>25.8111 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.5162 mL</td>
<td>2.5811 mL</td>
<td>5.1622 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.2581 mL</td>
<td>1.2906 mL</td>
<td>2.5811 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: ≥ 2.5 mg/mL (6.45 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
   Solubility: ≥ 2.5 mg/mL (6.45 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil  
   Solubility: ≥ 2.5 mg/mL (6.45 mM); Clear solution

### BIOLOGICAL ACTIVITY

**Description**  
Atuveciclib Racemate (BAY-1143572 Racemate) is the racemate mixture of Atuveciclib. Atuveciclib is a potent and highly selective, oral P-TEFb/CDK9 inhibitor which supresses CDK9/CycT1 with an IC₅₀ of 13 nM.

**IC₅₀ & Target**  
CDK9

**In Vitro**  
Atuveciclib (BAY-1143572) inhibits the proliferation of 7 MLL-rearrangements positive and negative AML cell lines.
with a median IC\textsubscript{50} of 385 nM (range 230-1100 nM) and induces apoptosis\cite{1}. Atuveciclib (BAY-1143572) has potent and highly selective PTEFb-kinase inhibitory activity in the low nanomolar range against PTEFb/CDK9 and an at least 50-fold selectivity against other CDKs. Atuveciclib (BAY-1143572) shows a favorable selectivity against a panel of non-CDK kinases. It shows broad antiproliferative activity against a panel of tumor cell lines with sub-micromolar IC\textsubscript{50} values. The concentration-dependent inhibition of the phosphorylation of the RNA polymerase II and downstream reduction of MYC mRNA and protein levels is observed\cite{2}.

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

### In Vivo

Atuveciclib (BAY-1143572) exhibits single agent efficacy at tolerated doses in 4 out of 5 AML xenograft tumor models in mice and in 2 out of 2 AML xenograft tumor models in rats upon once daily oral administration. Partial or even complete remissions could be achieved in several models\cite{1}. The inhibition of MYC mRNA is also observed in blood cells of Atuveciclib (BAY-1143572)-treated rats indicating the potential clinical utility of MYC in blood cells as a pharmacodynamic marker in clinical development. The in vivo efficacy of Atuveciclib (BAY-1143572) is significantly enhanced in combination with several chemotherapeutics in different solid tumor models\cite{2}.

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

### REFERENCES
