BMS-509744

Cat. No.: HY-11092  
CAS No.: 439575-02-7

Molecular Formula: $C_{32}H_{41}N_5O_4S_2$  
Molecular Weight: 623.83

Target: Itk
Pathway: Protein Tyrosine Kinase/RTK

Storage:
- Powder: -20°C 3 years, 4°C 2 years
- In solvent: -80°C 1 year, -20°C 6 months

SOLVENT & SOLUBILITY

In Vitro
DMSO: 21.9 mg/mL (35.11 mM; Need ultrasonic and warming)

<table>
<thead>
<tr>
<th>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>1.6030 mL</td>
<td>8.0150 mL</td>
<td>16.0300 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td>0.3206 mL</td>
<td>1.6030 mL</td>
<td>3.2060 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td>0.1603 mL</td>
<td>0.8015 mL</td>
<td>1.6030 mL</td>
</tr>
</tbody>
</table>

Preparing Stock Solutions

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 (4.01 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (4.01 mM); Clear solution

BIOLOGICAL ACTIVITY

Description
BMS-509744 is a potent, selective and ATP competitive Itk inhibitor with an IC$_{50}$ of 19 nM.

IC$_{50}$ & Target
IC$_{50}$: 19 nM [Itk]$^{[1]}$

In Vitro
BMS-509744 reduces T-cell receptor-induced functions including PLC$_{y1}$ tyrosine phosphorylation, calcium mobilization, IL-2 secretion, and T-cell proliferation in vitro in both human and mouse cells. BMS-488516 and BMS-509744 potently inhibit Itk in vitro with IC$_{50}$ values of 96 and 19 nM, respectively. Both compounds exhibit competitive kinetics with respect to ATP, suggesting that they bind to the ATP binding site of the Itk kinase domain$^{[1]}$.

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

BMS-509744 and BMS-488516 suppress the production of IL-2 induced by anti-T-cell receptor antibody administered to mice. BMS-509744 exhibits a 50% inhibitory capacity when dosed at 50 mg/kg, irrespective of the amount of induction antibody. BMS-509744 also significantly diminishes lung inflammation in a mouse model of ovalbumin-induced allergy/asthma[^1].

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**PROTOCOL**

**Kinase Assay[^1]**

BMS-509744 activity (IC\(_{50}\)) is determined by kinase assays. The kinase reactions are performed in the presence of 10 μM GST-SLP-76 and various concentrations of ATP for 10 min using 10 ng of enzyme. The concentrations of BMS-509744

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**Animal Administration[^1]**

Mice: Balb/c mice are injected subcutaneously with the compounds (BMS-509744 and BMS-488516) or vehicle (H\(_2\)O:ethanol:Tween 80 90:5:5) 15 min before intravenous administration of anti-CD3 antibody. Serum is collected for the analysis of IL-2 and compound levels at 90 min after anti-CD3 antibody administration. IL-2 is measured by ELISA, and compound levels are measured by mass spectrometry[^1].

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**CUSTOMER VALIDATION**

- Cancer Cell Int. 2019 Feb 14;19:32.
- Cancer Cell Int. 2019 Feb 14;19:32.
- Harvard Medical School LINCS LIBRARY

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**REFERENCES**


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Caution: Product has not been fully validated for medical applications. For research use only.

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