BPTES

Cat. No.: HY-12683
CAS No.: 314045-39-1
Molecular Formula: C₂₄H₂₄N₆O₂S₃
Molecular Weight: 524.68
Target: Glutaminase
Pathway: Metabolic Enzyme/Protease
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: 50 mg/mL (95.30 mM; Need ultrasonic)
H₂O: < 0.1 mg/mL (insoluble)

<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>1.9059 mL</td>
<td>9.5296 mL</td>
<td>19.0592 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td>0.3812 mL</td>
<td>1.9059 mL</td>
<td>3.8118 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td>0.1906 mL</td>
<td>0.9530 mL</td>
<td>1.9059 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 >> 90% corn oil
Solubility: ≥ 2.5 mg/mL (4.76 mM); Clear solution

BIOLOGICAL ACTIVITY

**Description**
BPTES is an allosteric and selective glutaminase inhibitor with an IC₅₀ of 0.16 μM.

**IC₅₀ & Target**
Glutaminase[¹]

**In Vitro**
BPTES (10 μM) exhibits inhibition of PDAC cell proliferation[¹]. BPTES preferentially slows growth of mutant IDH1 cells without inducing apoptosis. BPTES (10 μM) reduces glutaminase activity in both WT and mutant IDH1 expressing cells, diminishes glutamate and α-KG levels, and increases glycolytic intermediates while leaving total 2-HG levels unaffected[²]. BPTES (10 μM) shows a clear synergistic anti-cancer effect with 10 μM of 5-FU in A549 and EKVX cell lines, and results in a growth reduction response not only in EKVX and A549 but also in most of the NSCLC cell lines [³]. BPTES (10 μM) effectively reduces the levels of the metabolites of the TCA cycle, with no changes in the levels of...
metabolites in glycolysis and the pentose phosphate pathway. BPTES treatment reduces about 30% ATP production under normoxia, and an additional 10% reduction of ATP production is observed under hypoxia in EKVX.\[4\]

In Vivo

BPTES-NPs (BPTES nanoparticles, 1.2 mg BPTES in 100 µL nanoparticles, i.v.) significantly attenuates tumor growth in the patient-derived pancreatic orthotopic tumor model.\[1\]

PROTOCOL

Kinase Assay 2

DS4 cells are seeded in a T75 flask at $5 \times 10^5$ cells, and IDH1 expression is induced with doxycycline 48 hrs before assaying. Cells are collected and resuspended in PBS, 0.1% Triton X-100, and Halt-Protease Inhibitor. Cells are lysed for 30 min on ice and centrifuged for 30 min at 12000 rpm at 4°C. Protein concentration is measured using the BCA Assay. Varying amounts of protein are added to IDH activity assay buffer (33 mM Tris, pH 7.6, 0.33 mM EDTA, 0.1 mM NADP$, ^\text{+}$, 1.33 mM MnCl$_2$, and 1.3 mM isocitrate), and changes in absorbance at 340 nm after 5 min is documented for each protein amount.

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

Cell Assay 2

Cells are plated at a density of 500 cells/well in a 96-well black clear bottom plate. At 24 hrs, media is changed to the appropriate media (DMEM with 4.5 g/L, 1.5 g/L or 0.1 g/L glucose, 10% FBS, pencillin/streptomycin, and 4 mM glutamine with or without doxycycline). 48 hours after plating, compounds or DMSO are added. Media and alamarBlue is added to a volume of 200 µL in each well. Fluorescence is measured at 48 hrs or 72 hrs (EGCG) using a Victor3 plate-reader.

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Animal Administration 1

Four-week-old female Foxn1nuathymic nude mice are used for the assay. Freshly resected pancreatic tumor samples obtained from patients at the time of surgery are propagated from mouse to mouse as a live tumor bank. Once a tumor volume of 50 mm$^3$ is reached (4 wk postimplantation), mice are treated with 12.5 mg/kg BPTES by intraperitoneal injection, 200 mg/kg CB-839 twice per d by oral gavage, 54 mg/kg BPTES-NPs (1.2 mg BPTES in 100 µL nanoparticles per mouse) by intravenous injection, blank-NPs (100 µL per mouse) by intravenous injection, 25 mg/kg gemcitabine intraperitoneally, 250 mg/kg metformin intraperitoneally daily, or a combination of BPTES-NPs with gemcitabine or metformin. BPTES-NPs are injected once every 3 d for a total of six injections over 16 d.

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REFERENCES


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