**Capecitabine**

**Cat. No.:** HY-B0016

**CAS No.:** 154361-50-9

**Molecular Formula:** C₁₅H₂₂FN₃O₆

**Molecular Weight:** 359.35

**Target:** DNA/RNA Synthesis; Nucleoside Antimetabolite/Analog; Apoptosis

**Pathway:** Cell Cycle/DNA Damage; Apoptosis

**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 (278.28 mM; Need ultrasonic)

H₂O: ≥ 33.33 mg/mL (92.75 mM)

* "≥" means soluble, but saturation unknown.

### Preparing Stock Solutions

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Mass</th>
<th>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></td>
<td>2.7828 mL</td>
<td>13.9140 mL</td>
<td>27.8280 mL</td>
</tr>
<tr>
<td>5 mM</td>
<td></td>
<td></td>
<td>0.5566 mL</td>
<td>2.7828 mL</td>
<td>5.5656 mL</td>
</tr>
<tr>
<td>10 mM</td>
<td></td>
<td></td>
<td>0.2783 mL</td>
<td>1.3914 mL</td>
<td>2.7828 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: ≥ 10 mg/mL (27.83 mM); Clear solution

2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 10 mg/mL (27.83 mM); Clear solution

3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 10 mg/mL (27.83 mM); Clear solution

**BIOLOGICAL ACTIVITY**

**Description**

Capecitabine is an oral prodrug that is converted to its active metabolite, 5-FU, by thymidine phosphorylase.

**IC₅₀ & Target**

DNA/RNA Synthesis[¹]
Capecitabine is an anti-cancer chemotherapy drug. It is classified as an antimetabolite. Capecitabine is converted into 5′-deoxy-5-fluorocytidine (5′DFCR), 5′-deoxy-5-fluorouridine (5′DFUR) and 5-FU by carboxylesterases (CES1 and 2), cytidine deaminase (CDD), and thymidine phosphorylase (TP), in both liver and tumour. Capecitabine induces a significant cytotoxic effect in vitro only at high concentrations. Mean IC50 values vary from 860 μM in COLO205 cells to 6000 μM in HCT8 cells.

A pharmacokinetic/pharmacodynamic study is carried out in mice bearing HCT 116 xenografts receiving 0.52 and 2.1 mmol/kg/d of Capecitabine by oral gavage. Capecitabine administered at 0.52 mmol/kg/day induces partial control of HCT 116 xenografts tumour growth: growth rate =7.5±0.5 on day 21. Capecitabine 2.1 mmol/kg/day achieves complete control of tumor growth during the treatment period: growth rate =1±0.2 on day 21.

HCT 116, HT29, HCT8, HCT15, SW620 and COLO205 human colon cancer cells are used. Cells are plated on day 1 in 96-well plates at a density of 2500 cells/well for HCT 116, 3500 cells/well for HCT8 and HT29, 5000 cells/well for HCT15, 6000 cells/well for SW620 and 7000 cells/wells for COLO205 in a volume of 150 μL/well. All cell lines are treated on day 2 with increasing concentrations of Capecitabine (0.1-10 mM), 5′DFCR (10 nM-100 μM), 5′DFUR (2.5-500 μM) or 5-FU (0.5-250 μM) for 24 h. After drug exposure, cells are washed once with cold PBS and placed in 200 μL of drug-free medium for 72 h after the end of drug exposure. The cells are then fixed with trichloroacetic acid and stained with sulforhodamine B. Optical densities are measured at 540 nm with a Biohit BP-800. The results are based on three independent experiments performed in triplicate.

Six-week-old C57/Bl6 Nu/Nu mice are used. Bilateral HCT 116 xenografts are obtained by subcutaneous injection of 10^7 cells/flank. Animals bearing HCT 116 xenografts are treated with vehicle or Capecitabine 0.52 or 2.1 mmol/kg (563 and 2250 mg/m^2, respectively) given once daily for 5 consecutive days/week by oral gavage for 3 weeks (days 0-4, 7-11, 14-18). Animals are culled on day 0 at 15, 30 min, 1, 2, 4, 8 and 24 h, and prior to planned treatment on days 7 and 14 after the start of treatment. Three animals per time-point are analysed. At the time of collection, blood is collected in heparin, and plasma isolated and stored at −80°C. The liver is removed immediately and stored in RNAlater solution. Tumours are macro-dissected to remove fibrotic tissue and blood vessels and snap-frozen in liquid nitrogen.


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