Dicoumarol

Cat. No.: HY-N0645
CAS No.: 66-76-2
Molecular Formula: C₁₉H₁₂O₆
Molecular Weight: 336.29
Target: PDHK
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
H₂O : 50 mg/mL (148.68 mM; ultrasonic and adjust pH to 13 with NaOH)
DMSO : 3.67 mg/mL (10.91 mM; Need ultrasonic)
H₂O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Mass</th>
<th>1 mg</th>
<th>5 mg</th>
<th>10 mg</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂O</td>
<td>1 mM</td>
<td>2.9736 mL</td>
<td>14.8681 mL</td>
<td>29.7362 mL</td>
</tr>
<tr>
<td></td>
<td>5 mM</td>
<td>0.5947 mL</td>
<td>2.9736 mL</td>
<td>5.9472 mL</td>
</tr>
<tr>
<td></td>
<td>10 mM</td>
<td>0.2974 mL</td>
<td>1.4868 mL</td>
<td>2.9736 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 (7.43 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (7.43 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description
Dicoumarol is an inhibitor of both NAD(P)H:quinone oxidoreductase 1 (NQO1) and PDK1 with IC₅₀ of 0.37 and 19.42 μM, respectively.

IC₅₀ & Target
IC₅₀: 0.37 μM [NQO1][¹], 19.42 μM [PDK1][²]

In Vitro
Dicoumarol is an inhibitor of both NAD(P)H:quinone oxidoreductase 1 (NQO1) and PDK1 with IC₅₀ of 0.37±0.15 and 19.42±0.032 μM, respectively. The PDK1 activity is inhibited by Dicoumarol in a dose-dependent manner. The enzymatic activity of PDK1 is reduced by approximately 94% when treated with 200 μM Dicoumarol. Dicoumarol decreases the p-
PDHA1 level by 26% (100 μM Dicoumarol) and by 72% (200 μM Dicoumarol), with no statistical difference in the total PDHA1 level. Both 100 μM and 200 μM Dicoumarol markedly induce apoptosis of SKOV3 cells. Similarly, flow cytometric analysis of annexin V+PI+ cells reveals that 100 μM and 200 μM Dicoumarol treatments generate approximately 20.87% and 24.94% apoptotic cells, respectively, significantly higher than vehicle treatment[2]. It is also observed that treatment of MCF-7-TAMR cells with Dicoumarol, a known NQO1 inhibitor, reverses their tamoxifen-resistance phenotype[3].

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

| In Vivo | Dichloroacetate (DCA) at 100 mg/kg, Dicoumarol at 30 mg/kg, and Dicoumarol at 50 mg/kg all significantly reduce tumor volume and decrease tumor weight, when compare to tumors from control or vehicle groups. Total caspase-3 and total anti-poly (ADP-ribose) polymerase (PARP) are significantly decreased in Dicoumarol-treated SKOV3 xenografts, when compare to tumors from the control or vehicle group[2].

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|---|---|

### PROTOCOL

#### Cell Assay [2]

The in vitro cell viability is examined using the standard MTT assay. SKOV3 or A2780 cells are seeded in 96-well plates at 8000 cells/well. The next day, increasing concentrations of Dicoumarol (DIC) are added into each well, and the plate is incubated for 24 h. Then, 10 μL of 10 mg/mL MTT reagent in phosphate-buffered saline (PBS) is added into each well, and the plate is incubated for an additional 4 h. The formazan crystals are dissolved in 150 μL of DMSO, and after the plate is shaken for 5 min, the optical density at 570 nm is recorded by the reader[2].

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#### Animal Administration [2]

Twenty five female BALB/c-nu mice aged 5 to 6 weeks old and weighing approximately 15 g each are used. A total of 1×10⁷ SKOV3 cells are subcutaneously injected into the upper flank. After 10 days, when the tumor volume reaches approximately 100 mm³, the nude mice are randomized into five groups (n=5/group) and are given the following treatments intraperitoneally (i.p.) every other day, for a total of 12 days: control group, administered with 0.2 mL of 0.9% NaCl; vehicle group, administered with 1 mM NaOH; dichloroacetate (DCA) group, administered with 100 mg/kg DCA; Dicoumarol (DIC)-30 group, administered with 30 mg/kg Dicoumarol; and Dicoumarol-50 group, administered with 50 mg/kg Dicoumarol. The body weights and tumor volumes of each mouse are monitored every other day until sacrifice (on day 12 after the initial treatment)[2].

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#### CUSTOMER VALIDATION

- Neuroscience. 2020 Apr.

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### REFERENCES


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