## Product Data Sheet

### Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Product Name</strong></td>
<td>Simvastatin (Zocor)</td>
</tr>
<tr>
<td><strong>Cas No.</strong></td>
<td>79902-63-9</td>
</tr>
<tr>
<td><strong>M.Wt</strong></td>
<td>418.6</td>
</tr>
<tr>
<td><strong>Formula</strong></td>
<td>C25H38O5</td>
</tr>
<tr>
<td><strong>Chemical Name</strong></td>
<td>[(1S,3R,7S,8S,8aR)-8-[2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl]-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl] 2,2-dimethylbutanoate</td>
</tr>
<tr>
<td><strong>Canonical SMILES</strong></td>
<td>CCC(C)(C)(=O)OC1CC(C=C2C1C(C=C2)C)CCC3CC(CC(=O)O3)O)C</td>
</tr>
<tr>
<td><strong>Solubility</strong></td>
<td>&gt;20.95mg/mL in DMSO</td>
</tr>
<tr>
<td><strong>Storage</strong></td>
<td>Store at -20°C</td>
</tr>
<tr>
<td><strong>General tips</strong></td>
<td>For obtaining a higher solubility, please warm the tube at 37°C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.</td>
</tr>
</tbody>
</table>
| **Shopping Condition** | Evaluation sample solution : ship with blue ice  
All other available size: ship with RT, or blue ice upon request |

### Biological Activity

**Targets:** HMG-CoA Reductase  
**Pathways:** Metabolism >> HMG-CoA Reductase  
**Description:** Simvastatin (SIM), a lactone, is white, crystalline, nonhygroscopic and powdery, practically insoluble in water (30 mcg/ml), and 0.1 (N) HCl (60 mcg/ml). Its precursor is a fermentation product of Aspergillus terreus. It is used for treating coronary heart disease, hyperlipidemia,
hypercholesterolemia, atherosclerosis and stroke [1] [2]. SIM is biologically inactive. Oral ingestion hydrolyzed it into the β-hydroxyacid form which is an inhibitor of 3-hydroxy-3-methyl glutaryl coenzyme A (HMG CoA) reductase [2]. In human lung microvascular endothelial cells, it increased the amount of endothelial nitric oxide synthase mRNA [3]. Simvastatin had anti-cancer properties [1]. Its IC50 to inhibit P-glycoprotein is 9 μM [4].

HMG CoA reductase catalyses an early rate-limiting step in the biosynthesis of cholesterol [2]. In both cell lines HepG2 and Huh7, both doses of simvastatin (32 and 64 μM) had a significant inhibitory effect on tumor cell growth as compared to controls (p<0.05). This effect was time-dependent, a simvastatin pre-treatment for 48 h or 72 h significantly reduced cell growth as compared to 24 h pre-incubation (p<0.05). Simvastatin treatment for 48 or 72 h made HepG2 cells exhibit downregulation of CDK1, CDK2, CDK4 and cyclins D1 and E as compared to control tumor cells. Simvastatin treatment for 24, 48 and 72 h made relative expression of cyclin-dependent kinase inhibitors p19 and p27 enhance as compared to control tumor cells [1]. In patients with polygenic hypercholesterolemia and allocated to diet plus 20 mg/day simvastatin for 8 weeks, total cholesterol (-27%), low density lipoproteincholesterol (-33%), and monocyte expression of TNF (-49%) and IL-1( (-35%) significantly decreased (p<0.02) [5].

Reference:

Protocol

Cell experiment:

Cell lines Mouse L-M cells (fibroblast), rat H4IIE cells (liver) and human Hep G2 cells (liver)

Preparation method The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below - 20 °C for several months.

Reacting conditions
In mouse L-M cells (fibroblast), rat H4IIE cells (liver) and human Hep G2 cells (liver), Simvastatin inhibited cholesterol synthesis with the IC50 values of 19.3 nM, 13.3 nM and 15.6 nM, respectively.

Animal experiment [3]:

Animal models
Dogs

Dosage form
50 mg/kg/d; p.o.; q.d., for 1 month

Applications
Compared with L654,969 group, Simvastatin group showed a much lower serum cholesterol concentration. However, Simvastatin and Lovastatin showed equivalent cholesterol-lowering effects.

Other notes
Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

Reference:

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Shortterm storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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