Product Name: Gedunin
Catalog No.: 3387
Batch No.: 4
CAS Number: 2753-30-2
IUPAC Name: (1S,3aS,4aR,4bS,5R,6aR,10aR,10bR,12aS)-5-(Acetyloxy)-1-(3-furanyl)-1,5,6,6a,7,10a,10b,11,12,12a,decahydro-4b,7,7,10a,12a,-pentamethyloxireno[cl]phenanthro[1,2-d]pyran-3,8(3aH,4bH)-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{28}H_{34}O_{7}
Batch Molecular Weight: 482.57
Physical Appearance: White solid
Solubility: DMSO to 100 mM
ethanol to 10 mM with gentle warming
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: R_{f} = 0.5 (5:3:2 petrol:DCM:EtOAc)
HPLC: Shows >98.9% purity
^1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [\alpha]_D = +67.1 (Concentration = 1, Solvent = Methanol)
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
<th>Error</th>
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</thead>
<tbody>
<tr>
<td>Carbon</td>
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<tr>
<td>Hydrogen</td>
<td>7.1</td>
<td>7.15</td>
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</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Naturally occurring Hsp90 inhibitor. Induces Hsp90-dependent client protein degradation and displays antiproliferative activity in vitro (IC50 values are 3.22, 8.84 and 16.8 μM in SKBr3, MCF-7 and CaCo-2 cancer cell lines respectively). Decreases ovarian cancer cell proliferation in vitro and may enhance cisplatin-induced reduction in proliferation (CAT.No 3387). Also exhibits antimalarial activity against P. falciparum (IC50 values are 0.14 and 3.1 μM in parasite development and [H] -hypoxanthine uptake assays respectively).

Physical and Chemical Properties:
Batch Molecular Formula: C28H34O7
Batch Molecular Weight: 482.57
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ethanol to 10 mM with gentle warming

Stability and Solubility Advice:
Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:
SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.
SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References: