



Certificate of Analysis

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Product Name: Embelin Catalog No.: 2156 Batch No.: 1

CAS Number: 550-24-3 EC Number: 208-979-8

IUPAC Name: 2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{26}O_4$ Batch Molecular Weight: 294.39

Physical Appearance: Dark orange solid

Solubility: ethanol to 10 mM with gentle warming

DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

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2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows >98% purity

¹H NMR: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 69.36 8.9 Found 69.4 9.04



Product Information

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Print Date: Sep 16th 2016

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IUPAC Name: 2,5-Dihydroxy-3-undecyl-2,5-cyclohexadiene-1,4-dione

Description:

Cell-permeable, non-peptide inhibitor of X-linked inhibitor of apoptosis (XIAP) (IC $_{50}=4.1~\mu M$ in competition binding assay with Smac peptide); binds to the BIR3 domain, preventing XIAP interaction with caspase-9 and Smac. Inhibits cell growth, induces apoptosis and activates caspase-9 in prostate cancer cells (IC $_{50}$ 4 - 6 μM), but has a weaker effect on normal prostate cells (IC $_{50}=19$ - 20 μM). Overcomes the protective effect of XIAP on apoptosis in XIAP-transfected Jurkat cells. Anti-tumor, analgesic and anti-inflammatory in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₇H₂₆O₄ Batch Molecular Weight: 294.39 Physical Appearance: Dark orange solid

Minimum Purity: >98%

Batch Molecular Structure:

но

Storage: Store at +4°C

Solubility & Usage Info:

ethanol to 10 mM with gentle warming DMSO to 100 mM

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:

Modak et al (2013) Probing p300/CBP associated factor (PCAF)-dependent pathways with a small molecule inhibitor. ACS Chem.Biol. 8

Nikolovska-Coleska *et al* (2004) Discovery of embelin as a cell-permeable, small-molecular weight inhibitor of XIAP through structure-based computational screening of a traditional herbal medicine three-dimensional structure database. J.Med.Chem. *47* 2430. PMID: 15115387.

Chitra et al (1994) Antitumor, anti-inflammatory and analgesic property of embelin, a plant product. Chemotherapy 40 109. PMID: 7510605.