

Product Name: Docetaxel

Catalog No.: 4056

Batch No.: 3

CAS Number: 114977-28-5

IUPAC Name: [2a*R*-[2aα,4β,4aβ,6β,9α(α*R*^{*},β*S*^{*}),11α,12α,12aα,12bα]]-β-[[[(1,1-Dimethylethoxy)carbonyl]amino]-α-hydroxy-12b-(acetyloxy)-12-(benzyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester benzenepropanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₃H₅₃NO₁₄·¼H₂O

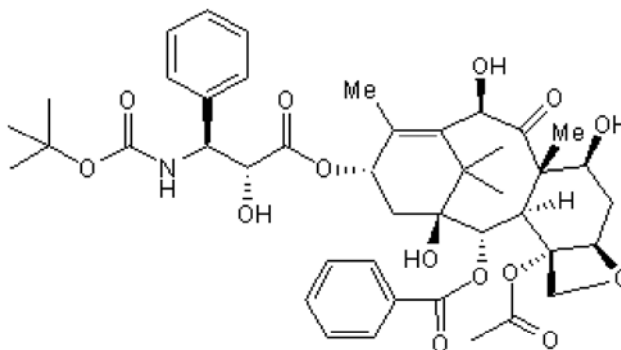
Batch Molecular Weight: 812.38

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.57	6.64	1.72
Found	63.35	6.54	1.87

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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CAS Number: 114977-28-5

IUPAC Name: [2a*R*-[2a α ,4 β ,4a β ,6 β ,9 α (α R*, β S*),11 α ,12 α ,12a α ,12b α]]- β -[[[1,1-Dimethylethoxy)carbonyl]amino]- α -hydroxy-12b-(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,6,11-trihydroxy-4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1*H*-cyclodeca[3,4]benz[1,2-*b*]oxet-9-yl ester benzenepropanoic acid

Description:

Binds and stabilizes microtubules; leads to cell cycle arrest and apoptosis. Displays significant antitumor activity in ovarian and gastric tumors. Prevents microtubule depolymerization and disassembly in the absence of GTP. Exhibits cytotoxic activity.

Physical and Chemical Properties:

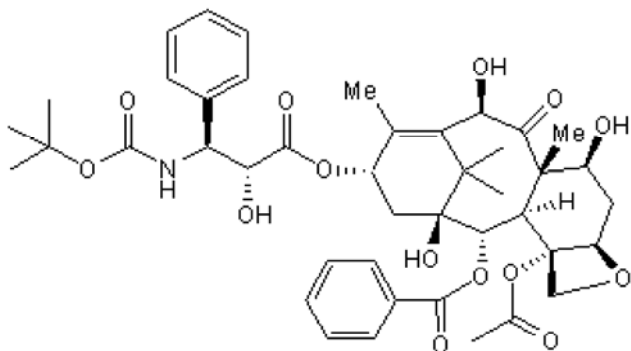
Batch Molecular Formula: C₄₃H₅₃NO₁₄·1/4H₂O

Batch Molecular Weight: 812.38

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Ramaswamy and Puhalla (2006) Docetaxel: a tubulin-stabilizing agent approved for the management of several solid tumors. *Drugs Today (Barc)* **42** 265. PMID: 16703123.

Lyseng-Williamson and Fenton (2005) Docetaxel: a review of its use in metastatic breast cancer. *Drugs* **65** 2513. PMID: 16296875.

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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.

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