

Certificate of Analysis

Product Name: Capecitabine

Catalog No.: 4799

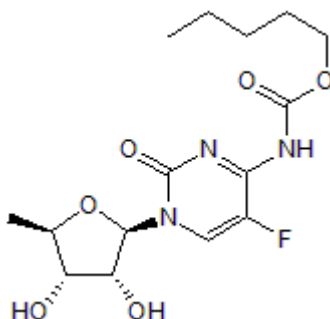
Batch No.: 2

CAS Number: 154361-50-9

IUPAC Name: 5'-Deoxy-5-fluoro-N-[(pentyloxy)carbonyl]cytidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₂₂FN₃O₆
Batch Molecular Weight: 359.35
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	50.14	6.17	11.69
Found	50.12	6.18	11.54

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

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IUPAC Name: 5'-Deoxy-5-fluoro-*N*-[(pentyloxy)carbonyl]cytidine

Description:

Prodrug of 5-Fluorouracil (5-FU) (Cat. No. 3257). Selectively activated in tumor cells by thymidine phosphorylase; inhibits DNA synthesis upon conversion to 5-FU. Orally available.

Physical and Chemical Properties:

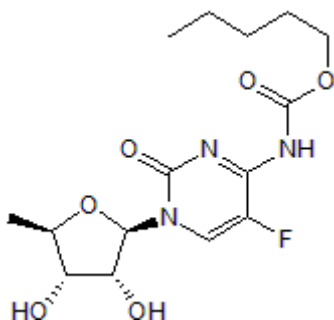
Batch Molecular Formula: C₁₅H₂₂FN₃O₆.

Batch Molecular Weight: 359.35

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Bhuyan *et al* (1972) Cell cycle phase specificity of antitumor agents. *Cancer Res.* **32** 398. PMID: 4258018.

Shimma *et al* (2000) The design and synthesis of a new tumor-selective fluoropyrimidine carbamate, *capecitabine*. *Bioorg.Med.Chem.Lett.* **8** 1697. PMID: 10976516.

Desmoulin *et al* (2002) Metabolism of capecitabine, an oral fluorouracil prodrug: ¹⁹F NMR studies in animal models and human urine. *Drug Metab.Dispos.* **30** 1221. PMID: 12386128.

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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