

Certificate of Analysis

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Product Name: Gemcitabine hydrochloride

Catalog No.: 3259

Batch No.: 3

CAS Number: 122111-03-9

IUPAC Name: (+)-2'-Deoxy-2',2'-difluorocytidine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₉H₁₁F₂N₃O₄.HCl

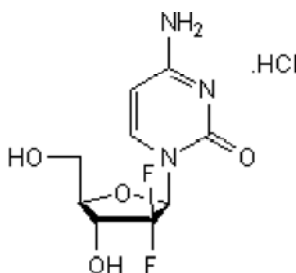
Batch Molecular Weight: 299.66

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 20 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +49.4 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	36.07	4.04	14.02
Found	36.07	3.92	13.77

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

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CAS Number: 122111-03-9

IUPAC Name: (+)-2'-Deoxy-2',2'-difluorocytidine hydrochloride

Description:

Gemcitabine hydrochloride is a deoxycytidine analog that inhibits DNA synthesis. Metabolized to form gemcitabine triphosphate (dFdCTP) and gemcitabine diphosphate (dFdCDP). dFdCTD inhibits ribonucleotide reductase causing a reduction in cellular nucleotides. dFdCTP is incorporated in DNA resulting in DNA strand termination. Displays antitumor activity in vitro and in vivo. Inhibits replication of MERS-CoV and SARS-CoV in vitro (EC₅₀ values are 1.216 and 4.957 μM, respectively).

Physical and Chemical Properties:

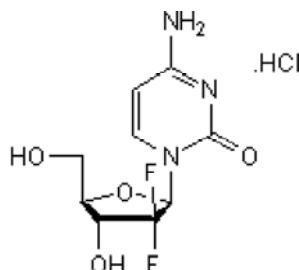
Batch Molecular Formula: C₉H₁₁F₂N₃O₄.HCl

Batch Molecular Weight: 299.66

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Dyall et al (2014) Repurposing of clinically developed drugs for treatment of Middle East Respiratory Syndrome coronavirus infection. *Antimicrob.Agents.Chemother.* **58** 4885. PMID: 24841273.

Heinemann et al (1995) Gemcitabine: a modulator of intracellular nucleotide and deoxynucleotide metabolism. *Semin.Oncol.* **22** (Suppl. 11) 11. PMID: 7481839.

Plunkett et al (1995) Preclinical characteristics of gemcit. *Anticancer Drugs* **6** (Suppl. 6) 7. PMID: 8718419.

Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 100 mM

DMSO to 20 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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