Print Date: Jan 15th 2013

Certificate of Analysis

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Product Name: **Trifluorothymidine** **Catalog No.: 4460** **Batch No.: 1**

CAS Number: 70-00-8

IUPAC Name: α,α,α-Trifluorothymidine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{10}H_{11}F_3N_2O_5$

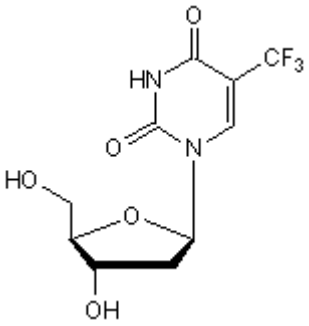
Batch Molecular Weight: 296.2

Physical Appearance: White solid

Solubility: water to 50 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +53.8 (Concentration = 1, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	40.55	3.74	9.46
Found	40.55	3.78	9.22

Product Information

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CAS Number: 70-00-8

IUPAC Name: α,α,α-Trifluorothymidine

Description:

Nucleoside analog; inhibitor of thymidylate synthase. Incorporation of the triphosphate form into DNA induces DNA fragmentation. Exhibits antitumor activity.

Physical and Chemical Properties:

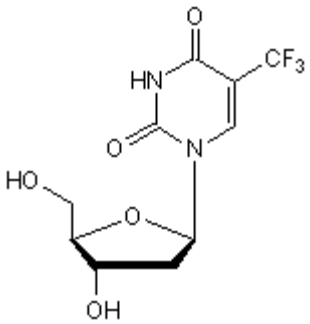
Batch Molecular Formula: $C_{10}H_{11}F_3N_2O_5$

Batch Molecular Weight: 296.2

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 50 mM
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:

Emura *et al* (2005) Potentiation of the antitumor activity of α, α, α-trifluorothymidine by the co-administration of an inhibitor of thymidine phosphorylase at a suitable molar ratio in vivo. Int.J.Oncol. ***27*** 449. PMID: 16010427.

Okayama *et al* (2012) Involvement of concentrative nucleoside transporter 1 in intestinal absorption of trifluorothymidine, a novel antitumor nucleoside, in rats. J.Pharmacol.Exp.Ther. ***340*** 457. PMID: 22076553.