

Certificate of Analysis

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Product Name: Methotrexate

Catalog No.: 1230

Batch No.: 3

CAS Number: 59-05-2

EC Number: 200-413-8

IUPAC Name: *N*-[4-[[[(2,4-Diamino-6-pteridiny)l)methyl]methylamino]benzoyl]-L-glutamic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₂N₈O₅·3H₂O

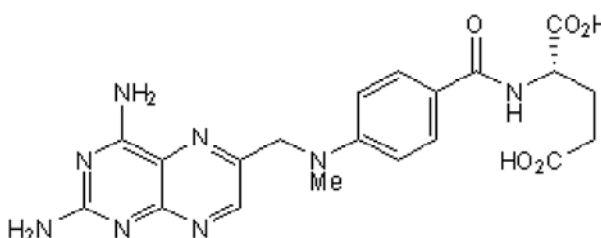
Batch Molecular Weight: 508.49

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +20.6 (Concentration = 1, Solvent = 0.05M Sodium Carbonate)

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

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Description:

Methotrexate is a cytotoxic agent. Inhibits thymidylate synthetase and de novo purine synthesis. Potent folic acid antagonist; inhibits dihydrofolate reductase. Also inhibits Ras carboxyl methylation in DKOB8 cells, leading to decreased p44 and Akt activation.

Physical and Chemical Properties:

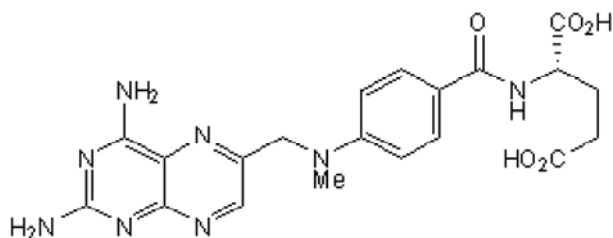
Batch Molecular Formula: C₂₀H₂₂N₈O₅·3H₂O

Batch Molecular Weight: 508.49

Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

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:

Winter-Vann et al (2003) Targeting Ras signaling through inhibition of carboxyl methylation: an unexpected property of methotr. *Proc.Natl.Acad.Sci.U.S.A.* **100** 6529. PMID: 12750467.

Chu et al (1990) Mechanism of thymidylate synthase inhibition by methotr. in human neoplastic cell lines and normal human myeloid progenitor cells. *J.Biol.Chem.* **265** 8470. PMID: 2341391.

Allegra et al (1987) Evidence for direct inhibition of *de novo* protein synthesis in human MCF-7 breast cells as a principal mode of metabolic inhibition by methotr. *J.Biol.Chem.* **262** 13520. PMID: 2443493.

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