

**Product Name:** Methotrexate

**Catalog No.:** 1230

**Batch No.:** 2

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:** C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>·3H<sub>2</sub>O

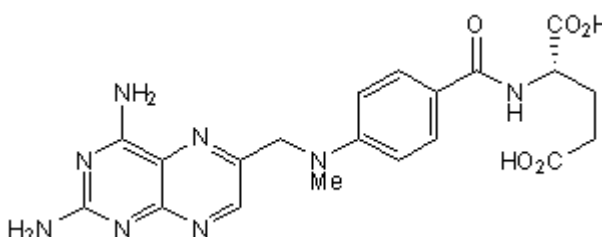
**Batch Molecular Weight:** 508.49

**Physical Appearance:** Orange solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.6% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +18.74 (Concentration = 1, Solvent = 0.05M Sodium Carbonate)

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	47.24	5.55	22.04
Found	47.53	5.45	22.08

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 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373  
[www.RnDSystems.com](http://www.RnDSystems.com)

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

**Description:**

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:**

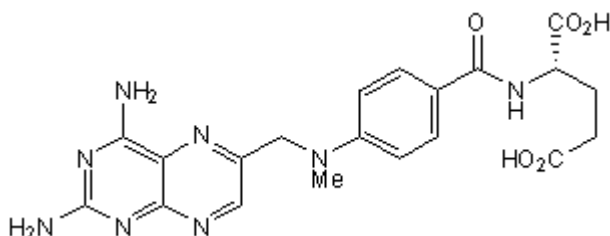
Batch Molecular Formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>·3H<sub>2</sub>O

Batch Molecular Weight: 508.49

Physical Appearance: Orange 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:**

**Jolivet et al** (1983) The pharmacology and clinical use of methotrexate. *N.Engl.J.Med.* **309** 1094. PMID: 6353235.

**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 methotrexate. *J.Biol.Chem.* **262** 13520. PMID: 2443493.

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

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

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