

Product Name: Phototrexate

Catalog No.: 7362

Batch No.: 2

CAS Number: 2268033-83-4

IUPAC Name: *N*-[4-[(1*E*)-2-(2,4-Diamino-6-quinazoliny)diazenyl]benzoyl]-L-glutamic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₁₉N₇O₅·1½H₂O

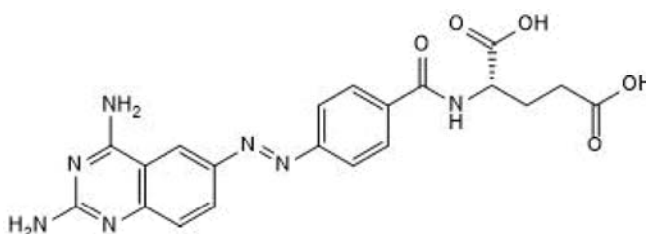
Batch Molecular Weight: 464.44

Physical Appearance: Brown solid

Solubility: DMSO to 4 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 96.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.72	4.77	21.11
Found	51.36	4.66	20.86

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

bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956

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IUPAC Name: N-[4-[(1E)-2-(2,4-Diamino-6-quinazoliny)diazenyl]benzoyl]-L-glutamic acid

Description:

Phototrexate is a photoswitchable potent inhibitor of human dihydrofolate reductase (DHFR). Phototrexate is a photochromic analog of Methotrexate (Cat. No. 1230). Antifolate activity is switched on (cis-Phototrexate) by UVA (375 nm) light; it can be switched off (trans-Phototrexate) by blue or white light and by thermal relaxation in the dark. cis-Phototrexate (IC₅₀ = 6 nM) significantly reduces the viability of HeLa cells compared with trans-Phototrexate (IC₅₀ = 34 μM).

Physical and Chemical Properties:

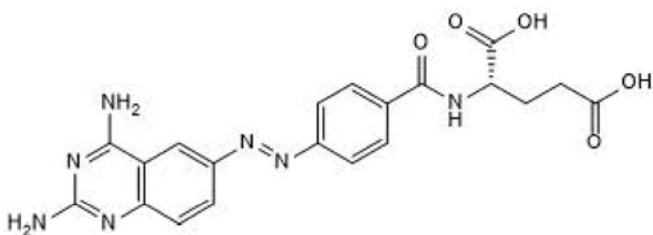
Batch Molecular Formula: C₂₀H₁₉N₇O₅·1½H₂O

Batch Molecular Weight: 464.44

Physical Appearance: Brown solid

Minimum Purity: ≥95%

Batch Molecular Structure:



References:

Mashita et al (2019) Light-wavelength-based quantitative control of dihydrofolate reductase activity by using a photochromic isostere of an inhibitor. *Chembiochem.* **20** 1382. PMID: 30656808.

Matera et al (2018) Photoswitchable antimetabolite for targeted photoactivated chemotherapy. *J.Am.Chem.Soc.* **140** 15764. PMID: 30346152.

Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 4 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.

Licensing Information:

Sold with permission of IBEC.

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North America

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