

Product Name: CI 898 trihydrochloride

Catalog No.: 2039

Batch No.: 3

CAS Number: 1658520-97-8

IUPAC Name: 5-Methyl-6-[[[(3,4,5-trimethoxyphenyl)amino]methyl]-2,4-quinazolinediamine trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₃N₅O₃·3HCl

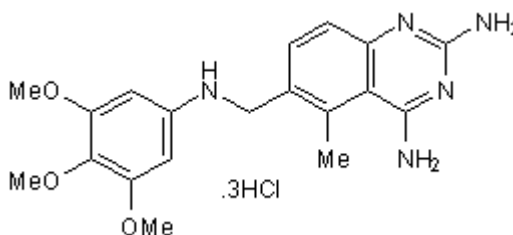
Batch Molecular Weight: 478.8

Physical Appearance: Pale yellow solid

Solubility: water to 20 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.65 (Dichloromethane:Methanol:Ammonia soln. [80:18.2])

HPLC: Shows 95.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.66	5.47	14.63
Found	47.72	5.77	14.47

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Description:

Potent lipophilic inhibitor of dihydrofolate reductase (DHFR) that displays antineoplastic and antiprotozoal properties. Inhibits protozoal, bacterial and human DHFR with IC₅₀ values of 1.4, 6.1 and 3.2 nM respectively. Affects G₁/S phase cell cycle progression.

Physical and Chemical Properties:

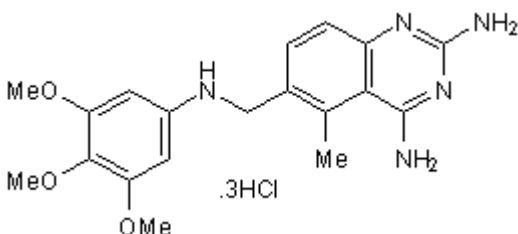
Batch Molecular Formula: C₁₉H₂₃N₅O₃.3HCl

Batch Molecular Weight: 478.8

Physical Appearance: Pale yellow solid

Minimum Purity: >95%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 20 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:

Chan and Anderson (2006) Towards species-specific antifolates. *Curr.Med.Chem.* **13** 377. PMID: 16475929.

Allegra et al (1987) Potent in vitro and in vivo antitoxoplasma activity of the lipid-soluble antifolate trimetrexate. *J.Clin.Invest.* **79** 478. PMID: 2948969.

Hook et al (1986) Cell cycle effects of trimetrexate (CI-898). *Cancer Chemother.Pharmacol.* **16** 116. PMID: 2936525.

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