

# **Data Sheet**

Product Name: Nolatrexed dihydrochloride

 Cat. No.:
 CS-0028903

 CAS No.:
 152946-68-4

 Molecular Formula:
 C14H14Cl2N4OS

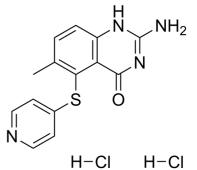
Molecular Weight: 357.26

Target: Thymidylate Synthase

Pathway: Apoptosis

Solubility: H2O: 50 mg/mL (139.95 mM; Need ultrasonic); DMSO: 41.67

mg/mL (116.64 mM; Need ultrasonic)



## **BIOLOGICAL ACTIVITY:**

Nolatrexed dihydrochloride (AG 337) is a non-competitive lipophilic inhibitor of **thymidylate synthase**, interacts at the folate cofactor binding site of the enzyme, with a  $\mathbf{K_i}$  of 11 nM for human thymidylate synthase<sup>[1]</sup>. Nolatrexed dihydrochloride (AG 337) induces cell cycle arrest in S phase of cancer cells. Anti-cancer activity<sup>[2]</sup>. IC50 & Target: Ki: 11 nM (Human Thymidylate Synthase)<sup>[1]</sup>

#### References:

- [1]. Webber S, et al. AG337, a novel lipophilic thymidylate synthase inhibitor: in vitro and in vivo preclinical studies. Cancer Chemother Pharmacol. 1996;37(6):509-17.
- [2]. McGuire JJ, et al. Characterization of the effect of AG337, a novel lipophilic thymidylate synthase inhibitor, on human head and neck and human leukemia cell lines.

### **CAIndexNames:**

4(1H)-Quinazolinone, 2-amino-6-methyl-5-(4-pyridinylthio)-, hydrochloride (1:2)

#### **SMILES:**

[H]CI.O=C1N=C(N)NC2=C1C(SC3=CC=NC=C3)=C(C)C=C2.[H]CI

Caution: Product has not been fully validated for medical applications. For research use only.

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