

Product Name: Dimethylenastron

Catalog No.: 5261

Batch No.: 1

CAS Number: 863774-58-7

IUPAC Name: 2,3,4,6,7,8-Hexahydro-4-(3-hydroxyphenyl)-7,7-dimethyl-2-thioxo-5(1H)-quinazolinone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₈N₂O₂S·¼H₂O

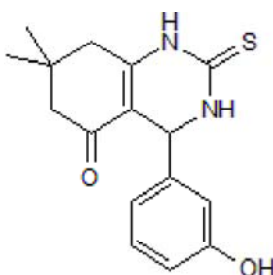
Batch Molecular Weight: 306.89

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.44 (Chloroform:Methanol [9:1])

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.62	6.08	9.13
Found	62.5	6.11	9.07

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

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Description:

Inhibitor of mitotic motor kinesin Eg5 (IC₅₀ = 200 nM). Arrests mitosis, triggers apoptosis and up-regulates Hsp-70 expression in multiple human myeloma cell lines. Also inhibits the growth of several types of cancer cell lines (EC₅₀ values are 330, 603, 743 and 881 nM in HCT116, Htert-HME1, BxPC3, K562 and NCI-H1299 cancer cells, respectively). Suppresses the migration and invasion of PANC1 cells in vitro. Cytoprotective.

Physical and Chemical Properties:

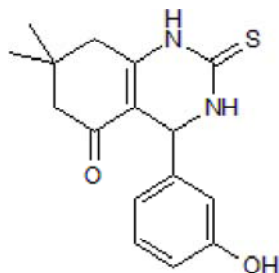
Batch Molecular Formula: C₁₆H₁₈N₂O₂S.¼H₂O

Batch Molecular Weight: 306.89

Physical Appearance: Pale yellow solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Sun et al (2011) Dimethylenastron suppresses human pancreatic cancer cell migration and invasion in vitro via allosteric inhibition of mitotic kinesin Eg5. *Acta.Pharmacol Sin.* **32** 1543. PMID: 21986572.

Kaan et al (2010) Structural basis for inhibition of Eg5 by dihydropyrimidines: stereoselectivity of antimetabolic inhibitors enastron, dimethylenastron and fluorastrol. *J.Med.Chem.* **53** 5676. PMID: 20597485.

Liu et al (2006) Inhibition of the mitotic kinesin Eg5 up-regulates Hsp70 through the phosphatidylinositol 3-kinase/Akt pathway in multiple myeloma cells. *J.Biol.Chem.* **281** 18090. PMID: 16627469.

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 100 mM

ethanol to 50 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.

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