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: $\text{C}_{16}\text{H}_{18}\text{N}_{2}\text{O}_{2}\text{S}\cdot\frac{1}{4}\text{H}_{2}\text{O}$
Batch Molecular Weight: 306.89
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM
ethanol to 50 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: $R_f = 0.44$ (Chloroform:Methanol [9:1])
HPLC: Shows 98.8% purity
$^1$H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>62.62</td>
<td>62.5</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.08</td>
<td>6.11</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.13</td>
<td>9.07</td>
</tr>
</tbody>
</table>

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, Ht-29, 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: C16H16N2O2S.¼H2O
Batch Molecular Weight: 306.89
Physical Appearance: Pale yellow solid
Minimum Purity: >99%

Batch Molecular Structure:

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.

References: