

**Product Name:** VER 155008

**Catalog No.:** 3803

**Batch No.:** 3

CAS Number: 1134156-31-2

IUPAC Name: 5'-O-[(4-Cyanophenyl)methyl]-8-[[[(3,4-dichlorophenyl)methyl]amino]-adenosine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>25</sub>H<sub>23</sub>Cl<sub>2</sub>N<sub>7</sub>O<sub>4</sub> · ½H<sub>2</sub>O

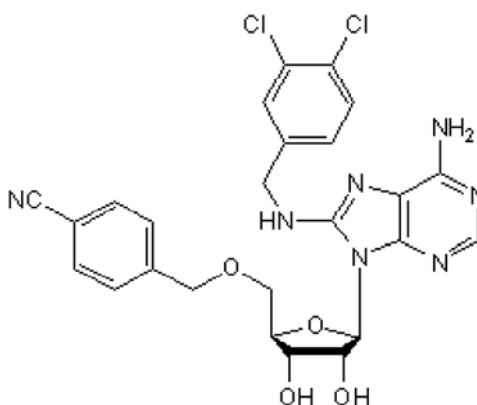
**Batch Molecular Weight:** 565.41

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.5% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 53.11  | 4.28     | 17.34    |
| Found       | 52.98  | 4.03     | 17.41    |

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

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**Description:**

Novel adenosine-derived inhibitor of Heat Shock Protein 70 (Hsp70) ( $IC_{50} = 0.5 \mu M$ ). Inhibits cell proliferation of multiple human tumor cell lines in vitro. Also binds Hsc70 and Grp78; displays selectivity against Hsp90 $\beta$  ( $IC_{50} > 200 \mu M$  for Hsp90 $\beta$ ).

**Physical and Chemical Properties:**

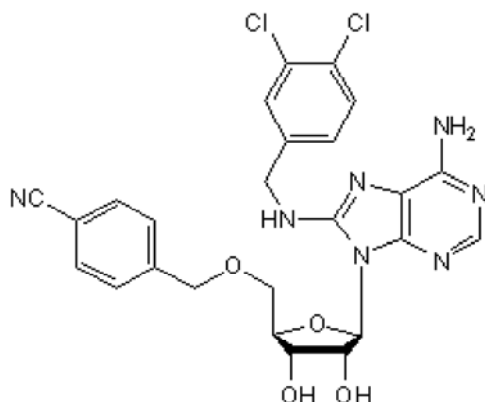
Batch Molecular Formula:  $C_{25}H_{23}Cl_2N_7O_4 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 565.41

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

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:**

**Macias *et al*** (2011) Adenosine-derived inhibitors of 78 kDa glucose regulated protein (Grp78) ATPase: insights into isoform selectivity. *J.Med.Chem.* **54** 4034. PMID: 21526763.

**Massey *et al*** (2010) ATPases as drug targets: insights from heat shock proteins 70 and 90. *J.Med.Chem.* **53** 7280. PMID: 20608738.

**Massey *et al*** (2009) A novel, small molecule inhibitor of Hsc70/Hsp70 potentiates Hsp90 inhibitor induced apoptosis in HCT116 colon carcinoma cells. *Cancer Chemother.Pharmacol.* **66** 535. PMID: 20012863.

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