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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **HA14-1** **Catalog No.: 1541** **Batch No.: 2**

CAS Number: 65673-63-4

IUPAC Name: 2-Amino-6-bromo-α-cyano-3-(ethoxycarbonyl)-4*H*-1-benzopyran-4-acetic acid ethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{17}BrN_2O_5$

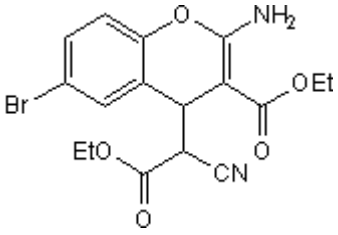
Batch Molecular Weight: 409.23

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.77 (Ethyl acetate:Petroleum ether [1:1])

Melting Point: Between 115 - 116°C

^{1}H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.89	4.19	6.85
Found	49.63	4.14	6.61

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Description:

Cell-permeable inhibitor of Bcl-2 protein (IC_{50} ~ 9 μM); acts by binding to the surface pocket. Disrupts Bax/Bcl-2 interaction and induces apoptosis of tumor cells. Also binds to the antiapoptotic Blc-2 proteins Bcl-XL and Bcl-w.

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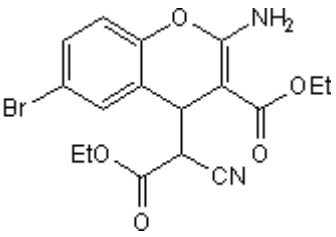

Storage: Desiccate at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

CAUTION - This product may be susceptible to decomposition when stored in solution. Therefore, we recommend that, as far as possible, solutions should be made up and used within 24 hours.

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:

Wang *et al* (2000) Structure-based discovery of an organic compound that binds Bcl-2 protein and induces apoptosis of tumor cells. Proc.Natl.Acad.Sci.U.S.A. ***97*** 7124. PMID: 10860979.

Milella *et al* (2002) Synergistic induction of apoptosis by simultaneous disruption of the Bcl-2 and MEK/MAPK pathways in acute myelogenous leukemia. Blood ***99*** 3461. PMID: 11964319.

Doshi *et al* (2006) Structure-activity relationship studies of ethyl 2-amino-6-bromo-4-(1-cyano-2-ethoxy-2-oxoethyl)-4H-chromene-3-carboxylate (HA 14-1), an antagonist for antiapoptotic Bcl-2 proteins to overcome drug resistance in cancer. J.Med.Chem. ***49*** 7731. PMID: 17181155.

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