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Certificate of Analysis

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Print Date: Jan 15th 2016

Product Name: AG 825 Catalog No.: 1555 Batch No.: 1

CAS Number: 149092-50-2

IUPAC Name: (E)-3-[3-[2-Benzothiazolythio)methyl]-4-hydroxy-5-methoxyphenyl]-2-cyano-2-propenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{19}H_{15}N_3O_3S_2$ **Batch Molecular Formula:**

Batch Molecular Weight: 397.47 Yellow solid **Physical Appearance:**

Solubility: DMSO to 100 mM Store at +4°C Storage:

Batch Molecular Structure:

2. ANALYTICAL DATA

 $R_f = 0.65$ (Ethyl acetate) TLC:

Melting Point: At 262°C(dec) **HPLC:** Shows 97.1% purity

¹H NMR: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 57.42 3.8 10.57 Found 57.4 3.85 10.2



Product Information

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Description:

Selective ErbB2 inhibitor (IC $_{50}$ values are 0.15 and 19 μ M at ErbB2 and ErbB1 respectively). Preferentially triggers p38 MAP kinase-dependent apoptosis in androgen-independent prostate cancer cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₉H₁₅N₃O₃S₂ Batch Molecular Weight: 397.47 Physical Appearance: Yellow solid

Batch Molecular Structure:

Storage: Store at +4°C

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:

Gazit *et al* (1993) Tyrphostins. 3. Structure-activity relationship studies of α -substituted benzylidenemalononitrile 5-S-aryltyrphostins. J.Med.Chem. **36** 3556. PMID: 7902440.

Osherov et al (1993) Selective inhibition of the epidermal growth factor and HER2/Neu receptors by tyrphostins. J.Biol.Chem. 268 11134. PMID: 8098709.

Murillo et al (2001) Tyrphostin AG825 triggers p38 mitogen-activated protein kinase-dependent apoptosis in androgen-independent prostate cancer cells C4 and C4-21. Cancer Res. 61 7408. PMID: 11606371.