



Certificate of Analysis

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Product Name: DPN Catalog No.: 1494 Batch No.: 7

CAS Number: 1428-67-7

IUPAC Name: 2,3-bis(4-Hydroxyphenyl)-propionitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{15}H_{13}NO_2$. ¹/₄ H_2O

Batch Molecular Weight: 243.77

Physical Appearance: Off-white solid

Solubility: 1eq. NaOH to 30 mM

ethanol to 100 mM DMSO to 100 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.37$ (Ethyl acetate:Hexane [1:1])

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 73.91 5.58 5.75 Found 74.21 5.43 5.95



Product Information

Print Date: Jan 8th 2016

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Description:

Highly potent estrogen ER β receptor agonist with a 70-fold selectivity over ER α (EC $_{50}$ values are 0.85 and 66 nM respectively). Relaxes mesenteric arteries in vitro. Shown to regulate expression of GluR1, GluR2 and GluR3 in rat hippocampus.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{15}H_{13}NO_2$. ¼ H_2O

Batch Molecular Weight: 243.77 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at -20°C

Solubility & Usage Info:

1eq. NaOH to 30 mM ethanol to 100 mM 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:

Meyers *et al* (2001) Estrogen receptor-β potency-selective ligands: structure-activity relationship studies of diarylpropionitriles and their acetylene and polar analogues. J.Med.Chem. *44* 4230. PMID: 11708925.

Montgomery et al (2003) Acute effects of oestrogen receptor subtype-specific agonists on vascular contractility. Br.J.Pharmacol. 139 1249. PMID: 12890703.

Harrington *et al* (2003) Activities of estrogen receptor alpha- and beta-selective ligands at diverse estrogen responsive gene sites mediating transactivation or transrepression. Mol.Cell.Endocrinol. **206** 13. PMID: 12943986.

Waters et al (2009) Estrogen receptor alpha and beta specific agonists regulate expression of synaptic proteins in rat hippocampus. Brain Res. 1290 1, PMID: 19596275.