# **Certificate of Analysis**

## www.tocris.com

Print Date: Dec 14th 2018

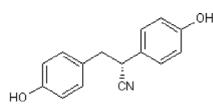
## Product Name: (R)-DPN

CAS Number: 524047-78-7 IUPAC Name: (*R*)-2,3-*bis*(4-Hydroxyphenyl)-propionitrile

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub> 239.27 White solid 1eq. NaOH to 25 mM DMSO to 100 mM ethanol to 100 mM Store at -20°C

# Storage: Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: HPLC: Chiral HPLC: <sup>1</sup>H NMR: Mass Spectrum: Optical Rotation: Microanalysis:  $\label{eq:Rf} \begin{array}{l} \mathsf{R_f} = 0.3 \mbox{ (Dichloromethane:Ethyl acetate:Petrol [3:2:5])} \\ \mathsf{Shows 100\% purity} \\ \mathsf{Shows >98.9\% purity} \\ \mathsf{Consistent with structure} \\ \mathsf{Consistent with structure} \\ [\alpha]_D = -9.2 \mbox{ (Concentration = 1.1, Solvent = Methanol)} \\ \\ \hline \\ \mathsf{Carbon Hydrogen Nitrogen} \\ \mathsf{Theoretical } 75.3 \qquad 5.48 \qquad 5.85 \\ \mathsf{Found} \qquad 75.13 \qquad 5.53 \qquad 5.97 \end{array}$ 

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# a biotechne brand

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Catalog No.: 4494 Batch No.: 1

# TOCRIS a biotechne brand

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Batch No.: 1

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#### Product Name: (R)-DPN

CAS Number: 524047-78-7 IUPAC Name: (*R*)-2,3-*bis*(4-Hydroxyphenyl)-propionitrile

#### **Description:**

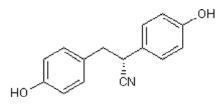
Enantiomer of DPN (Cat. No. 1494). Displays higher affinity for estrogen receptor (ER)  $\beta$  over ER $\alpha$  (K<sub>i</sub> values are 1.82 and 147 nM respectively).

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>15</sub>H<sub>13</sub>NO<sub>2</sub> Batch Molecular Weight: 239.27 Physical Appearance: White solid

#### Minimum Purity: >98%

**Batch Molecular Structure:** 



#### Storage: Store at -20°C

#### Solubility & Usage Info:

1eq. NaOH to 25 mM DMSO to 100 mM ethanol 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).

Catalog No.: 4494

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:**

**Carroll** *et al* (2011) Diarylpropionitrile (DPN) enantiomers: synthesis and evaluation of estrogen receptor  $\beta$ -selective ligands. J.Med.Chem. **55** 528. PMID: 22122563.

Weiser et al (2009) Estrogen receptor- $\beta$  agonist diarylpropionitrile: biological activities of *R*- and *S*-enantiomers on behavior and hormonal response to stress. Endocrinology **150** 1817. PMID: 19074580.

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