# TOCRIS a biotechne brand

#### Print Date: Jan 14th 2016

# **Certificate of Analysis**

# www.tocris.com

### Product Name: YE 120

Catalog No.: 4457 Batch No.: 1

CAS Number: IUPAC Name: 383124-82-1

2-[3-Cyano-5-(3,4-dichlorophenyl)-4,5-dimethyl-2(5H)-furanylidene]propanedinitrile

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C<sub>16</sub>H<sub>9</sub>Cl<sub>2</sub>N<sub>3</sub>O 330.17 White solid DMSO to 100 mM Store at -20°C

NC NC

## 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum: Microanalysis: Shows 99.8% purity Consistent with structure Consistent with structure

	Carbon	Hydrogen	Nitrogen
Theoretical	58.21	2.75	12.73
Found	58.08	2.68	12.74

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

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#### **Description:**

GPR35 agonist (EC<sub>50</sub> = 32 nM in DMR assays). Also displays partial agonist activity in a  $\beta$ -arrestin translocation assay (EC<sub>50</sub> = 10.2  $\mu$ M).

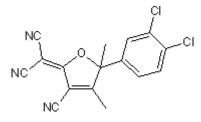
383124-82-1

### Physical and Chemical Properties:

Batch Molecular Formula: C<sub>16</sub>H<sub>9</sub>Cl<sub>2</sub>N<sub>3</sub>O Batch Molecular Weight: 330.17 Physical Appearance: White solid

#### Minimum Purity: >98%

**Batch Molecular Structure:** 



#### Storage: Store at -20°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).

Catalog No.: 4457

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:**

**Deng** *et al* (2011) Discovery of 2-(4-methylfuran-2(5*H*)-ylidene)malononitrile and thieno[3,2-*b*]thiophene-2-carboxylic acid derivatives as G protein-coupled receptor 35 (GPR35) agonists. J.Med.Chem. **54** 7385. PMID: 21950657.

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