



# **Certificate of Analysis**

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Product Name: YE 120 Catalog No.: 4457 Batch No.: 1

CAS Number: 383124-82-1

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{16}H_9Cl_2N_3O$ 

Batch Molecular Weight: 330.17
Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 99.8% purity

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.21 2.75 12.73 Found 58.08 2.68 12.74





# **Product Information**

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#### **Description:**

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

#### **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).

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.

