# TOCRIS a biotechne brand

#### Print Date: May 13th 2020

# **Certificate of Analysis**

## www.tocris.com

Batch No.: 2

Catalog No.: 4430

### Product Name: BAY 41-2272

CAS Number: 256376-24-6

IUPAC Name: 5-Cyclopropyl-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-4-pyrimidinamine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C<sub>20</sub>H<sub>17</sub>FN<sub>6</sub> 360.39 Off-white solid DMSO to 100 mM Store at +4°C

 $NH_2$ 

## 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 66.66 4.75 23.32			

Found

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66.22

4.75

22.93

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## **Product Information**

# Print Date: May 13<sup>th</sup> 2020

#### Product Name: BAY 41-2272

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IUPAC Name:

5-Cyclopropyl-2-[1-[(2-fluorophenyl)methyl]-1H-pyrazolo[3,4-b]pyridin-3-yl]-4-pyrimidinamine

#### **Description:**

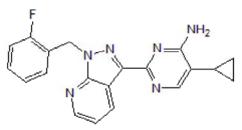
Activator of soluble guanylyl cyclase (sGC); acts at a nitric oxide (NO)-independent regulatory site in the sGC  $\alpha_1$  subunit. Inhibits platelet aggregation (IC<sub>50</sub> = 36 nM) and phenylephrine-induced contractions of rabbit aorta (IC<sub>50</sub> = 0.30  $\mu$ M). Also reduces vascular smooth muscle growth through cAMP- and cGMP-dependent PKA and PKG pathways.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>20</sub>H<sub>17</sub>FN<sub>6</sub> Batch Molecular Weight: 360.39 Physical Appearance: Off-white solid

#### Minimum Purity: ≥98%

#### **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:**

**Joshi** *et al* (2011) The soluble guanylate cyclase stimulator BAY 41-2272 inhibits vascular smooth muscle growth through the cAMP-dependent protein kinase pathways. J.Pharmacol.Exp.Ther. **339** 394. PMID: 21825001.

Stasch et al (2010) NO-independent regulatory site on soluble guanylate cyclase. Nature 410 212. PMID: 11242081.

**Mittendorf** *et al* (2009) Discovery of Riociguat (BAY 63-2521): a potent, oral stimulator of soluble guanylate cyclase for the treatment of pulmonary hypertension. ChemMedChem **4** 853. PMID: 19263460.

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## Catalog No.: 4430 B

Batch No.: 2