

**Product Name:** BAY 41-2272

**Catalog No.:** 4430

**Batch No.:** 1

**CAS Number:** 256376-24-6

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

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>20</sub>H<sub>17</sub>FN<sub>6</sub>·½H<sub>2</sub>O

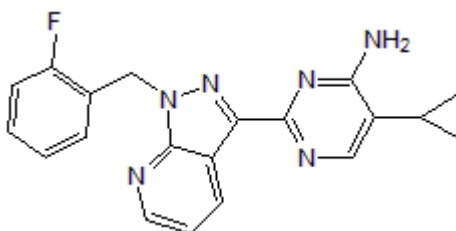
**Batch Molecular Weight:** 369.4

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	65.03	4.91	22.75
Found	65.09	4.73	22.64

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

**Product Name:** BAY 41-2272

**Catalog No.:** 4430

**Batch No.:** 1

CAS Number: 256376-24-6

IUPAC Name: 5-Cyclopropyl-2-[1-[(2-fluorophenyl)methyl]-1*H*-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 ( $IC_{50}$  = 36 nM) and phenylephrine-induced contractions of rabbit aorta ( $IC_{50}$  = 0.30  $\mu$ M). Also reduces vascular smooth muscle growth through cAMP- and cGMP-dependent PKA and PKG pathways.

**Physical and Chemical Properties:**

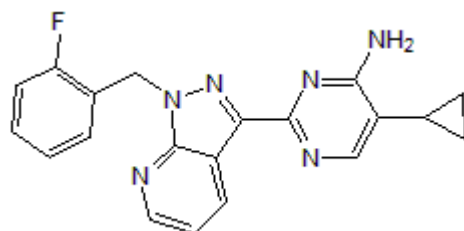
Batch Molecular Formula:  $C_{20}H_{17}FN_6 \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 369.4

Physical Appearance: 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:**

**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.

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

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

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