



**IUPAC Name:** 

# **Certificate of Analysis**

[4-[[6-Cyclopropyl-3-(1H-pyrazol-4-yl)imidazo[1,2-a]pyrazin-8-yl]amino]-3-fluorophenyl]-4-morpholinylmethanone

www.tocris.com

Product Name: P21d hydrochloride Catalog No.: 6073 Batch No.: 1

hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{23}H_{22}FN_7O_2.HCl.2H_2O$ 

**Batch Molecular Weight:** 519.96 **Physical Appearance:** White solid

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

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

HPLC: Shows >98.5% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.13 5.23 18.86 Found 53 5.14 18.93



## **Product Information**

Print Date: Jul 5<sup>th</sup> 2017

www.tocris.com

Product Name: P21d hydrochloride Catalog No.: 6073 Batch No.: 1

IUPAC Name: [4-[[6-Cyclopropyl-3-(1*H*-pyrazol-4-yl)imidazo[1,2-*a*]pyrazin-8-yl]amino]-3-fluorophenyl]-4-morpholinylmethanone

hydrochloride

#### **Description:**

Potent and selective breast tumor kinase (Brk) inhibitor (IC $_{50}$  = 30 nM). Exhibits >650-fold selectively for Brk over Aurora B kinase and Lck. Downregulates SNAIL protein, restores Ecadherin expression and suppresses migration in breast cancer cells. Also active in vivo and orally bioavailable.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>23</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>2</sub>.HCl.2H<sub>2</sub>O

Batch Molecular Weight: 519.96 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:

**Ito** et al (2016) PTK6 inhibition suppresses metastases of triple-negative breast cancer via SNAIL-dependent E-cadherin regulation. Cancer Res. **76** 4406. PMID: 27302163.

Zeng et al (2011) Discovery of novel imidazo[1,2-a]pyrazin-8-amines as Brk/PTK6 inhibitors. Bioorg.Med.Chem.Lett 21 5870. PMID: 21855335.