

# **Certificate of Analysis**

Print Date: Feb 11th 2022

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Product Name: 7rh Catalog No.: 5860 Batch No.: 3

CAS Number: 1429617-90-2

IUPAC Name: 4-Ethyl-*N*-[3-[(4-methyl-1-piperazinyl)methyl]-5-(trifluoromethyl)phenyl]-3-(2-pyrazolo[1,5-*a*]pyrimidin-6-ylethynyl)

benzamide

# 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{30}H_{29}F_3N_6O$ .

Batch Molecular Weight: 546.59

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 98.4% purity

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

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 65.92 5.35 15.38 Found 65.6 5.41 15.33

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



# **Product Information**

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#### **Description:**

7rh is a potent and selective DDR1 inhibitor (IC $_{50}$  = 6.8 nM). Exhibits selectivity for DDR1 over DDR2, Bcr-Abl and c-Kit (IC $_{50}$  values are 101.4 and 355 nM and > 10  $\mu$ M, respectively) and a range of other kinases. Inhibits proliferation of cancer cell lines expressing high levels of DDR1 in vitro and suppresses cancer cell invasion, adhesion and tumorigenicity. Orally bioavailable.

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

Batch Molecular Formula:  $C_{30}H_{29}F_3N_6O$ . Batch Molecular Weight: 546.59

Physical Appearance: Off 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:

**Gao** et al (2013) Discovery and optimization of 3-(2-(pyrazolo[1,5-a]pyrimidin-6-yl)ethynyl)benzamides as novel selective and orally bioavailable discoidin domain receptor 1 (DDR1) inhibitors. J.Med.Chem. **56** 3281. PMID: 23521020.

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