

Product Name: 7rh

Catalog No.: 5860

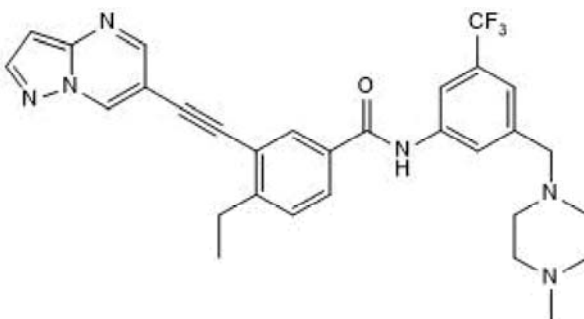
Batch No.: 1

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: C₃₀H₂₉F₃N₆O
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 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.92	5.35	15.38
Found	65.57	5.36	15.37

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

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Description:

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 μ 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:

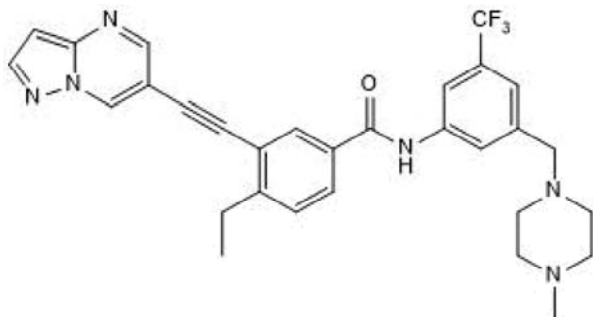
Batch Molecular Formula: $C_{30}H_{29}F_3N_6O$

Batch Molecular Weight: 546.59

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ 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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