

Product Name: GSK 429286

Catalog No.: 3726

Batch No.: 3

CAS Number: 864082-47-3

IUPAC Name: 4-[4-(Trifluoromethyl)phenyl]-N-(6-Fluoro-1H-indazol-5-yl)-2-methyl-6-oxo-1,4,5,6-tetrahydro-3-pyridinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₁₆F₄N₄O₂·¼H₂O

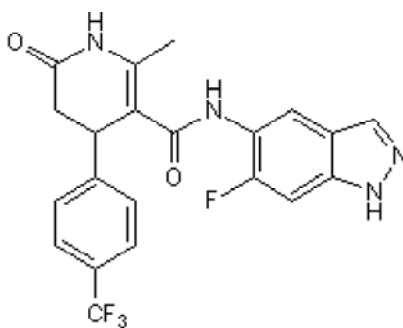
Batch Molecular Weight: 436.87

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.2 (Ethyl acetate:Petroleum ether [3:7])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.73	3.81	12.82
Found	57.53	3.74	12.7

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

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Description:

Selective Rho-kinase inhibitor (IC₅₀ values are 14, 780 and 1940 nM for ROCK1, RSK and p70S6K respectively). Reverses adrenalin-induced contraction of the rat aortic ring (IC₅₀ = 190 nM) and causes a dose-dependent decrease in mean arterial blood pressure in spontaneous hypertensive rats. Orally active.

Physical and Chemical Properties:

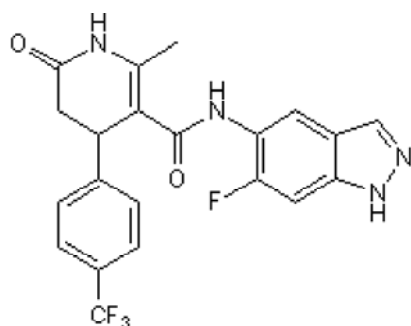
Batch Molecular Formula: C₂₁H₁₆F₄N₄O₂·½H₂O

Batch Molecular Weight: 436.87

Physical Appearance: White solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 25 mM

When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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.

Licensing Information:

Sold for research purposes under agreement from GlaxoSmithKline

References:

Nichols et al (2009) Substrate specificity and inhibitors of LRRK2, a protein kinase mutated in Parkinson's disease. *Biochem.J.* **424** 47. PMID: 19740074.

Goodman et al (2007) Development of dihydropyridone indazole amides as selective rho-kinase inhibitors. *J.Med.Chem.* **50** 6. PMID: 17201405.

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