

Product Name: Baricitinib

Catalog No.: 7222

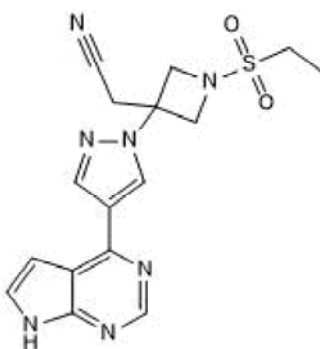
Batch No.: 1

CAS Number: 1187594-09-7

IUPAC Name: 1-(Ethylsulfonyl)-3-[4-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)-1H-pyrazol-1-yl]-3-azetidineacetonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₇N₇O₂S
Batch Molecular Weight: 371.42
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.74	4.61	26.4
Found	51.77	4.63	26.53

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

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Description:

Highly potent JAK1 and JAK2 inhibitor (IC₅₀ values are 5.9 and 5.7 nM, respectively). Also inhibits Tyk2 (IC₅₀ = 53 nM). Displays >100-fold selectivity for JAK1/2 over JAK3 (IC₅₀ = 53 nM for JAK3). Binds AAK1, BIKE, GAK and MPSK1 in vitro (K_d values are 17.2, 39.8, 134.4 and 68.5 nM, respectively). Inhibits IL-6-induced STAT phosphorylation and subsequent pro-inflammatory chemokine (MPC-1) and cytokine (IL-17 and IL-22) production in PBMCs and T-cells. Displays anti-inflammatory and disease modifying effects in the rat adjuvant arthritis model. In silico modelling predicts inhibition of SARS-CoV-2 cell entry. Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

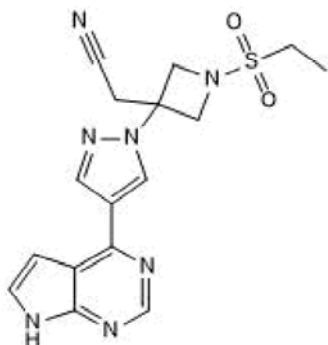
Batch Molecular Formula: C₁₆H₁₇N₇O₂S

Batch Molecular Weight: 371.42

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Richardson et al (2020) Baricitinib as potential treatment for 2019-nCoV acute respiratory disease. *Lancet*. **395** e30. PMID: 32032529.

Sorrell et al (2016) Family-wide structural analysis of human numb-associated protein kinases. *Structure*. **24** 401. PMID: 26853940.

Fridman et al (2010) Selective inhibition of JAK1 and JAK2 is efficacious in rodent models of arthritis: preclinical characterization of INCB028050. *J.Immunol.* **184** 5298. PMID: 20363976.

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.

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