bio-techne
TOCRIS

Print Date: Jul 27th 2023

Certificate of Analysis

www.tocris.com

Product Name: **Baricitinib** **Catalog No.: 7222** **Batch No.: 2**

CAS Number: 1187594-09-7

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{17}N_7O_2S$

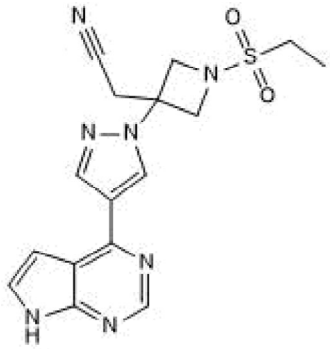
Batch Molecular Weight: 371.42

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.74	4.61	26.4
Found	51.85	4.54	26.23

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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Description:

Baricitinib is a highly potent JAK1 and JAK2 inhibitor (IC_{50} values are 5.9 and 5.7 nM, respectively). Also inhibits Tyk2 (IC_{50} = 53 nM). Displays >100-fold selectivity for JAK1/2 over JAK3 (IC_{50} = 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 specific page on www.tocris.com for full description.

Physical and Chemical Properties:

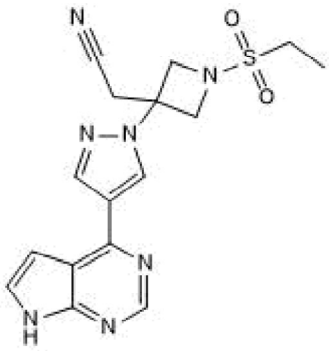
Batch Molecular Formula: $C_{16}H_{17}N_7O_2S$

Batch Molecular Weight: 371.42

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

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.