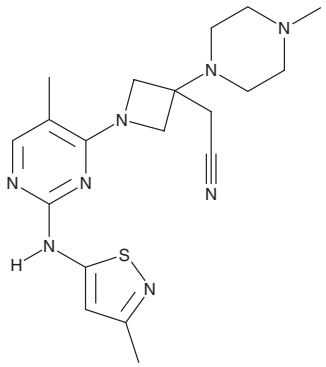
PRODUCT INFORMATION

JAK Inhibitor 31

Item No. 39387

CAS Registry No.:	2891469-99-9
Formal Name:	1-[5-methyl-2-[(3-methyl-5-isothiazolyl)amino]-4-pyrimidinyl]-3-(4-methyl-1-piperazinyl)-3-azetidineacetonitrile
Synonym:	Janus-Associated Kinase Inhibitor 31
MF:	$C_{19}H_{26}N_8S$
FW:	398.5
Purity:	≥98%
UV/Vis.:	λ_{max}: 226, 254, 286 nm
Supplied as:	A solid
Storage:	-20°C
Stability:	≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

JAK inhibitor 31 is supplied as a solid. A stock solution may be made by dissolving the JAK inhibitor 31 in the solvent of choice, which should be purged with an inert gas. JAK inhibitor 31 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of JAK inhibitor 31 in ethanol is approximately 10 mg/ml and approximately 30 mg/ml in DMSO and DMF.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of JAK inhibitor 31 can be prepared by directly dissolving the solid in aqueous buffers. JAK inhibitor 31 is slightly soluble in PBS (pH 7.2). We do not recommend storing the aqueous solution for more than one day.

Description

JAK inhibitor 31 is an inhibitor of JAK2 (IC_{50} = 3.9 nM).[1] It is selective for JAK2 over JAK3 (IC_{50}s = 70 nM), as well as Aurora B kinase, VEGFR2, Abl1, and GSK3β (IC_{50}s = 0.441, 1.5, 21.37, and 50 µM, respectively), but does inhibit JAK1 and TYK2 (IC_{50}s = 7 and 2.9 nM, respectively). JAK inhibitor 31 inhibits STAT3-mediated transcription of *IL6* in a secreted alkaline phosphatase (SEAP) reporter assay (IC_{50} = 162 nM). It reduces ocular inflammation, as well as decreases *Il6* expression in the meibomian glands, in a mouse model of allergic eye disease when used at concentrations of 1 or 3 mg/ml.

Reference

1. Gordhan, H.M., Miller, S.T., Clancy, D.C., *et al.* Eyes on topical ocular disposition: The considered design of a lead Janus kinase (JAK) inhibitor that utilizes a unique azetidin-3-amino bridging scaffold to attenuate off-target kinase activity, while driving potency and aqueous solubility. *J. Med. Chem.* **66(13)**, 8929-8950 (2023).

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