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	N N
Synonym:	Janus-Associated Kinase Inhibitor 31	
MF:	C ₁₉ H ₂₆ N ₈ S	Ń Ń
FW:	398.5	Ť
Purity:	≥98%	N S
UV/Vis.:	λ _{max} : 226, 254, 286 nm	H' II II
Supplied as:	A solid	
Storage:	-20°C	7
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 GSK3 β ($IC_{50}s$ = 0.441, 1.5, 21.37, and 50 μ M, respectively), but does inhibit JAK1 and TYK2 (IC₅₀s = 7 and 2.9 nM, respectively). JAK inhibitor 31 inhibits STAT3-mediated transcription of IL6 in a secreted alkaline phosphatase (SEAP) reporter assay $(IC_{50} = 162 \text{ nM})$. It reduces ocular inflammation, as well as decreases *II6* 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).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

SAFETY DATA This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 09/01/2023

CAYMAN CHEMICAL

1180 EAST ELLSWORTH RD ANN ARBOR, MI 48108 · USA PHONE: [800] 364-9897 [734] 971-3335 FAX: [734] 971-3640 CUSTSERV@CAYMANCHEM.COM WWW.CAYMANCHEM.COM