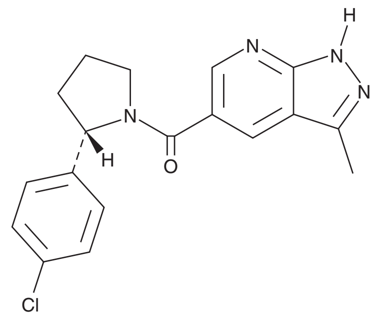
PRODUCT INFORMATION

MSC2530818

Item No. 29669

CAS Registry No.:	1883423-59-3
Formal Name:	[(2S)-2-(4-chlorophenyl)-1-pyrrolidinyl] (3-methyl-1H-pyrazolo[3,4-b]pyridin-5-yl)-methanone
MF:	$C_{18}H_{17}ClN_4O$
FW:	340.8
Purity:	≥98%
UV/Vis.:	λ_{max}: 223 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



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

Laboratory Procedures

MSC2530818 is supplied as a crystalline solid. A stock solution may be made by dissolving the MSC2530818 in the solvent of choice, which should be purged with an inert gas. MSC2530818 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of MSC2530818 in these solvents is approximately 10, 15, and 30 mg/ml, respectively.

MSC2530818 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, MSC2530818 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. MSC2530818 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

MSC2530818 is an orally bioavailable cyclin-dependent kinase 8 (Cdk8) inhibitor (IC_{50} = 2.6 nM).[1] It is selective for Cdk8 over a panel of 264 kinases at 1 µM but does inhibit glycogen synthase kinase 3α (GSK3α; IC_{50} = 691 nM). MSC2530818 inhibits STAT1 phosphorylation in SW620 colorectal cancer cells with an IC_{50} value of 8 nM. It also inhibits Wnt-dependent transcription in LS 174T, COLO 205, and PA-1 cancer cells (IC_{50}s = 32, 9, and 52 nM, respectively, in luciferase reporter assays). MSC2530818 (50 and 100 mg/kg) reduces tumor growth in a SW620 mouse xenograft model.

Reference

1. Czodrowski, P., Mallinger, A., Wienke, D., *et al.* Structure-based optimization of potent, selective, and orally bioavailable CDK8 inhibitors discovered by high-throughput screening. *J. Med. Chem.* **59(20)**, 9337-9349 (2016).

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