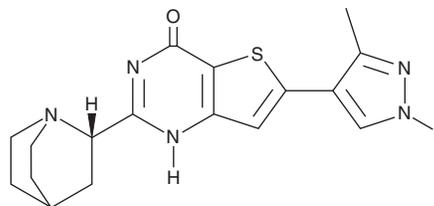


PRODUCT INFORMATION



Simurosertib Item No. 32519

CAS Registry No.: 1330782-76-7
Formal Name: 2-(2S)-1-azabicyclo[2.2.2]oct-2-yl-6-(3-methyl-1H-pyrazol-4-yl)-thieno[3,2-d]pyrimidin-4(3H)-one
Synonym: TAK-931
MF: C₁₇H₁₉N₅OS
FW: 341.4
Purity: ≥98%
Supplied as: A 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

Simurosertib is supplied as a solid. A stock solution may be made by dissolving the simurosertib in the solvent of choice, which should be purged with an inert gas. Simurosertib is soluble in DMSO.

Description

Simurosertib is an inhibitor of cell division cycle 7 (Cdc7) kinase (IC₅₀ = 0.26 nM).¹ It is selective for Cdc7 over cyclin-dependent kinase 2 (Cdk2) and Rho-associated kinase 1 (ROCK1; IC₅₀s = 6,300 and 430 nM, respectively). It inhibits phosphorylation of DNA replication licensing factor MCM2 in HeLa cells (IC₅₀ = 17 nM) and reduces proliferation of COLO 205 cells (EC₅₀ = 81 nM). Simurosertib induces replication stress, halts the cell cycle at the G₂/S phase, and inhibits the growth of a wide variety of cancer cells (GI₅₀s = 30.2->10,000 nM).² It reduces intratumor levels of phosphorylated MCM2 in COLO 205 and SW948 mouse xenograft models when administered at a dose of 80 mg/kg and reduces tumor growth in the same models when administered at doses of 40 or 60 mg/kg twice per day.

References

1. Kurasawa, O., Miyazaki, T., Homma, M., *et al.* Discovery of a novel, highly potent, and selective thieno[3,2-d]pyrimidinone-based Cdc7 inhibitor with a quinuclidine moiety (Tak-931) as an orally active investigational antitumor agent. *J. Med. Chem.* **63**(3), 1084-1104 (2020).
2. Iwai, K., Nambu, T., Dairiki, R., *et al.* Molecular mechanism and potential target indication of TAK-931, a novel CDC7-selective inhibitor. *Sci. Adv.* **5**(5), eaav3660 (2019).

WARNING

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

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, 12/02/2022

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