Product Datasheet

TAK-931

Catalog No. **BP-02140** · CAS **1330782-76-7** · Form **free base** · Physical state **other** · Color **white to off-white** · Version **1.0** · Revision **2026-09-02**

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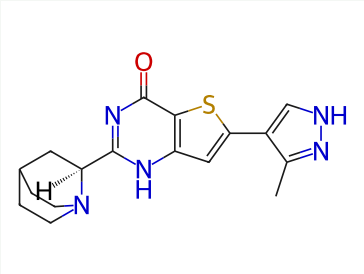
Target	Research area
CDK	**Cancer**

Molecular formula	**$C_{17}H_{19}N_5OS$**
Molecular weight	**341.4310**

STRUCTURE



DESCRIPTION

Simurosertib (TAK-931) is an orally active, selective and ATP-competitive cell division cycle 7 (CDC7) kinase inhibitor, with an IC50 of <0.3 nM. Simurosertib has anti-cancer activity.

BIOLOGICAL ACTIVITY

In Vitro

Simurosertib (TAK-931) potently inhibits CDC7 kinase activity (IC50 <0.3 nM) with a time-dependent ATP-competitive kinetics to its ATP-binding pocket. The selectivity studies using the 308 kinases reveals >120-fold selectivity of Simurosertib (TAK-931) for CDC7 kinase inhibition compared to other kinase inhibitions. Treatment with Simurosertib (TAK-931) suppresses the cellular MCM2 phosphorylation at Ser40 (pMCM2) in a dose-dependent manner, resulting in a delayed S phase progression, DNA-damage checkpoint activation, and caspase-3/7 activation.

In Vivo

In the COLO205-xenograft mouse model, oral administration of Simurosertib (TAK-931) inhibits pMCM2 of the xenografted COLO205 in dose- and time-dependent manners. Furthermore, Simurosertib (TAK-931) exhibits a significant antitumor activity in multiple xenograft models.

SOLUBILITY

Soluble in DMSO

In vitro	DMSO : 70 mg/mL

REFERENCES

[1]. K Iwai, et al. A novel CDC7-selective inhibitor TAK-931 with potent antitumor activity. European Journal of Cancer , 2016 , 69 (1) :S34.