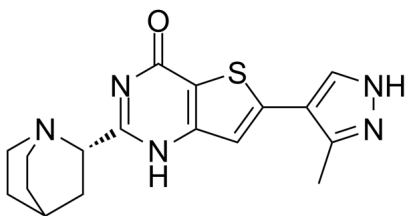


## Certificate of Analysis

Catalog Number	BP13498
Product Name	Simurosertib

## Physical and Chemical Properties

Synonyms	TAK-931
CAS No.	1330782-76-7
Chemical Formula	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> OS
Molecular Weight	341.43
Solubility	DMSO: 75 mg/mL (219.66 mM), Need ultrasonic
Storage	Powder: -20°C for 2 years In solvent: -80°C for 1 year
Chemical Structure OR Tested Image	

## Product Information

Description	Simurosertib is a selective and ATP-competitive cell division cycle 7 kinase inhibitor (IC <sub>50</sub> : <0.3 nM).
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Targets&IC50	Cdc7:<0.3 nM
In vitro	Simurosertib effectively inhibits CDC7 kinase activity (IC50 120-fold selectivity of Simurosertib for CDC7 kinase inhibition compared to other kinase inhibitions .
In vivo	Simurosertib (p.o.) inhibits pMCM2 of the xenografted COLO205 in a dose- and time-dependent manner in the COLO205-xenograft mouse model. Simurosertib shows a significant antitumor activity in multiple xenograft models .

## Analytical Data

HPLC	Shows Min >99% purity
H-NMR	Consistent with structure
Stability and Solubility Advice	Information on product stability, especially in solution, has rarely been reported and in most cases we can only provide a general guideline. We recommend that once the stock solution has been prepared, it be stored in equal quantities in sealed vials and used within 1 month. Avoid repeated freezing and thawing cycles. Storage conditions for some special products should be referred to their storage details.

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