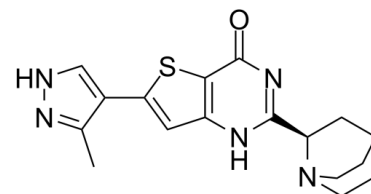


Data Sheet

Product Name:	(R)-Simurosertib
Cat. No.:	CS-0096221
CAS No.:	1330782-69-8
Molecular Formula:	C ₁₇ H ₁₉ N ₅ O ₂
Molecular Weight:	341.43
Target:	Others
Pathway:	Others
Solubility:	DMSO : 75 mg/mL (219.66 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

(R)-Simurosertib ((R)-TAK-931) is the (R)-enantiomer of Simurosertib, Simurosertib (TAK-931) is a selective cycle 7 (CDC7) kinase inhibitor, with an $IC_{50} < 0.3 \text{ nM}$ ^[1].

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.

CAIndexNames:

Thieno[3,2-d]pyrimidin-4(3H)-one, 2-(2R)-1-azabicyclo[2.2.2]oct-2-yl-6-(3-methyl-1H-pyrazol-4-yl)-

SMILES:

O=C1C=C(N2)C=C(C3=CN=C(C3)S1)N=C2[C@H]4CC5CCN4CC5

Caution: Product has not been fully validated for medical applications. For research use only.

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