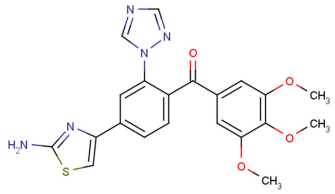
Data Sheet (Cat.No.T12823)

TargetMol
A DRUG SCREENING EXPERT

S516

Chemical Properties



CAS No.:	1016543-77-3
Formula:	C21H19N5O4S
Molecular Weight:	437.47
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	S516 is an active CKD-516 metabolite and is a potent inhibitor of tubulin polymerization(IC50 of 4.29 μM), has marked antitumor activity.
Targets(IC_{50})	tubulin polymerization: 4.29 μM
In vitro	S516 has potent cytotoxicity(HL-60, HCT116 and HCT15 cells with IC50s of 4.8 nM, 42.8 nM and 24.9 nM, respectively). S516 (30 nM; 16 hours; HL60 cells) treatmemt causes significant arrest of cells at the G2/M phase, resulting in apoptosis with concomitant loss of G0/G1 phase.
In vivo	In human LX-1 lung cancer and CX-1 colon cancer mouse xenografts,S516 (5-10 mg/kg; intraperitoneal injection; mice) treatment has promising antitumor activity (inhibition ratio (IR)> 63%) .

Solubility Information

Solubility	DMSO: 12.5 mg/mL (28.57 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.286 mL	11.429 mL	22.859 mL
5 mM	0.457 mL	2.286 mL	4.572 mL
10 mM	0.229 mL	1.143 mL	2.286 mL
50 mM	0.046 mL	0.229 mL	0.457 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Lee J, et al. Identification of CKD-516: a potent tubulin polymerization inhibitor with marked antitumor activity against murine and human solid tumors. J Med Chem. 2010 Sep 9;53(17):6337-54.

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