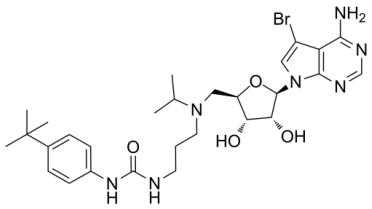
Data Sheet

Product Name:	SGC0946
Cat. No.:	CS-3531
CAS No.:	1561178-17-3
Molecular Formula:	C28H40BrN7O4
Molecular Weight:	618.57
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Solubility:	DMSO : ≥ 33 mg/mL (53.35 mM)



BIOLOGICAL ACTIVITY:

SGC0946 is a highly potent and selective DOT1L methyltransferase inhibitor with IC50 of 0.3 nM; selectively kill mixed lineage leukaemia cells. IC50 value: 0.3 nM(DOT1L) [1] Target: selective DOT1L inhibitor SGC 0946 is over 100-fold selective for other histone methyltransferases/HMTs. SGC 0946 potently reduces H3K79 dimethylation with IC50 of 2.6 nM in A431 cells, and 8.8 nM in MCF10A cells, which potently and selectively kills cells containing an MLL translocation. SGC 0946 is much more potent than its close analog EPZ004777, and serves as an excellent chemical probe for investigating DOT1L and further development of DOT1L inhibitors for cancer therapy.

References:

[1]. Yu W, et al. Catalytic site remodelling of the DOT1L methyltransferase by selective inhibitors. Nat Commun. 2012;3:1288. doi: 10.1038/ncomms2304.

CAIndexNames:

7H-Pyrrolo[2,3-d]pyrimidin-4-amine, 5-bromo-7-[5-deoxy-5-[[3-[[[[4-(1,1-dimethylethyl)phenyl]amino]carbonyl]amino]propyl](1-methylethyl)amino]-β-D-ribofuranosyl]-

SMILES:

NC1=NC=NC2=C1C(Br)=CN2[C@H]3[C@H](O)[C@H](O)[C@@H](CN(CCCNC(NC4=CC=C(C(C)(C)C)C=C4)=O)C(C)C)O3

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

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