

Product Data Sheet

Product Name: SGC0946 (trifluoroacetate salt)

Cat. No.: GC92040

Chemical Properties

Cas. No.

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

SMILES CC(C)(C)C1=CC=C(NC(NCCCN(C(C)C)C[C@@H]2[C@@H](O)[C@@H](O)[C@H](N3C(N=CN=C4N)=C4C(Br)=C3)O2)=O)C=C1.O=C(O)C(F)(F)F

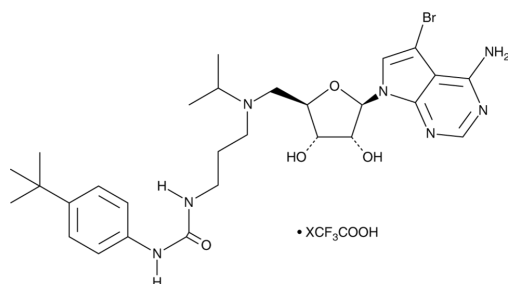
Formula $C_{28}H_{40}BrN_7O_4 \cdot XCF_3COOH$ M.Wt 618.6

Solubility DMSO: Slightly soluble: 0.1-1 mg/ml, Ethanol: Sparingly soluble: 1-10 mg/ml Storage -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

SGC0946 is an inhibitor of the non-SET domain-containing methyltransferase DOT1L ($IC_{50} = 0.3$ nM).¹ It is selective for DOT1L over a panel of 12 additional protein methyltransferases, DNA methyltransferase 1 (DNMT1), and a panel of 29 receptors and ion channels. SGC0946 reduces the levels of dimethylated lysine 79 on histone 3 (H3K79me2) in MCF-10A breast cancer cells ($IC_{50} =$

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8.8 nM). It selectively reduces the viability of isolated human cord blood cells transformed with an *MLL-AF9* fusion oncogene over those transformed with a *TLS-ERG* fusion oncogene when used at concentrations of 1 and 5 μ M. Adoptive transfer of isolated human CD3⁺ T cells pre-incubated with SGC0946 (0.5 μ M) prevents weight loss, increases survival, and reduces hepatic and colonic lymphocyte infiltration in a xenogeneic mouse model of graft versus host disease (GVHD).²

References:

- [1]. Yu, W., Chory, E.J., Wernimont, A.K., et al. Catalytic site remodelling of the DOT1L methyltransferase by selective inhibitors. *Nat. Commun.* 3:1288 (2012).
- [2]. Kagoya, Y., Nakatsugawa, M., Saso, K., et al. DOT1L inhibition attenuates graft-versus-host disease by allogeneic T cells in adoptive immunotherapy models. *Nat. Commun.* 9(1):1915 (2018).

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