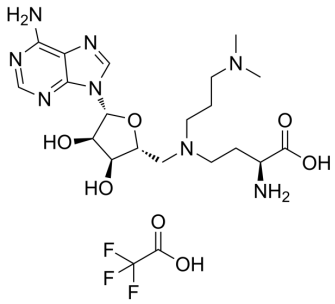
GSK2807 Trifluoroacetate

Cat. No.:	HY-104009A
CAS No.:	2245255-66-5
Molecular Formula:	$C_{21}H_{33}F_3N_8O_7$
Molecular Weight:	566.53
Target:	Histone Methyltransferase
Pathway:	Epigenetics
Storage:	4°C, sealed storage, away from moisture * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (176.51 mM; Need ultrasonic)

H_2O : ≥ 50 mg/mL (88.26 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.7651 mL	8.8257 mL	17.6513 mL
5 mM	0.3530 mL	1.7651 mL	3.5303 mL
10 mM	0.1765 mL	0.8826 mL	1.7651 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: PBS
   Solubility: 100 mg/mL (176.51 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.67 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (3.67 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (3.67 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

GSK2807 Trifluoroacetate is a potent, selective and SAM-competitive inhibitor of SMYD3, with a K_i of 14 nM and an IC_{50} of 130 nM[1][2].

IC_{50} & Target		
	SMYD3 14 nM (Ki)	SMYD3 130 nM (IC_{50})

In Vitro	A high-resolution crystal structure reveals that GSK2807 bridges the gap between the SAM-binding pocket and the substrate lysine tunnel of SMYD3. GSK2807 is 24-fold selective for SMYD3 in comparison with the closely related enzyme SMYD2 (K_i =14±6 nM and 345±36 nM, respectively)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Van Aller GS, et al. Structure-Based Design of a Novel SMYD3 Inhibitor that Bridges the SAM-and MEKK2-Binding Pockets. Structure. 2016 May 3;24(5):774-781.

[2]. Kaniskan HÜ, et al. Inhibitors of Protein Methyltransferases and Demethylases. Chem Rev. 2018 Feb 14;118(3):989-1068.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA