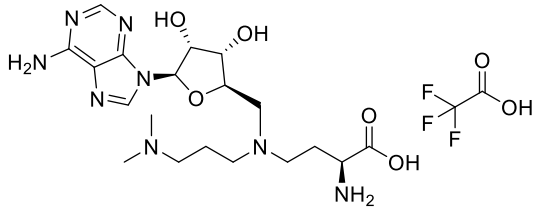
Product data sheet

MedKoo Cat#: 407994 Name: GSK2807 TFA CAS: 2245255-66-5 (TFA) Chemical Formula: $C_{21}H_{33}F_3N_8O_7$ Molecular Weight: 566.5392	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

GSK2807 is a potent and selective, SAM-competitive inhibitor of SMYD3 (Ki = 14 nM). GSK2807 bridges the gap between the SAM-binding pocket and the substrate lysine tunnel of SMYD3. GSK2807 may be useful for cancer treatment.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	250.0	441.28
Water	50.0	88.26

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.77 mL	8.83 mL	17.65 mL
5 mM	0.35 mL	1.77 mL	3.53 mL
10 mM	0.18 mL	0.88 mL	1.77 mL
50 mM	0.04 mL	0.18 mL	0.35 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Van Aller GS, Graves AP, Elkins PA, Bonnette WG, McDevitt PJ, Zappacosta F, Annan RS, Dean TW, Su DS, Carpenter CL, Mohammad HP, Kruger RG. Structure-Based Design of a Novel SMYD3 Inhibitor that Bridges the SAM-and MEKK2-Binding Pockets. Structure. 2016 May 3;24(5):774-781. doi: 10.1016/j.str.2016.03.010. Epub 2016 Apr 7. PMID: 27066749.

In vivo study

TBD

7. Bioactivity

Biological target:

GSK2807 Trifluoroacetate is a potent, selective and SAM-competitive inhibitor of SMYD3, with a Ki of 14 nM and an IC50 of 130 nM.

In vitro activity

These insights allowed for the design of GSK2807, a potent and selective, SAM-competitive inhibitor of SMYD3 (Ki = 14 nM). A high-resolution crystal structure reveals that GSK2807 bridges the gap between the SAM-binding pocket and the substrate lysine tunnel of SMYD3.

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Reference: Structure. 2016 May 3;24(5):774-781. https://pubmed.ncbi.nlm.nih.gov/27066749/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.