**Chemical Properties**

**Product Name:** EPZ031686  
**Cas No.:** 1808011-22-4  
**M.Wt:** 591.09  
**Formula:** C26H34ClF3N4O4S

**Chemical Name:** 6-chloro-2-oxo-N-((1R,3r,5S)-8-(((1-(4,4,4-trifluorobutyl)piperidin-4-yI)methyl)sulfonyl)-8-azabicyclo[3.2.1]octan-3-yl)indoline-5-carboxamide

**Canonical SMILES:** ClC1=CC(N2)=C(CC2=O)C=C1C(N[C@@](3([H])C[C@@]@)(N4S(CC(CC5CCN5CCCC(F)(F)F)(=O)=O)([H])CC[C@@]4([H])C3)=O

**Solubility:** Soluble in DMSO  
**Storage:** Store at -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.

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

**Biological Activity**

**Targets:** Chromatin/Epigenetics  
**Pathways:** Histone Methyltransferase  
**Description:**  
IC50: 3 nM  
EPZ031686 is the first SMYD3 inhibitor.  
Set and Mynd Domain containing 3 (SMYD3), a lysine methyltransferase (KMT) expressed at high
levels in a number of different cancer histologies, is reported to be associated with a poor clinical prognosis.

In vitro: EPZ031686 was the first SMYD3 inhibitor found to show double-digit nanomolar cellular activity. In addition, EPZ031686 displayed noncompetitive inhibition to both SAM and MEKK2 with a Ki = 1.2 and 1.1 nM, respectively. Moreover, EPZ031686 showed less than 30% inhibition against 16 histone methyltransferase targets at a 10 μM [1].

In vivo: Male mice i.v. administered a single dose of EPZ031686 at 1 mg/kg showed a moderate clearance of 27 mL/min/kg, which was in very good agreement with the microsomal data, with a volume of distribution at steady state of 2.3 L/kg, translating to a terminal half-life of 1.7 h. Around 20% of the administered dose was excreted unchanged in urine after 24 h, equivalent to a renal clearance of 5.3 mL/min/kg. Bioavailability of 48 and 69 was observed at 5 and 50 mg/kg, respectively, resulting in the EPZ031686 unbound blood concentration remaining above the SMYD3 IC50 value for more than 12 h after a 50 mg/kg p.o. administration [1].

Clinical trial: Up to now, EPZ031686 is still in the preclinical development stage.

Reference:

Caution

FOR RESEARCH PURPOSES ONLY.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most ApexBio products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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