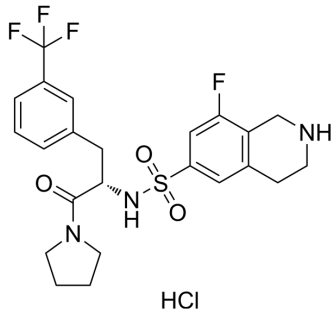
(S)-PFI-2 hydrochloride

Cat. No.:	HY-110196
CAS No.:	1627607-88-8
Molecular Formula:	$C_{23}H_{26}ClF_4N_3O_3S$
Molecular Weight:	535.98
Target:	Others
Pathway:	Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	(S)-PFI-2 hydrochloride is an inhibitor of lysine methyltransferase SETD7 and is approximately 500-fold more active than its enantiomer (R)-PFI-2. (R)-PFI-2 is a cofactor-dependent and substrate-competitive inhibitor. (R)-PFI-2 can occupy the substrate peptide binding groove of SETD7 (including the catalytic lysine binding channel) and interact with the cofactor The donor methyl group is in direct contact. However, (S)-PFI-2 was not observed to have the same interaction as (R)-PFI-2[1][2].
IC_{50} & Target	Lysine methyltransferase SETD7[1][2]
In Vitro	(S)-PFI-2 hydrochloride (10 μM; 2 h) cannot cause a dose-dependent increase in nuclear YAP in MCF7 cells or enhance the expression of YAP target genes AREG and CYR61; while (R)-PFI-2 can increase the expression of YAP, AREG and CYR61 expression[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Niu Y, et al. Revealing inhibition difference between PFI-2 enantiomers against SETD7 by molecular dynamics simulations, binding free energy calculations and unbinding pathway analysis. Sci Rep. 2017 Apr 18;7:46547.

[2]. Barsyte-Lovejoy D, et al. (R)-PFI-2 is a potent and selective inhibitor of SETD7 methyltransferase activity in cells. Proc Natl Acad Sci U S A. 2014 Sep 2;111(35):12853-8.

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