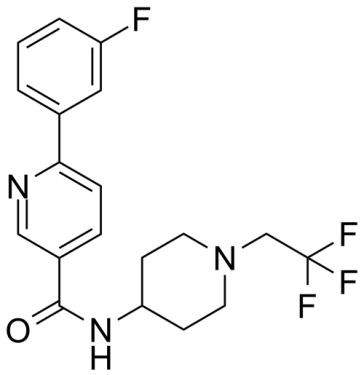
Data Sheet

Product Name:	HPGDS inhibitor 1
Cat. No.:	CS-1801
CAS No.:	1033836-12-2
Molecular Formula:	$C_{19}H_{19}F_4N_3O$
Molecular Weight:	381.37
Target:	PGE synthase
Pathway:	Immunology/Inflammation
Solubility:	DMSO : 50 mg/mL (131.11 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

HPGDS inhibitor 1 is a potent, selective and orally active **Hematopoietic Prostaglandin D Synthase (HPGDS)** inhibitor with an **IC_{50}** s of 0.6 nM and 32 nM in enzyme and cellular assays, respectively. HPGDS inhibitor 1 does not inhibit human L-PGDS, mPGES, COX-1, COX-2, or 5-LOX[1]. IC50 & Target: IC50: 0.6 nM (HPGDS in enzyme assays) and 32 nM (HPGDS in cellular assays)[1] **In Vitro:** HPGDS inhibitor 1 has equal potency against purified HPGDS from human, rat, dog, and sheep (IC_{50}, 0.5-2.3 nM)[1]. **In Vivo:** HPGDS inhibitor 1 (compound 8; 1 mg/kg) has excellent PK characteristics with 76% bioavailability, and the $T_{1/2}$ is 4.1 hours in rats[1]
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Rats dosed orally with 1 mg/kg and 10 mg/kg HPGDS inhibitor 1 (compound 8) are sacrificed at various times. Oral administration of HPGDS inhibitor 1 blocks PGD2 production in the rat spleen; inhibition of PGD2 is inversely correlated with the plasma concentration of HPGDS inhibitor 1 in a time- and dose-dependent manner[1].

HPGDS inhibitor 1 (compound 8; 1 mg/mL) illustrates efficacy in an in vivo sheep model of asthma[1].

References:

[1]. Chris P Carron, et al. Discovery of an Oral Potent Selective Inhibitor of Hematopoietic Prostaglandin D Synthase (HPGDS). ACS Med Chem Lett. 2010 Feb 2;1(2):59-63.

CAIndexNames:

3-Pyridinecarboxamide, 6-(3-fluorophenyl)-N-[1-(2,2,2-trifluoroethyl)-4-piperidinyl]-

SMILES:

O=C(NC1CCN(CC(F)(F)F)CC1)C2=CC=C(C3=CC=CC(F)=C3)N=C2

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