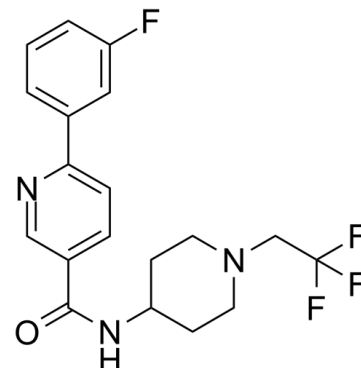


Data Sheet

Product Name:	HPGDS inhibitor 1
Cat. No.:	CS-1801
CAS No.:	1033836-12-2
Molecular Formula:	C ₁₉ H ₁₉ F ₄ N ₃ O
Molecular Weight:	381.37
Target:	PGE synthase
Pathway:	Immunology/Inflammation
Solubility:	DMSO : 50 mg/mL (131.11 mM; Need ultrasonic); H ₂ O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

HPGDS inhibitor 1 is a novel and selective Hematopoietic Prostaglandin D Synthase (HPGDS) inhibitor with an IC₅₀ Value of 0.7 nM. IC₅₀ Value: 0.7 nM [1] Target: HPGDS HPGDS inhibitor 1 was elected for further profiling based on its enzyme and cell potency. The compound illustrated equal potency against purified HPGDS from human, rat, dog, and sheep (IC₅₀, 0.5-2.3 nM). HPGDS inhibitor 1 was profiled in a panel of cellular assays to screen for activity against several relevant human enzyme targets. Those assay indicated that HPGDS inhibitor 1 does not inhibit human L- PGDS, m-PGDS, COX-1, COX-2 or 5 LOX (IC₅₀ values > 10000 nM). HPGDS inhibitor 1 had a solubility of 1.5 ug/ml (3.9 uM) at pH 6.5. The compound had excellent PK characteristics when dosed in rats at 1 mpk with 76% bioavailability. Rats dosed orally with 1 and 10 mpk HPGDS inhibitor 1 were sacrificed at various times, and plasma concentrations of HPGDS inhibitor 1 and spleen PGD₂ concentrations were measured. Oral administration of HPGDS inhibitor 1 blocked PGD₂ production in the rat spleen; inhibition of PGD₂ was inversely correlated with the plasma concentration of HPGDS inhibitor 1 in a time and dose-dependent manner. Spleen PGD₂ levels fall as HPGDS inhibitor 1 plasma levels increase over time; PGD₂ levels return to baseline levels as HPGDS inhibitor 1 plasma levels decline.

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, 1 (2), pp 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

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

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