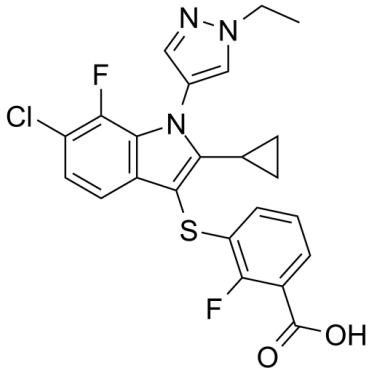
Data Sheet

Product Name:	PAT-505
Cat. No.:	CS-0030523
CAS No.:	1782070-22-7
Molecular Formula:	C23H18ClF2N3O2S
Molecular Weight:	473.92
Target:	Phosphodiesterase (PDE)
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : 48.33 mg/mL (101.98 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

PAT-505 is a potent, selective, noncompetitive and orally available **autotaxin** inhibitor, with an **IC_{50}** of 2 nM in Hep3B cells, 9.7 nM in human blood and 62 nM in mouse plasma. IC50 & Target: IC50: 2 nM (Autotaxin, Hep3B cell), 9.7 nM (Autotaxin, Human blood), 62 nM (Autotaxin, Mouse plasma)[1] **In Vitro:** PAT-505 is a potent, selective, noncompetitive and orally available autotaxin inhibitor, with an IC_{50} of 2 nM in Hep3B cells, 9.7 nM in human blood and 62 nM in mouse plasma. PAT-505 is selective for ATX versus other ENPP proteins, and shows marginal inhibition of radiolabeled agonist or antagonist binding to the adenosine A3 receptor, MT1 melatonin receptor, prostaglandin E2 EP4 receptor, 5-HT5a serotonin receptor, and GABA-gated Cl^- channel with 50%-70% inhibition at 10 μM[1]. **In Vivo:** PAT-505 suppresses ATX lysoPLD activity with an average IC_{50} value of 62 nM and an average IC_{90} value of 630 nM in mouse plasma, and the IC_{90} in rat plasma is □770 nM. PAT-505 (30 mg/kg, p.o.) significantly reduces fibrotic score, the percentage of PSR-positive area, and α-SMA immunoreactivity in mouse model of nonalcoholic steatohepatitis (NASH)[1].

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: [1]Mice[1]

NASH is induced in **male C57BL/6 mice**. Briefly, 5-week-old mice are acclimated for 1 week on normal chow before switching to a choline-deficient, l-amino acid-defined, high-fat diet (CDAHFD) containing 60% kcal% fat and 0.1% methionine. After 4 weeks of CDAHFD feeding, approximately 200 μL of blood is collected from each animal via a submandibular bleed and the serum analyzed for liver enzyme levels. Any animal with a total serum bilirubin level >1 mg/dL is removed from the study prior to compound dosing. Animals are fed CDAHFD for 5 weeks before randomization into treatment groups (n = 7-10 per group). Vehicle or **PAT-505 (3-30 mg/kg)** is administered by **oral gavage** in **0.5% methylcellulose (MC)** once daily from weeks 5 to 12[1].

References:

[1]. Bain G, et al. Selective Inhibition of Autotaxin Is Efficacious in Mouse Models of Liver Fibrosis. J Pharmacol Exp Ther. 2017 Jan;360(1):1-13. Epub 2016 Oct 17.

CAIndexNames:

Benzoic acid, 3-[[6-chloro-2-cyclopropyl-1-(1-ethyl-1H-pyrazol-4-yl)-7-fluoro-1H-indol-3-yl]thio]-2-fluoro-

SMILES:

O=C(O)C1=CC=CC(SC2=C(C3CC3)N(C4=CN(CC)N=C4)C5=C2C=CC(Cl)=C5F)=C1F

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

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