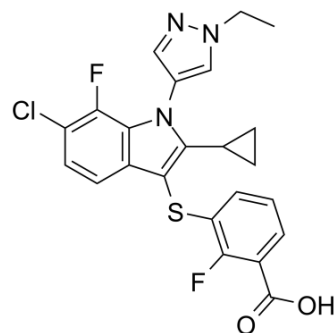


## PAT-505

<b>Cat. No.:</b>	HY-107781		
<b>CAS No.:</b>	1782070-22-7		
<b>Molecular Formula:</b>	C <sub>23</sub> H <sub>18</sub> ClF <sub>2</sub> N <sub>3</sub> O <sub>2</sub> S		
<b>Molecular Weight:</b>	473.92		
<b>Target:</b>	Phosphodiesterase (PDE)		
<b>Pathway:</b>	Metabolic Enzyme/Protease		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



### SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 48.33 mg/mL (101.98 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	<b>Preparing Stock Solutions</b>	1 mM	2.1101 mL	10.5503 mL	21.1006 mL
		5 mM	0.4220 mL	2.1101 mL	4.2201 mL
10 mM		0.2110 mL	1.0550 mL	2.1101 mL	
Please refer to the solubility information to select the appropriate solvent.					
<b>In Vivo</b>	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 4.83 mg/mL (10.19 mM); Clear solution  2. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 4.83 mg/mL (10.19 mM); Clear solution				

### BIOLOGICAL ACTIVITY

<b>Description</b>	PAT-505 is a potent, selective, noncompetitive and orally available autotaxin inhibitor, with an IC <sub>50</sub> of 2 nM in Hep3B cells, 9.7 nM in human blood and 62 nM in mouse plasma.		
<b>IC<sub>50</sub> &amp; Target</b>	Autotaxin 2 nM (IC <sub>50</sub> , In Hep3B cells)	Autotaxin 9.7 nM (IC <sub>50</sub> , In human blood)	Autotaxin 62 nM (IC <sub>50</sub> , In mouse plasma)
<b>In Vitro</b>	PAT-505 is a potent, selective, noncompetitive and orally available autotaxin inhibitor, with an IC <sub>50</sub> 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<sup>-</sup> channel with 50%-70% inhibition at 10 μM<sup>[1]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

#### In Vivo

PAT-505 suppresses ATX lysoPLD activity with an average IC<sub>50</sub> value of 62 nM and an average IC<sub>90</sub> value of 630 nM in mouse plasma, and the IC<sub>90</sub> 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)<sup>[1]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## PROTOCOL

#### Animal Administration <sup>[1]</sup>

Mice<sup>[1]</sup>

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<sup>[1]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## 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.

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

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