

Product Name	: Autotaxin inhibitor compound 1
Synonyms	: Autotaxin-IN-1
Cat No.	: M12375
CAS Number	: 1619971-30-0
Molecular Formula	: C ₂₁ H ₂₃ N ₇ O ₂
Formula Weight	: 405.46
Chemical Name	: 2-(2-(1H-1,2,3-triazol-4-yl)ethoxy)-1-(2-((2,3-dihydro-1H-inden-2-yl)amino)-5,7-dihydro-6H-pyrrolo[3,4-d]pyrimidin-6-yl)ethan-1-one
Description	Autotaxin inhibitor compound 1 (Autotaxin-IN-1) is a potent, selective, orally bioavailable inhibitor of autotaxin with IC₅₀ of 2.2 nM in ex vivo human whole blood assay, does not inhibit related proteins ENPP1 and ENPP7; demonstrates significant anti-inflammatory and analgesic effects in the carrageenan-induced paw inflammation and acetic acid-induced visceral pain tests, respectively; also significantly inhibits disease activity score in the dextran sodium sulfate-induced model of inflammatory bowel disease (IBD) and in autoimmune encephalomyelitis model of multiple sclerosis (MS).
Pathway	: Wnt/Notch/Hedgehog
Target	: Autotaxin
Receptor	: Autotaxin
Solubility	: —
SMILES	: <chem>O=C(N1CC2=NC(NC3CC4=C(C=CC=C4)C3)=NC=C2C1)COC(C=C1N=NN=C1)</chem>
Storage	: (-20°C)
Stability	: ≥ 2 years
Reference	:

1. Thirunavukkarasu K, et al. J Pharmacol Exp Ther. 2016 Oct;359(1):207-14. 2. Jones SB, et al. ACS Med Chem Lett. 2016 Aug 2;7(9):857-61.